YHAL N29
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N29

Quantum Mechanics
Physics 237 ~ 238
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1951 ~ 1952

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001

Quantum Mechanics

1951 Sept
~1952 June

Monday and Wednesday
11 ~ 12:20
Physics 329

Q. M. Ph. 237
Winter Session (1951~1952)

Q. M. Ph. 238
Spring Session (1952)

Appendix
Fock: Configuration Space and Second Quantization

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Reference:

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McGraw-Hill, 1949
Enrico Persico: Fundamentals of Q. M.
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Arthur March: Q. M. of Particles
and Wave Fields, 1951, John
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Chapter I.

Historical Development of Quantum Theory

Quantum ~~mechanics is a theory which had been~~ theory developed during the first quarter of the twentieth century ~~in such a way that~~ through several stages, until it became ~~the~~ a consisten

Quantum theory, which started in 1900, and had been was developed since then, was not a consistent theory, until ~~it to~~ q.m. appeared and completed during ~~the~~ nine years 1924~1927.

Let us look back briefly the most important points in the history of q.t.

1. The first ~~stage~~ is, of course, Planck's discovery of elementary quantum of action $h = 6.6 \times 10^{-27}$ erg. sec. This was first ~~when matter and~~ applied to quantization of motion harmonic oscillator, quantization of radiation.
2. Photons: Einstein
   duality of ~~matter and~~ wave and corpuscle
3. Atomic structure: Bohr
   Correspondence principle
   Ritz combination principle

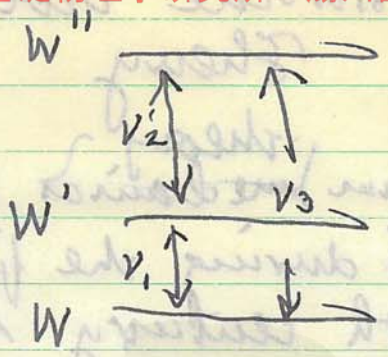
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$\nu_1 + \nu_2 = \nu_3$

$h\nu_1 = W' - W$

$h\nu_2 = W'' - W'$

$h\nu_3 = W'' - W$



stationary state
transition probability

4. de Broglie wave

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2meV}}$$ 非相対論

$$= \sqrt{\frac{150}{V}} \times 10^{-8} \text{ cm.}$$

5. Schrödinger wave eq. picture

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~~Problem~~ I. Prove that the eigenfunction of a linear ~~harmonic~~ oscillator belonging to the eigenvalue

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right)\hbar\nu$$

is given by

$$\psi_n = \left(2^n n! \sqrt{\pi}\right)^{-\frac{1}{2}} e^{-x^2/2} H_n(x)$$

$$n = 0, 1, 2, \cdots$$

where $H_n(x)$ is ~~the~~ the Hermite polynomial of the n-th degree as defined by

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n e^{-x^2}}{dx^n}.$$

Show also that the above ψ_n satisfies the normalization condition

$$\int_{-\infty}^{+\infty} \bar{\psi}_n \psi_n \, dx = 1$$

Hint: $\psi_n = N_n e^{-\frac{x^2}{2}} H_n(x)$

(i) $\Psi(x,t) = e^{-t^2+2xt} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n$

$$H_n(x) = \left(\frac{\partial^n \Psi}{\partial t^n}\right)_{t=0} = e^{-t^2+2xt}$$

$$= e^{x^2} \frac{\partial^n}{\partial t^n} \left(e^{-(t-x)^2}\right)_{t=0} = e^{x^2} (-1)^n \frac{d^n e^{-y^2}}{dy^n}\Big|_{y=x}$$

$t - x = -y$

$$= e^{x} (-1)^n \frac{d^n e^{-x^2}}{dx^n}.$$

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$$\frac{\partial \Psi}{\partial x} = 2t\Psi$$

$$\sum_n \frac{H_n'(x)}{n!} t^n = \sum_n \frac{H_n(x)}{n!} 2t^{n+1}$$

t^n: $\frac{1}{n!} H_n'(x) = \frac{1}{(n-1)!} H_{n-1}(x) \cdot 2$

$$H_n' = 2n H_{n-1}$$

$$\frac{\partial \Psi}{\partial t} = (2x - 2t)\Psi$$

$$\sum \frac{H_n'(x)}{n!} n t^{n-1} = 2x \sum \frac{H_n(x)}{n!} t^n - 2\sum \frac{H_n(x)}{n!} t^{n+1}$$

t^n: $\frac{1}{(n-1)!} H_{n-1}' = 2x \frac{1}{n!} H_n - 2 \frac{1}{(n-1)!} H_{n-1}$

$$H_{n+1}' = 2x H_n - 2n H_{n-1}$$

$$H_{n+1}' = 2x H_n' + 2H_n - 2n H_{n-1}'$$

$$H_n'' = 2n H_{n-1}'$$

$$= 2x H_n' + 2H_n - H_{n+1}'$$

$$= 2x H_n' + 2H_n - 2(n+1) H_n$$

$$= 2x H_n' - 2n H_n$$

(ii) $$\int_{-\infty}^{+\infty} H_n(x)(-1)^n \frac{d^n e^{-x^2}}{dx^n} dx$$

$$= \int_{-\infty}^{+\infty} H_n(x) \frac{d^n H_n(x)}{dx^n} e^{-x^2} dx$$

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$$H_n = (2x)^n - \frac{n(n-1)}{1!}(2x)^{n-2} + \cdots$$

$$\frac{d^n H_n}{dx^n} \sim 2^n \cdot n!$$

$$\int = 2^n n! \int_{-\infty}^{+\infty} e^{-x^2} dx$$

$$\simeq 2^n n! \sqrt{\pi}$$

$$N_n = (2^n n! \sqrt{\pi})^{-1/2}$$

Problem 2. Find the eigenfunctions of two dimensional h. o. in cylindrical coordinates r, θ:

$$x = r\cos\theta$$
$$y = r\sin\theta$$

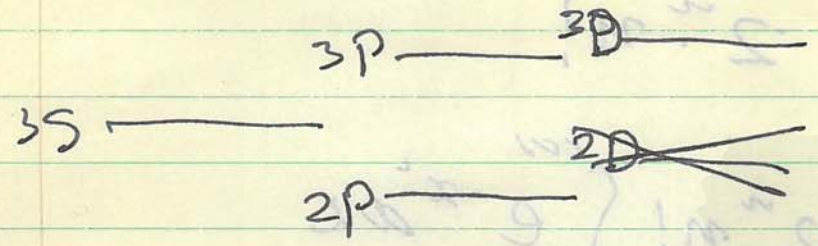
and compare them with those obtained in cartesian coordinates x, y.

Problem 2. Three dim. h. o.

Problem 3. Hydrogen atom in parabolic coordinates.

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Energy levels of alkali atoms



penetration of

$$\frac{\nu}{c} = -\frac{R}{(n+\Delta n)^2}$$

$$R = \frac{2\pi^2 m e^4}{c h^3}$$

$$= \frac{m e^4}{4\pi c \hbar^3}$$

(hydrogen-like atom $\nu = RZ^2\left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right)$)

$$E = -\frac{m e^4}{2\hbar^2} \frac{1}{(n+\Delta n)^2}$$

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Problem. Q.M. Virial theorem

Classical V.T.

$$r\cdot F = m\left[\frac{d}{dt}(r\dot r)-\dot r^2\right]$$

$$\frac{1}{\tau}\int_0^\tau (r\cdot F)\,dt = \frac{m}{\tau}\int_0^\tau\left\{\frac{d}{dt}(r\dot r)-\dot r^2\right\}dt$$

$$= \frac{m}{\tau}\left[r\cdot\dot r\right]_0^\tau - \frac{m}{\tau}\int_0^\tau \dot r^2\,dt$$

For periodic motion (bound state),

$$\overline{r\cdot F} = -2\overline{T} \quad \text{or} \quad \overline{r\cdot \operatorname{grad} V} = +2\overline{T}$$

$T = \frac{1}{2}mv^2$ V: pot. energy

Q.M.V.T.

$V = a/r$ $\quad \operatorname{grad} V = -\frac{ar}{r^2}$

$$r\cdot \operatorname{grad} V = -\frac{a}{r} = -V$$

$$\overline{V} = -2\overline{T}$$

$$\overline{E} = \overline{T}+\overline{V} = -\overline{T} = \frac{1}{2}\overline{V}$$

Q.M.V.T.

$$m\frac{\partial}{\partial t}\int r\dot r\,dv = \int r\cdot F|\psi|^2 dv + \int \psi^*(-\hbar^2\Delta\psi)\,dv$$

$$\overline{r\cdot F} = -2\overline{T} \qquad F = -\operatorname{grad} V$$

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Proof:

~~$m \int dv \cdot x \frac{\partial \dot{x}}{\partial t}$~~

~~$= x$~~

$$m x \frac{\partial \dot{x}}{\partial t} = -x \frac{\partial V}{\partial x} \hat{\psi} \psi$$

~~$x \sum \frac{\partial T_{\cdot}}{\partial x_{\cdot}}$~~

$$- x \sum_{l} \frac{\partial T_{xl}}{\partial x_l}$$

$$m x \frac{\partial \dot{x}}{\partial t} = -x \, \mathrm{grad} V \cdot \hat{\psi} \psi$$

$$= \sum_{j,l} x_j \frac{\partial T_{jl}}{\partial x_l}$$

$$T_{xx} = \frac{\hbar^2}{4m} \left(2 \frac{\partial \psi}{\partial x} \frac{\partial \hat{\psi}^{*}}{\partial x} - \hat{\psi} \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \hat{\psi}}{\partial x^2} \right)$$

$$T_{xy} = \frac{\hbar^2}{4m} \left(\frac{\partial \psi}{\partial x} \frac{\partial \hat{\psi}}{\partial y} + \frac{\partial \psi}{\partial y} \frac{\partial \hat{\psi}}{\partial x} - \hat{\psi} \frac{\partial^2 \psi}{\partial x \partial y} - \psi \frac{\partial^2 \hat{\psi}}{\partial x \partial y} \right)$$

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量子力学 p. 83

$$\Psi(q_1 \cdots q_n) = A e^{iS/\hbar}$$

$$e^{-iS/\hbar} \cdot i\hbar \frac{\partial}{\partial t}(A e^{iS/\hbar}) = H \cdot A e^{iS/\hbar}$$

$$i\hbar \frac{\partial A}{\partial t} + \frac{\partial S}{\partial t} A$$

$$= H(q_1 \cdots q_n, e^{-iS/\hbar}(-i\hbar \frac{\partial}{\partial q_1}) e^{iS/\hbar} \cdots) A$$

$$= H(q_1 \cdots q_n, -i\hbar \frac{\partial}{\partial q_1} + \frac{\partial S}{\partial q_1} \cdots) A$$

$$= H(q_1 \cdots q_n, \frac{\partial S}{\partial q_1}, \cdots) A$$

$+$

$$H = \sum_{r,s} C_{rs}(q_1 \cdots q_n) p_r p_s + f(q_1 \cdots q_n)$$

$C_{rs} = C_{sr}$

$$H(q_1 \cdots q_n, -i\hbar \frac{\partial}{\partial q_1} + \frac{\partial S}{\partial q_1} \cdots) A$$

$$= \sum_{r,s} C_{rs}(-i\hbar \frac{\partial}{\partial q_r} + \frac{\partial S}{\partial q_r})(-i\hbar \frac{\partial}{\partial q_s} + \frac{\partial S}{\partial q_s}) A + f(q_1 \cdots q_n) A$$

$$= \sum_{r,s} C_{rs} \left(\frac{\partial S}{\partial q_r}\right)\left(\frac{\partial S}{\partial q_s}\right) A + (-i\hbar) \underbrace{\sum C_{rs}} \left[\frac{\partial}{\partial q_r}\left\{\underline{\frac{\partial S}{\partial q_s}} \cdot A\right\} + \frac{\partial S}{\partial q_r} \cdot \frac{\partial A}{\partial q_s}\right] + f \cdot A$$

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$$\frac{\partial H(q_1 \cdots q_n, \frac{\partial S}{\partial q_1} \cdots \frac{\partial S}{\partial q_n})}{\partial(\frac{\partial S}{\partial q_s})}$$

$$= 2C_{ss}\left(\frac{\partial S}{\partial q_s}\right) + 2\sum_{\substack{s\neq r \\ r\neq s}} C_{rs}\left(\frac{\partial S}{\partial q_r}\right)$$

$$\sum_s \frac{\partial H}{\partial(\frac{\partial S}{\partial q_s})}\frac{\partial A}{\partial q_s} = 2\sum_s C_{ss}\frac{\partial S}{\partial q_s}\frac{\partial A}{\partial q_s}$$

$$+ 2\sum_{\substack{r\neq s \\ r,s}} C_{sr}\left(\frac{\partial S}{\partial q_r}\right)\left(\frac{\partial A}{\partial q_s}\right)$$

$$= 2\sum_{r,s} C_{rs}\left(\frac{\partial S}{\partial q_r}\right)\left(\frac{\partial A}{\partial q_s}\right)$$

$$\sum_{r,s} C_{rs}\frac{\partial}{\partial q_r}\left\{\frac{\partial S}{\partial q_s}A\right\}$$

$$= \sum_{r,s}\frac{\partial}{\partial q_r}\left(C_{rs}\frac{\partial S}{\partial q_s}A\right) - \sum_{r,s}\frac{\partial C_{rs}}{\partial q_r}\left(\frac{\partial S}{\partial q_s}A\right)$$

If C_{rs} are independent of $q_1 \cdots q_n$, we have

$$= 2\sum_r \frac{\partial}{\partial q_r}\left(\frac{\partial H}{\partial(\frac{\partial S}{\partial q_r})}A\right)$$

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$$\frac{\partial A}{\partial t} + \frac{1}{2}\sum_{r=1}^{n}\left\{\frac{\partial H(q_1 \cdots \frac{\partial S}{\partial q_r} \cdots)}{\partial\left(\frac{\partial S}{\partial q_r}\right)}\frac{\partial A}{\partial q_r} + \frac{\partial}{\partial q_r}\left\{\frac{\partial H}{\partial\left(\frac{\partial S}{\partial q_r}\right)} \cdot A\right\}\right] = 0$$

or

$$\frac{\partial A^2}{\partial t} + \sum_{r=1}^{n}\left(\frac{\partial H}{\partial\left(\frac{\partial S}{\partial q_r}\right)} \cdot A^2\right) = 0$$

~~$\frac{\partial H}{\partial}$~~ $p_r = \frac{\partial S}{\partial q_r}$

$$\frac{dq_r}{dt} = \frac{\partial H}{\partial\left(\frac{\partial S}{\partial q_r}\right)}$$

$$\frac{\partial A^2}{\partial t} + \sum_{r=1}^{n}\left(\frac{dq_r}{dt}\frac{\partial A^2}{\partial q_r}\right) = 0$$

$A=0$

$A=0$

$\frac{dA}{dt} = 0$

$A \neq 0$

$\frac{d(A^2)}{dt} = 0$ if $A^2 = 0$

$= -A^2\sum_{r=1}^{n}\frac{\partial}{\partial q_r}\left(\frac{dq_r}{dt}\right)$

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Heisenberg's approach to q.m.

~~D~~. $q_1 q_2 \cdots q_n$
$p_1 p_2 \cdots p_n$

Poisson bracket

$$(u,v) = \sum_{r=1} \left(\frac{\partial q_r}{\partial q_r} \frac{\partial v}{\partial p_r} - \frac{\partial u}{\partial p_r} \frac{\partial v}{\partial q_r} \right)$$

invariant with respect to canonical transformation

$$(u,v) = \sum_{r=1} \left(\frac{\partial u}{\partial Q_r} \frac{\partial v}{\partial P_r} - \frac{\partial u}{\partial P_r} \frac{\partial v}{\partial Q_r} \right)$$

Our problem is to find the q.m. ~~H.J. equivalent~~ counterpart of the P.B.

$$\frac{\partial W}{\partial t} + H\left(q_1 \cdots q_n, \frac{\partial W}{\partial q_1} \cdots \frac{\partial W}{\partial q_n}, t\right) = 0$$

~~$p_1 = \frac{\partial W}{\partial q_1}$~~

Complete solution

$$W(q_1 \cdots q_n, t, \alpha_1, \alpha_2 \cdots \alpha_n)$$

$$p_r = \frac{\partial W}{\partial q_r} \quad \& \quad r = 1, 2, \cdots n$$

$$\beta_r = \frac{\partial W}{\partial \alpha_r}$$

definite

q's and p's are functions of $(\alpha_1 \alpha_2 \cdots \alpha_n, \beta_1 \cdots \beta_n, t)$

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If H does not contain t explicitly,

$$W = S(q_1 \cdots q_n) - Et$$

$$H\left(q_1 \cdots q_n, \frac{\partial S}{\partial q_1} \cdots \frac{\partial S}{\partial q_n}\right) = E$$

where E is a constant which is nothing but the energy of the system.

Complete solution:

$$S(q_1 \cdots q_n, \alpha_1, \alpha_2 \cdots \alpha_n)$$

$\alpha_1 \equiv E$ or $\alpha_1 \equiv \phi_1(E)$ or $E(\alpha_1)$

$$p_r = \frac{\partial S}{\partial q_r} \qquad r = 1, 2, \cdots n$$

$$\beta_r = \frac{\partial S}{\partial \alpha_r} \qquad r = 2, \cdots n$$

$$\beta_1 = \frac{\partial S}{\partial \alpha_1} - \frac{\partial E}{\partial \alpha_1} t$$

$n = 1$ $\quad p_1 = p$, $q_1 = q$.

$$J = \int_C p\, dq \qquad S(q, \alpha) \quad \alpha_1 = \alpha, \ \beta_1 = \beta$$

$\alpha \equiv J$.

$$S(q, J)$$

$$p = \frac{\partial S}{\partial q}$$

$$\beta = \frac{\partial S}{\partial J} - \nu t \qquad \nu = \frac{\partial E}{\partial J}$$

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$$w = \frac{\partial S(q,J)}{\partial J}$$

$$w = \nu t + \beta$$

~~(J, w) is~~ the transformation from (q,p) to (w,J) satisfying

$$p = \frac{\partial S(q,J)}{\partial q}$$

$$w = \frac{\partial S(q,J)}{\partial J}$$

is a canonical or contact transformation, so that w and J form a pair of canonical variables.

$$\int_C dw = \int_C \frac{\partial w}{\partial q} dq$$

↓ diff. along C. (with fixed J)

$$= \int_C \frac{\partial S(q,J)}{\partial q \partial J} dq$$

$$= \frac{\partial}{\partial J} \int_C \frac{\partial S}{\partial q} dq = \frac{dJ}{dJ} = 1.$$

$$\int_C dw = \nu \int_C dt = \nu T = 1$$

$$\nu = \frac{1}{T}.$$

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$q(w,J)$, $p(w,J)$ are
periodic functions of w with period
1.

$$\left.\begin{aligned} q &= \sum_{n=-\infty}^{+\infty} q_n(J)\, e^{2\pi i n w} \\ &= \sum_{n=-\infty}^{+\infty} q_n(J)\, e^{2\pi i n \nu t} \\ p &= \sum_{n=-\infty}^{+\infty} p_n(J)\, e^{2\pi i n w} \end{aligned}\right\}$$

$$(q,p) = \frac{\partial q}{\partial w}\frac{\partial p}{\partial J} - \frac{\partial p}{\partial w}\frac{\partial q}{\partial J},$$

$$\downarrow$$

$$(\nu,\nu) = 2\pi i \sum_n \sum_m \left(n q_n \frac{\partial p_m}{\partial J} - n p_n \frac{\partial q_m}{\partial J} \right) \times e^{2\pi i (n+m) w}$$

$$\sum_n q_n e^{2\pi i n w} \to \left(q_{\alpha\beta}\, e^{2\pi i \nu_{\alpha\beta} t} \right)$$

$$\sum_m p_m e^{2\pi i m w} \to \left(p_{\alpha\beta}\, e^{2\pi i \nu_{\alpha\beta} t} \right)$$

$n \to \alpha - \gamma$, $m \to \gamma - \beta$

$$e^{2\pi i (-n+m) w} \to e^{2\pi i (\nu_{\alpha\beta} + \nu_{\beta\gamma}) t} = e^{2\pi i \nu_{\alpha\gamma} t}$$

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~~$J = n\hbar \qquad n = 0, 1, 2, \cdots$~~

$$(\alpha-\gamma) q_{\alpha\gamma} \frac{\partial p_{\gamma\beta}}{\partial J} - (\alpha-\gamma) p_{\alpha\gamma} \frac{\partial q_{\gamma\beta}}{\partial J}$$

$J = n\hbar \quad n = 0, 1, 2, \cdots$

~~$\frac{\partial p_{\gamma\beta}}{\partial J}$~~ $\rightarrow \dfrac{p_{\alpha,\alpha-\gamma+\beta} - p_{\gamma,\beta}}{(\alpha-\gamma)\hbar}$

w: fixed or $\nu_{\gamma\beta}$ or $\underline{\gamma-\beta : \text{fixed}}$

in $\dfrac{\partial p}{\partial J}, \dfrac{\partial q}{\partial J}$.

$(q,p) \rightarrow$

$$\frac{2\pi i}{\hbar} \sum_\gamma \Big(q_{\alpha\gamma} \underbrace{p_{\gamma\beta} \quad p_{\alpha,\alpha-\gamma+\beta}}_{\alpha-\delta+\beta \quad \delta} - q_{\alpha\gamma} p_{\gamma\beta} - p_{\alpha\gamma} q_{\gamma,\alpha-\gamma+\beta} + p_{\alpha\gamma} q_{\gamma\beta} \Big)$$

$$= -\frac{2\pi i}{\hbar} \sum_\gamma (q_{\alpha\gamma} p_{\gamma\beta} - p_{\alpha\gamma} q_{\gamma\beta})$$

$(q,p) \rightarrow -\dfrac{2\pi i}{\hbar}(qp - pq)$

or $-\dfrac{\hbar}{2\pi i} = i\hbar$

$$i\hbar\,(q,p) = (qp - pq)$$

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$i\hbar\,(u,v) \to [u,v] = uv - vu$

$(q,p) = 1.$

$\therefore (q,p) = \left(\frac{\partial q}{\partial q}\frac{\partial p}{\partial p} - \frac{\partial p}{\partial q}\frac{\partial q}{\partial p}\right)$

$= 1$

$[q,p] = i\hbar \underline{1}$

$\underline{1} = \begin{pmatrix} 1 & & 0 \\ & 1 & \\ 0 & & 1 \end{pmatrix}$

$1\,a = a\,1 = a$

Problem: Deduce the q.m. eq. of motion for a ~~charged~~ particle with el. charge $-e$ and mass m in the el. mag. field:

$$m\frac{d^2\mathbf{r}}{dt^2} = -e\mathbf{E} + \frac{1}{2}\frac{e}{c}\left\{\left[\frac{d\mathbf{r}}{dt}\times\mathbf{H}\right] - \left[\mathbf{H}\times\frac{d\mathbf{r}}{dt}\right]\right\}$$

as the consequence of

$$i\hbar\frac{d\mathbf{r}}{dt} = [\mathbf{r}, H]$$

$$i\hbar\frac{d\mathbf{p}}{dt} = [\mathbf{p}, H]$$

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~~W, K, B. method~~

where

$$H = \frac{1}{2m}\left(p + \frac{e}{c}A\right)^2 - eA_0$$

$$\left.\begin{aligned} E &= -\frac{1}{c}\frac{\partial A}{\partial t} - \operatorname{grad} A_0 \\ H &= \operatorname{curl} A \end{aligned}\right\}$$

$[x^2, p_x] = 2i\hbar x$ $\quad (= x[x, p_x] + [x, p_x]x)$

$[f(x), p_x^2] = i\hbar \dfrac{\partial f(x)}{\partial x}$

$[f(x), p_x^2] = 2i\hbar \dfrac{\partial f}{\partial x} p_x + \hbar^2 \dfrac{\partial^2 f}{\partial x^2}$

(See Schiff's book. p.135)

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Angular Momentum

$$m_x^2 + m_y^2 + m_z^2 = -\hbar^2 \left\{ \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right)^2 + \left(\quad \right)^2 + \left(\quad \right)^2 \right\}$$

$$= -\hbar^2 \Big(y^2\frac{\partial^2}{\partial z^2} + z^2\frac{\partial^2}{\partial y^2} - 2yz\frac{\partial^2}{\partial y \partial z} - y\frac{\partial}{\partial y} - z\frac{\partial}{\partial z} + z^2\frac{\partial^2}{\partial x^2} + x^2\frac{\partial^2}{\partial z^2} - 2zx\frac{\partial^2}{\partial z \partial x} - z\frac{\partial}{\partial z} - x\frac{\partial}{\partial x} + x^2\frac{\partial^2}{\partial y^2} + y^2\frac{\partial^2}{\partial x^2} - 2xy\frac{\partial^2}{\partial x \partial y} - x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y} \Big)$$

$$= -\hbar^2 \Big\{ (r^2 - x^2)\frac{\partial^2}{\partial x^2} + (r^2 - y^2)\frac{\partial^2}{\partial y^2} + (r^2 - z^2)\frac{\partial^2}{\partial z^2} - 2yz\frac{\partial^2}{\partial y \partial z} - 2zx\frac{\partial^2}{\partial z \partial x} - 2xy\frac{\partial^2}{\partial x \partial y} - 2x\frac{\partial}{\partial x} - 2y\frac{\partial}{\partial y} - 2z\frac{\partial}{\partial z} \Big\}$$

$$= -\hbar^2 \Big\{ r^2\Delta - \Big(r^2\frac{\partial^2}{\partial r^2} + \cdots\Big) - \Big(\frac{\partial^2}{\partial z^2}z^2 + \frac{\partial^2}{\partial x^2}x^2 + \frac{\partial^2}{\partial y^2}y^2\Big) \Big\}$$

$$\frac{\partial}{\partial x}\Big(r^2\frac{\partial}{\partial r}f\Big) = \Big(2x\frac{\partial}{\partial r} + x^2\frac{\partial^2}{\partial r^2}\Big)f$$

$$\frac{\partial}{\partial z}\Big(r^2\frac{\partial}{\partial r}f\Big) = \Big(2z\frac{\partial}{\partial r} + z^2\frac{\partial^2}{\partial r^2}\Big)f$$

$$\frac{\partial}{\partial y}\Big(r^2\frac{\partial}{\partial r}f\Big) = \Big(2y\frac{\partial}{\partial r} + y^2\frac{\partial^2}{\partial r^2}\Big)f$$

$$+ \Big(2x\frac{\partial}{\partial x} + 2y\frac{\partial}{\partial y} + 2z\frac{\partial}{\partial z}\Big)f$$

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$$\left(x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}+z\frac{\partial}{\partial z}\right)^2$$

$$= x^2\frac{\partial^2}{\partial x^2}+y^2\frac{\partial}{\partial y}+z^2\frac{\partial}{\partial z^2}$$

$$+x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}+z\frac{\partial}{\partial z}$$

$$+2xy\frac{\partial^2}{\partial x\partial y}+\cdots$$

$$\therefore M=-\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right.$$

$$\left.+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)$$

$$\{M_z, H\} = -i\hbar\frac{\partial}{\partial\varphi}\left(\frac{\hbar^2}{2m}\Delta+V(r)\right)$$

$$\left(-\frac{\hbar^2}{2m}\Delta+V(r)\right)\left(-i\hbar\frac{\partial}{\partial\varphi}\right)$$

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Problem

n-particles system

$x_1\ y_1\ z_1 \quad \cdots \quad x_n\ y_n\ z_n$

$p_{1x}\ p_{1y}\ p_{1z} \quad \cdots \quad p_{nx}\ p_{ny}\ p_{nz}$

$M_x = \sum_{i=1}^{n} m_{ix}$, $M_y = \sum_{i=1}^{n} m_{iy}$, ...

$L_x \quad m_{i3} = y_i p_{iz} - z_i p_{iy}$

etc.

prove that

$m_x m_y - m_y m_x = i\hbar m_z$

$L_x \quad L_y$ etc.

$L^2 M = m_x^2 + m_y^2 + m_z^2$

$M' = \hbar^2 \frac{k}{2}\left(\frac{k}{2}+1\right)$

$m_z' = -\frac{k}{2}\hbar, \cdots, +\frac{k}{2}\hbar$

$\frac{k}{2}$; integer $= l$

$2l+1 = k+1$; eigenvalues

Prove that if

$$H = \sum_{i=1}^{n} \frac{1}{2m_i}\left(p_{ix}^2 + p_{iy}^2 + p_{iz}^2\right) + V\left(r_{12}, r_{23}, \cdots\right)$$

$$r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2},$$

H is commutative with m_x, m_y, m_z.

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Hint. ~~$r_{12} = r_1 r_2 \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2)$~~

$$\left(\frac{\partial}{\partial\varphi_1} + \frac{\partial}{\partial\varphi_2}\right)\{\quad\} = 0.$$

$$r_{12} = \sqrt{(r_1 \sin\theta_1 \cos\varphi_1 - r_2 \sin\theta_2 \cos\varphi_2)^2 + (r_1 \sin\theta_1 \sin\varphi_1 - r_2 \sin\theta_2 \sin\varphi_2)^2 + (r_1 \cos\theta_1 - r_2 \cos\theta_2)^2}$$

$$= \sqrt{r_1^2 + r_2^2 - 2 r_1 r_2 \{\sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2) + \cos\theta_1 \cos\theta_2\}}$$

or $\sum_i \frac{\partial}{\partial\varphi_i} \cdot r_{12} = 0$

or $\sum_i \frac{\partial}{\partial\varphi_i} \cdot r_{jk} = 0$

Eigenfunction

$\psi_{L, L_z, \cdots}$

$L=$	
0	S
1	P
2	D
⋮	⋮

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n-particle system (with spin 1/2)

$\psi(x_1, y_1, z_1, \sigma_{12}; \cdots x_n y_n z_n \sigma_{n2})$

$H = \sum_i \frac{1}{2m} p_i^2 + V(r_1 - r_n, r_{12}, \cdots r_{n-1,n})$

$m_x = \sum_i m_{ix}$ etc,

$[m_{x2}, H] = 0$. etc.

$S_x = \sum_i \frac{\hbar}{2} \sigma_{i2}$

$[S_z, H] = 0$. etc.

$E(L, S, \cdots)$

$\mathbf{J} = \mathbf{L} + \mathbf{S}$

$J^2 : \hbar^2 j(j+1)$

$J_z : -j\hbar, \cdots +j\hbar$.

$j = l+s,\ l+s-1,\ \vdots,\ |l-s|$

$\sum_{j=|l-s|}^{l+s} (2j+1)$

$= \frac{\{2(l+s)+1 + 2|l-s|+1\}}{2} \times \{l+s-|l-s|+1\}$

$L_z : -l\hbar, \cdots +l\hbar$
$S_z : -s\hbar \cdots +s\hbar$) $(2l+1) \times (2s+1)$

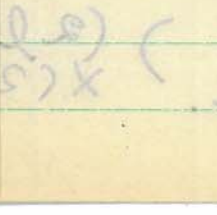
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$$LS = \frac{J(J+1) - L(L+1) - S(S+1)}{2}$$

$\therefore$ $J^2 = (L+S)^2$

$= L^2 + S^2 + 2LS$

Addition of Two Angular Momenta
(Vector Model)



$J^2 = j(j+1)\hbar^2$

$j = l+s \cdots l-s.$

$L^2 = l(l+1)\hbar^2$

$S^2 = s(s+1)\hbar^2$

1st repr:

$L^2, S^2; L_z, S_z$: diagonal rows and columns

$(2l+1)(2s+1)$

2nd repr:

$L^2, S^2; J^2, J_z$: diagonal rows and columns

$\sum_{j=|l-s|}^{l+s} (2j+1)$

δ-function

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Dirichlet's Theorem

$$\int \bar{\psi}\psi_{dv} = |c|^2 \int\cdots\int a(p_x' p_y' p_z')\,\bar{a}(p_x'' p_y'' p_z'') \exp\left\{\frac{i(p_x' - p_x'')x + \cdots}{\hbar}\right\} (dp')(dp'')(dx)$$

$$k_x = p_x' - p_x'', \quad \kappa_x = \frac{p_x' + p_x''}{2}$$

$$|c|^2 \cdot \int (d\kappa) \underbrace{\int f(k_x, k_y, k_z; \kappa_x, \kappa_y, \kappa_z) \exp\left(\frac{i k x + \cdots}{\hbar}\right)}_{(dk)(dx)}$$

$$\hbar \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(k_x\cdots) e^{ik_x x/\hbar}\, dk_x\, dx$$

$$k_x/\hbar = a.$$

$$= \hbar \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} g(a) e^{iax}\, da$$

$$= (\hbar) \lim_{X\to\infty} \int_{-\infty}^{+\infty} g(a)\, da \int_{-X}^{X} e^{iax}\, dx$$

$$= (\hbar) \lim_{X\to\infty} \int_{-\infty}^{+\infty} g(a) \frac{2\sin aX}{a}\, da$$

$$= (\hbar) \cdot 2\pi\, g(0) = \hbar\, g(0) = \hbar f(0; k_y \cdots)$$

$$\int \bar{\psi}\psi\, dv = \underbrace{|c|^2 \hbar^3}_{} \iiint |a(p_x' p_y' p_z')|^2\, dp_x'\, dp_y'\, dp_z'$$

$$c = \hbar^{-3/2}$$

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Uncertainty relation

Heisenberg, Physical principles

of the q. t. 1930.

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General Formalism
(general Transformation Theory)

Dirac
Jordan (1927)

Dirac, Principles of Q. M. 1947.

1. Representations of state — State-vector
coordinate representation* (Schröd. fn)
$\psi(q'_1, q'_2 \cdots q'_n, t)$.
momentum representation
$\psi(q'_1, q'_2 \cdots q'_n, t)$
$= h^{-\frac{n}{2}} \int \cdots \int a(p'_1 \cdots p'_n, t)\, e^{i\sum_{r=1}^{n} p'_r q'_r / h}\, dp'_1 \cdots dp'_n$

$a(p'_1 \cdots p'_n, t)$; wave fn in momentum space.

$$a(p'_1 \cdots p'_n, t) = h^{-\frac{n}{2}} \int \cdots \psi(q', t)\, e^{-i q' p'/h}\, dq'$$

$$\int_{-\infty}^{+\infty} e^{-i q' p'/h}\, dq' = 2\pi h \cdot \delta(p')$$

Both ψ and a can be regarded as different representations of

---

* $q'_1 q'_2 \cdots q'_n$: ~~eigen-values~~ numerical parameters which can take all possible values of coordinates.

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the same state, just as (x, y, z) and (r, θ, φ) ~~are (or~~ are or (x', y', z') are different representations of the same vector $\mathbf{r}$, the transformation function being $e^{\frac{i}{\hbar} \Sigma p_i r_i}$

in our case. Thus, the state can be visualized as a vector in a space, which is a complex space with infinitely many dimensions, in fact, continuous many dimensions.

More generally, we can expand $\psi(q_1 \cdots q_n, t)$ into a series of orth. and normalized eigenfunctions $\psi_j(q_1 \cdots q_n)$, $j = 1, 2, \cdots$

$$\psi = \sum_j c_j(t)\, \psi_j,$$

In that case, the state-vector can be represented by enumerably infinite number of coefficients (or coordinates) $c_j(t)$, which can change with time.

Since ψ, a, c_j are complex in general, ~~we~~ where are complex

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conjugate quantities $\hat{\psi}, \hat{a}, \hat{c}_j$.
And it is more convenient to
consider ~~the two~~ that there are
two vectors corresponding to
a ~~state~~ single state.
Dirac used the notations
ket $|\rangle \rightarrow |A\rangle$
and
bra $\langle| \rightarrow \xi\langle A|$.
in 3rd ed. but in former editions
he used more familiar notations
ψ and ϕ.

2.
a) Repeatability
b) Predictability

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Definition of Observable
Expansion into series of Eigenvectors
Compatibility of Measurements
Simultaneous measurements

Definition of operating on < 1 ;
(Self-adjoint operator)
$(\langle B|\alpha\rangle|A\rangle = \langle B|(\alpha|A\rangle)$

~~Adjoint~~ Hermitian conj. operator

$$\langle B|\alpha^*|A\rangle = \overline{\langle A|\alpha|B\rangle}$$

$$\alpha^*_{rs} = \tilde{\alpha}_{sr}$$

$$(\alpha\beta)^* = \beta^*\alpha^*$$

$$\therefore \langle B|(\alpha\beta)^*|A\rangle = \overbrace{\langle A|\alpha\beta|B\rangle}$$

Definition: Hermitian conjugate / ~~Adjoint~~ operator

$$\alpha|A\rangle = |B\rangle$$

$$\langle A|\tilde{\alpha}^* = \langle B|$$

$$\langle A|\tilde{\alpha}^*|C\rangle = \langle B|C\rangle$$

$$\langle C|\alpha^*|A\rangle = \underline{\langle C|B\rangle}$$

$$\langle A|\tilde{\alpha}^*|C\rangle = \overline{\langle C|\alpha|A\rangle}$$

Self-adjoint operator

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~~$\langle A | A \rangle =$~~

$(\langle B | \alpha) \cdot |A\rangle = \langle B | (\alpha | A \rangle)$

$\downarrow C \qquad \pi C \qquad \downarrow C$

$= \langle B | \alpha | A \rangle$

Basic Vectors : $\hat{i}, \hat{j}, \hat{k}$ $\qquad |a'\rangle$

Observables with
Continuous Eigenvalues

$\xi |\xi'\rangle = \xi' |\xi'\rangle$

ξ' : continuous

$$|A\rangle = \int C(\xi') |\xi'\rangle \, d\xi'$$

$$|\xi''\rangle = \int \langle \xi' | \xi'' \rangle \, |\xi'\rangle \, d\xi'$$

$$|\xi'\rangle = \int \langle \xi'' | \xi' \rangle \, |\xi''\rangle \, d\xi''$$

$$|A\rangle = \iint C(\xi') \langle \xi'' | \xi' \rangle \, |\xi''\rangle \, d\xi' d\xi''$$

$$= \iint C(\xi'') \langle \xi' | \xi'' \rangle \, |\xi'\rangle \, d\xi' d\xi''$$

$$\int C(\xi'') \langle \xi' | \xi'' \rangle \, d\xi'' = C(\xi')$$

for any continuous function $C(\xi')$

$\int \langle \xi' | \xi'' \rangle \, d\xi'' = 1$

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$\langle \xi' | \xi'' \rangle = \delta(\xi' - \xi'')$

condition

$\int \delta(\xi' - \xi'') \, d\xi'' = 1$

$\delta(\xi' - \xi'') = 0 \quad$ for $\xi' - \xi'' \neq 0$.

δ-function.

Normalization of $|\xi'\rangle$.

$\langle \xi'' | \xi' \rangle = \delta(\xi' - \xi'')$

$\int \tilde{\psi}_{\xi''}(q') \, \psi_{\xi'}(q') \, dq' = \delta(\xi' - \xi'')$

$\psi_{p'}(q') = h^{-1/2} \cdot e^{i p' q'/\hbar}$

$h^{-1} \int_{-\infty}^{+\infty} e^{i(p' - p'')q'/\hbar} \, dq' = \delta(p' - p'')$

Normalization:

$\langle A | f(q) | A \rangle$: exp. value

$f(q) | A \rangle = \int f(q') | q' \rangle \, dq' \langle q' | A \rangle$

$\langle A | f(q) | A \rangle = \int f(q') |\langle q' | A \rangle|^2 \, dq'$

only if $\langle q' | q'' \rangle = \delta(q' - q'')$

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Representation of observables

$|A\rangle = \int |q'\rangle dq' \langle q'|A\rangle$

$\alpha |q''\rangle = \int |q'\rangle dq' \langle q'|\alpha|q''\rangle$

~~$\beta \alpha |q''\rangle = \int$~~

$\alpha|q''\rangle = \int |q'''\rangle dq''' f(q''', q'')$

$\langle q'|\alpha|q''\rangle = f(q', q'')$

$\alpha\beta|q''\rangle = \alpha\{\int |q'''\rangle dq''' \langle q'''|\beta|q''\rangle\}$

$= \int |q'''\rangle dq''' \langle q'''|\alpha|q''\rangle dq'' \langle q''|\beta|q''\rangle$

$\langle q'|\alpha\beta|q''\rangle = \int \langle q'|\alpha|q''\rangle dq'' \langle q''|\beta|q''\rangle$

unit operator

$1|q''\rangle = \int |q'\rangle dq' \langle q'|1|q''\rangle$

$= |q''\rangle$

$\langle q'|1|q''\rangle = \delta(q'-q'')$

diagonal matrix

$f(q')\delta(q'-q'')$

$\langle q'|q|q''\rangle = q'\delta(q'-q'')$

$(\because \quad q|q''\rangle = q'|q'\rangle$

$= \int |q'\rangle dq' \langle q'|q|q''\rangle)$

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$$\langle q'|p|q''\rangle = i\hbar \frac{\delta(q'-q''+dq'')-\delta(q'-q'')}{dq''}$$

$$p|q''\rangle = +i\hbar \frac{|q''+dq''\rangle - |q''\rangle}{dq''}$$

$$\langle q'|p|q''\rangle = -i\hbar \cdot \delta'(q'-q'')$$

$$\langle q'|qp-pq|q''\rangle = i\hbar\,\delta(q'-q'') = i\hbar\langle q'|1|q''\rangle$$

$$\therefore = \int \langle q'|q|q'''\rangle dq''' \langle q'''|p|q''\rangle - \int \langle q'|p|q'''\rangle dq''' \langle q'''|q|q''\rangle$$

$$= -i\hbar \{ q'\delta'(q'-q'') - q''\delta'(q'-q'')\}$$

$$= -i\hbar (q'-q'')\delta'(q'-q'')$$

$$\int f(q')(q'-q'')\delta'(q'-q'')dq'$$

$$= -\int \frac{\partial}{\partial q'}\{f(q')(q'-q'')\}\delta(q'-q'')dq'$$

$$= -\int \frac{\partial f}{\partial q'}(q'-q'')\delta(q'-q'')dq'$$

$$-\int f(q')\delta(q'-q'')dq'$$

$$= -f(q'')$$

$$(q'-q'')\delta'(q'-q'') = -\delta(q'-q'')$$

more generally

$$\langle q'|p|q''\rangle = -i\hbar\delta'(q'-q'') + f(q')\delta(q'-q'')$$

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Example: Particle with spin

$x p_x - p_x x = i\hbar$ etc

$\sigma_x\sigma_y - \sigma_y\sigma_x = 2i\sigma_z$ etc

$\sigma_x^2 = 1$ etc

complete set of commuting observables:

(x, y, z, σ_z)

or $(p_x, p_y, p_z, \sigma_z)$

or $(r, \theta, \phi, \sigma_z)$

or (H, M, m_z, σ_z)

$H = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$

~~$\psi(x, y, z, \sigma_z)$~~

$H|r', M', m_z', \sigma_z'\rangle = E'|\cdots\rangle$

$M|r', M', m_z', \sigma_z'\rangle = M'|\cdots\rangle$

$m_z|\quad\cdots\quad\rangle = m_z'|\cdots\rangle$

$\sigma_z|\quad\cdots\quad\rangle = \sigma_z'|\cdots\rangle$

$\psi_{r'',l,m,\pm}(r', \theta', \varphi', \sigma_z') = \sum_{l+\frac{1}{2}} \delta(r'-r'') P_l^m(\cos\theta') e^{im\varphi'}$

$+:$ $\times\ \alpha(\sigma_z')$ $\quad \alpha(+1)=1,\ \alpha(-1)=0$

$-:$ $\times\ \beta(\sigma_z')$ $\quad \beta(+1)=0,\ \beta(-1)=1$

$\psi_A(r', \theta', \varphi', \sigma_z') = \sum_{\pm} \sum_{l,m} \int_0^\infty \chi^{(\pm)}_{l,m}(r'')\, \delta(r'-r'')\, P_l^m \cdot e^{im\varphi'} \cdots dr''$

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~~$\langle r'+r'' \rangle = \dfrac{\delta(r'-r'')}{r'^2}$~~

$$\psi_A(r',\theta',\varphi',\sigma_z') = \sum_{l,m} \chi^{(+)}_{l,m}(r')\, P_l^m(\cos\theta')\, e^{im\varphi'}\, \alpha(\sigma_z')$$

$$+ \sum_{l,m} \chi^{(-)}_{l,m}(r')\, P_l^m(\cos\theta')\, e^{im\varphi'}\, \beta(\sigma_z')$$

$\chi^{(\pm)}_{lm}(r')$: representation of arbitrary state with basic vectors

$|r', M', m_z', \sigma_z'\rangle$

$0 \le r' < \infty$

$M' = \hbar^2 l(l+1)$

$m_z' = m' \cdot \hbar$

$\sigma_z' = +1, -1$.

physical interpretation of

$|\chi^{(\pm)}_{lm}(r')|^2$.

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Schrödinger equation

$\psi_A(t) \equiv |A,t\rangle$

$\alpha_1 \alpha_2 \cdots \alpha_m$ i $\alpha_1' \alpha_2' \cdots \alpha_m'$ t

$$\frac{d\psi_A(t)}{dt} \equiv \frac{d}{dt}|A,t\rangle$$

$$= \lim_{\Delta t \to 0} \frac{|A,t+\Delta t\rangle - |A,t\rangle}{\Delta t}$$

$$i\hbar \frac{d|A,t\rangle}{dt} = H|A,t\rangle$$

$$|A,t\rangle = \int\cdots\int |q_1' \cdots q_n'\rangle \langle q_1' \cdots q_n'|A,t\rangle \, dq_1' \cdots dq_n' \quad (t_0)$$

$$i\hbar \frac{d}{dt}|A,t\rangle = \int\cdots\int |q_1' \cdots q_n'\rangle i\hbar \frac{\partial}{\partial t}\langle q_1' \cdots q_n'|A,t\rangle \, dq_1' \cdots dq_n'$$

$$H|A,t\rangle = \int\cdots\int |q_1'' \cdots q_n''\rangle \langle q_1'' \cdots q_n''|H|q_1' \cdots q_n'\rangle \langle q_1' \cdots q_n'|A,t\rangle \, dq_1' \cdots dq_n' \, dq_1'' \cdots dq_n''$$

$$i\hbar \frac{\partial}{\partial t}\langle q_1' \cdots q_n'|A,t\rangle$$

$$= \int \langle q_1' \cdots q_n'|H|q_1'' \cdots q_n''\rangle \langle q_1'' \cdots q_n''|A,t\rangle$$

$$i\hbar \frac{\partial}{\partial t}\psi(q_1' \cdots q_n', t) = H\left(q_1' \cdots q_n', -i\hbar \frac{\partial}{\partial q_1'} \cdots\right) \times \psi(q_1'' \cdots q_n'', t)$$

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Heisenberg eq. of motion

In Schrödinger rep. dynamical quantities which do not contain time explicitly are represented by matrices which time-independent coefficients.

On the contrary, in Heisenberg repr.

$$|A,t\rangle = \sum_{\alpha_1'\alpha_2'\cdots\alpha_n'} |\alpha_1'\alpha_2'\cdots\alpha_n' t\rangle \langle \alpha_1'\alpha_2'\cdots\alpha_n' t|A\rangle$$

where

$$i\hbar \frac{d}{dt} |\alpha_1'\alpha_2'\cdots\alpha_n' t\rangle = H |\alpha_1''\cdots\alpha_n'' t\rangle$$

$$\left(= \sum |\alpha_1''\cdots\alpha_n'' t\rangle \langle \alpha_1''\cdots\alpha_n''|H|\alpha_1'\cdots\alpha_n'\rangle\right)$$

then

$$i\hbar \frac{d}{dt}|A,t\rangle = \sum_{\alpha'',\alpha'} |\alpha_1''\cdots\alpha_n'' t\rangle\langle\alpha_1''\cdots\alpha_n''|H|\alpha_1'\cdots\alpha_n'\rangle \times \langle\alpha_1'\cdots\alpha_n' t|A\rangle$$

$$H|A,t\rangle =$$

$$= \sum_{\alpha_1'\cdots\alpha_n'} \left\{ i\hbar \frac{d}{dt} |\alpha_1'\alpha_2'\cdots\alpha_n' t\rangle \langle\alpha_1'\alpha_2'\cdots\alpha_n' t|A\rangle \right.$$

$$\left. + |\alpha_1'\alpha_2'\cdots\alpha_n' t\rangle i\hbar \frac{\partial}{\partial t} \langle\alpha_1'\cdots\alpha_n' t|A\rangle \right\}$$

$$H|A,t\rangle = \sum_{\alpha'} H|\alpha_1''\cdots\alpha_n'' t\rangle \cdot \langle\alpha_1'\cdots\alpha_n' t|A\rangle$$

or

$$\langle\alpha_1''\cdots\alpha_n''t| \quad \sum_{\alpha_1'\cdots\alpha_n'} |\alpha_1'\cdots\alpha_n' t\rangle \, i\hbar \frac{\partial}{\partial t} \langle\alpha_1'\cdots\alpha_n' t|A\rangle = 0$$

$$i\hbar \frac{\partial}{\partial t} \langle\alpha_1'\cdots\alpha_n' t|A\rangle = 0.$$

$$\therefore |A,t\rangle = \sum |\alpha_1'\cdots\alpha_n' t\rangle\langle\alpha_1'\alpha_2'\cdots\alpha_n'|A\rangle$$

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~~Problem of Measuring Process~~

$|\alpha_1' \cdots \alpha_m', t\rangle = e^{-iH(t-t_0)/\hbar} |\alpha_1' \cdots \alpha_m', t_0\rangle$

$|\alpha_1' \cdots \alpha_m', t\rangle = e^{-iHt/\hbar} |\alpha_1' \cdots \alpha_m', 0\rangle$

$i\hbar \frac{d}{dt} |\alpha_1' \cdots \alpha_m' t\rangle = H |\alpha_1' \cdots \alpha_m' t\rangle$

Now, if $\alpha_1, \alpha_2, \cdots \alpha_m$ are all commutative with H,

$|\alpha_1' \cdots \alpha_m', t\rangle = e^{-iE't/\hbar} |\alpha_1' \cdots \alpha_m'; 0\rangle$

because H is a function of $\alpha_1 \cdots \alpha_m$.

$E' = H(\alpha_1' \cdots \alpha_m')$.

$|A, t\rangle = \sum_{\alpha_1' \cdots \alpha_m'} |\alpha_1' \cdots \alpha_m' 0\rangle e^{-iE't/\hbar} \langle \alpha_1' \cdots \alpha_m' | A \rangle$

~~$\beta |\alpha_1' \cdots \alpha_m' t\rangle$~~

$\beta |\alpha_1'' \cdots \alpha_m'' t\rangle = \sum_{\alpha'} |\alpha_1' \cdots \alpha_m' t\rangle \cdot \langle \alpha_1' \cdots t | \beta | \alpha_1'' \cdots t \rangle$

~~$= \sum |\alpha_1' \cdots \alpha_m' 0\rangle e^{-iE't/\hbar} \langle \alpha_1' t | \beta | \alpha_1'' t \rangle$~~

~~$\langle \alpha_1''' \cdots t | \beta | \alpha_1'' \cdots \alpha_m'' t \rangle = \sum_{\alpha'} \langle \alpha_1''' \cdots t | \alpha_1' \cdots \alpha_m' 0 \rangle e^{-iE't/\hbar}$~~

~~$i\hbar \frac{d}{dt} \{ \beta |\alpha_1'' \cdots \alpha_m'' t\rangle \} =$~~

$\beta |\alpha_1'' \cdots \alpha_m'' 0\rangle = \sum_{\alpha'} |\alpha_1' \cdots \alpha_m' 0\rangle \langle \alpha_1' \cdots | \beta | \alpha_1'' \cdots \rangle$

$\beta |\alpha_1'' \cdots \alpha_m'' t\rangle e^{iE''t/\hbar} = \sum |\alpha_1' \cdots \alpha_m' t\rangle e^{iE't/\hbar} \langle \alpha_1' \cdots | \beta | \alpha_1'' \cdots \rangle$

$\langle \alpha_1' \cdots t | \beta | \alpha_1'' \cdots t \rangle = e^{i(E'-E'')t/\hbar} \langle \alpha_1' \cdots | \beta | \alpha'' \cdots \rangle$

Heisenberg rep.　　Schrödinger repr.

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Formally, one may write define

$\frac{d\beta}{dt}$ by

$$\frac{d\beta}{dt}\cdot|A\rangle = \frac{d}{dt}\{\beta|A\rangle\} - \beta\frac{d}{dt}|A\rangle$$

$$i\hbar\frac{d\beta}{dt}|A\rangle = H\beta - \beta$$

So the matrix $\langle\alpha_1'\cdots t|\beta|\alpha_1''\cdots t\rangle \equiv \beta$

satisfies the q.m.e. eq.

$$i\hbar\frac{d\beta}{dt} = [\beta, H]$$

where

$$\langle\alpha_1'\cdots t|H|\alpha_1'' \quad t\rangle = E'\delta_{\alpha_1'\alpha_1''}\cdots\delta_{\alpha_n'\alpha_n''}$$

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Problem of Measurement

Causal and Acausal Changes of the state

(i) $i\hbar \frac{d|A\rangle}{dt} = H|A\rangle$

$i\hbar \frac{\partial \psi}{\partial t} = H\psi$.

continuous and causal (predictable)

(ii) observation of $|A\rangle = |\alpha_1' \cdots \alpha_n' \, t\rangle$ ($\beta_1 \cdots \beta_n$ at time t)

$\rightarrow |\beta_1' \cdots \beta_n' \, t\rangle$

if the result $(\beta_1' \cdots \beta_n')$ is obtained

Contraction of wave packet

if β's are q's.

discontinuous and acausal

(unpredictable)

unknown change in the phase

(uncertainty)

Interference by disturbance

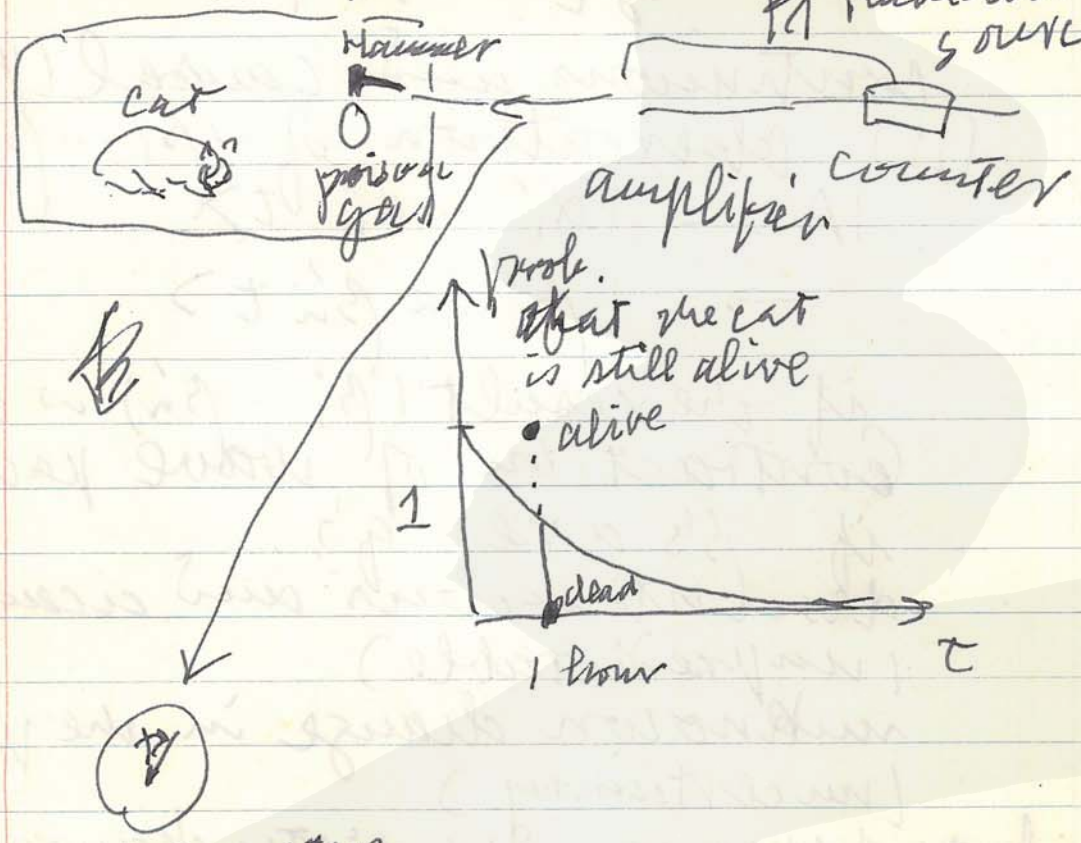
due to the act of measurement.

~~Does~~

Thus, ~~it seems that~~ the uncontrollable disturbance on the microscopic object is the origin of unpredictability of an ~~event.~~ atomic event, ~~so~~ Thus, one may conclude that the unpredictability ~~to refer~~ appears is inherent only in microscopic phenomena. However,

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This is not True:
Schrödinger's paradox
The fate of the cat can be observed without
any disturbance on the total system,
but still unpredictable.



electrometer
classical dynamical system

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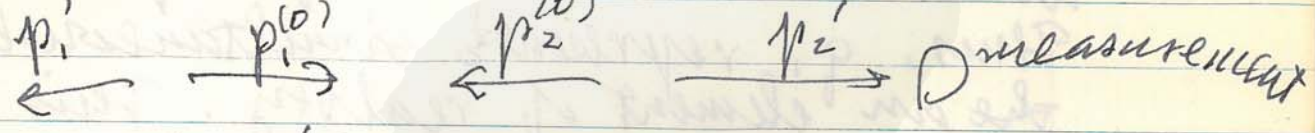
Einstein - Podolsky - Rosen's paradox.

Definition of reality: If a quantity α can be measured without disturbing the system, we think that α corresponds the physical reality.

Two particle system one dimensional motion. (object A, apparatus B)

$A(q_1, p_1)$, $B(q_2, p_2)$

$p_1 + p_2$: const. (0, any)



$p_1' + p_2' = 0$ or $p_1' = -p_2'$

State before the measurement

$$\psi(q_1', q_2') = \int_{-\infty}^{+\infty} \int a(p_1', p_2') e^{i(q_1' p_1' + q_2' p_2')/\hbar} dp_1' dp_2'$$

$$\delta(p_1' + p_2')$$

$$= \int_{-\infty}^{+\infty} a(p') e^{i(q_1' - q_2')p'/\hbar} dp'$$

p_1 represents an element of reality related to the first particle.

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If, in particular,

$$a(p') = \frac{1}{h} e^{iqp'}$$

$$\psi(q_1' q_2') = \frac{1}{h} \int_{-\infty}^{+\infty} \exp\{i(q_1' - q_2' + q_0)p'/\hbar\} dp'$$

$$= \delta(q_1' - q_2' + q_0)$$

Thus, if we measure q_2 and obtain a result q_2', we can conclude that

$$q_1' = q_2' - q_0$$

without disturbing the first particle. Thus, q_1 represents simultaneously ~~the~~ an element of reality. This seems to contradict ~~the~~ uncertainty principle.

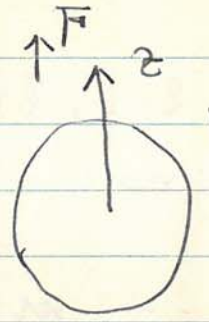
Now the requirements for a complete physical theory

1. Every ~~physical~~ element of physical reality must have a counterpart in the theory
2. ~~And~~ and separately existing elements of reality.
3. The world can be analysed in terms of distinct
4.

Wave fn does not provide a complete description because it contradict with the simultaneous definition of q_1 and p_1, both of which are elements of reality.

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Stark effect



$H' = eFz$

$V = -Fz$

n^2-fold degeneration

$$\begin{vmatrix} -W+W_n^{(0)} & +H_{12} & \cdots & +H_{1k} \\ +H_{21} & -W+W_n^{(0)} & & \\ \vdots & & \ddots & \\ +H_{k1} & & & -W+W_n^{(0)} \end{vmatrix} = 0 \qquad k = n^2$$

$n=2$: $l=1$ ($m=1,0,-1$), $l=0$ ($m=0$)

$n=1$: $l=0$ ($m=0$)

$\langle nlm | H' | n'l'm' \rangle$

$= eF \iiint \tilde{\psi}_{nlm}(r\theta\varphi)\, r\cos\theta \times \psi_{n'l'm'}(r\theta\varphi)\, r^2 dr \sin\theta d\theta d\varphi$

$N_l^m N_{l'}^{m'} \int\int \cos\theta\, P_l^m(\cos\theta)\, P_{l'}^{m'}(\cos\theta) \sin\theta d\theta d\varphi$

$= N_l^m N_{l'}^{m'} \int_0^{\pi} \left\{ \frac{l \pm m + 1}{2l+1} P_{l+1}^m(\cos\theta) + \frac{l \pm m}{2l+1} P_{l-1}^m(\cos\theta) \right\} P_{l'}^{m'}(\cos\theta) \sin\theta d\theta d\varphi$

$l' = l+1$:

$= \cdots \cdot \frac{l+|m|+1}{2l+1} \sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}} \sqrt{\frac{(2l+3)(l+1+|m|)!}{4\pi(l+1+|m|)!}}$

$= \cdots \cdot \frac{(l-|m|)!}{(l+|m|)!} \times \frac{4\pi}{2l+3}$

$= \sqrt{\frac{(l+|m|+1)^3}{(2l+1)(2l+3)(l-|m|)}}$

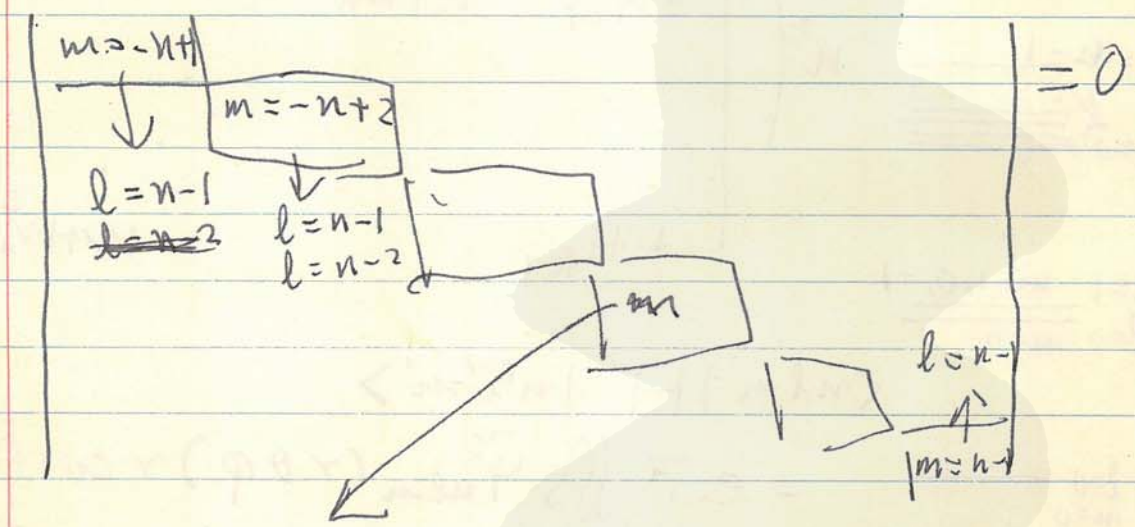
etc.

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$\langle n l m | H' | n'' l' m' \rangle$

$= 0$ unless $l' = l-1, l+1$
$m' = m$

~~$m = 0$~~ $-n+1$, $m = -n+2$, ... $m = n-1$



$|m| = \mu$:
$l = \mu, \mu+1, \cdots n-1$

$n-\mu$

$$\begin{vmatrix} W^{(0)} - W & H_{\mu,\mu+1} & 0 & 0 & \cdots \\ H_{\mu+1,\mu} & W^{(0)} - W & H_{\mu+1,\mu+2} & & \\ 0 & H_{\mu+2,\mu+1} & W^{(0)} - W & \ddots & H'_{n-2,n-1} \\ \cdots & & \ddots & H'_{n-1,n-2} & W^{(0)} - W \end{vmatrix} = 0$$

$n-\mu$

$H'_{l,l\pm1} \equiv$ ~~$R_{n,l,m}$~~ $\cdot \langle n,l,m | H' | n,l\pm1,m \rangle$

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Parabolic coordinates:

$\lambda_1 = r + z \quad 0 \le \lambda_1 < \infty$

$\lambda_2 = r - z \quad 0 \le \lambda_2 < \infty$

$0 \le \varphi < 2\pi$

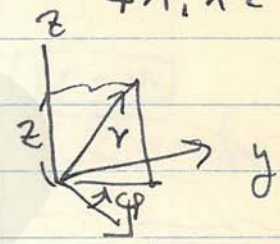
$$\Delta\psi = \frac{4}{\lambda_1+\lambda_2}\left\{\frac{\partial}{\partial\lambda_1}\left(\lambda_1\frac{\partial\psi}{\partial\lambda_1}\right)+\frac{\partial}{\partial\lambda_2}\left(\lambda_2\frac{\partial\psi}{\partial\lambda_2}\right)+\frac{\lambda_1+\lambda_2}{4\lambda_1\lambda_2}\frac{\partial^2\psi}{\partial\varphi^2}\right\}$$

$\varphi = \arctan\frac{y}{x}$

$$\frac{2m}{\hbar^2}V(r)\psi = -\frac{2mZe^2}{\hbar^2}\cdot\frac{4}{\lambda_1+\lambda_2}\quad \psi = \beta\frac{4}{\lambda_1+\lambda_2}\psi$$

$$\Delta\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

$$\frac{\partial}{\partial\lambda_1}\left(\lambda_1\frac{\partial\psi}{\partial\lambda_1}\right)+\frac{\partial}{\partial\lambda_2}\left(\lambda_2\frac{\partial\psi}{\partial\lambda_2}\right)+\frac{\lambda_1+\lambda_2}{4\lambda_1\lambda_2}\frac{\partial^2\psi}{\partial\varphi^2} - \left(\frac{\lambda_1+\lambda_2}{4r_0^2} - \beta\right)\psi = 0$$



$\psi = \Lambda_1\Lambda_2 e^{im\varphi}$

$$\frac{\partial}{\partial\lambda_1}\left(\lambda_1\frac{\partial\Lambda_1}{\partial\lambda_1}\right)+\left(\beta_1 - \frac{\lambda_1}{4r_0^2} - \frac{m^2}{4\lambda_1}\right)\Lambda_1 = 0$$

$$\frac{\partial}{\partial\lambda_2}\left(\lambda_2\frac{\partial\Lambda_2}{\partial\lambda_2}\right)+\left(\beta_2 - \frac{\lambda_2}{4r_0^2} - \frac{m^2}{4\lambda_2}\right)\Lambda_2 = 0$$

$\beta_1 + \beta_2 = \beta = \frac{mZe^2}{\hbar^2}$

$x = \frac{\lambda_1}{r_0} \quad y = \frac{\lambda_2}{r_0}$

$$\frac{\partial}{\partial x}\left(x\frac{\partial\Lambda_1}{\partial x}\right)+\left(\beta_1 r_0 - \frac{x}{4} - \frac{m^2}{4x}\right)\Lambda_1 = 0$$

$$\frac{\partial}{\partial y}\left(y\frac{\partial\Lambda_2}{\partial y}\right)+\left(\beta_2 r_0 - \frac{y}{4} - \frac{m^2}{4y}\right)\Lambda_2 = 0$$

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$$\Lambda_1^{(0)} = e^{-x/2} x^{\frac{|m|}{2}} L_{|m|+n_1}^{|m|}(x)$$

$$\Lambda_2^{(0)} = e^{-y/2} y^{\frac{|m|}{2}} L_{m+n_2}^{m}(y)$$

$$\frac{|m|}{2} + n_1 \simeq \beta_1 r_0 - \frac{1}{2}$$

$$\frac{|m|}{2} + n_2 \simeq \beta_2 r_0 - \frac{1}{2}$$

$$\beta r_0 = n_1 + n_2 + |m| + 1$$

$$\simeq n$$

$m=0$: $n_1 - n_2 = n-1$

$m=\pm 1$: $n_1 - n_2 = n-2$

$|m|=n-1$: $n_1 - n_2 = n-3$

$|m|=n-2$: $n-4$

$2n-3$: $n_1 - n_2 = 0$

n

$n_1 - n_2 = 1$

$n_1 - n_2 = -1$

$=n+2$

$n_1 - n_2 = -n+1$

$n_1 - n_2 = -n+1$

n

$$2\{1 + 3 + \cdots + (2n-1)\} - n^2$$

$$= n^2 - 2n + 1 = (n-1)^2$$

$$= n(n+1) - n = n^2 \text{ - states}$$

$2n-1$ - levels

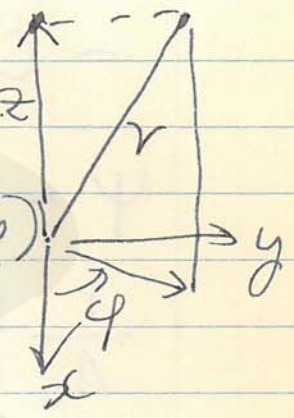
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Parabolic Coordinates

$\lambda_1 = r + z \qquad 0 \le \lambda_1 < \infty$

$\lambda_2 = r - z \qquad 0 \le \lambda_2 < \infty$

$\varphi = \arctan \frac{y}{x} \qquad 0 \le \varphi < 2\pi$



$$-\Delta\psi + \frac{2m}{\hbar^2}(E - V(r) - eFz)\psi = 0$$

$$V(r) = -\frac{Ze^2}{r} \qquad \psi(\lambda_1, \lambda_2, \varphi)$$

$$\frac{\partial}{\partial\lambda_1}\left(\lambda_1 \frac{\partial\psi}{\partial\lambda_1}\right) + \frac{\partial}{\partial\lambda_2}\left(\lambda_2 \frac{\partial\psi}{\partial\lambda_2}\right) + \frac{\lambda_1+\lambda_2}{4\lambda_1\lambda_2}\frac{\partial^2\psi}{\partial\varphi^2} + \left(-\frac{A}{4}(\lambda_1+\lambda_2) + B - \frac{C}{4}(\lambda_1^2 - \lambda_2^2)\right)$$

$$A = \frac{mE}{2\hbar^2} \quad \zeta = \frac{1}{r_0^2} \qquad B = \frac{mZe^2}{2\hbar^2} \qquad C = \frac{eF}{2}\frac{m}{\hbar^2}$$

$$\Delta\psi = \frac{4}{\lambda_1+\lambda_2}\left\{\frac{\partial}{\partial\lambda_1}\left(\lambda_1\frac{\partial\psi}{\partial\lambda_1}\right) + \frac{\partial}{\partial\lambda_2}\left(\lambda_2\frac{\partial\psi}{\partial\lambda_2}\right) + \frac{\lambda_1+\lambda_2}{4\lambda_1\lambda_2}\frac{\partial^2\psi}{\partial\varphi^2}\right\}$$

$$V = -\frac{Ze^2}{r} = \frac{-2Ze^2}{\lambda_1+\lambda_2} \qquad \frac{eFz}{V} = -\frac{\lambda_1^2 - \lambda_2^2}{2}\left(\frac{eF}{Ze^2}\right)$$

$$eFz = \frac{2eF}{2}(\lambda_1 - \lambda_2)$$

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$$\Psi \propto e^{i m \varphi}$$

$$\frac{\partial}{\partial \lambda_1}\left(\lambda_1 \frac{\partial \Psi}{\partial \lambda_1}\right) + \frac{\partial}{\partial \lambda_2}\left(\lambda_2 \frac{\partial \Psi}{\partial \lambda_2}\right) \pm \left(\frac{m^2}{4\lambda_1} + \frac{m^2}{4\lambda_2}\right)\Psi$$

$$- \frac{1}{4 r_0^2}(\lambda_1 + \lambda_2)\Psi + B\Psi$$

$$- C(\lambda_1^2 - \lambda_2^2)\Psi = 0$$

$$\Psi = \Lambda_1(\lambda_1)\Lambda_2(\lambda_2) e^{i m \varphi}$$

$$\frac{1}{\Lambda_1}\frac{d}{d\lambda_1}\left(\lambda_1 \frac{d\Lambda_1}{d\lambda_1}\right) + \frac{1}{\Lambda_2}\frac{d}{d\lambda_2}\left(\lambda_2 \frac{d\Lambda_2}{d\lambda_2}\right)$$

$$\pm \frac{m^2}{4\lambda_1} \pm \frac{m^2}{4\lambda_2} - \frac{1}{4 r_0^2}\lambda_1 - \frac{1}{4 r_0^2}\lambda_2$$

$$+ B - C\lambda_1^2 + C\lambda_2^2 = 0$$

$$\frac{d}{d\lambda_1}\left(\lambda_1 \frac{d\Lambda_1}{d\lambda_1}\right) - \left(\frac{1}{4 r_0^2}\lambda_1 \pm \frac{m^2}{4\lambda_1} - B_1 + C\lambda_1^2\right)\Lambda_1 = 0$$

$$\frac{d}{d\lambda_2}\left(\lambda_2 \frac{d\Lambda_2}{d\lambda_2}\right) - \left(\frac{1}{4 r_0^2}\lambda_2 + \frac{m^2}{4\lambda_2} - B_2 - C\lambda_2^2\right)\Lambda_2 = 0$$

$$B_1 + B_2 = B$$

$x = \lambda_1/r_0$:
$\Lambda_1 = e^{-x/2} v(x)$

$y = \lambda_2/r_0$
$\Lambda_2 = e^{-y/2} v(y)$

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$$\frac{d}{dx}\left(x\frac{d\Lambda_1}{dx}\right)+\left(\varepsilon_1-\frac{x}{4}-\frac{m^2}{4x^2}\right)\Lambda_1$$

$$-x\cdot x^2\Lambda_1=0$$

$$\frac{d}{dy}\left(y\frac{d\Lambda_2}{dy}\right)+\left(\varepsilon_2-\frac{y}{4}-\frac{m^2}{4y^2}\right)\Lambda_2$$

$$+x\,y^2\Lambda_2=0$$

$\varepsilon_1=B_1 r_0$ $\qquad \varepsilon_2=B_2 r_0$

$\varepsilon_1+\varepsilon_2=B r_0$

$x=C r_0^2=\frac{m}{\hbar^2}\frac{eF}{3}\cdot r_0^2$

Unperturbed system

$C=0$, $\kappa=0$ $\qquad \varepsilon_1=\varepsilon_1^{(0)}$, $\varepsilon_2=\varepsilon_2^{(0)}$

$\Lambda_1^{(0)}=e^{-x/2}u(x)$

$\Lambda_2^{(0)}=e^{-x/2}v(y)$

$u=x^{m/2}L_{m+n_1}^{m}(x)$

$v=y^{m/2}L_{m+n_2}^{m}(y)$

$\frac{m}{2}+n_1=\varepsilon_1^{(0)}-\frac{1}{2}$ $\qquad \varepsilon_1^{(0)}-\varepsilon_2^{(0)}$

$\frac{m}{2}+n_2=\varepsilon_2^{(0)}-\frac{1}{2}$ $\qquad =n_1-n_2$

$\varepsilon_1^{(0)}+\varepsilon_2^{(0)}=n\equiv m+n_1+n_2+1$

$B\cdot\left(\frac{\hbar}{\sqrt{2mE^{(0)}}}\right)=n$ $\qquad E^{(0)}=\frac{-\hbar^2 e^4 m}{2\pi^2 n^2}$

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$\varepsilon_1 = \varepsilon_1^{(0)} + x\varepsilon_1^{(1)}$

Perturbed system $\varepsilon_2 = \varepsilon_2^{(0)} + x\varepsilon_2^{(1)}$

$\Lambda_1(x) = \Lambda_1^{(0)}(x) + x\Lambda_1^{(1)} + \cdots$

$\Lambda_2(y) = \Lambda_2^{(0)}(y) + x\Lambda_2^{(1)} + \cdots$

$$\frac{d}{dx}\left(x\frac{d\Lambda_1^{(1)}}{dx}\right) + \left(\varepsilon_1^{(0)} - \frac{x}{4} - \frac{m^2}{4x^2}\right)\Lambda_1^{(1)} = (x^2 - \varepsilon_1^{(1)})\Lambda_1^{(0)}$$

$$\frac{d}{dy}\left(y\frac{d\Lambda_2^{(1)}}{dy}\right) + \left(\varepsilon_2^{(0)} - \frac{y}{4} - \frac{m^2}{4y^2}\right)\Lambda_2^{(1)} = -(y^2 + \varepsilon_2^{(1)})\Lambda_2^{(0)}$$

$$\int \Lambda_1^{(0)} \frac{d}{dx}\left(x\frac{d\Lambda_1^{(1)}}{dx}\right) dx = \int \Lambda_1^{(1)} \frac{d}{dx}\left(x\frac{d\Lambda_1^{(0)}}{dx}\right) dx$$

$$\int \Lambda_1^{(0)}(x^2 - \varepsilon_1^{(1)})\Lambda_1^{(0)} dx = 0$$

$$\varepsilon_1^{(1)} = \frac{\int x^2 (\Lambda_1^{(0)})^2 dx}{\int (\Lambda_1^{(0)})^2 dx} = 6(n_1+m)^2 + 6(n_1+m)(1-m) + (m-1)(m-2)$$

$$-\varepsilon_2^{(1)} = 6(n_2+m)^2 + 6(n_2+m)(1-m) + (m-1)(m-2)$$

$$\varepsilon_1^{(1)} + \varepsilon_2^{(1)} = 6\{(n_1+m)^2 - (n_2+m)^2\} + 6(n_1-n_2)(1-m) = 6n(n_1-n_2)$$

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$$B\left(\frac{\hbar}{\sqrt{-2mE}}\right) = \xi_1 + \xi_2$$

$$= n + 6\pi n(n_1 - n_2)$$

$$\frac{\hbar^2}{-2mE} = \frac{n^2}{B^2}\left(1 + \frac{eFmr_0^3}{8\hbar^2}(n_1 - n_2)\right)^2$$

$$-\frac{2mE}{\hbar^2} \fallingdotseq \frac{B^2}{n^2}\left(1 - \frac{eFmr_0^3}{4\hbar^2}(n_1 - n_2)\right)$$

$$r_0 = \frac{n}{B} \qquad B = \frac{mZe^2}{\hbar^2}$$

$$E = +E_0 + \frac{3eFmn(n_1 - n_2)}{2\cdot\hbar^2 B}$$

$$= E_0 + \frac{3}{2}\frac{\hbar^2 F}{meZ}n(n_1 - n_2)$$

Schwarzschild - Epstein's formula
linear Stark effect.

$n_1 - n_2 = \pm(n-\mu-1), \pm(n-\mu-3)$
$\cdots \quad \begin{cases} \pm 1 \\ 0 \end{cases}$

$\mu = 0, 1, 2, \cdots n-1$

$n_1 - n_2 = -n+1, -n+2, \cdots n-2, n-1$

$2n-1$

$(n_1 =$

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$(r+z)^{n_1}\ (r-z)^{n_2}$

$n_1 > n_2$

$(r^2-z^2)^{n_2}\ r^{n_1-n_2}\ (1+\cos\theta)^{n_1-n_2}$

$n-1 \geq n_1 \geq 0,\ n-1 \geq n_2 \geq 0$

$n-1 \geq n_1 - n_2 \geq 0.$

$$\int_0^{+\infty} e^{-x} x^{n_1} \left(L^{m}_{m+n_1}\right)^2 dx$$

$k = m+n_1$

$$= \int_0^{+\infty} e^{-x} x^{n_1} \left\{\frac{d^m}{dx^m}\left(e^x \frac{d^k}{dx^k}(x^k e^{-x})\right)\right\}^2 dx$$

$$L^{n_1}_k = \frac{d^m}{dx^m}\left\{e^x \frac{d^k}{dx^k}(x^k e^{-x})\right\}$$

$k = m+n_1$

$$= (-1)^m \int_0^{+\infty} \frac{d^m}{dx^m}\left\{e^{-x} x^m \frac{d^m}{dx^m}\left(e^x \frac{d^k}{dx^k}(x^k e^{-x})\right)\right\} \times e^x \cdot \frac{d^k}{dx^k}(x^k e^{-x})\, dx$$

k 階 : $ax^k + \cdots$

$$= (-1)^m \int_0^{\infty} (a x^k + \cdots) \frac{d^k}{dx^k}(x^k e^{-x})\, dx$$

$$= (-1)^k \int_0^{\infty} a\, k!\, x^k e^{-x} dx$$

$$= (-1)^k (k!)^2 a.$$

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$$x^m \frac{d^m}{dx^m}\left(e^x \frac{d^k}{dx^k}(x^k e^{-x})\right) = ax^k + bx^{k-1} + cx^{k-2} + \cdots$$

$$\int_0^\infty e^{-x} x^{2m+2} \left\{\frac{d^m}{dx^m}\left(e^x \frac{d^k}{dx^k}(x^k e^{-x})\right)\right\}^2 dx$$

$$= (-1)^m \int_0^\infty \frac{d^m}{dx^m}\left\{(ax^{k+2} + bx^{k+1} + cx^k)e^{-x}\right\} e^x \frac{d^k}{dx^k}(x^k e^{-x})\, dx$$

$$\frac{d^m}{dx^m}\left\{(a\underline{x}^{k+2} + b\underline{x}^{k+1} + c\underline{x}^k)e^{-x}\right\}$$

$$= (-1)^m \left\{a x^{k+2} - a\, m(k+2) x^{k+1} + a\frac{m(m-1)}{2}(k+2)(k+1)x^k + bx^{k+1} - bm(k+1)x^k + cx^k\right\} e^{-x}$$

$$\frac{d^k}{dx^k}\left\{ax^{k+2} - am(k+2)x^{k+1} + a\frac{m(m-1)}{2}(k+2)(k+1)x^k + bx^{k+1} - bm(k+1)x^k + cx^k\right\}$$

$$= a\frac{(k+2)!}{2!}x^2 - am(k+2)!\,x + a\frac{m(m-1)}{2}(k+2)! + b(k+1)!\,x - bm(k+1)! - c\,k!$$

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$$\int^{u} e^{-x} x^{m+2} \{\quad\}$$

$$= \sum_{k}^{v} (-1)^k \Big\{ a \frac{(k+2)!}{2} \{ (k+2)! - 2m(k+1)! + m(m-1)\, k! \} + b(k+1)! \{ (k+1)! - m\, k! \} + c\, k!\, k! \Big\}$$

$$= (-1)^k \{ (k!)^2 \{ \tfrac{1}{2}(k+2)(k+1)(k+2-m)(k+1-m) a + (k+1)(k+1-m) b + c \}$$

$$a_1^{(u)} = \frac{1}{2}(k+2)(k+1)(k+2-m)(k+1-m) + (k+1)(k+1-m)\frac{b}{a} + \frac{c}{a}$$

$$a x^k + b x^{k-1} + c x^{k-2} + \cdots$$

$$= x^m \frac{d^m}{dx^m} \left(e^x \frac{d^k}{dx^k} (x^k e^{-x}) \right)$$

$$= x^m \frac{d^m}{dx^m} (A x^k + B x^{k-1} + C x^{k-2} + \cdots)$$

$$= \frac{k!}{(k-m)!} A x^k + \frac{(k-1)!}{(k-m-1)!} B x^{k-1} + \frac{(k-2)!}{(k-m-2)!} C x^{k-2}$$

$$(k+2)(k+1) - 2m(k+1) + m(m-1)$$
$$= (k+2-m)(k+1) - m(k+2-m)$$
$$= (k+2-m)(k+1-m)$$

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$$Ax^k + Bx^{k-1} + Cx^{k-2} + \cdots$$

$$= e^x \frac{d}{dx^k}(x^k e^{-x})$$

$$= (-1)^k \{ x^k - k^2 x^{k-1} + \frac{k^2(k-1)^2}{2} x^{k-2} \cdots \}$$

$$A = (-1)^k \qquad B = -(-1)^k k^2 \qquad C = +\frac{k^2(k-1)^2}{2}$$

$$a = (-1)^k \frac{k!}{(k-m)!}$$

$$b = -(-1)^k \frac{k^2(k-1)!}{(k-m-1)!}$$

$$c = (-1)^k \frac{k^2(k-1)^2(k-2)!}{2(k-m-2)!}$$

$$\frac{b}{a} = -k(k-m)$$

$$\frac{c}{a} = \frac{1}{2} k(k-1)(k-m)(k-m-1)$$

$$a_1^{(1)} = \frac{1}{2}(k+2)(k+1)(k+2-m)(k+1-m)$$

$$-(k+1)\{k(k+1-m)(k-m)$$

$$+ \frac{1}{2} k(k-1)(k-m)(k-m-1)$$

$$= 2k\{(k+1)(k+1-m) - k(k-m)\}$$

$$+ (k+1)(k+1-m)(2-m)$$

$$+ k(k-m)m$$

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$$= 6k^2 + 6k(1-u) + (2-u)(1-u)$$

$$\lambda_1 \simeq r + z \simeq r(1+\cos\theta)$$

$$\lambda_2 \simeq r - z \simeq r(1-\cos\theta)$$

$$d\lambda_1 d\lambda_2 = \begin{vmatrix} \frac{\partial\lambda_1}{\partial r} & \frac{\partial\lambda_2}{\partial r} \\ \frac{\partial\lambda_1}{\partial\theta} & \frac{\partial\lambda_2}{\partial\theta} \end{vmatrix} dr\,d\theta = \begin{vmatrix} 1+\cos\theta & 1-\cos\theta \\ -r\sin\theta & +r\sin\theta \end{vmatrix} dr\,d\theta$$

$$= 2r\sin\theta\, dr\,d\theta$$

$$r^2\sin\theta\, dr\,d\theta = \frac{\lambda_1+\lambda_2}{4} d\lambda_1 d\lambda_2$$

Normalization:

$$N_{n_1 n_2 m}^2 \iiint \left| \Lambda_1^{(0)}(\lambda_1)\Lambda_2^{(0)}(\lambda_2) e^{im\varphi} \right|^2 \frac{\lambda_1+\lambda_2}{4} d\lambda_1 d\lambda_2 d\varphi = 1$$

Perturbation

$$H' = eFz = eF\frac{\lambda_1-\lambda_2}{2}$$

$$H'_{n_1 n_2 m; n_1' n_2' m} = eF \cdot N_{n_1 n_2 m} N_{n_1' n_2' m}$$

$$\times \iiint \left| \Lambda_1^{(0)}(\lambda_1)\Lambda_2^{(0)}(\lambda_2) e^{im\varphi} \right|^2 \frac{\lambda_1^2-\lambda_2}{8} d\lambda_1 d\lambda_2 d\varphi$$

$$= \frac{eF}{8} \frac{\int_{-\infty}^{+\infty} (\Lambda_1^{(0)})^2 \lambda_1^2 d\lambda_1 \int_{-\infty}^{\infty} (\Lambda_2^{(0)})^2 d\lambda_2 - \int_{-\infty}^{+\infty} (\Lambda_1^{(0)})^2 d\lambda_1 \int_{-\infty}^{\infty} (\Lambda_2^{(0)})^2 \lambda_2 d\lambda_2}{\int_{+\infty}^{+\infty} (\Lambda_1^{(0)})^2 \lambda_1 d\lambda_1 \int_{-\infty}^{\infty} (\Lambda_2^{(0)})^2 d\lambda_2 + \int_{+\infty}^{+\infty} (\Lambda_1^{(0)})^2 d\lambda_1 \int_{-\infty}^{\infty} (\Lambda_2^{(0)})^2 \lambda_2 d\lambda_2}$$

$x = \lambda_1/r_0$, $y = \lambda_2/r_0$

$$= \frac{eF}{8} r_0 \frac{\int_{-\infty}^{+\infty} (\Lambda_1^{(0)})^2 x^2 dx \int_{0}^{\infty} (\Lambda_2^{(0)})^2 dy - \int_{-\infty}^{+\infty} (\Lambda_1^{(0)})^2 dx \int_{0}^{\infty} (\Lambda_2^{(0)})^2 y\, dy}{\int_{-\infty}^{+\infty} (\Lambda_1^{(0)})^2 dx \int_{0}^{\infty} (\Lambda_2^{(0)})^2 dy}$$

$$\simeq \frac{eF}{8} r_0 \frac{}{\int_0^{\infty} (\Lambda_1^{(0)})^2 x\, dx \int_{-\infty}^{+\infty} \Lambda_2}$$

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$$H' = \frac{eF}{2} r_0 \frac{\int_0^{r_1} (\Lambda_1^{(0)})^2 x^2 dx}{\int_0^{r_1} (\Lambda_1^{(0)})^2 dx} \frac{\int_0^{r_2} (\Lambda_2^{(0)})^2 y^2 dy}{\int_0^{r_2} (\Lambda_2^{(0)}) dy}$$

$$\frac{\int_0^{r_1} (\Lambda_1^{(0)}) x^2 dx}{\int_0^{r_1} (\Lambda_1^{(0)}) dx} + \frac{\int_0^{r_1} (\Lambda_1^{(0)})^2 y dy}{\int_0^{r_1} (\Lambda_2^{(0)}) dy}$$

$$= \frac{eF}{2} r_0 \frac{6n(n_1 - n_2)}{2n}$$

$$= \frac{3eF}{2} \left(\frac{r_0}{n}\right) n(n_1 - n_2)$$

$$\frac{r_0}{n} = \frac{\hbar^2}{m^2 Z e^2}$$

$$H' = \frac{3}{2} \frac{\hbar^2 F}{meZ} n(n_1 - n_2)$$

$$\int_0^\infty e^{-x} x^{m+1} \left\{ \frac{d^m}{dx^m} \left(e^x \frac{d^k}{dx^k} (x^k e^{-x}) \right) \right\}^2 dx$$

$$= (-1)^m \int_0^\infty \frac{d^m}{dx^m} \left\{ (a x^{k+1} + b x^k) e^{-x} \right\} \times e^x \frac{d^k}{dx^k} (x^k e^{-x}) dx$$

$$= (-1)^m (-1)^m \int_0^\infty \left\{ a x^{k+1} - a m (k+1) x^k + b x^k \right\} \times \frac{d^k}{dx^k} (x^k e^{-x}) dx$$

$$= (-1)^k \int_0^\infty \frac{d^k}{dx^k} \left\{ a x^{k+1} - a m (k+1) x^k + b x^k \right\} \times x^k e^{-x} dx$$

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$$= (-1)^k \int_0^\infty \{(k+1)!\, a x - (k+1)!\, a m + k!\, b\} \times x^k e^{-x} dx$$

$$= (-1)^k \{(k+1)!^2 a - (k+1)!\, k!\, m a + (k!)^2 b\}$$

$$\int_0^\infty e^{-x} x^{m} \{\ \}^2 dx = (-1)^k (k!)^2 a$$

$$\frac{\int_0^\infty (\Lambda_n^{(0)})^2 x\, dx}{\int_0^\infty (\Lambda_1^{(0)})^2 dx} = (k+1)(k+1-m) + \frac{b}{a}$$

$$= (k+1)(k+1-m) - k(k-m)$$

$$= 2k - m + 1 = 2n_1 + m + 1$$

denominator $\simeq 2n_1 + m + 1 + 2n_2 + m + 1$

$$= 2n.$$

$$\int_0^\infty e^{-x} x^{m+2} \{\ \}^2 dx$$

$$\frac{}{\int_0^\infty e^{-x} x^{m} \{\ \}^2 dx} = 6\nu_1^2 + 6\nu_1(1-\mu) + (2-\mu)(1-\mu)$$

$$\nu_1 = n_1 + \mu$$

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$$W^{(1)} = \frac{3}{2}\frac{\hbar \mathcal{F}}{mcZ} n(n_1 - n_2)$$

$$= \frac{\mathcal{F}}{15590}\frac{n}{Z}(n_1 - n_2)\ cm^{-1}$$

$\mathcal{F}$: Volt/cm.

Rydberg energy

$$W^{(0)} = -\frac{Z^2 e^4 m}{2\hbar^2 n^2} \simeq -\frac{Z^2}{n^2} \times 10^5\ cm^{-1}$$

$\downarrow$ 1.097×10^5

$n = 5$; $\Delta W = 32 \cdot 5 \cdot 8 = 1280\ cm^{-1}$

$n_1 - n_2 = 2(n-1) = 8$, $Z = 1$

($n_1 = 4, n_2 = 0$; $n_1 = 0, n_2 = 4$)

for $\mathcal{F} = 5 \times 10^5$ Volt/cm.

$$W_n^{(0)} - W_{n'}^{(0)} = \left(\frac{1}{n'^2} - \frac{1}{n^2}\right) 2^2 \times 10^5\ cm^{-1}$$

$n' = 5$ $n = 6$

$= 1400\ cm^{-1}$.

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Transition between stationary states due to Perturbation

$$i\hbar \frac{\partial \psi(q_1, q_2 \cdots q_n, t)}{\partial t} = (H_0 + H')\psi .$$

$$\psi(q_1 \cdots q_n, t) = \sum_p a_p^{(t)} \psi_p(q_1 \cdots q_n)$$

$$\sum_r i\hbar \sum_p \dot{a}_p \psi_p = \sum_p a_p W_p \psi_p + \sum_p a_p H' \psi_p$$

$$i\hbar \dot{a}_r = W_r a_r + \sum_p H'_{rp} a_p$$

$$a_r(t) = c_r(t) e^{-iW_r t/\hbar}$$

$$i\hbar \dot{c}_r(t) = \sum_p H'_{rp} e^{i(W_r - W_p)t/\hbar} c_p(t)$$

$t=0$ $\quad c_p(0) = 0$ for $p \neq s$ $\quad c_s(0) = 1$ }

$$c_r(t) = -\frac{i}{\hbar} \int_0^t H'_{rs} e^{i(W_r - W_s)t/\hbar} dt$$

if t is sufficiently small.

$$c_r(t) = -\frac{H'_{rs}\left(e^{i(W_r - W_s)t/\hbar} - 1\right)}{W_r - W_s}$$

if H'_{rs} is indep of t.

etc.

If $H'_{rs}(t) = H'_{rs}(0) e^{\pm i\omega t}$

$$c_r(t) \simeq -\frac{H'_{rs}(0)\left(e^{i(W_r - W_s \pm \hbar\omega)t/\hbar} - 1\right)}{W_r - W_s \pm \hbar\omega}$$

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Relation between Two Methods

(i) S.M.: $E\, a_r(0) = W_r\, a_r(0) + \sum_p H'_{rp}\, a_p(0)$

with $a_p(t) = a_p(0)\, e^{-iE_p t/\hbar}$

for all p

(ii) n.s.m.: $a_p(t)$ changes with time in a more complicated way by starting from the initial condition

$a_p(0) = 1$ for $p = s$

$= 0$ otherwise

Applicability

(i) s.m.: discrete eigenvalues (bound state boundary cond.)
collision problems (boundary asymp. sol. condition)

(ii) n.s.m.: continuous eigenvalues
(Transition probability)

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Applications of Perturbation Theory

A. Sommerfeld, Atombau und Spektrallinien. (II. Band) (1939)
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H. Bethe, Quantenmechanik der Ein- und Zwei-Elektronenprobleme
(Handbuch der Physik, Vol 23
Part I. Chapter 3) (1933)

Collision Problems

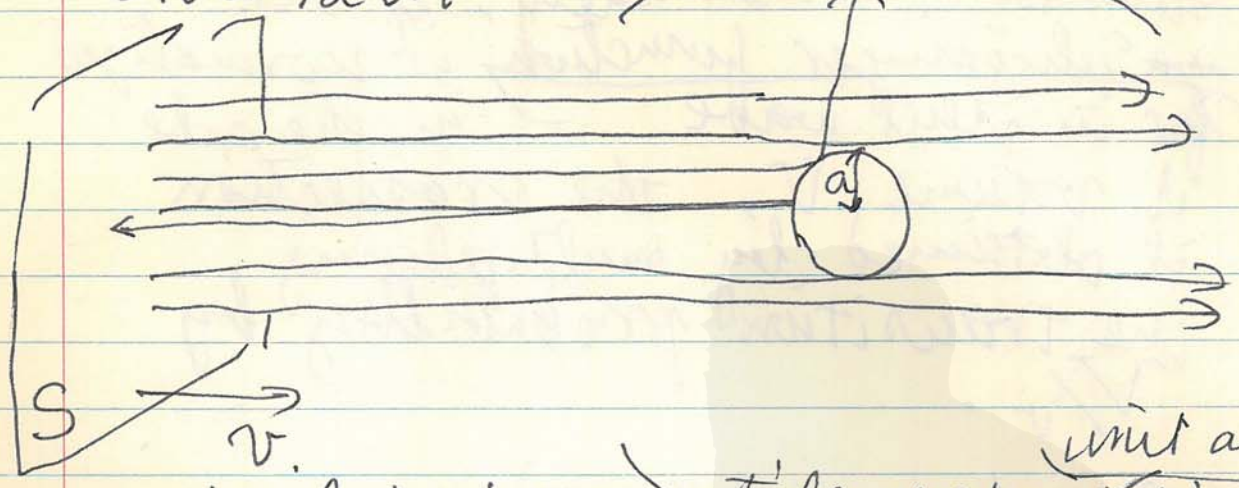
G. Wentzel, Wellenmechanik der Stoß- und Strahlungsvorgänge
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Mott and Massey, Theory of
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Collision Problems

Cross-section



number of incident particle per unit time per unit area = 1.
number of scattered particles per unit time

~~N~~ = ~~$n \cdot v \cdot \sigma$~~

$\sigma = \pi a^2$

Definition of total cross-section σ_t (or $\sigma(l^2)$):
number of scattered particles
per unit time (t^{-1}).
per unit incident particle
particle per unit area $((l^{-2})^{-1} = l^2)$
per unit time $((t^{-1})^{-1} = t)$

~~General definition~~
~~velocity~~ of incident particle v

v.

Definition of differential cross-section
$d\sigma$ = number of ~~insta~~ particles per unit time scattering into $d\Omega$ per unit particle per unit area per unit time

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Quantum-mechanically, if the ~~wa~~ Schrödinger function is normalized for incident wave in the cube of volume V, the crossection is obtained by multiplying the transition probability by V/v.

(Born's approximation)

Exact method for elastic scattering: collision:

$$\frac{d^2\chi_l}{dr^2} + \frac{2}{r}\frac{d\chi_l}{dr} + \left(\frac{2\mu W}{\hbar^2} - \frac{l(l+1)}{r^2}\right)\chi_l = 0$$

$$\chi_l = r^{-\frac{1}{2}} u_l$$

$$\frac{d\chi_l}{dr} = r^{-\frac{1}{2}}\frac{du_l}{dr} - \frac{1}{2} r^{-\frac{3}{2}} u_l$$

$$\frac{d^2\chi_l}{dr^2} = r^{-\frac{1}{2}}\frac{d^2u_l}{dr^2} - r^{-\frac{3}{2}}\frac{du_l}{dr} + \frac{3}{4} r^{-\frac{5}{2}} u_l$$

$$r^{-\frac{1}{2}}\left(\frac{d^2u_l}{dr^2} - \frac{1}{r}\frac{du_l}{dr} + \frac{3}{4r^2}u_l + \frac{2}{r}\frac{du_l}{dr} - \frac{1}{r^2}u_l + \frac{2\mu W}{\hbar^2}u_l - \frac{l(l+1)}{r^2}u_l\right) = 0$$

$$\frac{d^2u_l}{dr^2} + \frac{1}{r}\frac{du_l}{dr} + \left(k^2 - \frac{(l+\frac{1}{2})^2}{r^2}\right)u_l = 0$$

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$$k = \frac{\sqrt{2\mu W}}{\hbar}$$

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{du_\ell}{dr}\right) + \left(k^2 - \frac{(\ell+\frac{1}{2})^2}{r^2}\right)u_\ell = 0$$

or $x = kr$

$$\frac{1}{x}\frac{d}{dx}\left(x\frac{du_\ell}{dx}\right) + \left(1 - \frac{(\ell+\frac{1}{2})^2}{x^2}\right)u_\ell = 0$$

$$u_\ell(x) = J_{\ell+\frac{1}{2}}(x) \left(\sim \frac{1}{\Gamma(\ell+\frac{1}{2}+1)}\left(\frac{x}{2}\right)^{\ell+\frac{1}{2}} + \cdots \text{ for } x \ll 1\right)$$

$$\sim \sqrt{\frac{2}{\pi x}}\cos\left(x - \frac{(\ell+1)}{2}\pi\right) \text{ for } x \gg \ell$$

or $= J_{-\ell-\frac{1}{2}}(x) \left(\sim \frac{1}{\Gamma(-\ell-\frac{1}{2}+1)}\left(\frac{x}{2}\right)^{-\ell-\frac{1}{2}} + \cdots \text{ for } x \ll 1\right)$

$$\sim \sqrt{\frac{2}{\pi x}}\cos\left(x + \frac{\ell}{2}\pi\right)$$

$$\chi_\ell(r) = r^{-\frac{1}{2}}\left(A_\ell J_{\ell+\frac{1}{2}}(kr) + B_\ell J_{-\ell-\frac{1}{2}}(kr)\right)$$

$kr \gg 1$:

$$\psi(r,\theta) \cong \sqrt{\frac{2}{\pi k}}\frac{1}{r}\sum_{\ell=0}^{\infty} P_\ell(\cos\theta)$$

$$\left\{A_\ell \cos\left(kr - \frac{\ell+1}{2}\pi\right) + B_\ell \cos\left(kr + \frac{\ell}{2}\pi\right)\right\}$$

$A_\ell = C_\ell \cdots e^{i\xi_\ell}$ //

$B_\ell = C_\ell \cdot b_\ell e^{i\xi_\ell} \cdot e^{i}$

$$\frac{A_\ell e^{-i(\frac{\ell+1}{2})\pi} + B_\ell e^{i\frac{\ell\pi}{2}}}{2} e^{ikr} + \frac{A_\ell e^{i(\frac{\ell+1}{2})\pi} + B_\ell e^{-i\frac{\ell\pi}{2}}}{2} e^{-ikr}$$

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Condition of continuity:
intensity of ~~outgoing~~ divergent wave
= intensity of convergent wave

$$\left| A_l e^{-i(\frac{l+1}{2})\pi} + B_l e^{i l\pi/2} \right|^2$$

$$= \left| A_l e^{i(\frac{l+1}{2})\pi} + B_l e^{-i l\pi/2} \right|^2$$

$$\text{or} \quad A_l \tilde{B}_l e^{-i(l+\frac{1}{2})\pi} + \tilde{A}_l B_l e^{i(l+\frac{1}{2})\pi}$$

$$= A_l \tilde{B}_l e^{i(l+\frac{1}{2})\pi} + \tilde{A}_l B_l e^{-i(l+\frac{1}{2})\pi}$$

~~$A_l \tilde{B}_l = A_l \tilde{B}_l = \tilde{A}_l B_l$~~

~~$A_l = a_l e^{i\alpha_l}$~~

~~$B_l = b_l e^{i\beta_l}$~~

~~$a_l b_l e^{i(\alpha_l - \beta_l)} = a_l b_l e^{-i(\alpha_l - \beta_l)}$~~

~~$\alpha_l - \beta_l =$~~

~~$A_l \tilde{B}_l =$~~

$A_l = a_l e^{i\alpha_l}$, $B_l = b_l e^{i\beta_l}$

$e^{i(\alpha_l - \beta_l)} = e^{-i(\alpha_l - \beta_l)}$.

$e^{i(\alpha_l - \beta_l)} = \pm 1$.

$A_l = e^{i\alpha_l} \cdot C_l \cos\delta_l$

$B_l = e^{i\alpha_l}(\pm 1) C_l \sin\delta_l$

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* $\cos(x-\frac{\pi}{2}) = \cos x \cos\frac{\pi}{2} + \sin x \sin\frac{\pi}{2} = \sin x$

It is convenient to ~~take~~ put

$$A_l = e^{i\alpha_l} C_l \cos\delta_l$$

$$B_l = e^{i\alpha_l} (-1)^l C_l \sin\delta_l$$

$$A_l \cos(kr - \tfrac{l+1}{2}\pi) + B_l \cos(kr + \tfrac{l}{2}\pi)$$

$$= e^{i\alpha_l} \{ C_l \{ +\cos\delta_l \cos(kr - \sin(kr - \tfrac{l}{2}\pi) \}^* + (-1)^l \sin\delta_l \cos(kr + \tfrac{l}{2}\pi)$$

$$= \sin\delta_l \cos(kr - \tfrac{l}{2}\pi)^{**} \}$$

$$= e^{i\alpha_l} C_l \sin(kr - \tfrac{l}{2}\pi + \delta_l)$$

$$e^{ikz} = \sum_l A_l P_l(\cos\theta) \frac{J_{l+\frac{1}{2}}(kr)}{(kr)^{-\frac{1}{2}}} \sqrt{\frac{\pi}{2kr}}$$

$$\frac{2}{2l+1} A_l J_{l+\frac{1}{2}}(kr) = \int_{-1}^{+1} e^{ikrx} P_l(x)\, dx$$

$$\sqrt{\frac{\pi}{2kr}} \left(\frac{1}{kr}\right) = \frac{1}{ikr}\left[e^{ikr} P_l(1) - e^{-ikr} P_l(-1)\right]$$

$$O\left(\frac{1}{k^2r^2}\right) \rightarrow = \frac{1}{ikr} \int_{-1}^{+1} e^{ikrx} P_l'(x)\, dx$$

$P_l(1) = 1$, $P_l(-1) = (-1)^l = (+i)^{2l} = (i)^{-l} = e^{-i\frac{l\pi}{2}}$

Asymptotically:

$$\frac{2}{2l+1} A_l \sqrt{\frac{\pi}{2kr}} \sqrt{\frac{2}{\pi kr}} \sin(kx - \tfrac{l\pi}{2}) = \frac{2i^l}{kr} \sin(kr - \tfrac{l\pi}{2})$$

** $\cos(kr + \frac{l}{2}\pi) = \cos x \cos\frac{l}{2}\pi - \sin x$

$$\cos(kr - \tfrac{l}{2}\pi) \underset{(-1)^{\frac{l}{2}}}{\cos} l\pi - \sin(kr - \tfrac{l}{2}\pi) \underset{0}{\sin} l\pi$$

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Problem: ~~Screened Coulomb potential~~ square or a potential well

Scattering by a potential barrier:

$$V(r) = V_0 \ (>0) \quad (r<a)$$
$$= 0 \qquad (r>a)$$

S-wave:

$$J_{1/2}(x) = \sqrt{\frac{2}{\pi x}} \sin x$$
$$J_{-1/2}(x) = \sqrt{\frac{2}{\pi x}} (-1)^0 \cos x$$

$\chi =$

$r \lessgtr a$: $E > V_0$ $\qquad k' = \frac{\sqrt{2\mu E}}{\hbar}$

$\chi_0 = C \sin k'r / k'r$

$k' = \frac{\sqrt{2\mu(E-V_0)}}{\hbar}$

$$C \frac{\sin k'a}{k'a} = \frac{1}{\sqrt{a}} \left\{ \sqrt{\frac{2}{\pi a}} (A_0 \sin ka + B_0 \cos ka) \right\} \Rightarrow \begin{cases} \sin(ka+\delta_0) \\ \cos(ka+\delta_0) \end{cases}$$

$\frac{d}{dr}(r\chi_0)\Big|_{r=a} = \frac{d}{dr}(r\psi)\Big|_{r=a}$

$$+ Ck' \left(\cos k'a - \frac{\sin k'a}{k'a} \right) = \frac{k}{\sqrt{a}} \sqrt{\frac{2}{\pi a}} (A_0 \cos ka - B_0 \sin ka)$$

$$\frac{\frac{1}{k'} \tan k'a + \frac{\sin k'a}{k'^2 a^2}}{1 - \frac{\tan k'a}{k'a}} = \frac{1}{k} \frac{\frac{B_0}{A_0} + \tan ka}{1 - \frac{B_0}{A_0} \tan ka}$$

$$\frac{B_0}{A_0} \left(\frac{k}{k'} \tan k'a - \tan ka \right) = \frac{B_0}{A_0} \left(1 + \frac{k}{k'} \tan ka \right)$$

$$\tan \delta_0 = \frac{1 + \frac{k}{k'} \tan ka}{\frac{k}{k'} \tan k'a - \tan ka}$$

$V_0 \lesssim 0$: $ka \ll 1$:

$$\tan \delta_0 \simeq ka \left(\frac{\tan k'a}{k'a} - 1 \right)$$

$$\sigma_0 = 4\pi a^2 \left(\frac{\tan k'a}{k'a} - 1 \right)^2 \qquad \left(k' \simeq \frac{k_0 \simeq \sqrt{-2\mu V_0}}{\hbar} \right)$$

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$V_0 > E$:

$r < a$: $\chi_0 = \frac{C}{2ik'r}(e^{ik'r} - e^{-ik'r}) = C\frac{\sinh ik'r}{ik'r}$

$$\frac{d^2\chi_0}{dr^2} + \frac{2}{r}\frac{d\chi_0}{dr} + \frac{2\mu E}{\hbar^2}\chi_0 = 0$$

$$k' = \frac{\sqrt{2\mu E}}{\hbar}.$$

$$\frac{C}{2ik'a}\frac{\sinh ik'a}{ik'a} = \frac{1}{\sqrt{a}}\sqrt{\frac{2}{\pi a}}(A_0 \sin ka + B_0 \cos ka)$$

$$C k' \frac{\cosh ik'a}{ik'a} = \frac{k}{\sqrt{a}}\sqrt{\frac{2}{\pi a}}(A_0 \cos ka - B_0 \sin ka)$$

$$\frac{C \sin k'a}{k'a} = \frac{1}{\sqrt{a}}\sqrt{\frac{2}{\pi a}}(A_0 \sin ka + B_0 \cos ka)$$

$$C k' \frac{\cos k'a}{k'a} = \frac{k}{\sqrt{a}}\sqrt{\frac{2}{\pi a}}(A_0 \cos ka - B_0 \sin ka)$$

$$\frac{k}{k'}\tan k'a = \frac{\tan ka + \tan\delta_0}{1 - \tan ka \tan\delta_0}$$

$$= \tan(ka + \delta_0)$$

$$\delta_0 = \arctan\left(\frac{k}{k'}\tan k'a\right) - ka.$$

$ka \ll 1$,

$$\delta_0 \cong ka\left(\frac{\tan k'a}{k'a} - 1\right)$$

$$\sigma_0 = 4\pi a^2\left(\frac{\tan k'a}{k'a} - 1\right)^2$$

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$k'a \cong \frac{\pi}{2}(2n+1)$ σ : large

$k'a \cong n\pi$ σ : small.

$k'a \to 0$

$\sigma_0 \ll 4\pi a^2$ for $k_0 a \cong n\pi$

$\sigma_0 \gg 4\pi a^2$ for $k_0 a \cong \frac{\pi}{2}(2n+1)$

$\frac{k}{k'} \tanh k'a = \tan(ka + \delta_0)$

$\delta_0 = \arctan\left(\frac{k}{k'} \tanh k'a\right) - ka$

$ka \ll 1$:

$\delta_0 \cong ka\left(\frac{\tanh k'a}{k'a} - 1\right)$

$\sigma_0 = 4\pi a^2 \left(\frac{\tanh k'a}{k'a} - 1\right)^2$

$k' \to \infty$ $\delta_0 \to \infty$ $k' \to \infty$. $\tanh k'a \to 1$.

$\sigma_0 = 4\pi a^2$

~~$\tan\delta_0 \cong \frac{k}{k'} \tanh k'a$~~

$\tan\delta_0 = \tan\left(\frac{k}{k'} \tanh k'a - ka\right)$

$= \frac{\tan\left(\frac{k}{k'} \tanh k'a\right) - \tan ka}{1 - \tan(\quad)\tan ka}$

$\sim -\tan(ka)$

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Scattering in Coulomb field:

$$\Lambda_1(\lambda_1) = e^{ik\lambda_1/2} F\left(-\frac{B_1 i}{k} + \frac{1}{2}, 1, -ik\lambda_1\right)$$

$$\Lambda_2(\lambda_2) = e^{ik\lambda_2/2} F\left(-\frac{B_2 i}{2} + \frac{1}{2}, 1, -ik\lambda_2\right)$$

$$F(\alpha, \beta, x) = 1 + \frac{\alpha}{\beta \cdot 1} x + \frac{\alpha(\alpha+1)}{\beta(\beta+1)\cdot 2!} x^2 + \cdots$$

$$\frac{d}{d\lambda_1}\left(\lambda_1 \frac{d\Lambda_1}{d\lambda_1}\right) + \left(\frac{k^2}{4}\lambda_1 + B_1\right)\Lambda_1 = 0$$

$-ik\lambda_1 = x$. $-iB_1/k = b_1$

$$\frac{1}{-ik}\left\{\frac{d}{dx}\left(x\frac{d\Lambda_1}{dx}\right) + \left(-\frac{x}{4} - b_1\right)\Lambda_1 = 0\right.$$

$$\Lambda_1 = e^{-x/2} u_1(x)$$

$$\frac{d\Lambda_1}{dx} = e^{-x/2}\frac{du_1}{dx} - \frac{1}{2}e^{-x/2}u_1$$

$$\frac{d}{dx}\left(x\frac{d\Lambda_1}{dx}\right) = xe^{-x/2}\frac{d^2u_1}{dx^2} + e^{-x/2}\frac{du_1}{dx} - \frac{x}{2}e^{-x/2}\frac{du_1}{dx} - \frac{x}{2}e^{-x/2}\frac{du_1}{dx} - \frac{1}{2}e^{-x/2}u_1 + \frac{1}{4}xe^{-x/2}u_1$$

$$x\frac{d^2u_1}{dx^2} + (1-x)\frac{du_1}{dx} - (b_1 + \tfrac{1}{2})u_1 = 0$$

$$\Rightarrow u_1 = \sum_{\nu=0}^{\infty} a_\nu x^\nu$$

$$\mu(\mu-1) + \mu = 0 \quad \underline{\mu = 0}$$

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x^{ν} の係数:

$$(\nu+1)\nu\, a_{\nu+1} + (\nu+1)\, a_{\nu+1} - \nu\, a_\nu - (b_1+\tfrac{1}{2})\, a_\nu = 0$$

$$a_{\nu+1} = \frac{(b_1+\frac{1}{2}+\nu)}{(\nu+1)^2}\, a_\nu$$

$\alpha = b_1+\frac{1}{2}$

$$= \frac{\alpha(\alpha+1)\cdots(\alpha+\nu)}{\{(\nu+1)!\}^2}\, a_0$$

$$\sum_\nu a_\nu x^\nu = a_0\, F(\alpha, 1, x)$$

$$F(\alpha,\beta,x) = 1 + \frac{\alpha}{\beta\cdot 1!}x + \frac{\alpha(\alpha+1)}{\beta(\beta+1)\,2!}x^2 + \cdots + \frac{\alpha(\alpha+1)\cdots(\alpha+\nu-1)}{\beta(\beta+1)\cdots(\beta+\nu-1)\cdot\nu!}x^\nu$$

Confluent hypergeometric series

$|x| \gg 1$: asymptotic expression

$$F(\alpha,\beta,x) \cong \frac{(\beta-1)!}{\Gamma(\beta-\alpha)}(-x)^{-\alpha}\left\{1 + \frac{\alpha\beta}{1!}\frac{1}{x} + \cdots\right\}$$

$$+ \frac{(\beta-1)!}{\Gamma(\alpha)}x^{\alpha-\beta}e^x\left(1 + \frac{(1-\alpha)(\beta-\alpha)}{1!}\frac{1}{x} + \cdots\right)$$

$\Gamma(\alpha+1) = \alpha\,\Gamma(\alpha)$

$\Gamma(n+1) = n!$

$\Gamma(+1) = 1$
$\Gamma(0) = \infty$
$\Gamma(-1) = \infty$
⋮

$\Gamma(\alpha)\Gamma(1-\alpha) = \frac{\pi}{\sin\pi\alpha}$

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$$\Lambda_1(\lambda_1)\Lambda_2(\lambda_2) \cong e^{ikr}\left\{\frac{(+ik\lambda_1)^{-\alpha_1}}{\Gamma(1-\alpha_1)} + \frac{(-ik\lambda_1)^{\alpha_1-1}}{\Gamma(\alpha_1)} e^{-ik\lambda_1}\right\}$$

$$\times\left\{\frac{(ik\lambda_2)^{-\alpha_2}}{\Gamma(1-\alpha_2)} + \frac{(-ik\lambda_2)^{\alpha_2-1}}{\Gamma(\alpha_2)} e^{-ik\lambda_2}\right\}$$

$$\left.\begin{aligned}\alpha_1 &= -\frac{iB_1}{k} + \frac{1}{2}\\ \alpha_2 &= -\frac{iB_2}{k} + \frac{1}{2}\end{aligned}\right\}$$

$$\Lambda_1(\lambda_1)\Lambda_2(\lambda_2) \cong \left\{\frac{(ik\lambda_1)^{-\alpha_1}}{\Gamma(1-\alpha_1)} + \frac{(-ik\lambda_1)^{\alpha_1-1}}{\Gamma(\alpha_1)} e^{-ikz}\right\} e^{-ikr}$$

$$\times\left\{\frac{(ik\lambda_2)^{-\alpha_2}}{\Gamma(1-\alpha_2)} e^{ikr} + \frac{(-ik\lambda_2)^{\alpha_2-1}}{\Gamma(\alpha_2)} e^{ikz}\right\}$$

$\Gamma(\alpha_1) \neq \infty$ $\quad$ $\Gamma(1-\alpha_1) \neq 0$

$\alpha_1 = 0, -1, -2, \cdots$ (except $1-\alpha_1 \neq 1, 2, \cdots$)

$$-\frac{iB_1}{k} + \frac{1}{2} = 0, -1, -2, \cdots$$

However, if $\alpha_1 = -1, -2, \cdots$

$(ik\lambda_1)^{-\alpha_1} \to \infty$ for $\lambda_1 \to \infty$

So, the only possibility is

$\alpha_1 = 0$.

or $\dfrac{B_1 i}{k} = \dfrac{1}{2}$ $\qquad \alpha_2 = -\dfrac{iB_2}{k} + \dfrac{1}{2} = \dfrac{-Bi}{k} + 1$

$$\frac{B_2 i}{k} = \frac{Bi}{k} - \frac{1}{2}$$

$$\Lambda_1(\lambda_1)\Lambda_2(\lambda_2) \cong \frac{\{ik(r-z)\}^{-\alpha_2}}{\Gamma(Bi/k)} e^{ikr} + \frac{-ik}{} e^{ikz}$$

$$\left\{\frac{(-ik\lambda_2)^{-\alpha_2}}{\Gamma(1-\alpha_2)} e^{ikr} + \frac{(-ik\lambda_2)^{\alpha_2-1}}{\Gamma(\alpha_2)} e^{ikz}\right\}$$

$$\left(1 - \frac{\alpha_2}{ik\lambda_2}\right) \qquad \left(1 - \frac{(1-\alpha_1)^2}{ik\lambda_2}\right)$$

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$$\lambda_2 = r - z$$
$$= r(1-\cos\theta)$$
$$= 2r\sin^2\frac{\theta}{2}$$

$$\simeq \left\{\left(1 - \frac{B^2 i}{2k^3 r \sin^2\frac{\theta}{2}}\right)\frac{\{-ik(r-z)\}^{\alpha_2-1}}{\Gamma(\alpha_2)} e^{ikz}\right.$$
$$\left. + \frac{\{-ik(r-z)\}^{-\alpha_2+1}}{\Gamma(1-\alpha_2)} \cdot \frac{e^{ikr}}{-2ikr\sin^2\frac{\theta}{2}}\right\}$$

$$\{-ik(r-z)\}^{1-\alpha_2} = \{-ik(r-z)\}^{Bi/k}$$

$$= \exp\left\{\frac{Bi}{k}\log(-ik)\right.$$
$$\left. + \frac{Bi}{k}\log\left(2r\sin^2\frac{\theta}{2}\right)\right\}$$

$$\simeq \left(1 - \frac{B^2 i}{2k^3 r\sin^2\frac{\theta}{2}}\right)\exp i\left\{kr\cos\theta - \frac{B}{k}\log(\ )\right\}$$
$$\times \frac{(-ik)^{Bi/k}}{\Gamma\left(1-\frac{Bi}{k}\right)}$$

$-\frac{B}{ik} \simeq \alpha_2 + 1$

$$\simeq \frac{B}{2k^2 r\sin^2\frac{\theta}{2}} \frac{(-ik)^{-Bi/k}}{(1-\alpha_2)\Gamma(1-\alpha_2)} \exp i[kr\cos\theta + \cdots]$$

$$(1-\alpha_2)\Gamma(1-\alpha_2) = \Gamma(2-\alpha_2)$$
$$= \Gamma\left(1+\frac{Bi}{k}\right)$$

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$$(-ik)^{\beta i/k} = \exp\left\{\frac{\beta i}{k}\log(-ik)\right\}$$

$$= \exp\left\{\frac{\beta i}{k}\log(-i) + \frac{\beta i}{k}\log k\right\}$$

$$\log(-i) = -\frac{\pi}{2}$$

$$\simeq \exp\left(-\frac{\pi\beta i}{2k} + \cdots\right)$$

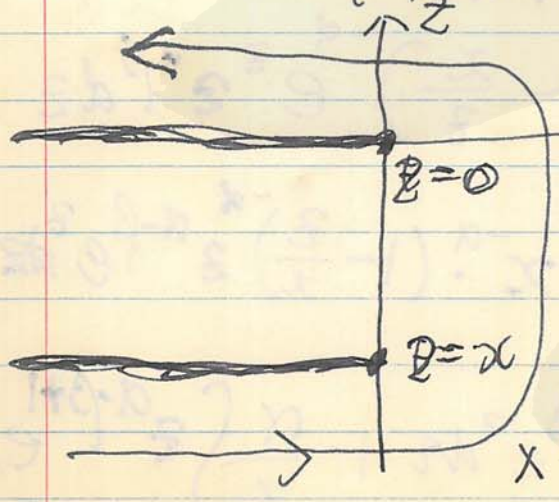
$$= e^{i\gamma}$$

$$\frac{\Gamma\left(1+\frac{\beta i}{k}\right)}{\Gamma\left(1-\frac{\beta i}{k}\right)} = e^{i\varepsilon}$$

Asymptotic expression of Confluent Geometric function $F(\alpha,\beta,x)$

$$x\frac{d^2F}{dx^2} + (\beta - x)\frac{dF}{dx} - \alpha F = 0$$

$$F(\alpha,\beta;x) = \frac{(\beta-1)!}{\Gamma(\beta)}\frac{1}{2\pi i}\int_C \left(1-\frac{x}{z}\right)^{-\alpha} e^z z^{-\beta}dz$$



$$x\frac{d^2F}{dx^2} + (\beta - x)\frac{dF}{dx} - \alpha F$$

$$= \frac{\alpha(\beta-1)!}{2\pi i}\int\left(1-\frac{x}{z}\right)^{-(\alpha+1)} e^z z^{-\beta}dz$$

$$\times\left\{\frac{(\alpha+1)x}{z^2}\left(1-\frac{x}{z}\right)^{-1} + \frac{(\beta-x)}{z} - \left(1-\frac{x}{z}\right)\right\}$$

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$$= \frac{-\alpha\cdot(\beta-1)!}{2\pi i}\int_C \left(1-\frac{x}{z}\right)^{-(\alpha+1)} e^z z^{-\beta} dz$$

$$\times \left\{ \frac{-(\alpha+1)\,x}{\Gamma(\beta)\, z^2}\left(1-\frac{x}{z}\right)^{-1} + 1 + \cdots \right\}$$

$$= \frac{-\alpha\cdot(\beta-1)!}{2\pi i}\int_C \frac{d}{dt}\left[\left(1-\frac{x}{z}\right)^{-(\alpha+1)} e^z z^{-\beta}\right] dz$$

$$= 0$$

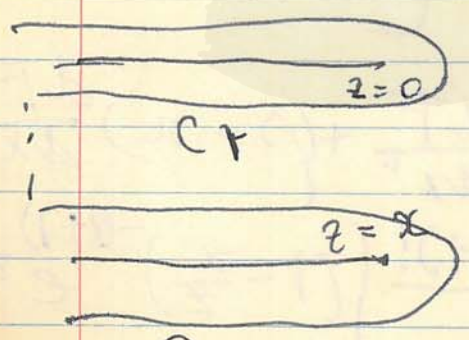
$|x/z| < 1$:

$$F(\alpha,\beta,z) = \frac{\Gamma(\beta)}{2\pi i}\left[\int e^z z^{-\beta} dt + \alpha x \int e^z z^{-(\beta-1)} dz + \cdots\right]$$

$$= \frac{\Gamma(\beta)}{\Gamma(\beta)} + \frac{\alpha\,\Gamma(\beta)}{\Gamma(\beta+1)} x + \cdots$$

$$= 1 + \frac{\alpha}{\beta} x + \cdots$$

$x = -ikx_1$ or $-ikx_2$:



$$\int_{C_1} \left(1-\frac{x}{z}\right)^{-\alpha} e^z z^{-\beta} dz$$

$$= \int_{C_1} x^{-\alpha}\cdot\left(1-\frac{z}{x}\right)^{-\alpha} z^{\alpha-\beta} e^z dz$$

$$= \sum_{k=0} x^{-\alpha-k} \int_{C_1} z^{\alpha-\beta} e^z dz + \frac{\alpha}{x}\int_{C_1} z^{\alpha-\beta+1} e^z dz + \cdots \Big\}$$

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$$\int_{C_2} \left(1-\frac{x}{z}\right)^{-\alpha} e^{z} z^{-\beta} dz$$

$z - x = u.$

$$= \int_{C_1} \left(\frac{u}{u+x}\right)^{-\alpha} e^{u+x} (u+x)^{-\beta} du$$

$$= e^{x} x^{\alpha-\beta} \left[\int_{C_1} e^{u} u^{-\alpha} du \right.$$

$$\left. + \frac{1}{x} \int_{C_1} (\alpha-\beta) e^{u} u^{-\alpha+1} du + \cdots \right]$$

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Examination　Physics 237

January 29, 1952　H. Yukawa

1. Give a quantum mechanical description (whatever description you think appropriate !) of what ~~had~~ would have happened in a cloud chamber, ~~before~~ when a track of a fast charged particle ~~was~~ is observed. State the reason why the particle behaved like a classical corpuscle.

2. Prove that the induced electric dipole moment of a hydrogen atom due to the uniform electric field of intensity F is given ~~by~~ approximately by

$$9/2\ (\hbar^2/me^2)^3 F$$

where m is the mass of the electron.

3. Show that the differential cross-section of scattering of an alpha-particle by another alpha-particle is given by

$$d\sigma = \left(\frac{4e^2}{Mv^2}\right)^2 \sin\theta\, d\theta\, d\varphi \left\{ \frac{1}{\sin^4\frac{\theta}{2}} + \frac{1}{\cos^4\frac{\theta}{2}} + \frac{2\cos\left(\frac{4e^2}{\hbar v}\log\tan^2\frac{\theta}{2}\right)}{\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}} \right\}$$

where M ~~is~~ is the mass ~~of the alpha-particle~~ of the alpha-particle, v the relative velocity and θ the angle of deflection in the centre of mass system.

What is the corresponding formula for the proton-proton scattering?

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Examination · Physics 237

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where M ~~is~~ the mass of the alpha-particle, v the relative velocity and θ the angle of deflection in the centre of mass system.

What is the corresponding formula for the proton-proton scattering?

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Examination ... Jan. 29, 9-12 a.m.
301 Pupin

you may ~~be~~ carry your note with you, but no other books, ~~since it is not fair~~, because ~~I am not sure whether~~ the answers to the problems ~~are~~ may be found in one book and ~~may~~ not in ~~the~~ other books. I cannot check that.

due to Coulomb repulsion

3. Show that the differential cross-section of scattering of an α-particle by another ~~helium nucleus~~ α-particle is given by

$$d\sigma = \left(\frac{4e^2}{M_\alpha v^2}\right)^2 \sin\theta\, d\theta\, d\varphi \times \left\{ \frac{1}{\sin^4\frac{\theta}{2}} + \frac{1}{\cos^4\frac{\theta}{2}} + \frac{2\cos\left(\frac{4e^2}{\hbar v}\log\tan^2\frac{\theta}{2}\right)}{\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}} \right\}$$

where M_α, v are the mass and the velocity of the α-particle and θ is the angle of deflection in the center of mass system. ~~What will be~~ Can you give the corresponding formula for ~~the proton~~ the scattering of a proton by another proton?

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1. Give a quantum mechanical description (whatever description you think appropriate!) of what had happened in a cloud chamber when a track of a charged particle was observed, fast (subatomic)
State the reason why the (subatomic) particle behaved like a classical corpuscle.

2. Prove that the magnitude of the induced electric dipole moment of a hydrogen atom due to the uniform electric field of intensity F is given approximately by

$$\frac{9}{2}\left(\frac{\hbar^2}{me^2}\right)^3 F$$

where m is the mass of the electron.

3. In what way is the Rutherford scattering formula modified in quantum mechanics for collision between α-particles?

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Phys. 237.

Exam. Jan. 29 9 a.m. 12 a.m.

048

301 pages 042

2. ~~How do Give whatever interpretation you like to the fact that~~

Give a quantum mechanical ~~description~~ description of what ~~the phenomena that is happened~~ in the ~~Wilson~~ cloud chamber, when a ~~the~~ track of a charged particle is observed.

(Subatomic) (whatever description you like) (subatomic)

State the reason why the particle behaved like a classical ~~particle~~ corpuscle.

2. Prove that the magnitude of the induced electric dipole-moment of a hydrogen atom due to the uniform electric field of intensity $\vec{F}$ is given by approximately by

$$\mu = \frac{9}{2}\left(\frac{\hbar^2}{me^2}\right)^3 F.$$

where m is the mass of the electron.

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$$-\frac{\hbar^2}{2m}\Delta\psi - \frac{e^2}{r}\psi + eFz\psi = E\psi$$

$$\left(\int ez(\psi^{(0)})^2 dv = 0\right)$$

$$\frac{\partial^2\psi^{(1)}}{\partial r^2} + \frac{2}{r}\frac{\partial\psi^{(1)}}{\partial r} + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi^{(1)}}{\partial\theta}\right)$$

$$+\frac{2}{ar}\psi^{(1)} - \frac{1}{a^2}\psi^{(1)} = \frac{2F}{ae}z\psi^{(0)}$$

$$a = \frac{\hbar^2}{me^2}$$

$$\psi^{(1)} = f_1(r)\cos\theta$$

$$\psi = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}\left\{1 - \frac{F}{e}\left(\frac{a^2}{2} + ar\right)\cos\theta\right\}$$

$$\mu = \iiint(-er\cos\theta)\psi^2 dv$$

$$= \frac{9}{2}a^3 F$$

$$(\lambda_1^{(1)} - \lambda_2^{(1)})$$

$$(\lambda_1^{(1)} + \lambda_2^{(1)})^2 (\lambda_1^{(1)} - \lambda_2^{(1)})$$

$$\lambda^{(1)}$$

Parabolic coordinates:

$$n = 0$$

$$\Lambda_1^{(0)} = e^{-\lambda_1/2r_0}$$

$$\Lambda_2^{(0)} = e^{-\lambda_2/2r_0}$$

$$n_1 = 0$$

$$n_2 = 0$$

$$r_0 = \frac{\hbar^2}{me^2}$$

$$\frac{d}{d\lambda_1}\left(\lambda_1\frac{d\Lambda_1^{(1)}}{d\lambda_1}\right) - \left(\frac{\lambda_1}{4r_0^2} - \beta_1\right)\Lambda_1^{(1)} = C\lambda_1^2\Lambda_1^{(0)}$$

$$\frac{d}{d\lambda_2}\left(\lambda_2\frac{d\Lambda_2^{(1)}}{d\lambda_2}\right) - \left(\frac{\lambda_2}{4r_0^2} - \beta_2\right)\Lambda_2^{(1)} = C\lambda_2^2\Lambda_2^{(0)}$$

$$\Lambda_2^{(0)} \propto (a\lambda_1^2 e^{-\lambda_1/2r_0}$$

$$+ b\lambda_1 + c)$$

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$$\frac{d}{d\lambda_1}\left(\lambda_1 \frac{d\Lambda_1^{(1)}}{d\lambda_1}\right) - \left(\frac{\lambda_1}{4r_0^2} - B_1\right)\Lambda_1^{(1)} = C\lambda_1^2 \Lambda_1^{(0)}$$

$$\Lambda_1^{(1)} = (a_1\lambda_1^2 + b_1\lambda_1 + c_1)\, e^{-\lambda_1/2r_0} \qquad \| \; e^{-\lambda_1/2r_0}$$

$$\frac{d}{d\lambda_1}\left\{\lambda_1\left(2a_1\lambda_1 + b_1 - \frac{a_1\lambda_1^2}{2r_0} - \frac{b_1\lambda_1}{2r_0} - \frac{c_1}{2r_0}\right)e^{-\lambda_1/2r_0}\right\}$$

$$\frac{d}{d\lambda_1}\left[\left\{-\frac{a_1}{2r_0}\lambda_1^3 + \left(2a_1 - \frac{b_1}{2r_0}\right)\lambda_1^2 + \left(b_1 - \frac{c_1}{2r_0}\right)\lambda_1\right\}e^{-\lambda_1/2r_0}\right]$$

$$= \left\{-\frac{3a_1}{2r_0}\lambda_1^2 + 2\left(2a_1 - \frac{b_1}{2r_0}\right)\lambda_1 + \left(b_1 - \frac{c_1}{2r_0}\right)\right.$$

$$\left. + \frac{a_1\lambda_1^3}{4r_0^2} - \frac{1}{2r_0}\left(2a_1 - \frac{b_1}{2r_0}\right)\lambda_1^2 - \frac{1}{2r_0}\left(b_1 - \frac{c_1}{2r_0}\right)\lambda_1\right\}e^{-\lambda_1/2r_0}$$

$$-\left(\frac{\lambda_1}{4r_0^2} - B_1\right)(a_1\lambda_1^2 + b_1\lambda_1 + c_1)\, e^{-\lambda_1/2r_0}$$

$$= \left\{-\frac{a_1\lambda_1^3}{4r_0^2} + \left(B_1 a_1 - \frac{b_1}{4r_0^2}\right)\lambda_1^2 + \left(B_1 b_1 - \frac{c_1}{4r_0^2}\right)\lambda_1 \right.$$

$$\left. + B_1 c_1\right\} e^{-\lambda_1/2r_0}$$

$$\left\{-\frac{1}{2r_0}\left(5a_1 - \frac{b_1}{2r_0}\right) + B_1 a_1 - \frac{b_1}{4r_0^2}\right\}\lambda_1^2 = C\lambda_1^2$$

$$\left\{4a_1 - \frac{3b_1}{2r_0} + \frac{c_1}{4r_0^2} + B_1 b_1 - \frac{c_1}{4r_0^2}\right\}\lambda_1 = 0$$

$$B_1 c_1 = 0$$

$$a_1 = C \Big/ \left(B_1 - \frac{5}{2r_0}\right)$$

$$b_1 = -4a_1 \Big/ \left(B_1 - \frac{3}{2r_0}\right)$$

$B_1 r_0 = \frac{1}{2}$

$B_2 r_0 = \frac{1}{2}$

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$$a_1 = -Cr_0/2$$

$$b_1 \simeq +4a_1 r_0 = -2Cr_0^2$$

$$e^{-\lambda_1/2r_0}\left(1 - Cr_0\left(\lambda_1^2/2 + 2r_0\lambda_1\right)\right)$$

$$\times\ e^{-\lambda_2/2r_0}\left(1 + Cr_0\left(\lambda_2^2/2 + 2r_0\lambda_2\right)\right)$$

$$\simeq e^{-r/r_0}\left(1 - Cr_0\left(\frac{\lambda_1+\lambda_2}{2} + 2r_0\right)(\lambda_1-\lambda_2)\right)$$

$$= e^{-r/r_0}\left(1 - Cr_0\left(r + 2r_0\right)\cancel{2}\, z\right)$$

$$2r\cos\theta$$

$$C = \frac{eF}{4\hbar^2} \qquad r_0 = \frac{\hbar^2}{me^2}$$

$$Cr_0 = \frac{F}{4e}$$

$$= e^{-r/r_0}\left(1 - \frac{F}{e}\left(\frac{r^2}{2} + r_0 r\right)\cos\theta\right)$$

$$\psi = \frac{1}{\sqrt{\pi r_0^3}}\, e^{-\frac{r}{r_0}}\left(1 - \frac{F}{e}\left(\frac{r^2}{2} + r_0 r\right)\cos\theta\right)$$

$$\int (-er\cos\theta)\,\psi^2\, r^2 dr \sin\theta\, d\theta\, d\varphi$$

$$\simeq \frac{2\pi}{\pi r_0^3}\cdot 2\cdot\cancel{F}\int\left(\frac{r^2}{2} + r_0 r\right) r^3 e^{-\frac{2r}{r_0}} dr$$

$$\times \int \cos^2\theta \sin\theta\, d\theta$$

$$\frac{2}{3}$$

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050

$x = \frac{2r}{r_0}$

$$\int_0^\infty \frac{r^5}{2} e^{-\frac{2r}{r_0}} dr = \left(\frac{r_0}{2}\right)^6 \frac{1}{2} \int e^{-x} x^5 dx$$

$$= \frac{1}{2}\left(\frac{r_0}{2}\right)^6 \cdot 5! = \left(\frac{r_0}{2}\right)^6 4! \cdot \frac{5}{2}$$

$$r_0 \int_0^\infty r^4 e^{-\frac{2r_0}{r_0}} dr = r_0 \left(\frac{r_0}{2}\right)^5 4!$$

$$= \left(\frac{r_0}{2}\right)^6 \cdot 4! \cdot 2$$

$$\left(\frac{r_0}{2}\right)^6 \cdot 4! \cdot \frac{9}{2}$$

$$\times \frac{2\cdot 4}{3 r_0^3} = r_0^3 \cdot \frac{2\cdot 2\cdot 3\cdot 4\cdot 4}{4\cdot 4\cdot 4\cdot 3} \cdot \frac{9}{2}$$

$$= \frac{9}{2} r_0^3$$

$H' = eF \cdot r\cos\theta$

$n=1,\ l=0,\ m=0 \rightarrow n=2,\ l=1,\ m=0$

$$\iiint \tilde{\psi} \cdot e r\cos\theta \cdot \psi \, dv$$

$$\psi = \psi_{0,0,0} + \sum_n \frac{H'_{n,1,0;0,0,0}}{E_n - E_0} \psi_{n,1,0}$$

$$\frac{\partial}{\partial F} \sum_n \frac{H'_{0,00;n,1,0} H'_{n,1,0;0,0,0}}{E_n - E}$$

$$H'_{0,00;n,10} = \frac{3}{2} eF \frac{n^4 a_1 \sqrt{n^2-1}}{\sqrt{3}}$$

$$E_n = \frac{-e^2}{2 a_1 n^2} \cdot \frac{n^2-1}{n^2}$$

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3. Show that the differential cross-section of scattering of an α-particle by another α-particle is given by

$$d\sigma = \left(\frac{4e^2}{M_\alpha v^2}\right)^2 \sin\theta\, d\theta\, d\varphi$$

$$\times \left\{ \frac{1}{\sin^4\frac{\theta}{2}} + \frac{1}{\cos^4\frac{\theta}{2}} + \frac{2\cos\left\{\frac{4e^2}{\hbar v}\log\left(\tan^2\frac{\theta}{2}\right)\right\}}{\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}} \right\}$$

where M_α, v are the mass and the velocity of the α-particle and θ is the angle of deflection in the centre of mass system. What ~~will be~~ is the corresponding formula for the proton-proton scattering.

$$\frac{1}{\sqrt{2}}\{\psi(\theta) + \psi(\pi-\theta)\} \longrightarrow \longleftarrow$$

$$= \{ e^{ikr\cos\theta} + \frac{B e^{i\frac{B}{k}\log\left(\sin^2\frac{\theta}{2}\right)}}{2k^2 r \sin^2\frac{\theta}{2}} e^{ikr} + e^{ikr\sin\theta} + \frac{B e^{i\frac{B}{k}\log\left(\cos^2\frac{\theta}{2}\right)}}{2k^2 r\cos^2\frac{\theta}{2}} e^{ikr} \}$$

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$$= \{ e^{ikr\cos\theta} + e^{ikr\sin\theta} \}$$

$$+ \frac{B}{2k^2} \quad f(\theta) \cdot \frac{e^{ikr}}{r}$$

$$|f(\theta)|^2 = \left(\frac{B}{2k^2}\right)^2 \left\{ \frac{1}{\sin^4\frac{\theta}{2}} + \frac{1}{\cos^4\frac{\theta}{2}} \right.$$

$$\left. - \left[\frac{e^{i\frac{B}{k}\{\log(\sin^2\frac{\theta}{2}) - \log(\cos^2\frac{\theta}{2})\}} - \cdots}{\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}} + e \right] \right\}$$

$$2\cos\frac{B}{k}\log(\tan^2\frac{\theta}{2})$$

$$B = \frac{4\mu e^2}{\hbar^2} \qquad \frac{B}{k} = \frac{4e^2}{\hbar v}$$

$$k = \frac{\mu v}{\hbar}$$

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$$\sum \frac{|H'_{n,10;1,0,0}|^2}{E_n - E_0}$$

$$|H'_{n,1,0;1,0,0}|^2 = \frac{9}{4} e^2 F^2 a_1^2 \frac{n^2(n^2-1)}{3}$$

$$E_n - E_k = \frac{-e^2}{2a_1 n^2} + \frac{e^2}{2a_1}$$

$$= \frac{e^2}{2a_1}\left(\frac{n^2-1}{n^2}\right)$$

$$\sum_{n=2} \frac{|H'|^2}{E_n - E_1} = \frac{3}{2} a_1^3 F^2 \sum n^4$$

$$\Delta W = -\frac{n^4}{16}\left(\frac{\hbar^2}{me^2}\right)^3 F^2 \{17n^2 - 3(n_1-n_2)^2 - 9m'^2 + 19\}$$

$n=1$, $n_1 = n_2 = m' = 0$.

$$-\frac{\partial(\Delta W)}{\partial F} = \frac{9}{2}\left(\frac{\hbar^2}{me^2}\right)^3 F$$

G. Wentzel, ZS. 38 (1926), 527
F. Waller, ibid. 635
P. S. Epstein, Phys. Rev. 28 (1926), 695

$$\frac{3\hbar^2}{2me} F n (n_1 - n_2)$$

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052

Quantum Mechanics (Ph 238)
Spring Session (1952)

052

What we know already:

(i) Bound states (Discrete Energy States)
H-atom, He-atom etc

(ii) Continuous Energy States
Collision processes

(iii) Effect of static El. ~~and~~ Mg. fields, (Zeeman Stark

What we don't know yet:

(iii) Fine structure in energy levels due to relativistic effects

(iv) Effect of radiation
(Effect of time-dependent el. mg. field on atomic system)

Program

I. Theory of Radiation { semi-classical
II. Theory of Electron
(Dirac's theory)

III. Methods of Approximation
(i) W. K. B. method
(ii) Methods based on variation principle

IV. Group theoretical considerations

V. Quantization of Wave Fields

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Reference

(I, II) { Schiff, Q. M.
Heitler, Q. T. of Radiation

Semi-classical theory of (radiation) dispersion

Problem. Show that

$$\sum_j f_{jk} \simeq 1$$

and hence the dispersion formula reduces to the classical Thomson formula

$$n^2 - 1 \simeq -\frac{Ne^2}{\pi m \nu^2}$$

in the limit $\nu \gg \nu_{jk}$ for all j.

Oscillator strength

$$m(\ddot{y} + \omega_s^2 y) = -eE. \qquad E = E_0 \sin \omega t$$

$$y = \frac{eE}{m(\omega^2 - \omega_s^2)}$$

$$\ddot{y} = \frac{-\omega^2 e E}{m(\omega^2 - \omega_s^2)}$$

$$m(\ddot{y} + \omega_s^2 y) = -eE$$

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$$P = -\sum_s \frac{N f_s \cdot e^2}{m(\omega^2 - \omega_s^2)} E$$

classical

$N f_s$: number of oscillators with the eigen-frequency ω_s.

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Radiation and Matter

Classical Electromagnetic field

$$A = \sum_\lambda q_\lambda^{(t)} A_\lambda^{(t)} + \sum_\lambda q_\lambda^{(\ell)} A_\lambda^{(\ell)}$$

$$A_0 = \sum a_\lambda^{(t)} \varphi_\lambda$$

$$\Delta (A_\lambda^{(t)}, A_\lambda^{(\ell)}, \varphi_\lambda) + \frac{\omega_\lambda^2}{c^2} (A_\lambda^{(t)}, A_\lambda^{(\ell)}, \varphi_\lambda) = 0$$

div ~~curl~~ $A_\lambda^{(t)} = 0$

curl $A_\lambda^{(\ell)} = 0$

$A_\lambda^{(\ell)} = \frac{c}{\omega_\lambda} \operatorname{grad} \varphi_\lambda$ }

$$\int A_\lambda^{(t),(\ell)} A_\mu^{(t),(\ell)} dv = 4\pi c^2 \delta_{\ell\ell} \delta_{\lambda\mu}$$

$$\int \varphi_\lambda \varphi_\mu dv = 4\pi c^2 \delta_{\lambda\mu}$$

Lorentz condition, $\left(\operatorname{div} A + \frac{1}{c} \frac{\partial A_0}{\partial t} = 0 \right)$

$$(L)^0 \quad \omega_\lambda q_\lambda^{(\ell)} = a_\lambda$$

Field eq.:

$$(I) \quad \ddot{q}_\lambda^{(t)} + \omega_\lambda^2 q_\lambda^{(t)} = \frac{1}{c} \sum_k \dot{e}_k A_\lambda^{(t)}(r_k)$$

$$(II) \quad \ddot{q}_\lambda^{(\ell)} + \omega_\lambda^2 q_\lambda^{(\ell)} = \frac{1}{c} \sum_k \dot{e}_k A_\lambda^{(\ell)}(r_k)$$

$$(III) \quad \ddot{a}_\lambda + \omega_0^2 a_\lambda = \sum_k e_k \varphi_\lambda(r_k)$$

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Maxwell condition

$$\mathrm{div}\, E = 4\pi\rho$$

(M) $\omega_\lambda \dot{q}_\lambda + \omega_\lambda^2 a_\lambda = \sum_k e_k \varphi(r_k)$

(M) and (III)

(IV) $\omega_\lambda \dot{q}_\lambda = \ddot{a}_\lambda$

~~$\omega_\lambda \ddot{q}_\lambda = \dddot{a}_\lambda$~~

Conservation law of charge

~~$\frac{\partial \rho}{\partial t} + \mathrm{div}\, I = 0$~~

~~or~~ (C) $\underline{i_k = e_k \dot{r}_k}$

$$\sum_k i_k \,\mathrm{grad}\, \varphi_\lambda(r_k) = \sum_k e_k \dot{r}_k \,\mathrm{grad}\, \varphi_\lambda(r_k)$$

$$\omega_\lambda A_\lambda^{(l)} = \sum_k e_k \frac{d\varphi_\lambda(r_k)}{dt} = \frac{d}{dt} \sum_k e_k \varphi_\lambda(r_k)$$

or by (II) and (III)

$$\omega_\lambda \ddot{q}_\lambda^{(l)} + \omega_\lambda^3 q_\lambda^{(l)} = \dddot{a}_\lambda + \omega_\lambda^2 \dot{a}_\lambda$$

by (IV),

(V) $\omega_\lambda \ddot{q}_\lambda^{(l)} = \dddot{a}_\lambda$

Problem. Prove that (V), so that the relations ~~(I), (II), (III)~~, (L), ~~(M), (C) are~~ compatible with (I), (II), (III), if (M), (C) hold.

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$$\omega_\lambda \overset{\cdots(t)}{q_\lambda} = \overset{\cdots}{a_\lambda}$$

$$-\omega_\lambda^2 q_\lambda^{(t)} + \frac{1}{c}\sum_k \dot{r}_k A_\lambda^{(t)}(r_k) + \dot{r}_k (\dot{r}_k \cdot \operatorname{grad}) A_\lambda^{(t)}(r_k)$$

$$= \operatorname{grad}\varphi \qquad \varphi$$

Classical charged particles

$$H_k = \frac{1}{2m_k}\left(p_k - \frac{e_k}{c}A(r_k)\right)^2 + e_k A_0(r_k)$$

$$m_k \dot{r}_k = p_k - \frac{e_k}{c}A(r_k)$$

Hamiltonian;

$$H = H_{\text{elmg}} + \sum_k H_k$$

Canonical variables

(x_k, p_k)

$(q_\lambda^{(t)}, p_\lambda^{(t)})$

$(q_\lambda^{(l)}, p_\lambda^{(l)})$

$(q_\lambda a_\lambda, b_\lambda)$

$$H_{\text{elmg}} = \sum_\lambda \frac{1}{2}\left\{(p_\lambda^{(t)})^2 + \omega_\lambda^2 (q_\lambda^{(t)})^2\right\} = H^{(t)}$$

$$+ \sum_\lambda \frac{1}{2}\left\{(p_\lambda^{(l)})^2 + \omega_\lambda^2 (q_\lambda^{(l)})^2\right\} \Big\} H^{(l)}$$

$$- \sum_\lambda \frac{1}{2}\left\{b_\lambda^2 + \omega_\lambda^2 a_\lambda^2\right\}$$

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$$\dot{x}_k = \frac{\partial H}{\partial p_{xk}}$$

$$\dot{p}_{xk} = -\frac{\partial H}{\partial x_k}$$

$$\dot{q}_\lambda^{(t)} = \frac{\partial H}{\partial p_\lambda^{(t)}} = p_\lambda^{(t)}$$

$$\dot{p}_\lambda^{(t)} = -\frac{\partial H}{\partial q_\lambda^{(t)}} = -\omega_\lambda^2 q_\lambda^{(t)}$$

$$+\sum_k \frac{e_k}{m_k c} p_k A_\lambda^{(t)}(r_k) - \sum_k \frac{e_k^2}{m_k}\cdots$$

$$\sum_k \frac{e_k}{c} \dot{r}_k A_\lambda^{(t)}(r_k)$$

$$\dot{q}_\lambda^{(l)} = p_\lambda^{(l)}$$

$$\dot{p}_\lambda^{(l)} = -\omega_\lambda^2 q_\lambda^{(l)} + \frac{1}{c}\sum_k e_k \dot{r}_k A_\lambda^{(l)}(r_k)$$

$$\dot{a}_\lambda = \frac{\partial H}{\partial b_\lambda} = -b_\lambda$$

$$\dot{b}_\lambda = -\frac{\partial H}{\partial a_\lambda} = \omega_\lambda^2 a_\lambda - \sum_k e_k \varphi_\lambda(r_k)$$

$$H_k = \sum_k \frac{1}{2m_k} p_k^2 - \frac{e_k}{2m_k c}(p_k A(r_k) + A(r_k) p_k)$$

$$+ \frac{e_k^2}{2m_k c^2} A^2(r_k) + e_k A_0(r_k)$$

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Lorentz condition : (L') $\boxed{\omega_\lambda q_{p\lambda}^{(l)} = -b_\lambda}$

$$H^{(l)} = \sum_\lambda \frac{1}{2}\{(p_\lambda^{(l)})^2 - \omega_\lambda^2 a_\lambda^2\}$$

Maxwell

$$(M')\quad \boxed{\omega_\lambda p_\lambda^{(l)} = \omega_\lambda \dot{q}_\lambda^{(l)} = -\omega_\lambda^2 a_\lambda + \sum_k e_k \varphi_\lambda(r_k)}$$

$$H^{(l)} + \sum_k e_k A_0(r_k)$$

$$= \sum_\lambda \frac{1}{2}\{(p_\lambda^{(l)})^2 - \omega_\lambda^2 q_\lambda^2\} + \sum_\lambda \sum_k e_k \varphi_\lambda(r_k)\, a_\lambda$$

$$= \sum_\lambda \left[\frac{1}{2}\left\{-\omega_\lambda a_\lambda + \frac{1}{\omega_\lambda}\sum_k e_k \varphi_\lambda(r_k)\right\}^2 - \frac{1}{2}\omega_\lambda^2 q_\lambda^2 + \sum_k e_k a_\lambda \varphi_\lambda(r_k)\right]$$

$$= \sum_\lambda \frac{1}{2\omega_\lambda^2} \sum_{k,l} e_k e_l \varphi_\lambda(r_k)\varphi_\lambda(r_l)$$

$$F(r_k, r_l) \equiv \sum_\lambda \frac{1}{\omega_\lambda^2} \varphi_\lambda(r_k)\varphi_\lambda(r_l)$$

$$\Delta_k F = \sum_\lambda \frac{1}{\omega_\lambda^2} \Delta_k \varphi_\lambda(r_k)\cdot \varphi_\lambda(r_l)$$

$$= -\frac{1}{c^2}\sum_\lambda \varphi_\lambda(r_k)\varphi_\lambda(r_l)$$

$$= -4\pi\delta(r_i - r_k)$$

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$$F(r_k - r_l) = \frac{1}{r_{kl}} \left(+ f(r_k, r_l) \right)^{*}$$

$$H = H^{(t)} + \sum_k H_k + \sum_{k<l} \frac{e_k e_l}{r_{kl}} + \frac{1}{2} \sum_k \frac{e_k^2}{r_{kk}}$$

Self-energy : divergent

Problem. Prove directly that

$$F = \frac{1}{r_{kl}}$$

by taking

$$\varphi_\lambda = \sqrt{8\pi c^2} \begin{pmatrix} \cos(k_\lambda r) \\ \sin(k_\lambda r) \end{pmatrix}$$

under the restriction that $-k_\lambda$ is omitted, if k_λ is already counted.

$$\frac{1}{2} \int_0^\infty \iiint \frac{\cos(K r_{kl} \cos\theta)}{K^2} K^2 dK \sin\theta \, d\theta \, d\varphi$$

$$\left(\frac{1}{2\pi}\right)^3 = \frac{2\pi}{(2\pi)^2}$$

$$= \frac{1}{2} \int \frac{\sin K r_{kl}}{K r_{kl}} dK$$

$$= \frac{1}{2} \frac{2\pi}{r_{kl}} \int_0^\infty \frac{\sin x}{x} dx = \frac{1}{4\pi} \frac{1}{r_{kl}} \cdot \frac{1}{2} \cdot \pi$$

* $\Delta_k f = \partial_l f = 0$

$f = \text{const.} = 0$

$\therefore \left(\frac{1}{2}\right) \sum_k \cdot \frac{\sin k r_k \sin k r_l + \cos k r_k \cos k r_l}{\omega_\lambda^2}$

$= \frac{1}{2} \sum_k \cos k (r_k - r_l) / k^2 c^2$

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Elimination of longitudinal wave

$H(q_k, p_k, q_\lambda^{(t)}, p_\lambda^{(t)}, q_\lambda^{(l)}, q_\lambda^{(l)})$

Hamilton-Jacobi

$$\frac{\partial S}{\partial t} = H\left(q_k, \frac{\partial S}{\partial q_k}, \cdots\right)$$

$$S(q_k, q_\lambda^{(t)}, q_\lambda^{(l)}, t)$$

$$= S_1 + S_2$$

$$S_2 = \sum q_\lambda^{(l)} \sum_k e_k \frac{\varphi_\lambda(r_k)}{\omega_\lambda}$$

$\left(\frac{\partial S_2}{\partial t} = 0\right)$ $\qquad A_\lambda^{(l)} = \frac{c}{\omega_\lambda} \operatorname{grad} q_\lambda$

$$H_k = \frac{1}{2m_k}\left(p_k - \frac{e_k}{c} A(r_k)\right)^2$$

$$= \frac{1}{2m_k}\left(\operatorname{grad}_k S_1 + \operatorname{grad}_k S_2 - \frac{e_k}{c} A(r_k)\right)^2$$

$$= \frac{1}{2m_k}\left(\operatorname{grad}_k S_1 + \frac{e_k}{c}\sum_\lambda q_\lambda^{(l)} A_\lambda^{(l)}(r_k) - \frac{e_k}{c} A(r_k)\right)^2$$

$$= \frac{1}{2m_k}\left(\operatorname{grad}_k S_1 - \frac{e_k}{c}\sum_\lambda q_\lambda^{(t)} A_\lambda^{(t)}(r_k)\right)^2$$

$$\frac{\partial S_1}{\partial t} = H'\left(q_k, \frac{\partial S_1}{\partial q_k}; q_\lambda^{(t)}, \frac{\partial S_1}{\partial q_\lambda^{(t)}}\right)$$

$$H' = \sum H_k + H^{(t)} + \sum_{k<l} \frac{e_k e_l}{r_{kl}}$$

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$$H_k = \frac{1}{2m_k}\left(p_k - \frac{e_k}{c}\sum_\lambda q_\lambda^{(t)} A_\lambda^{(t)}\right)^2$$

External field: $A^{(e)}$, $A_0^{(e)}$

Emission of Photon

one electron ~ photon system

$$H = \frac{1}{2m}\left(p + \frac{e}{c}A^{(t)}(r)\right)^2 + \sum_\lambda \hbar\omega_\lambda (N_\lambda + \tfrac{1}{2}) \quad + V(r)$$

$$A(r,t) = \sum_\lambda \sqrt{\frac{\hbar}{2\omega_\lambda}}\left(a_\lambda A_\lambda + a_\lambda^* \bar{A}_\lambda\right)$$

$$A_\lambda = \sqrt{\frac{4\pi c^2}{L^3}}\, e_\lambda\, e^{i k_\lambda r}$$

$$A(r,t) = \sum_\lambda \sqrt{\frac{2\pi\hbar c^2}{\omega_\lambda L^3}}\left(a_\lambda e^{i k_\lambda r} + a_\lambda^* e^{-i k_\lambda r}\right) e_\lambda$$

$\Psi(r, n_1, n_2, \cdots n_\lambda \cdots, t)$

$N_\lambda = a_\lambda^* a_\lambda$

$H = H_0 + H'$

$$H_0 = \frac{1}{2m}p^2 + V(r) + \sum_\lambda \hbar\omega_\lambda (N_\lambda + \tfrac{1}{2})$$

$N_\lambda = n_\lambda$

$$H' = \frac{e}{2mc}(p\cdot A(r) + A(r)\, p) + \frac{e^2}{2mc^2}A^2(r)$$

$$= \frac{e}{mc}A(r)(-i\hbar\,\mathrm{grad}) + \frac{e^2}{2mc^2}A^2(r)$$

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$$\chi_{n_1' n_2' \cdots n_\lambda' \cdots}(n_1, n_2, \cdots n_\lambda \cdots) = \delta_{n_1 n_1'} \delta_{n_2 n_2'} \cdots \delta_{n_\lambda n_\lambda'} \cdots$$

Initial state

$$H_0 \Psi_A = W_A \Psi_A$$

$$\Psi_A = \psi_a(r) \cdot \chi_{n_1' n_2' \cdots n_\lambda' \cdots}(n_1, n_2 \cdots n_\lambda \cdots) e^{-iE_a t/\hbar} \, e^{-i(n_1'\omega_1' + \cdots + n_\lambda'\omega_\lambda' + \cdots)t}$$

$$\left\{ \frac{1}{2\mu} p^2 + V(r) \right\} \psi_a(r) = E_a \psi_a(r)$$

$$W_A = E_a + n_1' \hbar\omega_1' + \cdots + n_\lambda' \hbar\omega_\lambda' + \cdots$$

Final state

$$\Psi_B = \psi_b(r) \chi_{n_1' n_2' \cdots n_\lambda' + 1 \cdots}(n_1, n_2 \cdots n_\lambda \cdots) \, e^{-iE_b t/\hbar} \, e^{-i(n_1'\omega_1 + n_2'\omega_2 + \cdots (n_\lambda' + 1)\omega_\lambda' + \cdots)t}$$

$$W_B = E_b + n_1' \hbar\omega_1 + \cdots + (n_\lambda' + 1)\hbar\omega_\lambda' + \cdots$$

Transition probability

$$W_{BA}^{(\lambda)} d\Omega = \frac{2\pi}{\hbar} |H'_{BA}|^2 \rho_W \, d\Omega$$

$$W = W_A = W_B .$$

$$H' \rightarrow \frac{e}{\mu\omega} \sqrt{\frac{2\pi\hbar\alpha}{\omega_\lambda L^3}} (e_\lambda \cdot p) \, a_\lambda^* \, e^{-ik_\lambda r}$$

$d\Omega$ k_λ

$$H'_{BA} = \frac{e}{\mu\omega} \sqrt{\frac{2\pi\hbar\alpha}{\omega_\lambda L^3}} \sqrt{n_\lambda' + 1} \int \tilde{\psi}_b \, e^{-ik_\lambda r} \times (e_\lambda \cdot p) \psi_a \, dv$$

$$\rho_W \, dW \, d\Omega = \left(\frac{L}{2\pi}\right)^3 k^2 \, dk \, d\Omega$$

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$$= \left(\frac{L}{2\pi c}\right)^3 \omega^2 d\omega\, d\Omega$$

$$W = \hbar\omega$$

$$\rho_W d\Omega = \left(\frac{L}{2\pi c}\right)^3 \frac{\omega^2 d\omega d\Omega}{\hbar}$$

$$W_{BA}^{(\lambda)} d\Omega = \frac{e^2}{m^2 c^3 \cdot \hbar} \frac{\omega}{2\pi} (\bar{n}'_\lambda + 1) \times \left| \int \tilde{\psi}_b e^{-i k_\lambda r} (e_\lambda p) \psi_a dv \right|^2$$

$\bar{n}'_\lambda$: average number of photons (before the transition) with the wave number k_λ which is about equal to k_λ.

$$\hbar c k_\lambda'' = E_a - E_b$$

$x = 1/k_\lambda$ > r_0 (size of the atom)

$$\int \tilde{\psi}_b e^{-i k_\lambda r} (e_\lambda p) \psi_a dv$$

$$\cong m \int \tilde{\psi}_b (e_\lambda p) \psi_a dv$$

$$= \frac{m\, i(E_b - E_a)}{\hbar} \int \tilde{\psi}_b (e_\lambda r) \psi_a dv$$

Heisenberg repr

$$p_{ba}^{(H)} = \int \tilde{\psi}_b^e p \psi_a^e dv \underbrace{e^{i(E_b - E_a)t/\hbar}}_{} = m \frac{d}{dt}(r_{ba}^{(H)})$$

$$= \frac{m \cdot i(E_b - E_a)}{\hbar} r_{ba}^{(H)}$$

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Problem: Show that directly from Schrö. eq. that

$(-i\hbar)\iiint \tilde{\psi}_b \operatorname{grad} \psi_a \, dw = \frac{m}{\omega} \iiint \tilde{\psi}_b \dot{\psi}_a \, dw$ $\quad \omega = \frac{E_a - E_b}{\hbar}$

Schrödinger repr.

$$p^{(s)}_{ba} = \frac{m \cdot i(E_b - E_a)}{\hbar} x^{(s)}_{ba}$$

$$\| \qquad \| \qquad \|$$

$$p_{ba} = -imw \, x_{ba}$$

$$W^{(\lambda)}_{BA} d\Omega = \frac{e^2 \omega^4 d\Omega}{2\pi \cdot \hbar c^3} |e_\lambda x_{ba}|^2 (\bar{n}'_\lambda + 1)$$

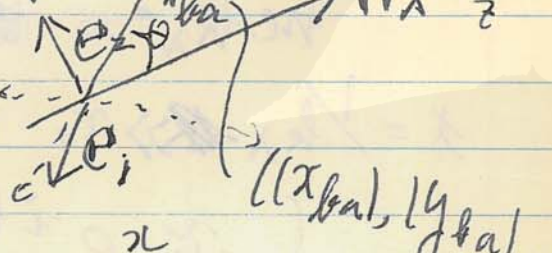
$\bar{n}_\lambda \to \bar{n}_\omega$

$$W_{BA} d\Omega = \frac{e^2 \omega^4 d\Omega}{2\pi \hbar c^3} \sum |e_\lambda x_{ba}|^2 (\bar{n}'_\omega + 1)$$

Spontaneous emission $\int \omega d. \; (\bar{n}_\omega = 0)$

x_{ba}: complex in general

$x'_{ba} \simeq x_{ba}$ if x_{ba}: real



~~$|x_{ba,x}|^2 + |x_{ba}|^2$~~

$|x_{ba}|^2 + |y_{ba}|^2$

$= |r_{ba}|^2 \cdot \sin^2\theta \to 2/3$

$|x'_{ba}|^2 = |r_{ba}|^2$

$$W_{BA} d\Omega \simeq \frac{e^2 \omega^4 d\Omega}{2\pi \hbar c^3} |r_{ba}|^2 \sin^2\theta \to 2/3$$

Intensity of light

$$S_{BA} d\Omega = \frac{e^2 \omega^4}{2\pi c^3} d\Omega \, |r_{ba}|^2 \sin^2\theta \to 2/3$$

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If we integrate over all directions of emitted photons, total intensity of light emitted per unit time is,

$$\overline{S_{BA}} = \frac{4}{3}\frac{e^2\omega^4}{c^3}|r_{ba}|^2$$

Absorption

$$W^{(\lambda)}_{AB}\,d\Omega = \frac{e^2\omega^3 d\Omega}{2\pi\hbar c^3}|e_\lambda r_{ba}|^2 \cdot \bar{n}_\lambda$$

Intensity of light: (polarized)

$$I_\omega d\omega = \hbar\omega \cdot c \cdot \frac{\bar{n}'_\lambda}{L^3} \cdot \frac{\omega^2 d\omega d\Omega}{(2\pi c)^3}$$

$$= \bar{n}'_\lambda \cdot \frac{\hbar\omega^3 d\omega d\Omega}{(2\pi c)^3}$$

Energy which is absorbed per unit time:

$$\overline{S_{AB}} = \frac{4\pi^2 e^2 \omega}{\hbar c}|e_\lambda r_{ba}|^2$$

On the average

$$= \frac{4\pi^3}{3}\frac{e^2\omega}{\hbar c}|r_{ba}|^2$$

When eigenvalues E_a, E_b are both degenerate g_a, g_b.

$$a \to b \quad |r_{ba}|^2 \to \frac{1}{g_a}\sum_{\beta,\alpha}\sum_{e_\lambda}|r_{\beta\alpha}|^2$$

$\sum_{pol} e_\lambda$

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$b \to a \to |(e_\lambda r_{ab})|^2$ e_λ r

$\sum_{p\alpha} |r_{ab}|^2 \to \frac{1}{g_b} \sum_{\gamma\alpha} \frac{1}{g_b} \sum_{\alpha,\beta} |r_{\alpha\beta}|^2$

~~$|r_{\beta a}|^2 |r_{\alpha\beta}|^2$~~ $|e_\lambda r_{\beta a}|^2 = |e_\lambda r_{\alpha\beta}|^2$

$$\frac{W_e}{W_a} = \frac{\bar{n}'_\omega + 1}{\bar{n}'_\omega} \cdot \frac{g_b}{g_a}$$

Boltzmann statistics.

$g_a e^{-E_a/kT}$

$g_b e^{-E_b/kT}$

Equilibrium condition

$$g_a e^{-E_a/kT} \cdot W_e = g_b e^{-E_b/kT} W_a$$

$$\frac{\bar{n}_\omega + 1}{\bar{n}_\omega} = e^{\hbar\omega/kT}$$

$\hbar\omega = E_a - E_b$

~~Einstein~~ $\bar{n}_\omega = \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1}$

Q.M. foundation of Einstein's derivation of Planck's formula: Energy density

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$$u(\omega)d\omega = \frac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}} \pm 1} 2\cdot\left(\frac{1}{2\pi c}\right)^3 \cdot \omega^2 d\omega \cdot 4\pi$$

$2\pi\nu = \omega$

$$u(\nu)d\nu = \frac{8\pi h\nu^3 d\nu}{c^3} \cdot \frac{1}{e^{\frac{h\nu}{kT}} \pm 1}$$

Scattering (2nd-order terms)
Raman $\quad \frac{e^2}{mc^2}$ or α in H',
Compton $\quad$ or α^2 in transition prob.
(Photo-electric effect
ψ_a : continuous state)

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Problem 1. Prove that the transition between two states of ~~equation~~ each number l, with the azimuthal quantum number m and magnetic quantum number m and (l', m') respectively is by emitting or absorbing the dipole radiation is possible only if

$$l' = l \pm 1, \quad m' = m, m \pm 1,$$

(Selection Rule
$\Delta l = \pm 1$
$\Delta m = 0, \pm 1$)

Problem 2. When there is a weak homogeneous magnetic field H in z-direction, the el. mag. wave emitted in z-direction due to the transition of an atom has the frequencies

$$\nu_0 \pm \frac{\omega_L}{2\pi}, \qquad \omega_L = \frac{eH}{2mc},$$

where ν_0 is the freq. in the abs. of H and, while the wave emitted in x or y-direction has the frequencies

$$\nu_0, \quad \nu_0 \pm \frac{\omega_L}{2\pi}$$

(Normal Zeeman Effect)

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Problem #3.

If the spin of the electron is taken into account, the Hamiltonian has the extra term

$$\frac{e\hbar}{2mc}\sigma H$$

in non-relativistic approximation. The transition probability per unit time of an electron atom from a state a to another state b by emitting a magnetic dipole radiation is given by

$$\frac{4}{3}\frac{e^2\omega^3}{\hbar c^3}.$$

$$\frac{e^2\omega^3 d\Omega}{2\pi\hbar}\left(\frac{\hbar}{mc}\right)^2\left|[e_\lambda \times p^{(0)}_\lambda],\sigma_{ba}\right|^2(\bar{n}_\lambda+1)$$

where $p^{(0)}_\lambda$ is the unit vector in the dir. of p_λ.

Hint: $\frac{e}{mc}Ap \to \frac{e\hbar}{2mc}\sigma H$

$$A = \sum_\lambda \sqrt{\frac{\hbar}{2\omega_\lambda}}\sqrt{\frac{2\pi\hbar}{\omega_\lambda L^3}}\cdot c e_\lambda\left(a_\lambda e^{ikr} + a^*_\lambda e^{-ikr}\right)$$

$$i(k_x e_{\lambda y} - k_y e_{\lambda x})$$

$$H = \operatorname{curl} A = \sum_\lambda \sqrt{\frac{2\pi\hbar}{\omega_\lambda L^3}}\, c\cdot i[k_\lambda e_\lambda]\left(\quad,\quad\right)$$

$$\frac{e}{mc}(e_\lambda p_{ba}) = \frac{-im\omega_{e_\lambda}}{\frac{e}{mc}} r_{ba} = -i\frac{e\omega}{c(e_\lambda)} r_{ba}$$

$$\to -i\frac{e\hbar}{mc}[e_\lambda k_\lambda]\sigma_{ba}$$

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or

$$e_\lambda r_{ba} \to \frac{\hbar}{mc}\frac{c}{\omega}[e_\lambda k_\lambda]\sigma_{ba}$$

~~$\to \frac{\hbar}{mc} e_\lambda [\sigma_{ba} k_\lambda$~~

$$w_{BA}\,d\Omega = \left(\frac{e}{mc}\right)^2\left(\frac{\hbar}{mc}\right)^2 \cdot k_\lambda^{(\omega)}$$

$$\frac{e^2\omega^3 d\Omega}{2\pi\hbar}\cdot\left(\frac{\hbar}{mc}\right)^2 \left|[e_\lambda, k_\lambda]\sigma_{ba}\right|^2 (\bar{n}_\lambda + 1)$$

the int. of

* Show that the m. d. r. is smaller than that of el. dip. rad. by a factor of the order of

$$\left(\frac{\hbar}{mc}\right)^2 / r_0^2,$$

where r_0 is the radius of the atom.

$$\sigma_{ba} = \int \tilde{\psi}_b \sigma \psi_a$$

$$\sigma_{ba,x} = \int\int \tilde{\psi}_b(r,+1)\psi_a(r,-1) + \tilde{\psi}_b(r,-1)\psi_a(r,+1)\,dx\,dy\,dz$$

$$\psi_a = \chi_a \cdot \alpha \to \begin{pmatrix}1\\0\end{pmatrix} \qquad \psi_b = \chi_b \cdot \beta \to \begin{pmatrix}0\\1\end{pmatrix}$$

$$\sigma_{ba,x} = \int \tilde{\chi}_b \chi_a\,dx\,dy\,dz$$

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Relativistic Theory of Electron

Non-relativistic

Problem. 1. Pauli approximation

$$\left\{\frac{W}{c} - \alpha p - \beta mc\right\}\psi = 0$$

$$W/c = \pm\sqrt{m^2c^2 + p^2}$$

If $p \ll mc$, $(W>0)$, ψ_3, ψ_4 is smaller than ψ_1, ψ_2 by a factor p/mc.

If $p \ll mc$, $(W<0)$, ψ_1, ψ_2 is smaller than ψ_3, ψ_4 by a factor p/mc.

Problem 2.

~~Problem. 2. Pauli approximation.~~

$W>0$. If $W - mc^2 \ll mc^2$.

$W - mc^2 = E$, ~~$A_x = A_y = A_z = 0$~~

$$\left(E + \frac{e}{c}A_0\right)\psi_1 + \left\{i\hbar\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right) - \frac{e}{c}(A_x - iA_y)\right\}\psi_4 + \left\{i\hbar\frac{\partial}{\partial z} - \frac{e}{c}A_z\right\}\psi_3 = 0$$

$$\left(E + \frac{e}{c}A_0\right)\psi_2 + \left\{i\hbar\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) - \frac{e}{c}(A_x + iA_y)\right\}\psi_3 - \left\{i\hbar\frac{\partial}{\partial z} - \frac{e}{c}A_z\right\}\psi_4 = 0$$

$$\psi_3 \cong \frac{-1}{2mc}\left[\left\{i\hbar\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right) - \frac{e}{c}(A_x - iA_y)\right\}\psi_2 + \left\{i\hbar\frac{\partial}{\partial z} - \frac{e}{c}A_z\right\}\psi_1\right]$$

$$\psi_4 \cong -\frac{1}{2mc}\left[\left\{i\hbar\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) - \frac{e}{c}(A_x + iA_y)\right\}\psi_1 - \left\{i\hbar\frac{\partial}{\partial z} - \frac{e}{c}A_z\right\}\psi_2\right]$$

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$$\left(E + \frac{e}{c}A_0\right)\psi_1 + \qquad \psi = (\varphi, \chi)$$

$$E + e$$

$$\left(E - mc + \frac{e}{c}A_0\right)\psi = (\sigma, p + \frac{e}{c}A)\chi$$

$$\left(E + 2mc + \frac{E}{c} + \frac{e}{c}A_0\right)\chi = (\sigma, p + \frac{e}{c}A)\psi$$

$$E = mc^2 + E$$

$$\left(E/c + \frac{e}{c}A_0\right)\psi = (\sigma, p + \frac{e}{c}A)$$

$$\times \frac{1}{2mc}(\sigma, p + \frac{e}{c}A)\psi$$

$$\left\{\frac{E}{c} + \frac{e}{c}A_0 - \frac{i\sigma_z}{2mc}\right.$$

$$\left. \sigma_x\sigma_y\{(p_x + \frac{e}{c}A_x)(p_y + \frac{e}{c}A_y) - (p_y + \frac{e}{c}A_y)(p_x + \frac{e}{c}A_x)\}\right.$$

$$-ih$$

$$E\psi = \left\{-\frac{e}{2mc}A_0 + \frac{1}{2mc}\left(p^{2m} + \frac{e}{c}A\right)^2\right.$$

$$\left. + \frac{eh}{2mc}\sigma_z\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\right\}\psi$$

$$+ \cdots$$

$$E\psi = \cancel{-eA_0}\, H\psi$$

$$H = \frac{1}{2mc}\left(p + \frac{e}{c}A\right)^2 - eA_0 + \frac{eh}{2mc}\sigma H$$

$$\chi = \frac{1}{2mc}\left(1 + \frac{E + \frac{e}{c}A_0}{2mc^2}\right)^{-1}(\sigma, (p + \frac{e}{c}A)\psi$$

$$\simeq \frac{1}{2mc}(\sigma, (p + \frac{e}{c}A)\psi - \frac{1}{4m^2c^3}(E + eA_0)$$

$$\times (\sigma, (p + \frac{e}{c}A)\psi$$

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$$\simeq \frac{1}{2mc}(\sigma(p+\frac{e}{c}A))\psi$$

$$-\frac{1}{4m^2c^3}(E+eA_0)(\sigma p)\cdot\psi$$

$$(E/c+\frac{e}{c}A_0)\psi = \frac{1}{2mc}((\sigma p)+\frac{e}{c}A)^2\psi$$

$$\cancel{m} - \frac{1}{4m^2c^3}(\sigma p)\cdot(E+eA_0)(\sigma p)\cdot\psi$$

$$-\frac{1}{4m^2c^3}(E+eA_0)p^2 + \frac{e}{4m^2c^3}(\sigma \operatorname{grad} A_0)(\sigma \operatorname{grad})\psi$$

$$= -\frac{1}{4m^2c^3}(E+eA_0)p^2 + \frac{e\hbar^2}{4m^2c^3}\operatorname{grad}A_0\operatorname{grad}\psi$$

$$\frac{p^2}{2m}$$

$$+\frac{ie\hbar^2}{4m^2c^3}\sigma[\operatorname{grad}A_0 \times \operatorname{grad}\psi]$$

$$-eA_0 = V(r)$$

$$(\operatorname{grad}V)\cdot\operatorname{grad} = \frac{dV}{dr}\frac{\partial}{\partial r}$$

$$\operatorname{grad}V = \frac{r}{r}\frac{dV}{dr}$$

$$+\frac{\hbar}{4m^2c^3}\sigma\cdot[r\times p]\cdot\psi\left(\frac{1}{r}\frac{dV}{dr}\right)$$

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$$E\psi = \left\{ \frac{1}{2m}\left(p + \frac{e}{c}A\right)^2 - \frac{p^4}{8m^3c^2} + \frac{e\hbar}{2mc}\sigma H \right.$$

$$\left. + V(r) - \frac{\hbar^2}{4m^2c^2}\frac{dV}{dr}\frac{\partial}{\partial r} \qquad \frac{e}{2mc}sH \right.$$

$$\left. + \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\,s\cdot m \right\}\psi$$

$$s = \frac{\hbar}{2}\sigma$$

$$m = [r \times p]$$

$$\frac{\hbar}{4m^2c^2}\sigma$$

$$E\psi = \left\{ \frac{1}{2m}\left(p + \frac{e}{c}A\right)^2 - \frac{p^4}{8m^3c^2} + V(r) \right.$$

$$\left. + \frac{e\hbar}{2mc}\sigma H - \frac{\hbar^2}{4m^2c^2}\frac{dV}{dr}\frac{\partial}{\partial r} \right.$$

$$\left. + \frac{\hbar}{4m^2c^2}\frac{1}{r}\frac{dV}{dr}(\sigma \cdot m) \right\}\psi$$

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L. L. Foldy and S. A. Wouthuysen, P. R. 78 (1950), 29.

$$\Psi' = e^{iS}\Psi$$

$$H' = e^{iS} H e^{-iS}$$

$$i\frac{\partial \Psi'}{\partial t} = H'\Psi'$$

$$S = -(i/2m)\beta\alpha\cdot p\cdot w(p/m)$$

$$H' \Longrightarrow H = \beta m + \alpha p$$

$$e^{iS} = \sum \left(\frac{m}{2m}\right)^n \frac{1}{n!} (\beta\alpha p)^n w^n(p/m)$$

$$(\beta\alpha p)^2 = -p^2$$

$$\beta\alpha_x \beta\alpha_x = -1 \qquad \beta\alpha_x\beta\alpha_y = -\beta^2\alpha_x\alpha_y$$

$$= \beta^2\alpha_y\alpha_x = -\beta\alpha_y\beta\alpha_x$$

$$e^{iS} = \sum_n \left(\frac{1}{2m}\right)^{2n} \frac{(-1)^{2n}}{n!} p^{2n} w^{2n}(p/m)$$

$$+ \frac{\beta\alpha p}{p} \sum_n \left(\frac{1}{2m}\right)^{2n+1} \frac{(-1)^{2n+1}}{n!} p^{2n+1} w^{2n+1}(p/m)$$

$$= \cos\left(\frac{pw}{2m}\right) + \frac{\beta\alpha p}{p}\sin\left(\frac{pw}{2m}\right)$$

$$\beta(\alpha p) = -(\alpha p)\beta$$

$$\beta\{\beta(\alpha p)\} = -\{\beta(\alpha p)\}\beta$$

$$(\alpha p)\{\beta(\alpha p)\} = -\{\beta(\alpha p)\}(\alpha p)$$

$$e^{+iS} H e^{-iS} = e^{2iS} H.$$

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$$= \left\{ \cos\left(\frac{pw}{m}\right) + \left(\frac{\beta \alpha p}{p}\right) \sin\left(\frac{pw}{m}\right) \right\} \times \left\{ \beta m + (\alpha p) \right\}$$

$$= \beta \left\{ m \cos\left(\frac{pw}{m}\right) + p \sin\left(\frac{pw}{m}\right) \right\} + \frac{(\alpha p)}{p} \left\{ p \cos\left(\frac{pw}{m}\right) - m \sin\left(\frac{pw}{m}\right) \right\}$$

$$\tan\left(\frac{pw}{m}\right) = \frac{p}{m}$$

$$\frac{pw}{m} = \arctan(p/m)$$

$$w = \frac{m}{p} \arctan(p/m)$$

$$\cos\left(\frac{pw}{m}\right) = \frac{1}{\sqrt{1+\tan\left(\frac{pw}{m}\right)^2}} = \frac{1}{\sqrt{1+\left(\frac{p}{m}\right)^2}}$$

$$H' = \frac{\beta m}{\sqrt{1+\left(\frac{p}{m}\right)^2}} \left\{ 1 + \frac{p}{m} \cdot \frac{p}{m} \right\}$$

$$= \beta \sqrt{p^2+m^2} = \beta E_p$$

$$r = e^{iS} R e^{-iS} \qquad p = e^{iS} p e^{-iS}$$

$$R = r + \frac{i\beta\alpha}{2E_p} - \frac{i\beta(\alpha p)p + [\alpha \times p]p}{2E_p(E_p+m)p}$$

$$\frac{dr}{dt} = i[H', r] = \beta p / E_p$$

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$$\sigma = e^{iS} \sum e^{-iS}$$

$$\sum = \sigma - \frac{i}{E_v}\beta[\alpha \times p\sigma] - \frac{[p\sigma \times [\sigma \times p\sigma]]}{E_p[E_p + m]}$$

$$H = \beta m + \mathcal{E} + \mathcal{O} \qquad \mathcal{E} = -e\varphi$$

$$H' = e^{iS} H e^{-iS} \qquad \mathcal{O} = \alpha(p - eA)$$

$$S \approx -i/2m \cdot \beta \mathcal{O}$$

$$H' = \beta m + \mathcal{E} + \frac{\beta}{2m}\mathcal{O}^2 - \frac{1}{8m^2}[\mathcal{O},[\mathcal{O},\mathcal{E}]]$$

$$+ \frac{1}{2m}\beta[\mathcal{O},\mathcal{E}]\mathcal{O} - \frac{1}{3m^2}\mathcal{O}^3$$

$$S_1 = -\frac{i}{2m}\beta\alpha(p - eA)$$

$$H_1 \approx \beta m - e\varphi + \frac{\beta}{2m}(p - eA)^2$$

$$- \frac{e}{2m}\beta\sigma H - \frac{e}{4m^2}\sigma E \times (p - eA)$$

$$+ \frac{e}{8m^2} d\omega E + \mathcal{O}_1 + \mathcal{O}_2$$

$$S_2 = -\frac{i}{2m}\beta\mathcal{O}_1 \quad \text{etc}$$

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Majorana Representation

In Dirac representation,

$$\left.\begin{aligned}\tilde{\alpha}_x &= \alpha_x \\ \tilde{\alpha}_y &= -\alpha_y \\ \tilde{\alpha}_z &= \alpha_z \\ \tilde{\beta} &= \beta\end{aligned}\right\} \qquad \left.\begin{aligned}\alpha_x^{\dagger} &= \alpha_x \\ \alpha_y^{\dagger} &= -\alpha_y \\ \alpha_z^{\dagger} &= \alpha_z \\ \beta^{\dagger} &= \beta.\end{aligned}\right\}$$

One may interchange α_y and β:

$$\left.\begin{aligned}\tilde{\alpha}_x &= \alpha_x^{\dagger} = \alpha_x \\ \tilde{\alpha}_y &= \beta^{\dagger} = \beta \\ \tilde{\beta} &= \alpha_y^{\dagger} = \alpha_y \\ \tilde{\alpha}_z &= \alpha_z^{\dagger} = \alpha_z\end{aligned}\right\} \text{ real elements}$$

$\tilde{\beta} = \beta^{\dagger} = -\beta$. imaginary el.

$$\left\{\frac{i\hbar}{c}\frac{\partial}{\partial t} + i\hbar(\alpha \operatorname{grad}) - \beta\varkappa c\right\}\psi = 0$$

or $\left\{\frac{1}{c}\frac{\partial}{\partial t} + (\alpha \operatorname{grad}) - i\beta\varkappa\right\}\psi = 0 \quad (M)$

$$\varkappa = \frac{mc}{\hbar},$$

$$i\beta = \beta' \qquad \beta'^2 = -1$$

$$(\beta')^* = -\beta'$$

$$\tilde{\beta}' = \beta'^{\dagger} = -\beta' \qquad \beta' \text{ , } \quad \beta'^{\dagger} = -\beta'$$

Now, if ψ is a solution of (M), ψ^* is also a solution.

$$\psi = u \exp i(\mathbf{k}\mathbf{r} - k_0 ct)$$

$$\left\{-ik_0 + \alpha\mathbf{k} + \beta\varkappa\right\}u$$

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$$\begin{pmatrix} k_0-k_y & 0 & k_z & k_x-ix \\ 0 & k_0-k_y & k_x+ix-k_z & \\ k_z & k_x-ix & k_0+k_y & 0 \\ k_x+ix & -k_z & 0 & k_0+k_y \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = 0$$

k_z $\quad k_z u_3 + (k_x - ix) u_4 = -(k_0 - k_y) u_1$

$(k_x - ix)$ $\quad (k_x + ix) u_3 - k_z u_4 = -(k_0 - k_y) u_2$

$$-(k_0 + k_y) u_3 = k_z u_1 + (k_x - ix) u_2$$

$$-(k_0 + k_y) u_4 = (k_x + ix) u_1 - k_z u_2$$

$1 + \overline{(k_0 + k_y)^2}$

$$k^2 u_3 = -(k_0 - k_y)(k_z u_1 - (k_x - ix) u_2)$$

or $$u_3 = \frac{-(k_0 - k_y)\{k_z u_1 - (k_x - ix) u_2\}}{k_0^2 - k_y^2}$$

$$u_4 = \frac{-(k_0 - k_y)\{(k_x + ix) u_1 - k_z u_2\}}{k_0^2 - k_y^2}$$

	$k_0 > 0$	$k_0 > 0$	$k_0 < 0$	$k_0 < 0$
u_1	1	0	1	0
u_2	0	1	0	1
u_3	$\frac{-k_z}{k_0 + k_y}$	$\frac{k_x - ix}{k_0 + k_y}$	$\frac{k_z}{-k_0 + k_y}$	$\frac{k_x - ix}{-k_0 + k_y}$
u_4	$\frac{-(k_x + ix)}{k_0 + k_y}$	$\frac{k_z}{k_0 + k_y}$	$\frac{-(k_x + ix)}{-k_0 + k_y}$	$\frac{k_z}{-k_0 + k_y}$
	$\Psi^{(1)}_k(k, k_0)$	$\Psi^{(2)}_k(k, k_0)$	$\Psi^{(3)}_k(k, -k_0)$	$\Psi^{(4)}_k(k, -k_0)$

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$$\tilde{\Psi}^{(1)}_{\alpha}(k, k_0) = \Psi^{(3)}_{\beta}(-k, -k_0)$$

$$\tilde{\Psi}^{(2)}_{\alpha}(k, k_0) = \Psi^{(4)}_{\alpha}(-k, -k_0)$$

$$\Psi = \sum_{j=1}^{2} a_j(k, k_0) \Psi^{(j)}(k, k_0) + \sum_{j=3}^{4} b_j \Psi^{(j)}(k, -k_0)$$

$$= \sum_{j=1}^{2} a_j(k, k_0) \Psi^{(j)}(k, k_0) + \sum_{j=1}^{2} b_j(-k, -k_0) \tilde{\Psi}^{(j)}(k, k_0)$$

Ψ : Hermitian.

$$b_j(k, -k_0) = a_j^*(k, k_0)$$

$$\Psi = \sum_{j=1}^{2} \{ a_j(k, k_0) \Psi^{(j)}(k, k_0) + a_j^*(k, k_0) \tilde{\Psi}^{(j)}(k, k_0) \}$$

$$= \sum_{j=1}^{2} \{ a_{j,k} \Psi^{(j)}(k) + a^*_{j,k} \tilde{\Psi}^{(j)}(k) \}$$

This applies only for neutral particles, because for charged particles, Majorana

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equations become complex and
α_j and β_j ~~must be different~~ are
~~not~~ hermitian conjugate to
each other.

$$\alpha_x = \rho_1 \sigma_x \qquad \alpha_x = \rho_1 \sigma_x$$
$$\alpha_y = \rho_1 \sigma_y \qquad \alpha_y = \rho_1 \sigma_y \rho_3$$
$$\alpha_z = \rho_1 \sigma_z \qquad \sigma_z = \rho_1 \sigma_z$$
$$\beta = \rho_3 \qquad \beta = \rho_1 \sigma_y$$

$\alpha_x\alpha_y\alpha_z\beta = i\rho_1\rho_3 = \rho_2$ ~~is Hermitian~~ $\qquad \alpha_x\alpha_y\alpha_z\beta = -i\rho_2\sigma_x \cdot i\rho_2 = -\rho_2$

Pseudoscalar ~~interaction~~ leads
purely imaginary matrix elements.
both scalar and

s. ps. pv. : $\tilde{A} = A^\dagger = -A = -A^*$

~~t. : $\tilde{T} = T$~~
~~$T^\dagger = -T$~~

v. $V = \tilde{V} = V^\dagger = V^*$

t: $(\alpha_x\alpha_y)^* = \alpha_y^*\alpha_x^* = \alpha_y\alpha_x = -(\alpha_x\alpha_y)$

~~$i\alpha_x\alpha_y$~~

$(\alpha_x\alpha_y)^\dagger = -(\alpha_x\alpha_y)$

$\{i(\alpha_x\alpha_y)\}^\dagger = -i(\alpha_x\alpha_y)$

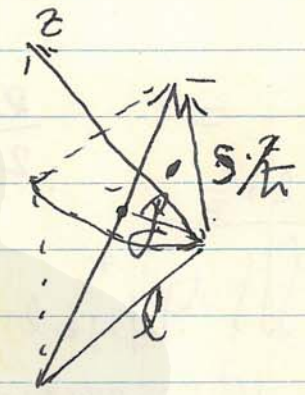
~~$\{i(\alpha_x\beta)\}^\dagger =$~~

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Problem. Anomalous Zeeman Effect

$$-\frac{e\hbar}{2mc}(m_s + 2s_z)H$$

$$m_s + 2s_z = j_z + s_z$$



~~$j^2 + \left(\frac{S}{\hbar}\right)^2 - l^2$~~

$$j\hbar = l\hbar + S$$

$$j^2 + (S/\hbar)^2 - l^2 = 2j\cdot(S/\hbar)$$

$$\overline{s_z} = \frac{j(S/\hbar)\cdot\sqrt{\frac{S}{\hbar}\left(\frac{S}{\hbar}+1\right)}}{\sqrt{j(j+1)}\sqrt{\frac{S}{\hbar}\left(\frac{S}{\hbar}+1\right)}}\cdot\frac{j_z}{\sqrt{j(j+1)}}$$

$$= \frac{j_z}{2j(j+1)}\left[j(j+1) - l(l+1) + \frac{S}{\hbar}\left(\frac{S}{\hbar}+1\right)\right]$$

$$j_z + s_z = j_z\left(1 + \frac{j(j+1) - l(l+1) + \frac{S}{\hbar}\left(\frac{S}{\hbar}+1\right)}{2j(j+1)}\right)$$

$$= j_z\,\frac{2j(j+1) - l(l+1) + \frac{1}{2}\cdot\frac{3}{2}}{2j(j+1)} \qquad -\left(l+\tfrac{3}{2}\right)\left(l-\tfrac{1}{2}\right)$$

$j = l + \frac{1}{2}$:

$$j_z\,\frac{3\left(l+\frac{1}{2}\right)\left(l+\frac{3}{2}\right) - l(l+1) + \frac{1}{2}\frac{3}{2}}{2\left(l+\frac{1}{2}\right)\left(l+\frac{3}{2}\right)}$$

$$= j_z\,\frac{3\left(l+\frac{1}{2}\right) - l + \frac{3}{4}}{2\left(l+\frac{1}{2}\right)} = j_z\,\frac{2l+2}{2\left(l+\frac{1}{2}\right)} = j_z\,\frac{j+\frac{1}{2}}{l+\frac{1}{2}}$$

$j = l - \frac{1}{2}$:

$$j_z\,\frac{3\left(l-\frac{1}{2}\right)\left(l+\frac{1}{2}\right) - \left(l+\frac{3}{2}\right)\left(l-\frac{1}{2}\right)}{2\left(l+\frac{1}{2}\right)\left(l+\frac{1}{2}\right)} = j_z\,\frac{j+\frac{1}{2}}{l+\frac{1}{2}}$$

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Problem: Prove that

$$\iiint \psi^{**}_{j,j_z,l}\ \frac{e\mathcal{H}}{2\mu c}(m_z+2s_z)\,\psi_{j,j_z,l}\,dxdydz$$

$$= \frac{e\hbar}{2\mu c}\mathcal{H}\, j_z\cdot\frac{2j+1}{2l+1}.$$

$j=l+\frac{1}{2}$

$$\iiint \psi^{*}_{j,j_z,l}\, s_z\, \psi_{j,j_z,l} = \frac{\hbar}{2}\times$$

$$\times\iiint\Big[(l+\mu+\tfrac{1}{2})\,\tilde{u}_l(r)\,\tilde{Y}_{l,\mu-\frac{1}{2}}(\theta,\varphi)\,u_l(r)\,Y_{l,\mu-\frac{1}{2}}(\theta,\varphi)$$

$$-(l-\mu+\tfrac{1}{2})\,u_l(r)\,\tilde{Y}_{l,\mu+\frac{1}{2}}(\theta,\varphi)\,u_l(r)\,Y_{l,\mu+\frac{1}{2}}(\theta,\varphi)\Big]\,dxdydz$$

$$=\frac{\hbar}{2}\cdot\frac{2\mu}{2l+1}$$

$$\hbar\left(j_z+\frac{\hbar j_z}{2l+1}\right)=\hbar j_z\frac{2l+2}{2l+1}$$

$$=\hbar j_z\frac{2j+1}{2l+1}$$

$j=l-\frac{1}{2}$

$$\frac{l-\mu+\frac{1}{2}-(l+\mu+\frac{1}{2})}{l-\mu+\frac{1}{2}+(l+\mu+\frac{1}{2})}=\frac{-2\mu}{2l+1}$$

$$\hbar j_z\frac{2l+1-1}{2l+1}=\hbar j_z\frac{2j+1}{2l+1}$$

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$$S_z M^2 = S_z (M_x^2 + M_y^2 + M_z^2)$$

$$= M_z (S_x M_x + S_y M_y + S_z M_z)$$

$$+ (S_z M_x - M_z S_x) M_x + (S_z M_y - M_y S_y) M_y$$

$$+ (S_z M_z - M_z S_z) M_z$$

$$= M_z \cdot \frac{1}{2} \cdot \frac{j(j+1) + l(l+1) + \frac{1}{2}(\frac{1}{2}+1)}{j(j+1)}$$

+ non diagonal terms

because

$$\gamma_x = S_z M_y - M_z S_y = m_y S_z - m_z S_y$$

$$\gamma_y = M_z S_x - S_x M_x = m_z S_x - m_x S_z$$

$$\gamma_z = m_x S_y - m_y S_x$$

$$M\gamma = 0$$

$$\left.\begin{aligned} [M_z, \gamma_x] &= \gamma_y \\ [M_z, \gamma_y] &= -\gamma_x \\ [M_z, \gamma_z] &= 0 \end{aligned}\right\}$$

---

strong field ignore multiplet separation:

j_z, S_z : constants of motion

$$\frac{e\hbar}{2mc} H (m_z + 2S_z)$$

integer

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Problem. Fine structure of Hydrogen atom in Pauli Approximation

$$E_1 = -\frac{1}{2}\frac{\alpha^2 Z^4}{n^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right)$$

$$\alpha = \frac{e^2}{\hbar c} \simeq \frac{1}{137}.$$

$j = l+\frac{1}{2}$

ΔE_1

$j = l-\frac{1}{2}$

Hint: $A_0 = \frac{e^* Z}{r}$ $\quad \frac{dA_0}{dr} = -\frac{e^2 Z}{r^2}$ Schrödinger.

$$E_1 = -\frac{1}{2mc^2}\int_0^\infty \left(E_0 + \frac{e^2 Z}{r}\right)^2 (u_l^{(0)})^2 r^2 dr$$

$$+ \frac{e^2\hbar^2 Z}{4m^2c^2}\int_0^\infty u_l^{(0)} \frac{dl}{r^2}\left(\frac{du_l^{(0)}}{dr} - [j(j+1) - l(l+1) - s(s+1)]\frac{u_l^{(0)}}{r}\right) \times r^2 dr$$

$$\Delta E_1 = +\frac{1}{2}\frac{\alpha^2 Z^4}{n^3}\left(\frac{1}{l} - \frac{1}{l+1}\right) = \frac{1}{2}\frac{\alpha^2 Z^4}{n^3}\cdot\frac{1}{l(l+1)}$$

$$j(j+1) - l(l+1) - s(s+1)$$
$$= (l \pm \tfrac{1}{2})(l \pm \tfrac{1}{2} + 1) - l(l+1) - \frac{3}{4}$$
$$= (l \pm \tfrac{1}{2})(l \pm \tfrac{1}{2} + 1) - (l - \tfrac{1}{2})(l + \tfrac{3}{2})$$
$$= \begin{cases} -(l-\frac{1}{2}) \\ (l+\frac{3}{2}) \end{cases} \begin{cases} (l+\frac{3}{2}) \\ -(l-\frac{1}{2}) \end{cases} \qquad l \geq 1$$

$l = 0$. $\quad \frac{1}{2}(\frac{1}{2}+1) - \frac{1}{2}\cdot\frac{3}{2} = 0$.

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Hydrogen atom in Dirac theory, I,

$$A_0 = \frac{2e}{r} \qquad A = 0$$

$$\frac{1}{c}\left(W + \underbrace{\frac{2e^2}{r}}_{(-mc^2)}\right)\psi_+ = (\sigma p)\psi_-$$

$$\frac{1}{c}\left(W + \frac{2e^2}{r} + mc^2\right)\psi_- = (\sigma p)\psi_+$$

$$\sigma p = -i\hbar \begin{pmatrix} \frac{\partial}{\partial z} & \frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} & -\frac{\partial}{\partial z} \end{pmatrix}$$

$$\frac{1}{\hbar c}\left(W + \frac{2e^2}{r} - mc^2\right)\begin{pmatrix}\psi_1 \\ \psi_2\end{pmatrix} = \begin{pmatrix} \frac{\partial \psi_3}{\partial z} + \left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\psi_4 \\ \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\psi_3 - \frac{\partial \psi_4}{\partial z} \end{pmatrix}$$

$$\frac{i}{\hbar c}\left(W + \frac{2e^2}{r} + mc^2\right)\begin{pmatrix}\psi_3 \\ \psi_4\end{pmatrix} = \begin{pmatrix} \cdot \\ \cdot \end{pmatrix}$$

$j = l + \frac{1}{2}$:

$$\psi_1 = g(r)\sqrt{\frac{l+\mu+\frac{1}{2}}{2l+1}}\, Y_{l,\mu-\frac{1}{2}}(\theta,\varphi)$$

$$\psi_2 = g(r)\sqrt{\frac{l-\mu+\frac{1}{2}}{2l+1}}\, Y_{l,\mu+\frac{1}{2}}(\theta,\varphi)$$

$$\frac{i}{\hbar c}\left(W + \frac{2e^2}{r} + mc^2\right)\psi_3$$

$$= \sqrt{\frac{l-\mu+\frac{3}{2}}{2l+3}}\left(\frac{dg}{dr} - l\frac{g}{r}\right) Y_{l+1,\mu-\frac{1}{2}}$$

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$$r=\sqrt{x^2+y^2+z^2} \qquad \cos\theta=\frac{z}{r} \qquad z=r\cos\theta$$

$$x=r\sin\theta\cos\varphi \qquad y=r\sin\theta\sin\varphi \qquad \tan\varphi=\frac{y}{x} \qquad e^{i\varphi}=\frac{x+iy}{\sqrt{x^2+y^2}}$$

$$\frac{\partial}{\partial x}=\frac{x}{r}\frac{\partial}{\partial r}-\frac{xz}{r^2}\frac{\partial}{\partial(\theta\cos\theta)}$$

$$+\left(\frac{1}{\sqrt{x^2+y^2}}-\frac{x+iy}{x^2+y^2}\right)\frac{\partial}{\partial(e^{i\varphi})} \qquad -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}$$

$$=-i e^{i\varphi}\frac{\partial}{\partial\varphi}$$

$$=\sin\theta\cos\varphi\frac{\partial}{\partial r}+\cos\theta\cos\varphi\frac{\partial}{\partial\theta}$$

$$-ie^{-i\varphi}\left(\frac{1}{r\sin\theta}-\frac{e^{i\varphi}\cos\varphi}{r\sin^2\theta}\right)\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial y}=\sin\theta\sin\varphi\frac{\partial}{\partial r}+\cos\theta\sin\varphi\frac{\partial}{\partial\theta}$$

$$-ie^{-i\varphi}\left(\frac{+i}{r\sin\theta}-\frac{e^{i\varphi}\sin\varphi}{r\sin\theta}\right)\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}=\sin\theta e^{i\varphi}\frac{\partial}{\partial r}+\cos\theta e^{i\varphi}\frac{\partial}{\partial\theta}$$

$$+\frac{ie^{i\varphi}}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}=\sin\theta e^{-i\varphi}\frac{\partial}{\partial r}+\cos\theta e^{-i\varphi}\frac{\partial}{\partial\theta}$$

$$-\frac{ie^{-i\varphi}}{r\sin\theta}\frac{\partial}{\partial\varphi}$$

$$-\frac{1}{2}\frac{(x+iy)2x}{\left(\sqrt{x^2+y^2}\right)^3}=-e^{i\varphi}\frac{r\sin\theta\cdot\cos\varphi}{r^2\sin^2\theta}$$

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$$\cos\theta\, e^{i\varphi}\frac{\partial}{\partial\theta}Y_{\ell,m} = -\cos\theta\sin\theta\, e^{i\varphi}\frac{\partial Y_{\ell,m}}{\partial(\cos\theta)}$$

$$= -\cos\theta(\sin\theta)^{\frac{|m|}{2}+1}\frac{d^{|m|+1}}{dx^{|m|+1}}P_\ell(x)\cdot e^{i(m+1)\varphi}$$

$$-\cos\theta(\sin\theta)\left(-\frac{|m|}{2}\right)(1-x^2)^{\frac{|m|}{2}-1}\frac{d^{|m|}P_\ell}{dx^{|m|}}e^{i(m+1)\varphi}$$

$$= -x(1-x^2)^{\frac{|m|}{2}+1}\frac{d^{|m|+1}}{dx^{|m|+1}}P_\ell(x)\cdot e^{i(m+1)\varphi}$$

$$-x^2(1-x^2)^{\frac{|m|}{2}-\frac{1}{2}}\frac{d^{|m|}}{dx^{|m|}}P_\ell(x)\,e^{\cdots}$$

$$\frac{d^{|m|+1}}{dx^{|m|+1}}(x\cdot P_\ell) =$$

$$P_\ell' = (\ell+1)\frac{P_{\ell+1}-xP_\ell}{x^2-1}$$

$$(1-x^2)\frac{d}{dx}P_\ell^m = (\ell+1)xP_\ell^m - (\ell-m+1)P_{\ell+1}^m$$

① $$\frac{d}{d\theta}P_\ell^m = m\frac{\cos\theta}{\sin\theta}P_\ell^m - P_\ell^{m+1}$$

② $$\cos\theta\, P_\ell^m = \frac{\ell-m+1}{2\ell+1}P_{\ell+1}^m + \frac{\ell+m}{2\ell+1}P_{\ell-1}^m$$

①′ $$\cos\theta\frac{d}{d\theta}P_\ell^m = m\frac{(1-\sin^2\theta)}{\sin\theta}P_\ell^m - \cos\theta\, P_\ell^{m+1}$$

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$$= \frac{m}{\sin\theta} P_l^m - m\cot\theta P_l^m - \cos\theta P_l^{m+1}$$

(3) $$\sin\theta P_l^m = \frac{P_{l+1}^{m+1}}{2l+1} - \frac{P_{l-1}^{m+1}}{2l+1}$$

$$\cos\theta \frac{d}{d\theta} P_l^m = \frac{m}{\sin\theta} P_l^m - \frac{m}{2l+1} P_{l+1}^{m+1}$$

$$+ \frac{m}{2l+1} P_{l+1}^{m+1} - \frac{l-m+1}{2l+1} P_{l+1}^{m+1} - \frac{l+m+1}{2l+1} P_{l-1}^{m+1}$$

$$= \frac{m}{\sin\theta} P_l^m - \frac{l}{2l+1} P_{l+1}^{m+1} + \frac{l+1}{2l+1} P_{l-1}^{m+1}$$

$$\frac{dg}{dr} \sin\theta e^{i\varphi} P_l e^{im\varphi} + \frac{g}{r} \cos\theta e^{i\varphi} \frac{dP_l^m}{d\theta} e^{im\varphi}$$

$$+ \frac{ig}{r} \frac{e^{i\varphi}}{\sin\theta} P_l^m \cdot \frac{d}{d\varphi} e^{im\varphi}$$

$$= \frac{dg}{dr} \left(\frac{P_{l+1}^{m+1} e^{i(m+1)\varphi}}{2l+1} - \frac{P_{l-1}^{m+1} e^{i(m+1)\varphi}}{2l+1} \right)$$

$$+ \frac{g}{r} e^{i(m+1)\varphi} \left(\frac{m}{\sin\theta} P_l^m - \frac{l}{2l+1} P_{l+1}^{m+1} - \frac{l+1}{2l+1} P_{l-1}^{m+1} \right)$$

$$- \frac{g}{r} \frac{m}{\sin\theta} e^{i(m+1)\varphi} P_l^m$$

$$= \frac{1}{2l+1} P_{l+1}^{m+1} e^{i(m+1)\varphi} \left(\frac{dg}{dr} - l\frac{g}{r} \right)$$

$$- \frac{1}{2l+1} P_{l-1}^{m+1} e^{i(m+1)\varphi} \left(\frac{dg}{dr} + (l+1)\frac{g}{r} \right)$$

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$$\frac{\partial}{\partial z} = \frac{z}{r}\frac{\partial}{\partial r} + \frac{\frac{1}{z}}{r}\frac{\partial}{\partial(\cos\theta)}$$

$$= \cos\theta \frac{\partial}{\partial r} - \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}$$

$$\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\psi_1 + \frac{\partial\psi_2}{\partial z}$$

$$= \left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) g\sqrt{\frac{l+\mu+\frac{1}{2}}{2l+1}}\, P_{l,\mu-\frac{1}{2}}$$

$$\pm \frac{\partial}{\partial z} g\sqrt{\frac{l-\mu+\frac{1}{2}}{2l+1}}\, P_{l,\mu+\frac{1}{2}}$$

$$= -\frac{1}{2l+1}\sqrt{\frac{l+\mu+\frac{1}{2}}{2l+1}}\, P_{l+1,\mu+\frac{1}{2}}\,(\quad)$$

$$+ \frac{l}{2l+1}\sqrt{\frac{l\pm\mu+\frac{1}{2}}{2l+1}}\, P_{l-1,\mu+\frac{1}{2}}\,(\quad)$$

$$\mp \frac{1}{2l+1}\sqrt{\frac{l-\mu+\frac{1}{2}}{2l+1}}\cdot P_{l+1,\mu+\frac{1}{2}}\,(\quad)$$

$$- \frac{1}{2l+1}\sqrt{\frac{l-\mu+\frac{1}{2}}{2l+1}}\, P_{l-1,\mu+\frac{1}{2}}\,(\quad)$$

$$=$$

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Definition and Properties of Spherical Harmonics

H. Bethe, Handb. d. Phys. XXIV. 1.
Kap. 3. S. 551.

$$Y_{lm}(\theta,\varphi) = \frac{1}{\sqrt{2\pi}} P_{lm} e^{im\varphi}$$

$$P_{lm} = \sqrt{\frac{2l+1}{2}\cdot\frac{(l-m)!}{(l+m)!}}\, P_l^m$$

$$P_l^m = \frac{1}{2^l\cdot l!}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l \qquad (1-x^2)^{m/2}$$

$$\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\varphi\, |Y_{lm}|^2 = 1$$

$m<0$ $\quad Y_{lm} = (-1)^m \overline{Y_{lm}}^*$; $\quad Y_{lm}^* = P_{l,|m|}\, e^{im\varphi}$ / $\frac{1}{\sqrt{2\pi}}$

P_{lm} = 2

$\therefore$ $\quad P_l = \frac{1}{2^l\cdot l!}\frac{d^l(x^2-1)^l}{dx^l}$

$$P_l(x) = \frac{(2l)!}{2^l\cdot(l!)^2}(x^l - \cdots)$$

$$P_{lm} = \frac{(2l)!}{2^l l!(l-m)!}\sqrt{\frac{2l+1}{2}\cdot\frac{(l-m)!}{(l+m)!}}(1-x^2)^{m/2}(x^{l-m} - \cdots)$$

$$= \frac{(2l)!}{2^l l!(l+m)!}\sqrt{\frac{2l+1}{2}\frac{(l+m)!}{(l-m)!}}(-1)^m(1-x^2)^{\frac{m}{2}}(x^{l+m} - \cdots)$$

$$= (-1)^m P_{l,-m}$$

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$$\sin\theta \cdot P_{\ell m}(\cos\theta) = \sqrt{\frac{(\ell+m+1)(\ell+m+2)}{(2\ell+1)(2\ell+3)}}\, P_{\ell+1,m+1} - \sqrt{\frac{(\ell-m)(\ell-m-1)}{(2\ell+1)(2\ell-1)}}\, P_{\ell-1,m+1}$$

$$\sin\theta P_{\ell m} = -\sqrt{\frac{(\ell-m+1)(\ell-m+2)}{(2\ell+1)(2\ell+3)}}\, P_{\ell+1,m-1} + \sqrt{\frac{(\ell+m)(\ell+m-1)}{(2\ell+1)(2\ell-1)}}\, P_{\ell-1,m-1}$$

$$\cos\theta P_{\ell m} = +\sqrt{\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)}}\, P_{\ell+1,m} + \sqrt{\frac{(\ell+m)(\ell-m)}{(2\ell+1)(2\ell-1)}}\, P_{\ell-1,m}$$

$$\frac{dP_{\ell m}}{d\theta} = \sqrt{(\ell+m)(\ell-m+1)}\, P_{\ell,m-1} - m\cot\theta \cdot P_{\ell,m}$$

$$\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)(f\bar{Y}_{\ell m}) = \sqrt{\frac{(\ell+m+2)(\ell+m+1)}{(2\ell+3)(2\ell+1)}}\, \bar{Y}_{\ell+1,m+1}\left(\frac{df}{dr} - \ell\frac{f}{r}\right) - \sqrt{\frac{(\ell-m)(\ell-m-1)}{(2\ell+1)(2\ell-1)}}\, \bar{Y}_{\ell-1,m+1}\left(\frac{df}{dr} + (\ell+1)\frac{f}{r}\right)$$

$$\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)(f\bar{Y}_{\ell m}) = -\sqrt{\frac{(\ell-m+2)(\ell-m+1)}{(2\ell+3)(2\ell+1)}}\, \bar{Y}_{\ell+1,m-1}\left(\frac{df}{dr} - \ell\frac{f}{r}\right)$$

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$$\mp\sqrt{\frac{(l+m)(l+m-1)}{(2l+1)(2l-1)}}\,\bar{Y}_{l-1,m-1}\left(\frac{d}{dr}\mp(l+1)\frac{1}{r}\right)$$

$$\frac{\partial}{\partial z}(f\bar{Y}_{l,m}) = \sqrt{\frac{(l+m+1)(l-m+1)}{(2l+3)(2l+1)}}\,\bar{Y}_{l+1,m}\left(\frac{d}{dr}-l\frac{1}{r}\right)$$

$$\mp\sqrt{\frac{(l+m)(l-m)}{(2l+1)(2l-1)}}\,\bar{Y}_{l-1,m}\left(\frac{d}{dr}+(l+1)\frac{1}{r}\right)$$

$$\sum_{l,m}\bar{Y}^{*}_{lm}(\Theta,\Phi)\,\bar{Y}_{lm}(\vartheta,\varphi) = \delta(\vartheta-\Theta,\varphi-\Phi)$$

$$\bar{Y}_{l0}(0)\,\bar{Y}_{l0}(\vartheta') = \sum_{m}\bar{Y}^{*}_{lm}(\Theta,\Phi)\,\bar{Y}_{lm}(\vartheta,\varphi)$$

$$\cos\vartheta' = \sin\vartheta\sin\Theta\cos(\varphi-\Phi)+\cos\vartheta\cos\Theta$$

$$\sum_{m}|\bar{Y}_{lm}(\Theta,\Phi)|^2 = (\bar{Y}_{l0}(0))^2 = \frac{2l+1}{4\pi}$$

$j=l+\frac{1}{2}$:

$$\left.\begin{aligned}
\psi_1 &= g(r)\sqrt{\frac{l+\mu+\frac{1}{2}}{2l+1}}\,\bar{Y}_{l,\mu-\frac{1}{2}}(\theta,\varphi)\\
\psi_2 &= \mp g(r)\sqrt{\frac{l-\mu+\frac{1}{2}}{2l+1}}\,\bar{Y}_{l,\mu+\frac{1}{2}}(\theta,\varphi)\\
\psi_3 &= -if(r)\sqrt{\frac{l-\mu+\frac{3}{2}}{2l+3}}\,\bar{Y}_{l+1,\mu-\frac{1}{2}}(\theta,\varphi)\\
\psi_4 &= \mp if(r)\sqrt{\frac{l+\mu+\frac{3}{2}}{2l+3}}\,\bar{Y}_{l+1,\mu+\frac{1}{2}}(\theta,\varphi)
\end{aligned}\right\}$$

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$j = l - \frac{1}{2}$

$$\left.\begin{aligned}
\psi_1 &= g(r)\sqrt{\frac{l-\mu+\frac{1}{2}}{2l+1}}\,\overline{Y}_{l,\mu-\frac{1}{2}} \\
\psi_2 &= g(r)\sqrt{\frac{l+\mu+\frac{1}{2}}{2l+1}}\,\overline{Y}_{l,\mu+\frac{1}{2}} \\
\psi_3 &= \mp i f(r)\sqrt{\frac{l+\mu-\frac{1}{2}}{2l-1}}\,\overline{Y}_{l-1,\mu-\frac{1}{2}} \\
\psi_4 &= i f(r)\sqrt{\frac{l-\mu-\frac{1}{2}}{2l-1}}\,\overline{Y}_{l-1,\mu+\frac{1}{2}}
\end{aligned}\right\}$$

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Hydrogen Atom in Dirac's theory, II.

$$\left\{\frac{W+eA_0}{c} - \rho_1(\sigma p + \tfrac{e}{c}A) - \rho_3 mc\right\}\psi = 0$$

$$W\psi = H\psi$$

$$H = -eA_0 + c\rho_1\sigma(p + \tfrac{e}{c}A) + \rho_3 mc^2$$

$A_0(r)$, $\quad A = 0$.

$$K = \rho_3\{(\sigma m) + \hbar\}$$

$\Rightarrow [K, H] = 0$.

$\because$ $(\sigma m)(\sigma p) = i(\sigma, [m \times p])$

$(\sigma m p)(\sigma m) = i(\sigma [p \times m])$

$(\sigma m)(\sigma p) + (\sigma p)(\sigma m)$

$= i\sum \sigma_x \{m_y p_z - m_z p_y + p_y m_z - p_z m_y\}$

$= i\sum \sigma_x \; 2i\hbar p_x = -2\hbar(\sigma p)$

$$K^2 = (\sigma m)^2 + 2\hbar(\sigma, m) + \hbar^2$$

$$= m^2 + i(\sigma(m \times m)) + 2\hbar(\sigma m) + \hbar^2$$

$(m \times m) = i\hbar m$

$$= m^2 + \hbar(\sigma, m) + \hbar^2$$

$$= \left(m + \frac{\hbar}{2}\sigma\right)^2 + \frac{1}{4}\hbar^2$$

Eigenvalues of K^2 are

$$\{j(j+1) + \tfrac{1}{4}\}\hbar^2 = (j+\tfrac{1}{2})^2\hbar^2$$

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$K = -k_K t$

$k = \pm(j + \frac{1}{2}) = \pm 1, \pm 2, \cdots\cdots$

positive or negative integer excluding 0.

$\textcircled{H} = \rho_1 (\sigma, \frac{r}{r})$

~~is also commutative with H.~~

$\sum^2 = (\sigma, \frac{r}{r})^2 = \frac{r^2}{r^2} = 1$

$(\sigma, \frac{r}{r})(\sigma, p) = (\frac{r}{r} p) + i\sigma[\frac{r}{r}, p]$

$= p_r + i \sum \sigma_x (\frac{y}{r} p_z - \frac{z}{r} p_y)$

$= p_r + i \frac{(\sigma m)}{r}$

$\textcircled{H} \cdot \rho_1 (\sigma p) = p_r + i \frac{(\sigma m)}{r}$

or $\rho_1 (\sigma p) = \textcircled{H} \cdot p_r + i \textcircled{H} \frac{(\sigma m)}{r}$

$\sigma m \approx \rho_3 K - t$

$\rho_1 (\sigma p) = \textcircled{H} \cdot p_r + i \textcircled{H} \cdot \frac{\rho_3 K - t}{r}$

$H \approx -eA_0 + c \cdot \textcircled{H} (p_r + i \frac{\rho_3 K - t}{r}) + \rho_3 mc^2$

$r(A_0), p_r, K$; $\textcircled{H}, \rho_3$

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$$[\mathcal{H}, K] = \beta_3\left(\frac{r}{r}, m\right) + i\sigma\left[\frac{r}{r} \times m\right] + \hbar\left(\sigma, \frac{r}{r}\right) = 0$$

$$= \beta_3 \

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$$\frac{W}{\hbar c} = \text{[illegible]}$$

$$\left.\begin{aligned} (\varepsilon - \kappa + \frac{\alpha Z}{r}) g &= -\frac{df}{dr} + \frac{k+1}{r} f \\ (\varepsilon + \kappa + \frac{\alpha Z}{r}) f &= \frac{dg}{dr} + \frac{k+1}{r} g \end{aligned}\right\}$$

$j = l + \frac{1}{2}$.

$$\left.\begin{aligned} (\varepsilon - \kappa + \frac{\alpha^2}{r}) g &= -\frac{df}{dr} - \frac{l+2}{r} f \\ (\varepsilon + \kappa + \frac{\alpha^2}{r}) f &= \frac{dg}{dr} - \frac{l}{r} g \end{aligned}\right\}$$

$$\underline{k = -l-1 \quad = -(j + \tfrac{1}{2})}$$

$\tilde{j} = l - \frac{1}{2}$

$$\left.\begin{aligned} (\varepsilon - \kappa + \frac{\alpha^2}{r}) g &= -\frac{df}{dr} + \frac{l-1}{r} f \\ (\varepsilon + \kappa + \frac{\alpha^2}{r}) f &= \frac{dg}{dr} + \frac{l+1}{r} g \end{aligned}\right\}$$

$$\underline{k = +l \quad = +(j + \tfrac{1}{2})}$$

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Problem. 1.

Prove that

$$(\sigma, B)(\sigma, C) = (B \cdot C) + i(\sigma(B \times C))$$

for any two vectors B, C which commute with σ

$$(\sigma, B)(\sigma, C) = \sum \sigma_i^2 B_i C_i + \sum \sigma_1 \sigma_2 B_1 C_2 + \sum \sigma_2 \sigma_1 B_2 C_1$$
$$= (BC) + i \sum \sigma_3 (B_1 C_2 - B_2 C_1)$$

Problem. 2.

Prove that

$$\{(\sigma m) + t\}\{(\sigma p) + (\sigma p)\}\{(\sigma m) + t\} = 0$$

Problem 3.

Prove that

$$[H, K] = 0$$
$$[H, p_r] = 0$$

$$\left[\frac{1}{r}, p_x\right] = i\hbar\left(-\frac{x}{r^3}\right)$$

$$\left[\frac{x}{r}, p_x\right] = x\left[\frac{1}{r}, p_x\right] + \left[x, p_x\right]\frac{1}{r}$$
$$= -i\hbar\frac{x^2}{r^3} + i\hbar\frac{1}{r}$$

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Problem. 4.

Show that the wave functions for $j = l + \frac{1}{2}$, $l - \frac{1}{2}$ ~~correspon~~ are the eigenstates of

$$K = \beta_3 \{(\sigma \cdot \mathbf{l}) + 1\}$$

with the eigenvalues

$-kh = (l+1)h$ and $-lh$
$\underbrace{\qquad\qquad\qquad\qquad}$
$-kh =$

respectively.

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$$n' = \frac{\alpha Z \varepsilon}{\sqrt{1-\varepsilon^2}} - \sqrt{k^2 - \alpha^2 Z^2} = \frac{\alpha^2 Z \varepsilon}{\sqrt{1-\varepsilon^2}} - \gamma$$

$$a_\nu = (-1)^\nu \frac{(n'-1)\cdots(n'-\nu)}{\nu!\,(2\gamma+1)\cdots(2\gamma+\nu)} a_0$$

$$b_\nu = (-1)^\nu \frac{n' \cdot -(n'-\nu+1)}{\nu!\,(2\gamma+1)\cdots(2\gamma+\nu)} b_0$$

$n' = 0$: ~~$\varphi_1 \propto r^{\gamma+n'}$~~

$$\left(\gamma + k\frac{\alpha\varepsilon Z}{\sqrt{1-\varepsilon^2}}\right) a_0 + \left(k + \frac{\alpha^2 Z}{\sqrt{1-\varepsilon^2}}\right) b_0 = 0$$

$$\left(k - \frac{\alpha^2 Z}{\sqrt{1-\varepsilon^2}}\right) a_0 + \left(\gamma - \frac{\alpha\varepsilon Z}{\sqrt{1-\varepsilon^2}}\right) b_0 = 0$$

~~If~~ $k - \frac{\alpha^2 Z}{\sqrt{1-\varepsilon^2}}$ $\quad k > 0.$

$$k^2 - \alpha^2 Z^2 = \frac{\alpha^2 Z^2 \varepsilon^2}{1-\varepsilon^2}$$

$$k = \frac{\alpha Z}{\sqrt{1-\varepsilon^2}}$$

~~$\sqrt{k}$~~ $\quad \frac{\alpha Z \varepsilon}{\sqrt{1-\varepsilon^2}} + \frac{\alpha^2 Z^2 \varepsilon}{1-\varepsilon^2} \neq 0$

$k > 0$:

$a_0 = b_0 = 0$ or $a_0 \neq 0$ $b_0 \neq 0$

then $\varphi_1 = \rho^\gamma \sum_{\nu=0}^{\infty} a_\nu \rho^\nu$

increases like e^ρ for $r \to \infty$.

which is not permitted.

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$k<0$.　$a_0=0$,　$b_0\neq 0$

$\therefore$　$k+\frac{\alpha^2 Z}{\sqrt{1-\alpha^2}}=0$,　$\gamma-\frac{\alpha\varepsilon Z}{\sqrt{1-\alpha^2}}=0$

$n'=0$　　$j=l+\frac{1}{2}$

$$W=\frac{mc^2}{\sqrt{1+\left(\frac{\alpha Z}{n-|k|+\sqrt{k^2-\alpha^2Z^2}}\right)^2}}$$

$$=mc^2\left\{1-\frac{1}{2}\left(\frac{\alpha Z}{n-|k|+\sqrt{k^2-\alpha^2Z^2}}\right)^2+\frac{\left(-\frac{1}{2}\right)\left(-\frac{1}{2}-1\right)}{2}\left(\frac{\alpha Z}{n-|k|+\sqrt{k^2-\alpha^2Z^2}}\right)^4+\cdots\right\}$$

$$\simeq mc^2-\frac{1}{2}\frac{me^4Z^2}{\hbar^2}\frac{1}{n^2}$$

$$-\frac{1}{2}mc^2\left(\frac{\alpha Z}{n}\right)^2\left(1-\frac{|k|-\sqrt{k^2-\alpha^2Z^2}}{n}\right)^2+\frac{1}{4}mc^2\frac{3}{8n^4}\alpha^4Z^4$$

$$\simeq mc^2\left\{1-\frac{1}{2}\frac{\alpha^2Z^2}{n^2}-\frac{1}{2}\frac{\alpha^4Z^4}{n^3}\frac{1}{|k|}+\frac{3\alpha^4Z^4}{8n^4}+\cdots\right\}$$

$$\sqrt{k^2-\alpha^2Z^2}=|k|-\frac{1}{2}\frac{\alpha^2Z^2}{|k|}$$

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Lamb Shift

Non-relativistic approximation

$$\Delta E = \sum_I \frac{H'_{0I} H'_{I0}}{W_0 - W_I}$$

$$H_{I0} = \frac{e}{mc}\sqrt{\frac{2\pi\hbar c}{k_\lambda \mathcal{V}}} \int \tilde{\psi}_I e^{-ik_\lambda r} (e_\lambda p) \psi_0 \, dv$$

$$\Delta E = \frac{e^2}{m^2c^2} \frac{2\pi\hbar c}{\mathcal{V}} \sum_I \frac{\left| \int \tilde{\psi}_I e^{-ik_\lambda r} (e_\lambda p) \psi_0 dv \right|^2}{k_\lambda (E_0 - E_I - \hbar k_\lambda c)}$$

$W_0 = E_0$ $\quad\therefore\quad W_I = E_I + \hbar k_\lambda c$

$$\sum_I \cdots \to \iiint \frac{k^2 dk}{(2\pi)^3} \sin\theta d\theta d\varphi$$

$$\Delta E_{free} = -\frac{e^2}{m^2c^2} \int_0^K k dk \sum_I \frac{|p_{I0}|^2}{(k\hbar c + E_I - E_0)}$$

$E_I - E_0 = 0$

$$\left(\frac{\hbar c}{(2\pi)^2}, \frac{8\pi}{3}\right)$$

$$= -\frac{2e^2}{3\pi} \frac{|p_{I0}|^2}{mc} K$$

$\omega_I = E_I/\hbar c$

$\omega_0 = E_0/\hbar c$

$\cdot\, p_0^2/m^2c^2$

$$\Delta E = \Delta E_{bound} - \Delta E_{free}$$

$$= -\frac{2e^2}{3\pi} \frac{1}{m^2c^2} \int_0^K k dk \sum_I \left(\frac{|p_{I0}|^2}{k + \omega_I - \omega_0} - \frac{|p_{I0}|^2}{k} \right)$$

$$= \frac{2e^2}{3\pi} \frac{1}{m^2c^2} \sum_I |p_{I0}|^2 \left\{ \frac{(\omega_I - \omega_0)}{\frac{E_I - E_0}{\hbar c}} \right\} \log \frac{K}{(\omega_I - \omega_0)}$$

Ans.

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$$S \simeq \sum_I \frac{|\psi_{I0}|^2 (E_I - E_0)}{\hbar^2 c^2} = \frac{1}{2}\left(\frac{\hbar}{mc}\right)^2 \int \nabla^2 V \cdot \psi_0^2 \, dv$$

$V = -\frac{Ze^2}{r}$: $\quad \nabla^2 V = Ze^2 \cdot 4\pi\delta$

$$S \simeq 2\pi \left(\frac{\hbar}{mc}\right)^2 e^2 Z \psi_0^2(0)$$

$$= 4 \left(\frac{e^2}{\hbar c}\right)^2 \frac{Z^4}{n^3} Ry$$

$$\frac{\Delta E}{h} \simeq \frac{8}{3\pi}\left(\frac{e^2}{\hbar c}\right)^3 Ry \frac{Z^4}{n^3} \log \frac{mc^2/h}{16.721\, Ry\, Z^2}$$

$\simeq 1,040$ for $2S_{1/2}$ megacycles.

$$Ry = \frac{1}{4\pi} \cdot \frac{me^4}{\hbar^3} = \frac{4,1342 \times 10^{16}}{4\pi} \sec^{-1}.$$

$Z=1$:

$$\Rightarrow E \propto \alpha^3 Ry/8 = (137)^{-3} \frac{4.13 \times 10^{16}}{4\pi \cdot 8}$$

$$\propto 4.13 \times 10^8 \times \log(\ )$$

$$\propto 400 \text{ megacycles} \times \log(\ )$$

Reference: Bethe, P. R. 72 (1947), 339.

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$$S = \sum_I \frac{\sum_I p_{oI} p_{Io} \cdot H}{m^2 c^2}$$

$$\simeq p_{oI} \frac{d p_{Io}}{dt} = p_{oI} (-\mathrm{grad} V)_{Io}$$

$$\simeq \frac{1}{2} \frac{d}{dt} \sum_I p_{oI} p_{Io}$$

$$\simeq \frac{1}{2} \frac{d}{dt} \psi_0^* \circ \psi_0 = \frac{d}{dt} \psi_0 V \psi_0$$

$$= \sum_I \int \cdot \mathrm{grad}\psi_0 \cdot \psi_I \, dw \int \psi_I (-\mathrm{grad}) \psi_0$$

$$= \int \mathrm{grad}\psi_0 \cdot (-\mathrm{grad} V) \psi_0$$

$$\to \frac{1}{2} \int \{ \mathrm{grad}\psi_0 (-\mathrm{grad} V) \psi_0 + \psi_0 (-\mathrm{grad}) \cdot \mathrm{grad}\psi_0 \}$$

$$\to \frac{1}{2} \int \psi_0 (\Delta^2 V) \psi_0 \, dw$$

$$S = \sum_I \int \tilde{\psi}_0 (-i\hbar \mathrm{grad}\psi_I)(E_I - E_0) \int \tilde{\psi}_I (-i\hbar \mathrm{grad}) \psi_0$$

$$= -\int (\tilde{\psi}_0 H)(-i\hbar \mathrm{grad}\psi_I) \int \tilde{\psi}_I (-i\hbar \mathrm{grad}) \psi_0$$

$$+ \int \tilde{\psi}_0 (-i\hbar \mathrm{grad} H \psi_I) \int \tilde{\psi}_I (-i\hbar \mathrm{grad}) \psi_0$$

$$= (-i\hbar) \int \tilde{\psi}_0 (\mathrm{grad} V) \psi_I \int \tilde{\psi}_I (-i\hbar) \mathrm{grad}\psi_0$$

$$= -\hbar^2 \int \tilde{\psi}_0 (\mathrm{grad} V) \mathrm{grad}\psi_0 \quad \mathrm{grad}(\tilde{\psi}_0 \psi_0) \;\; \mathrm{grad} V \psi_0 //$$

$$= -\frac{1}{2} \hbar^2 \int \psi_0 \mathrm{grad}\tilde{\psi}_0 \cdot (\mathrm{grad} V) \psi_0 + \cdots$$

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Problem. 1. Show that, in the case of the free electron, the negative energy solution

$$\psi' = \rho_2 \sigma_y \tilde{\psi}$$

represents ~~corresponds~~ the state with $-p', -W', \downarrow$,
if ψ represents the state with $p', W', \uparrow$.

$$\rho_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}$$

$$\rho_2 \sigma_y = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & +1 & 0 \\ 0 & +1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$$\psi = \begin{pmatrix} 1 \\ 0 \\ p'_z/\mu \\ (p'_x + i p'_y)/\mu \end{pmatrix} \cdot \exp\, i(p'r - W't)/\hbar$$

$$\psi' = -\begin{pmatrix} (+p'_x - i p'_y)/\mu \\ -p'_z/\mu \\ 0 \\ 1 \end{pmatrix} \cdot \exp\, -i(p'r - W't)/\hbar$$

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Relativistic formulation of Dirac Equation

$-x^4 = ct = x_4$, $x' = x = x_1$, $y = y = x_2$, $z = x_3$

$W/c \equiv p_4 = i\hbar \frac{\partial}{\partial x_4} = -p^4$ x_μ: Covariant

$+p_x = p_1 = -i\hbar \frac{\partial}{\partial x_1} = p^1$ x^μ: contravariant

$+p_y = p_2 = -i\hbar \frac{\partial}{\partial x_2} = p^2$

$+p_z = p_3 = -i\hbar \frac{\partial}{\partial x_3} = p^3$

$x^\mu = g^{\mu\nu} x_\nu$ $g^{\mu\nu} = g_{\mu\nu}$ $x_\mu = g_{\mu\nu} x^\nu$

$A_0 = A_4$, $A_x = A_1$, $A_y = A_2$, $A_z = A_3$

$\left\{ \sum_\mu \alpha_\mu^\mu \left(p_\mu + \frac{e}{c} A_\mu\right) + \beta mc \right\} \psi = 0$

$-\alpha^0 = \alpha_0 = 1$

$\alpha^1 = \alpha_1 = \alpha_x$

$\alpha^2 = \alpha_2 = \alpha_y$

$\alpha^3 = \alpha_3 = \alpha_z$

$g_{\mu\nu} = (+1, +1, +1, -1)$

$x'_\mu = \sum_\nu a_\mu{}^\nu x_\nu$, $x_\nu = \sum_\kappa b_\nu{}^\kappa x'_\kappa$

$x_\mu x'^\mu = x_\mu x^\mu = (-x_4^2 + x_1^2 + x_2^2 + x_3^2)$

$\sum_{\mu\nu} x'_\mu x'_\nu = \sum_{\mu\nu} g_{\mu\nu} x_\mu x_\nu$

$\sum_{\mu\nu} a_\mu{}^\kappa x_\kappa \cdot a_\nu{}^\lambda x_\lambda$

$= g_{\mu\nu} a_\mu{}^\kappa a_\nu{}^\lambda x_\kappa x_\lambda = g_{\kappa\lambda} x_\kappa x_\lambda$

$g_{\mu\nu} a_\mu{}^\kappa a_\nu{}^\lambda = g_{\kappa\lambda}$

$a_\mu{}^\nu b_\nu{}^\kappa = \delta_{\mu\kappa}$

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$$\bar{\psi}'\{\gamma\sum\alpha^\mu(p'_\mu+\tfrac{e}{c}A'_\mu)+\beta mc\}\psi'=0$$

$$\psi'=S\psi\ ,\quad \bar{\psi}'=\psi\bar{S}$$

$\bar{S}$: Hermitian conjugate of S

$$\psi=S^{-1}\psi'\qquad \bar{\psi}=\bar{\psi}'\bar{S}^{-1}$$

~~$\bar{S}\alpha^\mu S$.~~

$$\{\bar{S}\alpha^\mu S\cdot a_\mu{}^\nu(p_\nu+\tfrac{e}{c}A_\nu)+\bar{S}\beta S mc\}\psi=0$$

$b_\nu{}^\kappa$:
$$\left.\begin{aligned}\bar{S}\alpha^\mu S\cdot a_\mu{}^\nu&=\alpha^\nu\\ \bar{S}\beta S\cdot&=\beta\end{aligned}\right\}$$

$\varepsilon_{\mu\kappa}\,b_\kappa{}^\kappa$

$$\left.\begin{aligned}\bar{S}\alpha^\mu S&=\alpha^\nu b_\nu{}^\kappa\\ \bar{S}\beta S&=\beta\end{aligned}\right\}$$

$$\{\alpha^\mu b_\mu{}^\nu(p'_\nu+\tfrac{e}{c}A'_\nu)+\beta mc\}S^{-1}\psi'=0$$

$$\bar{S}^{-1}\{\alpha^\mu b_\mu{}^\nu(\ \ )+\beta mc\}S^{-1}\psi'=0$$

$$\left.\begin{aligned}\bar{S}^{-1}\alpha^\mu S^{-1}b_\mu{}^\nu&=\alpha^\nu\\ \bar{S}^{-1}\beta S^{-1}&=\beta\end{aligned}\right\}$$

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$$\left\{+\left(\frac{W+eA_0}{c}\right)\mp\alpha\left(p\mp\frac{e}{c}A\right)\mp\beta mc\right\}\psi=0$$

$$+i\beta = +i\rho_3 = \gamma^4,\quad -i\rho_3=\gamma_4$$

$$-i\beta\alpha = \rho_2\sigma = (\gamma_1,\gamma_2,\gamma_3)=(\gamma^1,\gamma^2,\gamma^3)$$

$$\left\{\gamma^\mu\left(p_\mu+\frac{e}{c}A_\mu\right)-imc\right\}\psi=0$$

$$-\bar\psi\gamma^4\left\{\gamma^\mu\left(p_\mu+\frac{e}{c}A_\mu\right)-imc\right\}=0$$

$$\gamma^\mu\gamma^\nu+\gamma^\nu\gamma^\mu = g^{\mu\nu}=g_{\mu\nu}$$

$$-\bar\psi\gamma^4=\psi^+ \qquad \bar\psi=\psi^+\gamma^4$$

$$p'_\mu+\frac{e}{c}A'_\mu = a_\mu{}^\nu\left(p_\nu+\frac{e}{c}A_\nu\right)$$

$$\psi'=S\psi \qquad \psi=S^{-1}\psi' \qquad p_\mu+\frac{e}{c}A_\mu = b_\mu{}^\nu\left(p'_\nu+\frac{e}{c}A'_\nu\right)$$

$$b_\mu{}^\nu a_\nu{}^\lambda=\delta_{\mu\lambda}$$

$$\left\{S\gamma^\mu S^{-1},\ b_\mu{}^\nu\left(p'_\nu+\frac{e}{c}A'_\nu\right)-imc\right\}\psi'=0$$

$$S\gamma^\mu S^{-1}\cdot b_\mu{}^\nu = \gamma^\nu$$

$$S\gamma^\mu S^{-1}\cdot b_\mu{}^\nu a_\nu{}^\lambda = \gamma^\nu a_\nu{}^\lambda$$

$$S\gamma^\mu S^{-1}=\gamma^\nu a_\nu{}^\mu$$

$$x'^\mu = x^\nu c_\nu{}^\mu$$

$$x'^\mu x'_\mu = x^\nu c_\nu{}^\mu a_\mu{}^\lambda x_\lambda = x^\nu x_\nu$$

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$c_\nu{}^\mu a_\mu{}^\lambda = \delta_\nu{}^\lambda$

$c_\nu{}^\mu \equiv b_\nu{}^\mu$

$\psi'^\dagger = \psi^\dagger S^{-1}$ $\quad \psi^\dagger = \psi'^\dagger S$

$\psi'^\dagger \psi' = \psi^\dagger \psi$ invariant (scalar)

$\psi'^\dagger \{ \gamma^\mu (p_\mu' + \frac{e}{c} A_\mu') - i m c \} = 0.$

$\psi^\dagger \gamma^\mu \psi' = \psi^\dagger S \gamma^\mu S^{-1} \psi' b_\mu{}^\nu$

$= \psi^\dagger \gamma^\mu \psi b_\mu{}^\nu$

$\psi^\dagger \gamma^\mu \psi$: contravariant vector

$= \bar\psi \gamma^4 \gamma^\mu \psi = (-\bar\psi\psi, \bar\psi \alpha \psi)$

$\psi^\dagger \gamma^\mu \gamma^\nu \psi$: contrav. tensor

(antisymmetric)

(∵ $S \gamma^\mu \gamma^\nu S^{-1} = b_\mu{}^\kappa b_\nu{}^\lambda$

$(S S^{-1})$

$= \gamma^\kappa \gamma^\lambda$

$\psi'^\dagger S \gamma^\mu \gamma^\nu S^{-1} \psi' b_\mu{}^\kappa b_\nu{}^\lambda = \psi^\dagger \gamma^\kappa \gamma^\lambda \psi'$

$\psi^\dagger \gamma^\mu \gamma^\nu \psi \, b_\mu{}^\kappa b_\nu{}^\lambda = \psi^\dagger \gamma^\kappa \gamma^\lambda \psi$)

$\psi^\dagger \gamma^\lambda \gamma^\mu \gamma^\nu \psi$: pseudovector

$\pm i \psi^\dagger \gamma^\kappa \gamma^\lambda \gamma^\mu \gamma^\nu \psi = \pm \psi^\dagger \gamma^5 \psi = \pm \psi^* \rho_2 \psi$

$\gamma^5 = i \gamma^1 \gamma^2 \gamma^3 \gamma^4 = i \cdot i \rho_3 \rho_2 \sigma_x \cdot \rho_2 \sigma_y \cdot \rho_2 \sigma_z$

$= -i \rho_1$

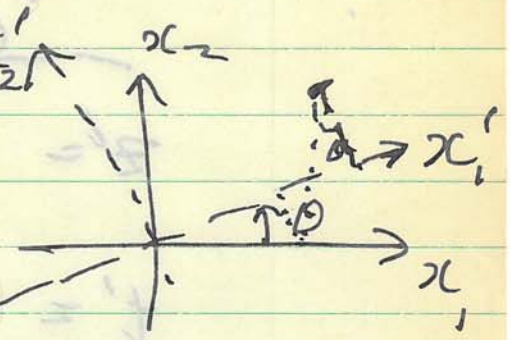
$\gamma^\kappa \gamma^5 = -i \rho_3 \rho_1 = \rho_2$

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a_1' a_2^2

$$\begin{cases} x_1' = x_1\cos\theta + x_2\sin\theta \\ x_2' = -x_1\sin\theta + x_2\cos\theta \\ x_3' = x_3 \\ x_4' = x_4 \end{cases}$$

x_2' a_2'



$$S = \cos\frac{\theta}{2} + \gamma_1'\gamma_2'\sin\frac{\theta}{2}$$

$$S^{-1} = \cos\frac{\theta}{2} - \gamma_1'\gamma_2'\sin\frac{\theta}{2}$$

$$\therefore SS^{-1} = \left(\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\right) = 1$$

$$S\gamma^\mu S^{-1} = \gamma^\nu a_{\nu\mu}$$

$$\left.\begin{aligned} S\gamma^1 S^{-1} &= \gamma^1\cos\theta - \gamma^2\sin\theta \\ S\gamma^2 S^{-1} &= \gamma^1\sin\theta + \gamma^2\cos\theta \end{aligned}\right\}$$

$$\left(\cos\frac{\theta}{2} + \gamma_1'\gamma_2'\sin\frac{\theta}{2}\right)\gamma^1\left(\cos\frac{\theta}{2} - \gamma_1'\gamma_2'\sin\frac{\theta}{2}\right)$$

$$= \gamma^1\left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right) - \gamma^2 2\sin\frac{\theta}{2}\cos\frac{\theta}{2}$$

$$\left(\cos\frac{\theta}{2} + \gamma^1\gamma^2\sin\frac{\theta}{2}\right)\gamma^2\left(\cos\frac{\theta}{2} - \gamma^1\gamma^2\sin\frac{\theta}{2}\right)$$

$$= \gamma^1 2\sin\frac{\theta}{2}\cos\frac{\theta}{2} + \gamma^2\left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right).$$

$$\begin{cases} x_1' = x_1, \quad x_2' = x_2 \\ x_3' = x_3\cosh\theta - x_4\sinh\theta \\ x_4' = -x_3\sinh\theta + x_4\cosh\theta \end{cases}$$

$$\cosh\theta = \frac{1}{\sqrt{1-\left(\frac{v}{c}\right)^2}} = \frac{1}{\sqrt{1-\beta^2}} \qquad \sinh\theta = \frac{\beta}{\sqrt{1-\beta^2}}$$

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$$\theta = \log\sqrt{\frac{1+\beta}{1-\beta}} = \log\sqrt{\frac{c+v}{c-v}}.$$

$$\left.\begin{aligned} z' &= \frac{z - vt}{\sqrt{1-\left(\frac{v}{c}\right)^2}} \\ t' &= \frac{t - \frac{vz}{c^2}}{\sqrt{1-\left(\frac{v}{c}\right)^2}} \end{aligned}\right\}$$

$$S = \cosh\frac{\theta}{2} + \gamma^3\gamma^4 \sinh\frac{\theta}{2}$$

$$S^{-1} = \cosh\frac{\theta}{2} - \gamma^3\gamma^4 \sinh\frac{\theta}{2}$$

$$S\gamma^3 S^{-1} = \gamma^3 \cosh\theta + \gamma^4 \sinh\theta$$

$$S\gamma^4 S^{-1} = -\gamma^3 \sinh\theta + \gamma^4 \cosh\theta$$

$$\left(\cosh\frac{\theta}{2} + \gamma^3\gamma^4 \sinh\frac{\theta}{2}\right)\gamma^3$$

$$\left(\cosh\frac{\theta}{2} + \gamma^3\gamma^4 \sinh\frac{\theta}{2}\right)$$

$$= \gamma^3\left(\cosh^2\frac{\theta}{2} + \sinh^2\frac{\theta}{2}\right)$$

$$+ \gamma^4\left(2\sinh\frac{\theta}{2}\cosh\frac{\theta}{2}\right)$$

$$\left(\cosh\frac{\theta}{2} + \gamma^3\gamma^4 \sinh\frac{\theta}{2}\right)\gamma^4$$

$$\left(\cosh\frac{\theta}{2} - \gamma^3\gamma^4 \sinh\frac{\theta}{2}\right)$$

$$= \gamma^4\left(\cosh^2\frac{\theta}{2} + \sinh^2\frac{\theta}{2}\right) - \gamma^3\left(2\sinh\frac{\theta}{2}\cosh\frac{\theta}{2}\right)$$

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$x_1' \Rightarrow -x_1$

$x_2' = x_2$, $x_3' = x_3$, $x_4' = x_4$

$S = \gamma^2\gamma^3\gamma^4$ $\quad S^{-1} = \gamma^4\gamma^3\gamma^2$

$S\gamma^1 S^{-1} = -\gamma^2\gamma^3\gamma^4\gamma^1\gamma^4\gamma^3\gamma^2 = \gamma^2\gamma^3\gamma^4$

$= -\gamma^1$

$S\gamma^2 S^{-1} = \gamma^2$ etc

ambiguity

$S = \epsilon\gamma^2\gamma^3\gamma^4$

$S^2 = C^2 = \pm 1$

~~$\psi'' + \psi = \psi' S(S^{-1})^2 \psi'$~~

Problem 1. Show that

$$\begin{pmatrix} 1/\mu & & & \\ & 0 & & \\ & & p_z/\mu & \\ & & & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} \exp i(p_z z - W' t)/\hbar$$

can be obtained from

$u_1 = 1, \quad u_2 = u_3 = u_4 = 0$

for the electron at rest by a Lorentz transformation

$x_3' = x_3 \cosh\theta + x_4 \sinh\theta$

$x_4' = + x_3 \sinh\theta + x_4 \cosh\theta$

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Problem 2. Prove that ψ_μ / ψ^μ a contrav. vector.

contr. $x'_\mu = a_\mu{}^\nu x_\nu$

cov. $x'^\mu = x^\nu b_\nu{}^\mu$ } where $b_\mu{}^\nu a_\nu{}^\lambda = \delta_\mu{}^\lambda$

Prove that the inverse transformation is given by

$x_\mu = b_\mu{}^\nu x'_\nu$

$x^{\prime\mu} = x'^\nu a_\nu{}^\mu$ }

$\therefore$ ~~$x'_\mu = a_\mu{}^\nu b_\nu{}^\lambda x'_\lambda$~~

~~$a_\mu{}^\nu b_\nu{}^\lambda = \delta_\mu{}^\lambda$~~

(i) ~~$x'_\mu = a_\mu{}^\nu x_\nu$~~ $x_\mu = c_\mu{}^\nu x'_\nu = c_\mu{}^\nu a_\nu{}^\lambda x'_\lambda$

~~$x_\mu = a_\mu{}^\nu c_\nu{}^\lambda x'_\lambda$~~

~~$a_\mu{}^\nu c_\nu{}^\lambda = \delta_\mu{}^\lambda$~~

$c_\mu{}^\nu a_\nu{}^\lambda = \delta_\mu{}^\lambda$

(ii) $x'^\mu x'_\mu = x^\mu x_\mu$

or $x^\mu b_\mu{}^\nu a_\nu{}^\lambda x_\lambda = x^\mu x_\mu$

$b_\mu{}^\nu a_\nu{}^\lambda = \delta_\mu{}^\lambda$

$\therefore c_\mu{}^\nu = b_\mu{}^\nu$

$x'^\mu = x'^\nu d_\nu{}^\mu = x^\kappa b_\kappa{}^\nu d_\nu{}^\mu$

~~$d_\mu{}^\nu b_\nu{}^\lambda = \delta_\mu{}^\lambda$~~

or $b_\kappa{}^\nu d_\nu{}^\mu = \delta_\kappa{}^\mu$ $\therefore d_\nu{}^\mu = a_\nu{}^\mu$

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Problem 3. ~~$a_\lambda{}^\kappa = g^{\kappa\nu} b_\nu{}^\mu g_{\mu\lambda}$~~ and hence

Prove that $\| a_\mu{}^\nu \| = \| b_\mu{}^\nu \|$ (= +1 or −1) or both −1

~~$a_\mu{}^\nu a_\nu{}^\lambda = \delta_{\mu\lambda}$~~ and that $\| a_\mu{}^\nu \| \cdot \| b_\mu{}^\nu \| = 1$

Hint: $\| b_\mu{}^\nu \| \cdot \| a_\nu{}^\lambda \| = 1$

~~$x'_\mu = a_\mu{}^\nu x_\nu$~~

$g_{\kappa\mu}$ $x'^\mu = x^\nu b_\nu{}^\mu$ $x^\nu = g^{\nu\kappa} x_\kappa$

$x'_\lambda = x^\nu b_\nu{}^\mu g_{\lambda\mu}$

$= x^\nu g_{\kappa\nu} g^{\kappa\nu} b_\nu{}^\mu g_{\mu\lambda}$

$= a_\lambda{}^\kappa x_\kappa$

$a_\lambda{}^\kappa = g^{\kappa\nu} b_\nu{}^\mu g_{\mu\lambda}$

$\| a_\lambda{}^\kappa \| = \| g^{\kappa\nu} \| \cdot \| b_\nu{}^\mu \| \cdot \| g_{\mu\lambda} \|$

$= -1 \cdot \| b_\nu{}^\mu \| \cdot -1$

$\therefore \| a_\lambda{}^\kappa \| = \| b_\nu{}^\mu \|$

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Problem 4. ~~Show that~~ ~~The quantity with the comp.~~

$$\varepsilon_{\kappa\lambda\mu\nu} = +1 \quad \text{if } \kappa\lambda\mu\nu : \text{even}$$
$$= -1 \quad \text{if odd}$$
$$= 0 \quad \text{otherwise}$$

is an antisymmetric tensor of the ~~fourth~~ rank.

~~Show that~~

$\frac{1}{24}\varepsilon_{\kappa\lambda\mu\nu}F^{\kappa\lambda\mu\nu}$: scalar

$\frac{1}{6}\varepsilon_{\kappa\lambda\mu\nu}F^{\lambda\mu\nu}$: vector

$\frac{1}{2}\cdot\varepsilon_{\kappa\lambda\mu\nu}F^{\mu\nu}$: dual tensor

where F's are all antisym. tensors and $\varepsilon_{\kappa\lambda\mu\nu}$ is defined by

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Vectors and tensors (Spinors)

Spinors

$x'_\mu (x_1 x_2 x_3 x_4)$

$$dx'_\mu = \frac{\partial x'_\mu}{\partial x_\nu} dx_\nu = a_\mu{}^\nu (x_1, x_2, x_3, x_4)\, dx_\nu$$

contravariant vector

$f(x_1 x_2 x_3 x_4) = f(x'_1 x'_2 x'_3 x'_4)$

: scalar, invariant

$$\frac{\partial f}{\partial x'_\mu} = \frac{\partial x_\nu}{\partial x'_\mu} \frac{\partial f}{\partial x_\nu}$$

$$p'^\mu = \frac{\partial x'_\mu}{\partial x_\nu} p^\nu$$

covariant vector

$$\frac{\partial f}{\partial x'_\mu} dx'_\mu = \frac{\partial f}{\partial x_\mu} dx_\mu$$

invariant

(scalar product)

Metric tensor

$$ds^2 = g^{\mu\nu} dx_\mu dx_\nu = g'^{\mu\nu} dx'_\mu dx'_\nu$$

$g^{\mu\nu}$: covariant tensor (metric)

$dx^\mu = g^{\mu\nu} dx_\nu$: contravariant vector

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu$$

$g_{\mu\nu}$: contravariant metric tensor

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Minkowski space

$$ds^2 = dx_1^2 + dx_2^2 + dx_3^2 - dx_4^2$$

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$ds^2 = (dx^1)^2 + (dx^2)^2 + (dx^3)^2 + (dx^4)^2$$

$\therefore dx^\mu = g^{\mu\nu} dx_\nu$

$dx^1 = dx_1 \quad \cdots \quad dx^4 = -dx_4$

$$\underline{g^{\mu\nu} = g_{\mu\nu}}$$

(x_1, x_2, x_3, x_4)

$(0,0,0,0)$

$$g^2 = x_1^2 + x_2^2 + x_3^2 - x_4^2$$

$$= x_1'^2 + x_2'^2 + x_3'^2 + x_4'^2$$

$x'_\mu = a_\mu{}^\nu x_\nu$

$$\underline{a_\mu{}^\nu a_\kappa{}^\lambda = g_{\mu\kappa}}$$

$x'^\mu = x^\nu c_\nu{}^\mu$

$x'^\mu x'_\mu = x^\nu c_{\nu\mu} a_\mu{}^\kappa x_\kappa$

$c_\nu{}^\mu a_\mu{}^\kappa = \delta_{\nu\kappa}$

$x_\nu = b_{\nu\mu} x'^\mu$

$b_{\nu\mu} a_\mu{}^\kappa = \delta_{\nu\kappa}$

$$\underline{c_{\nu\mu} = b_{\nu\mu}}$$

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Antisymmetric tensor

2nd rank:

$$\left.\begin{aligned} \overline{F}_{\mu'\nu'} &= a_{\mu}{}^{\kappa} a_{\nu}{}^{\lambda} F_{\kappa\lambda} \\ \overline{F}_{\kappa\lambda} &= -\overline{F}_{\lambda\kappa} \end{aligned}\right\}$$

$$H_x = \frac{\partial A_3}{\partial x_2} - \frac{\partial A_2}{\partial x_3} = F_{23}$$

$$H_y = F_{31}, \quad H_z = F_{12}$$

$$E_x = -\frac{1}{c}\frac{\partial A_1}{\partial t} - \frac{\partial A_0}{\partial x}$$

$$= \frac{\partial A_1}{\partial x^4} - \frac{\partial A_4}{\partial x^1} = F_{41}$$

$$E_y = F_{42}, \quad E_z = F_{43}$$

$$(F_{\mu\nu}) = \begin{pmatrix} 0 & H_z & -H_y & -E_x \\ -H_z & 0 & H_x & -E_y \\ H_y & -H_x & 0 & -E_z \\ E_x & E_y & E_z & 0 \end{pmatrix}$$

3rd rank: ~~pseudo-vector~~ ~~Pseudo-tensor~~

$$\left.\begin{aligned} F_{\lambda\mu\nu} &= -\overline{F}_{\lambda\nu\mu} = -F_{\mu\lambda\nu} \\ &= \overline{F}_{\nu\lambda\mu} = -F_{\nu\mu\lambda} = F_{\mu\nu\lambda} \end{aligned}\right\}$$

$(F_{123}, F_{124}, F_{134}, F_{234})$

$\Leftrightarrow$ (G^4, G^3, G^2, G^1)

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4th rank ; pseudoscalar

$F_{\kappa\lambda\mu\nu}$ $\quad F_{1234} = -F_{1243} = \cdots$

$\varepsilon_{\kappa\lambda\mu\nu}$ $\quad \varepsilon_{1234} = 1 \quad \varepsilon_{1243} = -1$

$\varepsilon_{1111} = 0$ etc.

$$F'_{\alpha\beta\gamma\delta} = a_\alpha{}^\kappa a_\beta{}^\lambda a_\gamma{}^\mu a_\delta{}^\nu F_{\kappa\lambda\mu\nu}$$

~~$\varepsilon'_{\alpha\beta\gamma\delta} = a_\alpha{}^\kappa a_\beta{}^\lambda a_\gamma{}^\mu a_\delta{}^\nu \varepsilon_{\kappa\lambda\mu\nu}$~~

$$F'_{1234} = a_1{}^\kappa a_2{}^\lambda a_3{}^\mu a_4{}^\nu F_{\kappa\lambda\mu\nu}$$
$$= a_1{}^\kappa a_2{}^\lambda a_3{}^\mu a_4{}^\nu \varepsilon_{\kappa\lambda\mu\nu} \cdot F_{1234}$$
$$= \begin{Vmatrix} a_1{}^1 & a_1{}^2 & a_1{}^3 & a_1{}^4 \\ a_2{}^1 & a_2{}^2 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & a_4{}^4 \end{Vmatrix} F_{1234}$$
$$= \| a_\mu{}^\nu \| F_{1234}$$
$$= \pm F_{1234}$$

$$\varepsilon'_{1234} = \pm \varepsilon_{1234}$$

$$\varepsilon_{\kappa\lambda\mu\nu} = -\varepsilon^{\kappa\lambda\mu\nu}$$

$$\frac{1}{4!} \varepsilon^{\kappa\lambda\mu\nu} F_{\kappa\lambda\mu\nu} = F$$

~~pseudoscalar~~.

$$\frac{1}{3!} \varepsilon_{\kappa\lambda\mu\nu} F^{\lambda\mu\nu} = F_\kappa$$ ~~pseudovector~~

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dual tensor

$$\tilde{F}_{\kappa\lambda} = \frac{1}{2}\varepsilon_{\kappa\lambda\mu\nu}F^{\mu\nu}$$

$$\tilde{F}_{12} = \frac{1}{2}(\varepsilon_{1234}F^{34} + \varepsilon_{1243}F^{43})$$

$$= \frac{1}{2}F^{34} \qquad \text{for } \varepsilon_{1234} = 1.$$

$$= -\frac{1}{2}F_{34}$$

$$\tilde{F}_{34} = \varepsilon_{3412}F^{12} = F_{12}$$

$$(\tilde{F}_{\mu\nu}) = \begin{pmatrix} 0 & E_z & -E_y & H_x \\ -E_z & 0 & E_x & H_y \\ E_y & -E_x & 0 & H_z \\ -H_x & -H_y & -H_z & 0 \end{pmatrix}$$

self-dual tensor

$$G_{\mu\nu} = (F_{\mu\nu} + i\tilde{F}_{\mu\nu}) = \begin{pmatrix} 0 & H_z + iE_z & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot \\ \cdot & \cdot & 0 & -E_z + iH_z \\ \cdot & \cdot & \cdot & 0 \end{pmatrix}$$

$$\bar{G}_{\mu\nu} = \bar{F}_{\mu\nu} - i\bar{\tilde{F}}_{\mu\nu} = -iG_{\mu\nu}$$

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Spinor

$\psi' = S\psi$ $\qquad$ $\psi'^{\dagger} = \psi^{\dagger} S^{-1}$

scalar $\psi^{\dagger}\psi$

vector $\psi^{\dagger}\gamma^{\mu}\psi$

tensor $\psi^{\dagger}\gamma^{\mu}\gamma^{\nu}\psi$ (not linearly indep. of $\psi^{\dagger}\psi$)

antisymmetric tensor

$F^{\mu\nu} = \frac{1}{2}\psi^{\dagger}(\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu})\psi$

or

$\psi^{\dagger}(\frac{1}{2}\varepsilon_{\kappa\lambda\mu\nu}\gamma^{\mu}\gamma^{\nu})\psi$

(dual antisym. tensor)

pseudovector

$\psi^{\dagger}\frac{1}{6}(\gamma^{\lambda}\gamma^{\mu}\gamma^{\nu} - \gamma^{\lambda}\gamma^{\nu}\gamma^{\mu} + \gamma^{\nu}\gamma^{\lambda}\gamma^{\mu} - \gamma^{\nu}\gamma^{\mu}\gamma^{\lambda} + \gamma^{\mu}\gamma^{\nu}\gamma^{\lambda} \mp \gamma^{\mu}\gamma^{\lambda}\gamma^{\nu})\psi$

$F'_{\alpha\beta\gamma} = a_{\alpha}{}^{\lambda} a_{\beta}{}^{\mu} a_{\gamma}{}^{\nu} F_{\lambda\mu\nu}$

$F'_{234} = a_2{}^{\lambda} a_3{}^{\mu} a_4{}^{\nu} F_{\lambda\mu\nu}$

$a_4{}^{4} = (a_2{}^{1} a_3{}^{2} a_4{}^{3} - a_2{}^{2} a_3{}^{1} a_4{}^{3} - \cdots + \cdots - \cdots + \cdots - \cdots) F_{123}$

$\begin{vmatrix} a_2{}^{1} & a_2{}^{2} & a_2{}^{3} \\ a_3{}^{1} & a_3{}^{2} & a_3{}^{3} \\ a_4{}^{1} & a_4{}^{2} & a_4{}^{3} \end{vmatrix} = A_4 = (\quad) F_{124} + (a_2{}^{2} a_3{}^{3} a_4{}^{4} - \cdots) F_{234}$

$F'_1 = A_1{}^{4} F_4 + A_1{}^{3} F_3 + \cdots$

$F_{234} = G^{1}$, $F_{134} = -G^{2}$, $F_{124} = G^{3}$, $F_{123} = -G^{4}$

$F'^{\mu\nu} = G^{\mu} A_{\mu\nu}$

$a_{\lambda}{}^{\mu} A_{\mu}{}^{\nu} = \| a_{\lambda}{}^{\mu} \| \delta_{\lambda\nu}$

$G'^{\mu\nu} = G^{\mu} b_{\mu}{}^{\nu} \| a_{\lambda}{}^{\mu} \|$

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$(F')^{\alpha\rho\sigma} = F^{\lambda\mu\nu} b_\lambda{}^\alpha b_\mu{}^\beta b_\nu{}^\gamma$

$F^{\lambda\mu\nu} = \pm G_\kappa$

$= + G_\kappa$ if $\kappa, \lambda, \mu\nu$ is an even element of 1, 2, 3, 4.

$= - G_\kappa$ ∴ odd ∴

$G'_\rho = A_\rho{}^\nu G_\kappa$

~~$A_\mu{}^\nu = \pm |b_\lambda|$~~

$$A_1' = \begin{vmatrix} b_2{}^2 & b_2{}^3 & b_2{}^4 \\ b_3{}^2 & b_3{}^3 & b_3{}^4 \\ b_4{}^2 & b_4{}^3 & b_4{}^4 \end{vmatrix}$$

$$A_2' = (-)\begin{vmatrix} b_2{}^1 & b_2{}^3 & b_2{}^4 \\ b_3{}^1 & b_3{}^3 & b_3{}^4 \\ b_4{}^1 & b_4{}^3 & b_4{}^4 \end{vmatrix} \qquad A_1^2 = (-)\begin{vmatrix} b_1{}^2 & b_1{}^3 & b_1{}^4 \\ b_3{}^2 & b_3{}^3 & b_3{}^4 \\ b_4{}^2 & b_4{}^3 & b_4{}^4 \end{vmatrix}$$

$b_\lambda{}^\mu A_\mu{}^\nu = \| b_\lambda{}^\mu \| \delta_{\lambda\nu}$

$= \| a_\lambda{}^\mu \| \delta_{\lambda\nu}$

$A_\mu{}^\nu = \| a_\mu{}^\nu \| a_\mu{}^\nu$

($\| a_\mu{}^\nu \| = \| b_\mu{}^\nu \|$ ∵ $\| a_\lambda{}^\mu b_\mu{}^\nu \| = 1$

$\| a_\mu{}^\nu \| = \| b_\mu{}^\nu \| = 1$

or $\| a_\mu{}^\nu \| = \| b_\mu{}^\nu \| = -1$)

$G'_\mu = \| a_\mu{}^\nu \| a_\mu{}^\nu G_\nu$

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pseudoscalar

$$F^{\pi\lambda\mu\nu} = \psi^\dagger \frac{1}{24} \epsilon(\gamma^\pi\gamma^\lambda\gamma^\mu\gamma^\nu)\psi \cdot$$

$$F'^{\alpha\beta\gamma\delta} = F^{\pi\lambda\mu\nu} b_\pi^\alpha b_\lambda^\beta b_\mu^\gamma b_\nu^\delta$$

$$F'^{1234} = \| b_\pi^\alpha \| F^{1234}$$

$$G' = \| a_\mu^\nu \| G.$$

Invariant Lagrangian

$$L = -\frac{1}{16\pi} \cdot F_{\mu\nu}F^{\mu\nu} = \frac{1}{8\pi}(E^2 - H^2)$$

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092

Interaction between Dirac electron and radiation.

Problem. Prove that the probab. of spontaneous emission of dipole radiation is given by the same formula as in the case of non-relativistic electron in which r_{ba} is defined by

$$r_{ba} = \int \bar{\psi}^{(b)} r \psi^{(a)} dv$$

where Dirac wave function $\psi^{(a)}$, $\psi^{(b)}$ are Dirac wave functions for initial and final states.

Hint

$$c.\alpha^{(H)} = \frac{dr^{(H)}}{dt}$$

or $\sum \int \bar{\psi}^{(b)(H)} \alpha \psi^{(a)(H)} dv = \sum \int \left(\frac{\partial \bar{\psi}^{(b)(H)}}{\partial t} r \psi^{(a)(H)} + \bar{\psi}^{(b)(H)} r \frac{\partial \psi^{(a)(H)}}{\partial t} \right) dv$

$\because \frac{dr}{dt}$

$$= \frac{i(W_a - W_b)}{\hbar} \sum \int \bar{\psi}^{(b)} r \psi^{(a)} dv$$

(Problem: Photo-electric effect)

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Weisskopf-Wigner's Method.

Reference : Heitler,

electron : initial state $n_\lambda = 0$ $\psi^{(a)}(r) e^{-iW_a t/\hbar}$ energy W_a

photon { final state $n_\lambda = 1$ $\psi^{(b)}(r) e^{-iW_b t/\hbar}$ W_b

$\Psi(r; n_1, n_2, \cdots n_\lambda \cdots t)$

$= C_{a0}(t) \psi^{(a)}(r) \delta_{n_1,0} \delta_{n_2,0} \cdots \delta_{n_\lambda,0} \cdots e^{-iW_a t/\hbar}$

$+ \sum_\lambda C_{b\lambda}(t) \psi^{(b)}(r) \delta_{n_1,0} \cdots \delta_{n_\lambda,1} \cdots e^{-i(W_b + \hbar\omega_\lambda)t/\hbar}$

$+ \cdots$ ⟶ small

$$i\hbar \frac{dC_{a0}}{dt} = \sum_\lambda H'_{a0,b\lambda} C_{b\lambda} \exp(-i(\omega_\lambda - \omega_0)t)$$

$$\omega_0 = (W_a - W_b)/\hbar$$

$$H'_{a0,b\lambda} = ec\sqrt{\frac{2\pi\hbar}{\omega_\lambda V^3}} \int \bar{\psi}^{(a)} (\alpha e_\lambda) \psi^{(b)} e^{-ikr} dv$$

$$i\hbar \frac{dC_{b\lambda}}{dt} = H'_{b\lambda,a0} C_{a0} \exp(i(\omega_\lambda - \omega_0)t)$$

$$H'_{b\lambda,a0} = \tilde{H}'_{a0,b\lambda}$$

initial condition : $C_{a0}(0) = 1$, $C_{b\lambda}(0) = 0$ $\lambda = 1, 2, \cdots$

$C_{a0}(t) = e^{-\gamma t/2}$ $\tau = \frac{1}{\gamma}$.

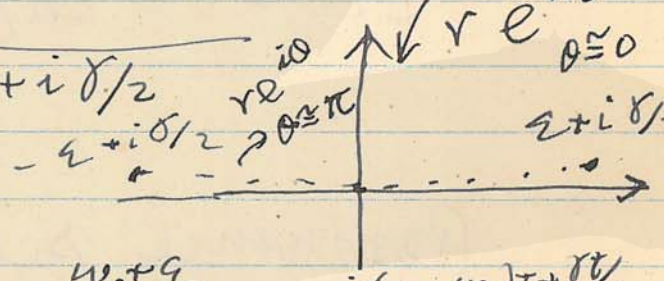
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$$C_{b\lambda}(\tau) = \frac{H'_{b\lambda,a0}}{\hbar} \frac{1-e^{i(\omega_\lambda-\omega_0)t-\gamma t/2}}{(\omega_\lambda-\omega_0+i\gamma/2)}$$

$$\frac{i\hbar\gamma}{2} = \sum_{(\theta_\lambda,\varphi_\lambda)} \frac{|H'_{a0,b\lambda}|^2}{\hbar} \frac{1-e^{-i(\omega_\lambda-\omega_0)t+\gamma t/2}}{(\omega_\lambda-\omega_0+i\gamma/2)}$$

$$\gamma = \frac{1}{i\pi} \sum_{\varphi_\lambda} \int w_e(\omega_\lambda)\, d\omega_\lambda\, d\Omega \frac{1-e^{-i(\omega_\lambda-\omega_0)t+\gamma t/2}}{(\omega_\lambda-\omega_0+i\gamma/2)}$$

$$\int_0^\infty w_e(\omega_\lambda) \frac{1-e^{-i(\omega_\lambda-\omega_0)t+\gamma t/2}}{\omega_\lambda-\omega_0+i\gamma/2}$$

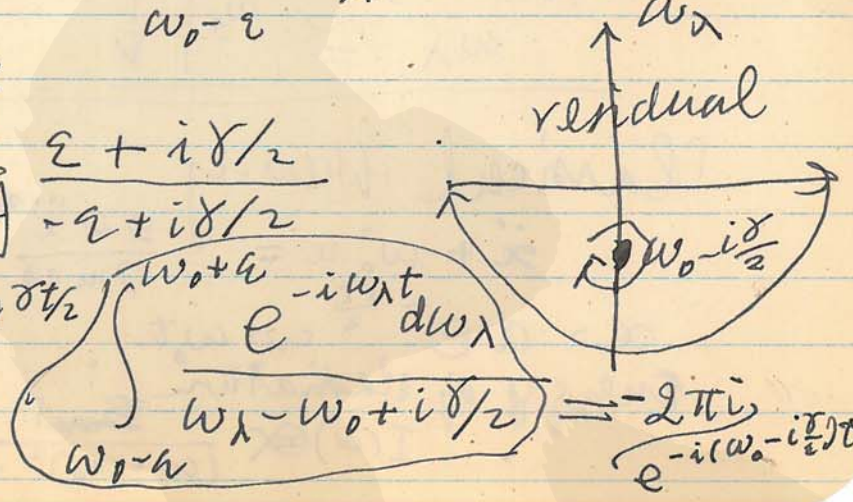


$\gamma \ll \omega_0 \rightarrow \varepsilon \gg \gamma$

$$\int_{\omega_0-\varepsilon}^{\omega_0+\varepsilon} \frac{w_e(\omega_\lambda)\,d\omega_\lambda}{\omega_\lambda-\omega_0+i\gamma/2} - \int_{\omega_0-\varepsilon}^{\omega_0+\varepsilon} \frac{w_e(\omega_\lambda)\,e^{-i(\omega_\lambda-\omega_0)t+\gamma t/2}\,d\omega_\lambda}{\omega_\lambda-\omega_0+i\gamma/2}$$

$$= w_e(\omega_0) \log \frac{\varepsilon+i\gamma/2}{-\varepsilon+i\gamma/2} \quad (-i\pi)$$

$$- w_e(\omega_0)\, e^{i\omega_0 t+\gamma t/2} \int_{\omega_0-\varepsilon}^{\omega_0+\varepsilon} \frac{e^{-i\omega_\lambda t}\,d\omega_\lambda}{\omega_\lambda-\omega_0+i\gamma/2}$$



$$= -2\pi i\, e^{-i(\omega_0-i\frac{\gamma}{2})t}$$

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$$= -\pi i w_e(\omega_0) + 2\pi i w_e(\omega_0)$$

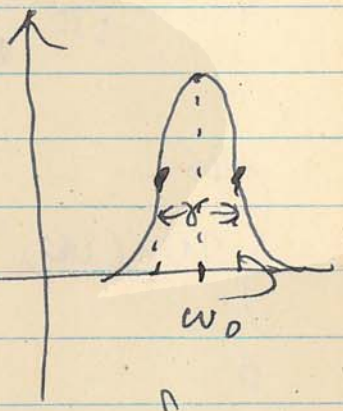
$$\gamma = \sum_{e_\lambda} \int w_e(\omega_0)\, d\Omega$$

$$[C_{n\lambda}^{(a)}]^2 = \frac{|H'_{n\lambda,a0}|^2}{\hbar} \frac{1}{(\omega_\lambda - \omega_0)^2 + \gamma^2/4}$$

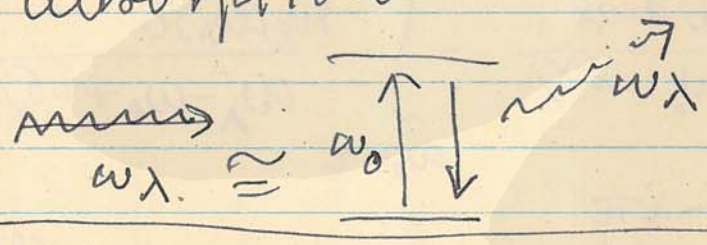
Natural line breadth

$$\omega = \omega_0 \pm \gamma/2$$

$$I(\omega)\, d\omega = \frac{\gamma}{2\pi} \frac{\pi \omega_0\, d\omega}{(\omega-\omega_0)^2 + \gamma^2/4}$$



Resonance scattering and absorption



Classical theory

$$\ddot{x} + \omega_0^2 x = \frac{2e}{3mc^3} \dddot{x}$$

$$x = a e^{-\frac{\gamma t}{2}} \cos \omega_0 t \qquad \gamma = \frac{2e^2\omega_0^2}{3mc^3} \ll \omega_0$$

Energy of Radiation:

$$I(\omega) \propto \frac{\text{Energy}}{(\omega-\omega_0)^2 + (\frac{\gamma}{2})^2}$$

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Problem 1.

Show that γ is very small compared with ω_0, provided that $|r_{ba}|$ is of the order of the atomic radius a (or 10^{-8} cm) and ω_0 is of the order $\frac{e^2}{\hbar a}$.

$$\gamma = \sum_{e,\lambda} \int W_e(\omega_0)\, d\Omega$$

$$\sim \frac{e^2\omega_0^3}{2\pi\hbar c^3} |r_{ba}|^2 \cdot 4\pi$$

$$\frac{\hbar^2}{e^2 m} = \left(\frac{\hbar c}{e^2}\right)\left(\frac{\hbar}{mc}\right)$$

$$\frac{\gamma}{\omega_0} \sim \left(\frac{e^2}{\hbar c}\right)^3$$

In classical theory,

$$\frac{\gamma}{\omega_0} \sim \frac{2e^2}{3mc^3}\omega_0$$

$$\omega_0 \sim \frac{e^2}{\hbar a} \sim \left(\frac{e^2}{\hbar c}\right)^2 \frac{mc^2}{\hbar}$$

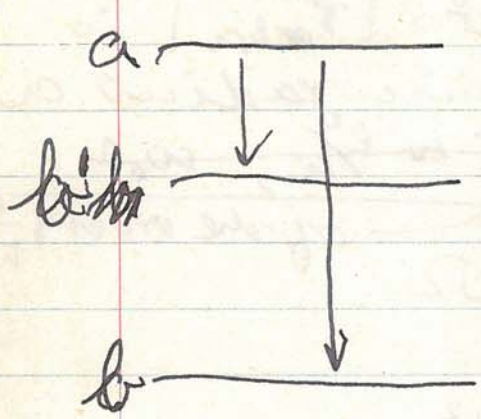
$$a = \frac{\hbar^2}{e^2 m}$$

$$\frac{\gamma}{\omega_0} \sim \left(\frac{e^2}{\hbar c}\right)^3$$

Show that the above qualitive result agrees ~~qualitively~~ with that of the classical theory, ~~only if~~

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Problem 2. Show that (b is the ground state), if there is an excited state b' which has the smaller energy $W_{b'}$ than W_a, the natural line-breadth γ_a of spectral line due to the transition from a to b is given by



$$\gamma_a = \gamma_{b'a} + \gamma_{ba}$$

where $\gamma_{b'a}$, γ_{ba} are the probabilities per unit time of the spontaneous transition $a \to b'$ and $a \to b$ respectively.

$$\Psi = c_{a0}(t)\,\psi^{(a)}(x)\,\delta_{n_1,0}\cdots\delta_{n_\nu,0}\cdots \exp(-iW_a t/\hbar)$$
$$+ \sum_\lambda c_{b\lambda}(t)\,\psi^{(b)}(x)\,\delta_{n_1,0}\cdots\delta_{n_\lambda,1}\cdots\delta_{n_\nu,0}\cdots \exp\left[-i\left(\frac{W_a}{\hbar}+\omega_\lambda\right)t\right]$$
$$+ \sum_\mu c_{a'\mu}(t)\,\psi^{(a')}(x)\,\delta_{n_1,0}\cdots\delta_{n_\lambda,0}\cdots\delta_{n_\mu,1}\cdots \times \exp\left(-i\left(\frac{W_{a'}}{\hbar}+\omega_\mu\right)t\right)$$

$$i\hbar\frac{dc_{a0}}{dt} = \sum_\lambda H'_{a0,b\lambda}\,c_{b\lambda}\exp(-i(\omega_\lambda-\omega_0)t) + \sum H'_{a0,b'\mu}\,c_{b'\mu}\exp(-i(\omega_\mu-\omega_0')t)$$
$$\omega_0' = \frac{W_a - W_{b'}}{\hbar}$$

$$i\hbar\frac{dc_{b\lambda}}{dt} = H'_{b\lambda,a0}\,c_{a0}\exp(i(\omega_\lambda-\omega_0)t)$$

$$i\hbar\frac{dc_{b'\mu}}{dt} = H'_{b'\mu,a0}\,c_{a0}\exp(i(\omega_\mu-\omega_0')t)$$

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Problem 2.
Show that the energy of radiation in the frequency range $(\omega, \omega+d\omega)$ $(\omega = 2\pi\nu)$ absorbed per unit time due to the transition $b \to a$ of the atom is

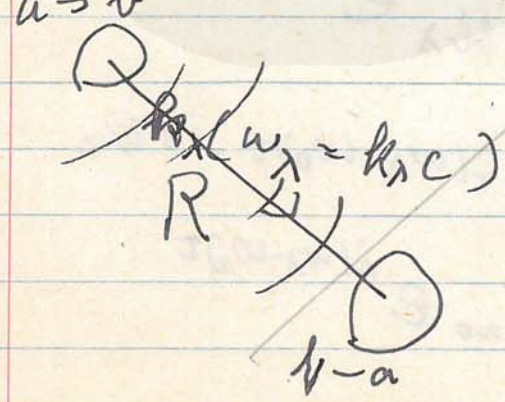
$$S(\omega)d\omega = \frac{\pi c^2 \gamma^2}{2\omega_0^2} \frac{I(\omega_0)d\omega}{(\omega-\omega_0)^2 + (\gamma/2)^2}$$

$$C_{a0}(t) = e^{-\gamma_a t/2}$$

$$\frac{i\hbar\gamma_a}{2} = \sum_\lambda + \sum_\mu$$

$$\gamma_\mu = \gamma_{ba} + \gamma_{b'a}$$

Problem 3. A Quantum mechanical proof ~~derivation~~ of the statement that the light propagates with the velocity c: Prove that, when there are two atoms at a distance R in the states a, b respectively at $t=0$, the ~~second atom~~ probability that the second atom is excited to the state b while the first is in the ground state a is different from 0, only if $t \geq \frac{R}{c}$,



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provided that R is large compared with the wave length of the light emitted by the first atom.

$$\Psi(r_1, r_2; n_1, n_2, \cdots n_\lambda \cdots; t)$$
$$= c_{abo}(t)\,\psi^{(a)}(r_1)\psi^{(b)}(r_2)\,\delta_{n_1,0}\cdots\delta_{n_\lambda,0}\cdot e^{-i(W_a+W_b)t/\hbar}$$
$$+\sum_\lambda c_{bb\lambda}(t)\,\psi^{(b)}(r_1)\psi^{(b)}(r_2)\,\delta_{n_1,0}\cdots\delta_{n_\lambda,1}\cdots e^{-i(W_b+\hbar\omega_\lambda+W_b)t/\hbar}$$
$$+\; c_{ba\lambda}(t)\,\psi^{(b)}(r_1)\psi^{(a)}(r_2)\,\delta_{n_1,0}\cdots\delta_{n_\lambda,0}\cdots e^{-i(W_a+W_b)t/\hbar}$$

$$c_{abo}(t) = e^{-\gamma t/2} \qquad c_{bb\lambda}(0) = c_{ba\lambda}(0) = 0.$$

$$H' = \sum_{\alpha_\lambda}(\cdot)^{\alpha_\lambda}\left(\alpha_1 e_\lambda\, e^{\pm i k_\lambda r_1} + (\alpha_2 e_\lambda) e^{\pm i k_\lambda r_2}\right)$$

$$i\hbar\frac{dc_{abo}}{dt} = \sum_\lambda H'_{ao;b\lambda}\, c_{bb\lambda}\, e^{-i(\omega_\lambda-\omega_0)t}$$

$$i\hbar\frac{dc_{bb\lambda}}{dt} = H'_{b\lambda;ao}\, c_{abo}\, e^{i(\omega_\lambda-\omega_0)t} + H'_{b\lambda;ao}\, c_{bao}\, e^{i(\omega_\lambda-\omega_0)t}$$

$$i\hbar\frac{dc_{bao}}{dt} = \sum_\lambda H'_{ao;b\lambda}\, c_{bb\lambda}\, e^{-i(\omega_\lambda-\omega_0)t}$$

$$i\hbar\frac{dc_{bb\lambda}}{dt} = H'_{b\lambda;ao}\, e^{i(\omega_\lambda-\omega_0)t-\gamma t/2} + H'_{b\lambda;ao}\, c_{bao}\, e^{i(\omega_\lambda-\omega_0)t}$$

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$$i\hbar \frac{dC_{a\omega_0}}{dt} = \sum_{\lambda} H'_{a\omega_0;b\lambda} C_{b\omega_\lambda} e^{-i(\omega_\lambda - \omega_0)t}$$

$$i\hbar \frac{dC_{b\omega_\lambda}}{dt} = H'_{b\omega_\lambda;a\omega_0} C_{a\omega_0} e^{i(\omega_\lambda - \omega_0)t}$$

~~H'~~

Fermi, R. M. P.
Kikuchi, ZS. f. Phys.

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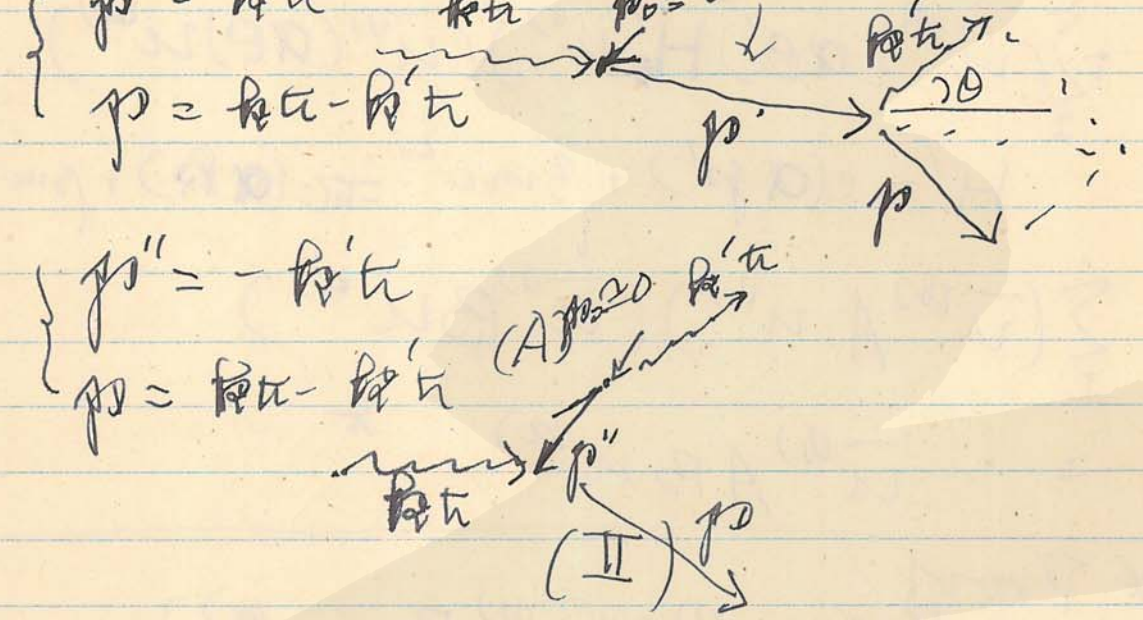
Compton Effect:

$$i\hbar \frac{dC_B}{dt} = V_{BA} e^{i(E_B - E_A)t/\hbar} C_A \Big\}$$

$C_A = 1$

$$V_{BA} = \sum_I \frac{H'_{BI} H'_{IA}}{E_A - E_I} + \sum_{II} \frac{H'_{BII} H'_{IIA}}{E_A - E_{II}}$$

(A) (I) (B)



$$\begin{cases} p' = \hbar k' \\ p = \hbar k - \hbar k' \end{cases}$$

$$\begin{cases} p'' = -\hbar k' \\ p_0 = \hbar k - \hbar k' \end{cases}$$

$$V_{BA} = \frac{2\pi e^2 \hbar c^2}{\sqrt{\omega \omega' L^3}} \left\{ \sum_I \frac{(\bar{u}^{(b)}(\alpha e')u^{(i)})(\bar{u}^{(i)}(\alpha e)u^{(a)})}{mc^2 + \hbar\omega - W'} + \sum_{II} \frac{(\bar{u}^{(b)}(\alpha e)u^{(i)})(\bar{u}^{(i)}(\alpha e')u^{(a)})}{mc^2 - \hbar\omega' - W''} \right\}$$

$$\left.\begin{aligned} W' &= \pm c\sqrt{m^2c^2 + p'^2} \\ W'' &= \pm c\sqrt{m^2c^2 + p''^2} \end{aligned}\right\}$$

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$$\sum_I \frac{(\bar{u}^{(b)}(\alpha e)u^{(1)})(\bar{u}^{(1)}(\alpha e)u^{(a)})}{mc^2+\hbar\omega-W'}$$

$$\frac{1}{mc^2+\hbar\omega-W'} = \frac{mc^2+\hbar\omega+W'}{(mc^2+\hbar\omega)^2-(W')^2}$$

$$\sum_I (mc^2+\hbar\omega+W')(\bar{u}^{(b)}(\alpha e')u^{(1)})(\bar{u}^{(1)}(\alpha e)u^{(a)})$$

$$= (mc^2+\hbar\omega)\sum_I (\bar{u}^{(b)}(\alpha e')u^{(1)})(\bar{u}^{(1)}(\alpha e)u^{(a)})$$

$$+\sum_I (\bar{u}^{(b)}(\alpha e')H'_e u^{(1)})(\bar{u}^{(1)}(\alpha e)u^{(a)})$$

$$H' = c(\alpha p') + \beta mc^2 = \hbar c(\alpha k) + \beta mc^2$$

$$\sum_{\pm}(\bar{u}^{(b)} A u^{(1)})(\bar{u}^{(1)} B u^{(a)})$$

$$= \bar{u}^{(b)} AB u^{(a)} \quad *$$

---

* Proof:

$$\sum_{\pm}(\bar{u}^{(b)}_i A_{ij} u^{(1)}_j)(\bar{u}^{(1)}_k B_{kl} u^{(a)}_l)$$

$$\sum_{\pm} u^{(1)}_j \bar{u}^{(1)}_k = \delta_{jk} \quad \text{(completeness)}$$

	$k_0>0$	$k_0>0$	$k_0<0$	$k_0<0$
u_1	1	0	$-p_z/\mu$	$-(p_x-ip_y)/\mu$
u_2	0	1	$-(p_x+ip_y)/\mu$	p_z/μ
u_3	p_z/μ	$(p_x-ip_y)/\mu$	1	0
u_4	$(p_x+ip_y)/\mu$	$-p_z/\mu$	0	1

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$$W'^2 = c^2(\hbar^2 k^2 + m^2 c^2)$$

$$(mc^2 + \hbar\omega)^2 - W'^2 = 2mc^2 \cdot \hbar\omega$$

$$\sum_{\mathrm{I}} \frac{\bar{u}^{(b)}(\alpha e')\, K'(\alpha e)\, u^{(a)}}{2mc^2 \cdot \hbar\omega}.$$

$$K' = mc^2 + \hbar\omega + H' = (1+\beta)mc^2 + \hbar\omega + (\alpha \hbar k) \quad (\hbar c)$$

$$-\sum_{\mathrm{II}} \frac{\bar{u}^{(b)}(\alpha e')\, K''(\alpha e')\, u^{(a)}}{2mc^2 \cdot \hbar\omega'}$$

$$K'' = mc^2 - \hbar\omega' + H''$$

$$H'' = c(\alpha p'') + \beta mc^2 = -\hbar c(\alpha k') + \beta mc^2$$

$$K'' = (1+\beta)mc^2 - \hbar\omega' - \hbar c(\alpha k').$$

$$\sum_{\mathrm{I}} + \sum_{\mathrm{II}} = \frac{1}{2mc^2}\left[\frac{\bar{u}^{(b)}(\alpha e')K(\alpha e)u^{(a)}}{\hbar\omega} - \frac{\bar{u}^{(b)}(\alpha e)K(\alpha e)u^{(a)}}{\hbar\omega'}\right]$$

$$\sum_j u_j^{(r)} u_j^{(s)} = \delta_{rs}$$

$$u_{pk}^{(s)} = u_j^{(r)}$$

$$S_{ir} u_j^{(r)} \cdots u_j^{(s)} S_{sk} =$$

$$u_j^{(s)} = \sum_r C_{sr} u_j^{(r)} \qquad \sum_s u_k^{(s)} u_j^{(s)} = \sum C_{sr}$$

$$\langle (1 + \rho(W')) \frac{W'}{|W'|} | p_3, \sigma_2 \rangle$$

σ_2,

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Summation over spin directions of final electron and average over spin directions of initial electron.

$$\frac{1}{2}\sum_B \sum_A \left|\left\{\sum_{\mathrm{I}} + \sum_{\mathrm{II}}\right\}\right|^2$$

$$\sum_B (\bar{u}^{(a)} C u^{(b)})(\bar{u}^{(b)} D u^{(a)})$$

$$= \bar{u}^{(a)} C \frac{H+|W|}{2|W|} D u^{(a)}$$

$$H = c(\alpha p) + \beta m c^2$$

$$= \bar{u}^{(a)} C \frac{H+W}{2W} D u^{(a)} \quad \text{for } W > 0$$

$$\frac{1}{2}\sum_A (\bar{u}^{(a)} C \frac{H+W}{2W} D u^{(a)})$$

$$= \frac{1}{8W \cdot mc^2} \sum_{A,i,j} \bar{u}_i^{(a)} C (H+W) D (H_0 + mc^2)_{ij} u_j^{(a)}$$

$$\sum_A \bar{u}_i^{(a)} u_j^{(a)} = \delta_{ij} \qquad \underline{H_0 = \beta m c^2}$$

$$= \frac{1}{8W \cdot mc^2} \underset{\text{Trace}}{Sp} \left(C(H+W) D (H_0 + mc^2)\right)$$

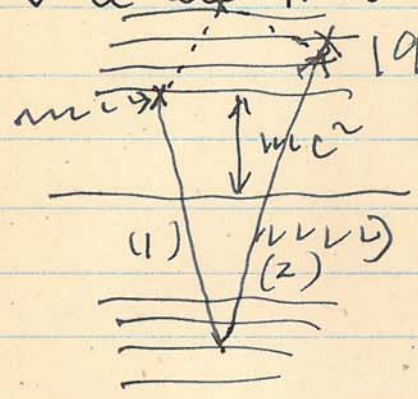
~~$Sp(\quad) = mc^2$~~

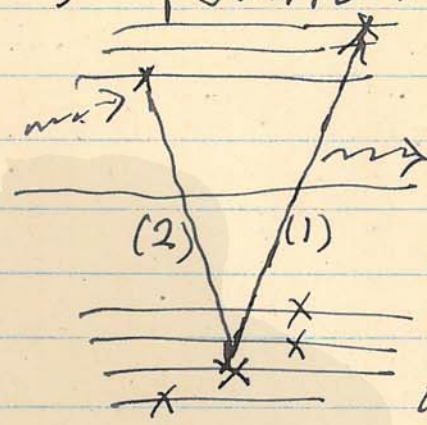
$$mc^2 \cdot Sp\{(\alpha e^m) K'(\alpha e')(H+W)(\alpha e') K'(\alpha e)(1+\beta)\}$$

etc.

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One electron theory → Positron theory





virtual creation and annihilation of pair

→ T.S.F. theory

(Q.F.T. →

(Quantization of Electron Field or Feynmen theory)

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Methods of Approximation

B. Variation method

(1)

Schiff, p. 169

$\psi(q_1, q_2 \cdots q_n)$, $H(q_1 \cdots q_n, -i\hbar\frac{\partial}{\partial q_1}, \cdots)$

$$\bar{H} = \int\cdots\int \tilde{\psi} \cdot H \psi \, dq_1 dq_2 \cdots dq_n \quad (= \langle H \rangle)$$

$$\delta \bar{H} = 0.$$

under the condition

$$\int\cdots\int \tilde{\psi} \psi \, dq_1 \cdots dq_n (= \text{const}) = 1$$

$$\delta \int\cdots\int (\tilde{\psi} H \psi - E \cdot \tilde{\psi} \psi) \, dq_1 dq_2 \cdots dq_n = 0$$

$$\left.\begin{aligned} \delta\tilde{\psi}: \quad & H\psi - E\psi = 0 \\ \delta\psi: \quad & \tilde{\psi} H - \tilde{\psi} E = 0 \end{aligned}\right\} \quad (1)$$

(provided that ψ is stable at ∞)

For $\psi, \tilde{\psi}$ satisfying (1), we obtain

$$\int \tilde{\psi} \cdot H \psi \, dq_1 \cdots dq_n = E.$$

or more generally

$$E = \int \tilde{\psi} H \psi \, dq_1 \cdots dq_n \Big/ \int \tilde{\psi} \psi$$

Thus, the eigenvalue E is obtained as the extremum ~~of the value~~ of $\bar{H}$.

Now suppose that we know the complete set of eigenfunctions $\psi_0, \psi_1, \psi_2, \ldots$ belonging respectively to eigenvalues $E_0 \leq E_1 \leq E_2 \leq \cdots$,

$$\psi = \sum_i C_i \psi_i$$

$$\bar{H} = \langle H \rangle = \sum_{i=0}^{\infty} E_i |C_i|^2$$

The right hand side takes the minimum

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value E_0, ~~for~~ if
$|C_0|=1$, $C_1=0$, $C_2=0$, $C_3=0$ ... .
Thus, the eigenvalue of the lowest energy state is the minimum of $\overline{H}$.

This argument helps us very much in obtaining an approximate value for the low energy value together with the appr. eigen-fn, in the cases when Schrödinger eq. can not be solved rigorously. For example, choose a trial function ψ with a number of indeterminate parameters and adjust the values of the parameters in such a way that the value of $\overline{H}$ becomes minimum. This minimum E_{min} cannot be smaller than the true eigenvalue E_0, but ~~because~~ but comes closer and closer to E_0, as the trial function becomes nearer to the true eigenfunction.

In particular, if we start from ~~a~~ a system of complete set of orthogonal and normalized functions $\varphi_1, \varphi_2, \ldots$ and choose the trial function

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$$\psi = \sum_{i=1}^{n} c_i \varphi_i$$

with a certain finite integral value n
the coefficients $c_1, c_2, \ldots c_n$ can
be so adjusted that $\overline{H}$ becomes
minimum. This method is called
Ritz's method. If we increase n,
the accuracy will be better, but the
computation will be more complicated.
One must make some compromise
between complexity and accuracy*.
Let us consider one example of
helium at ground state of the
helium atom.

$$H = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) - 2e^2\left(\frac{1}{r_1} + \frac{1}{r_2}\right) + \frac{e^2}{r_{12}}$$

If we ignore the last term, the solution
of Schrödinger eq. for the ground state
is

$$\psi(r_1, r_2) = \frac{Z^3}{\pi a_0^3} \cdot e^{-\left(\frac{Z}{a_0}\right)(r_1 + r_2)}$$

$$Z = 2 \qquad a_0 = \frac{\hbar^2}{e^2 m} = \alpha\left(\frac{\hbar}{mc}\right)$$

Now let us start from the trial function
with Z as a parameter which is not
necessarily be equal to 2.

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$$\bar{H} = \left(\frac{e^2Z^2}{2a_0} + \frac{e^2Z^2}{2a_0}\right) - \left(\frac{2e^2Z}{a_0} + \frac{2e^2Z}{a_0}\right)$$

(H.I: 正)

K.E. $4\pi \int \chi \left(\frac{d^2\chi}{dr^2} + \frac{2}{r}\frac{d\chi}{dr}\right) r^2 dr$

$= 4\pi \int e^{-\frac{2Z}{a_0}r} \left(\frac{2Z}{a_0}\right)^2 r^2 dr$

$= 2\left[\left(\frac{2Z}{a_0}\right) e^{-\frac{2Z}{a_0}r} r\, dr \right] \frac{Z^3}{\pi a_0^3}$

$= \frac{Z^2}{2a_0^2}\left[\int e^{-x} x^2 dx - 4\int e^{-x} x\, dx\right]$

$= \frac{Z^2}{2a_0^2}\left[2 - 4\right] = \frac{2^2}{a_0^2}$

K.E. $-\frac{\hbar^2}{2m}\left(-\frac{Z^2}{a_0^2}\right) = \frac{e^2Z^2}{2a_0}$

P.E. $4\pi \int \chi^2 \frac{2e^2}{r} r^2 dr$

$= 4\pi \int e^{-2Z/a_0 \cdot r} r\, dr \cdot 2e^2 \frac{Z^3}{\pi a_0^3}$

$= \frac{2e^2Z}{a_0} \int e^{-x} x\, dx = \frac{2e^2Z}{a_0}$

E.I $\int\int \psi^2(r_1, r_2) \frac{e^2}{r_{12}} dv_1 dv_2 =$

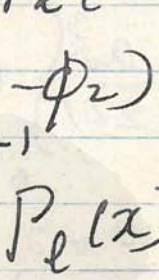
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(3)

$$= \left(\frac{Z^3}{\pi a_0^3}\right)^2 e^2 \int\cdots\int \frac{1}{r_{12}} e^{-\left(\frac{2Z}{a_0}\right)(r_1+r_2)} \, dv_1 dv_2$$

$$\frac{1}{r_{12}} = \frac{1}{r_1} \sum_{l=0}^{\infty} \left(\frac{r_2}{r_1}\right)^l P_l(\cos\theta) \qquad r_1 > r_2$$

$$= \frac{1}{r_2} \sum_{l=0}^{\infty} \left(\frac{r_1}{r_2}\right)^l P_l(\cos\theta) \qquad r_1 < r_2$$



$$\cos\theta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2)$$

$$\frac{1}{\sqrt{1-2sx+s^2}} = \sum_{l=0}^{\infty} P_l(x) s^l \qquad s<1$$

$$\frac{1}{\sqrt{r_1 - 2r_1 r_2 \cos\theta + r_2^2}} = \frac{1}{r_1} \frac{1}{\sqrt{1-2bx+b^2}}$$

for $r_1 > r_2$ $\quad s = \frac{r_2}{r_1}$ $\quad x = \cos\theta_1$

Addition theorem:

$$P_l(\cos\theta) = P_l(\cos\theta_1) P_l(\cos\theta_2)$$

$$+ 2 \sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} P_l^m(\cos\theta_1) P_l^m(\cos\theta_2) \times \cos m(\phi_1 - \phi_2)$$

$$\int_{m=0} P_l^m(\cos\theta) \sin\theta \, d\theta \to \int_{-1}^{+1} P_l(x)\, dx = 2 \quad \text{for } l=0.$$

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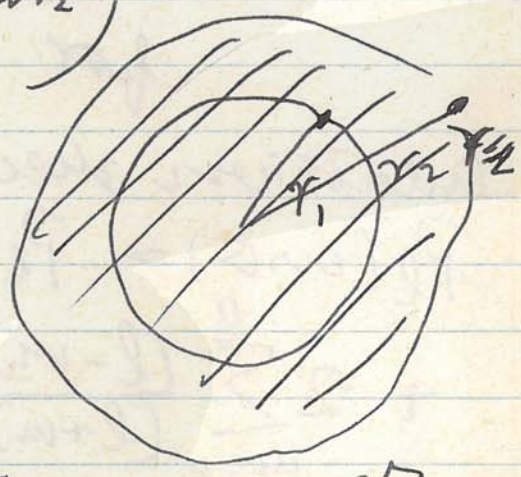
$$F.I_1 = \left(\frac{Z^3}{\pi a_0^3}\right)^2 e^2 \cdot (4\pi)^2$$

$$\times \int_0^\infty \left[\frac{1}{r_1}\int_0^{r_1} e^{-\frac{2Z}{a_0}(r_1+r_2)} r_2^2 dr_2 + \int_{r_1}^\infty \frac{1}{r_2} e^{-\frac{2Z}{a_0}(r_1+r_2)} r_2^2 dr_2\right] r_1^2 dr_1$$

$$\left(\int_0^\infty \left(\int_{r_1}^\infty \frac{1}{r_2} e^{-\frac{2Z}{a_0}(r_1+r_2)} r_2^2 dr_2 \right) r_1^2 dr_1 \right.$$



$$\left. = \int_0^\infty \left(\frac{1}{r_2} \int_0^{r_2} e^{\cdots} r_1^2 dr_1 \right) r_2^2 dr_2 \right)$$



$$\int_0^{r_1} e^{-\frac{2Z}{a_0} r_2} r_2^2 dr_2$$

$$= \left(\frac{a_0}{2Z}\right)^3 \int_0^{x_1} e^{-x_2} x_2^2 dx_2 \qquad x_1 = \frac{2Z}{a_0} r_1$$

$$= \left(\frac{a_0}{2Z}\right)^3 \cdot \left[-e^{-x_1} x_1^2 - 2e^{-x_1} x_1 + 2\int_0^{x_1} e^{-x_2} dx_2 \right]$$

$$= \left(\frac{a_0}{2Z}\right)^3 \left[-e^{-x_1} x_1^2 - 2e^{-x_1} x_1 + 2 - 2e^{-x_1} \right]$$

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$$E.I_1 = \frac{2e^2}{a_0} \int_0^\infty e^{-x}\left(2 - 2e^{-x} - 2e^{x}x^0 - e^{-x}x^2\right) x\,dx$$

$$\simeq \frac{2e^2}{a_0}\left\{2 - \frac{1}{2} - \frac{1}{2} - \frac{6}{16}\right\} \quad \frac{1}{16}$$

$$= \frac{2e^2}{a_0}\left\{\frac{16-4-4-3}{8}\right\} = \frac{2e^2}{a_0}\frac{5}{8}$$

$$\bar{H} \simeq \frac{e^2}{a_0}\left(Z^2 - 4Z - \frac{5}{8}Z\right)$$

$$\simeq + \frac{e^2}{a_0}\left(Z^2 - \frac{27}{8}Z\right)$$

$$\frac{\partial \bar{H}}{\partial Z} = 2Z - \frac{27}{8} = 0 \qquad 2 \times \frac{11}{8}$$

$$Z = \frac{27}{16} = 1.69 \left(= Z_0 - \frac{5}{16}\right) \qquad = \frac{11}{4}$$

$$\bar{H} = -\frac{e^2}{a_0}\cdot\left(\frac{27}{16}\right)^2$$

$$\simeq -2.85\,\frac{e^2}{a_0}$$

$$\left(Z = 2 : \quad \bar{H} \simeq \frac{e^2}{a_0}\cdot 2\left(2 - \frac{27}{8}\right)\right.$$

$$\left. \simeq -2.75\,\frac{e^2}{a_0}\right)$$

(to remove both electrons)

Experimental value $E_0 = -2.904\,\frac{e^2}{a_0}$

only two percent higher

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Hylleraas: Next approximation
this means that each electron
screens the nuclear charge acting
on the other electron, so that the
effective charge is reduced by
an amount $\frac{5}{16}e$. from $2e$

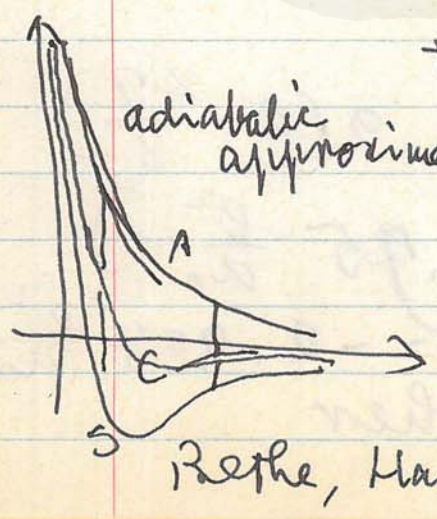
Problem.
Show that if we regard $\frac{e^2}{r_{12}}$
as perturbation, we obtain
in the first approximation

$$E_0 = -\frac{4e^2}{a_0} + \frac{5}{4}\frac{e^2}{a_0}$$

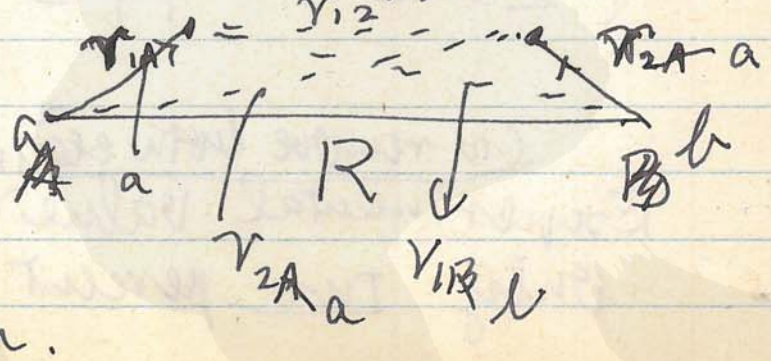
$$= -2.75\,\frac{e^2}{a_0}$$

The second example: Modification of Ritz's method
Two hydrogen atom
Heitler-London's approximation

$$H = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) - \frac{e^2}{r_{1a}} - \frac{e^2}{r_{2b}}$$
$$+ \frac{e^2}{R} + \frac{e^2}{r_{12}} - \frac{e^2}{r_{1b}} - \frac{e^2}{r_{2a}}$$



Bethe, Handbuch.



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(5)

$$\psi = \frac{1}{\pi a_0^3} e^{-r_{1a}/a_0} e^{-r_{2b}/a_0} = u_1$$

$$\frac{1}{\pi a_0^3} e^{-r_{1b}/a_0} e^{-r_{2a}/a_0} \Big\} u_2$$

$$\psi = \frac{1}{\pi a_0^3}\left(c_1 e^{-(r_{1a}+r_{2b})/a_0} + c_2 e^{-(r_{1b}+r_{2a})/a_0}\right)$$

(they are not orthogonal to each other)

$\delta H = 0$ $\delta(\int \psi H \psi - E \int \psi\psi) = 0$

$H = H_{11}c_1^2 + H_{22}c_2^2 + (H_{12} + H_{21})c_1c_2$

$H_{11} = H_{22}$

$H_{12} = H_{21}$ (real)

$H_{11}c_1 + H_{12}c_2 = E(c_1 + c_2 S^2)$

$H_{12}c_1 + H_{11}c_2 = E(c_1 S^2 + c_2)$

$$\begin{vmatrix} H_{11}-E & H_{12}-ES^2 \\ H_{12}-ES^2 & H_{11}-E \end{vmatrix} = 0 \qquad E = \frac{H_{11} \pm H_{12}}{1 \pm S^2}$$

$(H_{11}-E)^2 = (H_{12}-ES^2)^2$

$H_{11} - E = \pm(H_{12} - ES^2)$

$c_1 = \pm c_2$

$\psi \propto e^{-(r_{1a}+r_{2b})/a_0} u_1 \pm e^{-(r_{1b}+r_{2a})/a_0} u_2$

symmetric and antisym.

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Electron spin:

$$\psi = \psi_S \cdot \frac{1}{\sqrt{2}}\big(\alpha(1)\beta(2) - \beta(1)\alpha(2)\big)$$

$\alpha(1)\alpha(2)$

$$\psi_A \begin{cases} \frac{1}{\sqrt{2}}\big(\alpha(1)\beta(2) + \beta(1)\alpha(2)\big) \\ \beta(1)\beta(2) \end{cases}$$

$$\psi_S = \frac{1}{\sqrt{2(1+S^2)}}\left\{\frac{1}{\pi a_0^3}\left(e^{-(r_{a1}+r_{b2})/a_0} + e^{-(r_{1b}+r_{2a})/a_0}\right)\right.$$

$u_1 + u_2$

$$\left.\psi_A = \frac{1}{\sqrt{2(1-S^2)}}\{\quad , \quad - \quad , \quad \}\right.$$

$u_1 - u_2$

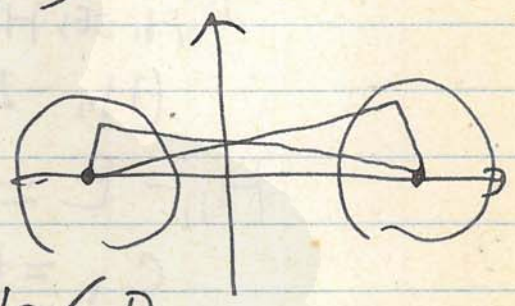
$$S = \left(\frac{1}{\pi a_0^3}\right)^2 \int\int e^{-(r_{1a}+r_{2b}+r_{1b}+r_{2a})/a_0} \times dv_1\, dv_2$$

or $$S = \left(\frac{1}{\pi a_0^3}\right) \int e^{-(r_{1a}+r_{1b})/a_0}\, dv_1$$

$$= \left(1 + R + \frac{1}{3}R^2\right)e^{-R}$$

Exchange Integral

$H_{12} < 0$



$$H_{12} = \int u_2 H' u_1\, dv_1 dv_2 < 0$$

corresponding to the fact that

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$\begin{cases} E_s(R_{min}) = -3.2 \text{ volt} \\ E_{exp} = -4.6 \text{ volt} \end{cases}$ $R_{min} = 0.74 \times 10^{-8}$ cm.

the attractions between the nuclei and electron is slightly larger than that the repulsions between electrons and between nuclei.

Problem 1.

Find the best approximation of the form Show that

$$\psi \approx C e^{-\mu^2 r^2} \qquad \mu: \text{parameter}$$

for the ground state of the hydrogen atom ~~and show that~~ is given by the value

$$\mu = \frac{2}{3}\sqrt{\frac{2}{\pi}}\frac{me^2}{\hbar^2} = 0.532/a_0$$

and that the energy is

$$\overline{H}_{\mu=0.532 a_0} = -\frac{4}{3\pi}\frac{me^4}{\hbar^2} = -0.435\frac{me^4}{\hbar^2}$$

whereas the true eigenvalue is $-\frac{1}{2}\cdot\frac{me^4}{\hbar^2}$,

$$\overline{H} = \frac{\int \psi H \psi r^2 dr}{\int \psi^2 r^2 dr} = 8\sqrt{\frac{2}{\pi}}\cdot\mu^3\left\{\frac{\hbar^2}{2m}\int_0^\infty (-6\mu^2 r^2 + 4\mu^4 r^4) e^{-2\mu^2 r^2} dr - e^2 \int_0^\infty e^{-2\mu^2 r^2} r dr\right.$$

$$= \frac{3\hbar^2}{2m}\mu^2 - 2\sqrt{\frac{2}{\pi}}e^2\cdot\mu$$

$$= \frac{3\hbar^2}{2m}\left(\mu - \frac{2me^2}{3\hbar^2}\sqrt{\frac{2}{\pi}}\right)^2 - \frac{4}{3\pi}\frac{me^4}{\hbar^2}$$

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X Problem 2.

Deuteron problem:

$$H = \frac{\hbar^2}{M}\left(\frac{d}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) - g^2\frac{e^{-\pi^2 r^2}}{r}$$

$$\psi = Ce^{-\mu^2 r^2}$$

$$\bar{H} = \frac{3\hbar^2}{M}\mu^2 - 8\sqrt{\frac{2}{\pi}}\cdot\mu^3 g^2 \int e^{-(2\mu^2+\pi^2)r^2} r\,dr$$

$$= \frac{3\hbar^2}{M}\mu^2 - 2\sqrt{\frac{2}{\pi}}\frac{\mu^3 g^2}{(\mu^2+\frac{\pi^2}{2})}$$

$$\delta\bar{H} = 0$$

$$\frac{3\hbar^2}{M}\mu - 2\sqrt{\frac{2}{\pi}}g^2\frac{(\mu^2+\frac{\pi^2}{2})3\mu^2 - 2\mu^4}{(\mu^2+\frac{\pi^2}{2})^2}$$

$$= 2\cdot\frac{\frac{3\hbar^2}{M}\mu - \sqrt{\frac{2}{\pi}}g^2\cdot\mu^2(\mu^2+\frac{3}{2}\pi^2)}{(\mu^2+\frac{\pi^2}{2})^2} = 0$$

$$3\mu(\mu^2+\tfrac{\pi^2}{2})^2$$

$$\frac{3\hbar^2}{M}(\mu^2+\frac{\pi^2}{2})^2 - \sqrt{\frac{2}{\pi}}g^2\mu(\mu^2+\frac{3}{2}\pi^2) = 0$$

$\mu^2 \ll \pi^2$

$$\mu \sim \frac{\hbar^2}{3Mg^2}\sqrt{\frac{\pi}{2}}\cdot\frac{\pi^2}{2}$$

$$\bar{H} = \frac{3\cdot\hbar^6}{M^3 g^4}\frac{\pi}{2}\frac{\pi^4}{4} - \frac{2\hbar^6}{M^3 g^4}\frac{\pi}{2}\frac{\pi^4}{24}$$

$$\int e^{-(2\mu^2+\pi^2)r^2} r\,dr = \frac{\int e^{-x}dx}{2(2\mu^2+\pi^2)} = \frac{1}{2(2\mu^2+\pi^2)}$$

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Bethe, H.B.: S. 535.

$$U_1 = u_a(1)\,u_b(2) = \frac{1}{\pi a_0^3} e^{-(r_{1a}+r_{2b})/a_0}$$

$$U_2 = u_b(1)\,u_a(2) = \frac{1}{\pi a_0^3} e^{-(r_{1b}+r_{2a})/a_0}$$

$$\left.\begin{aligned} U_s &= \frac{1}{\sqrt{2(1+S^2)}}(U_1+U_2) \\ U_a &= \frac{1}{\sqrt{2(1-S^2)}}(U_1-U_2) \end{aligned}\right\}$$

$$S = \frac{1}{\pi a_0^3}\int e^{-(r_{1a}+r_{2b})/a_0}\, dv_1$$

$$\Psi = c_1 U_1 + c_2 U_2$$

$$\int \tilde{\Psi}\Psi = \tilde{c}_1 c_1 + \tilde{c}_2 c_2 + 2(\tilde{c}_1 c_2 + \tilde{c}_2 c_1) S^2$$

$$\bar{H} = H_{11}\tilde{c}_1 c_1 + H_{12}\tilde{c}_1 c_2 + H_{21}\tilde{c}_2 c_1 + H_{22}\tilde{c}_2 c_2$$

$$H_{11} = H_{22} = \int U_1 H U_1\, dv_1 dv_2$$

$$H_{12} = H_{21} = \int U_2 H U_1\, dv_1 dv_2$$

$$H_{11}c_1 + H_{12}c_2 = Ec_1 + ES^2 c_2$$

$$\begin{vmatrix} H_{11}-E & H_{12}-ES^2 \\ H_{12}-ES^2 & H_{22}-E \end{vmatrix} = 0$$

$$E = \frac{H_{11} \pm H_{12}}{1 \pm S^2} =$$

$$c_1 = \pm c_2$$

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$$A = \int u_a^2(1) u_b^2(2) e^2 \left(\frac{1}{R} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}} + \frac{1}{r_{12}} \right) dv_1 dv_2$$

$$B = \int u_a(1) u_b(1) u_a(2) u_b(2) e^2 \left(\frac{1}{R} - \frac{1}{r_{a2}} - \frac{1}{r_{b1}} + \frac{1}{r_{12}} \right) dv_1 dv_2$$

$$\left(-\frac{\hbar^2}{2m} \Delta_1 - \frac{e^2}{r_{12}} \right) u_a(1) = W_0 u_a(1)$$

$$H_{11} = 2W_0 + A$$

$$H_{12} = 2W_0 S^2 + B.$$

$$E = \frac{A \pm BS^2}{1 \pm S^2}$$

$$E \simeq 2W_0 + \frac{A \pm B}{1 \pm S^2}$$

$$= 2W_0 + A \pm \frac{B - AS^2}{1 \pm S^2}$$

$$A(R) = e^{-2R/a_0} e^2 \left(\frac{1}{R} - \frac{5}{8} - \frac{3}{4} R - R^2 \right) < 0$$

for not to small values of R.

$B(R)$: negative and $|B(R)|$ is larger than AS^2.

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* Ritz's method.

$$I = \int \tilde{\psi} H \psi \, dq - E \int \tilde{\psi} \psi \, dq$$

$$\delta I = 0$$

$$\psi = \sum_{k=1}^{n} c_k \varphi_k \qquad \left(\sum_j \tilde{c}_j c_j = 1 \right)$$

$$I = \sum_{j,k=1}^{n} \tilde{c}_j H_{jk} c_k - E \sum_j \tilde{c}_j c_j \qquad H_{jk} = \int \tilde{\varphi}_j H \varphi_k \, dq$$

$$\sum_{k=1}^{n} H_{jk} c_k = E c_j \qquad (1)$$

$$\| H_{jk} - E \delta_{jk} \| = 0$$

modification

φ_k : not orthogonal

$$I = \sum \tilde{c}_j H_{jk} c_k - E \sum_{j,k} c_k \Delta_{jk} c_k$$

$$\Delta_{jk} = \int \tilde{\varphi}_j \varphi_k \, dq$$

$$\| H_{jk} - E \Delta_{jk} \| = 0.$$

$$\sum_{k=1}^{n} H_{jk} c_k = E \sum_k \Delta_{jk} c_k$$

The simultaneous equations (1) have the same form as those which appeared in perturbation theory, but the choice of $\varphi_1, \varphi_2 \cdots \varphi_n$, i.e. we have much wider the solution tends to $n \to \infty$, we have the exact solution.

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Variation Method for excited states

$$\psi = \sum_{i=0}^{\infty} c_i \psi_i$$

$$\bar{H} = \sum_{i=0}^{\infty} E_i |c_i|^2$$

Additional Condition:

$$\int \tilde{\psi}_0 \psi \, dq = 0.$$

$$c_0 = 0$$

or

$$\bar{H} = \sum_{i=1}^{\infty} E_i |c_i|^2 \geq E_1 \sum_{i=1}^{\infty} |c_i|^2 \geq E_1$$

Minimum of $\bar{H}$ is E_1 for

$c_0 = 0$, $c_1 = 1$, $c_2 = 0$, ...

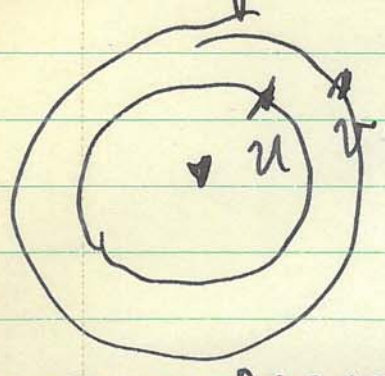
If the eigenfunction of the ground state φ_0 is ~~approximated~~ sufficiently well known, say by φ_0, then

$$\psi' = \psi - \varphi_0 \int \tilde{\varphi}_0 \psi \, dq$$

is orthogonal to φ_0. Thus, by applying the variation method to ~~the trial function~~ ψ' ~~of the~~ with the trial function ψ, we can compute the upper limit of the lowest excited state.

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Example: Excited states of He atom



$U_1 = u(r_1)\,v(r_2)$

$U_2 = v(r_1)\,u(r_2)$

$\int \tilde{u}(r_1)\,v(r_1)\,dV_1 = 0$

First Approximation:

$\psi \cong c_1 U_1 + c_2 U_2$

$$H = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) + \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}}$$

$$H_{11}c_1 + H_{12}c_2 = E c_1$$
$$H_{21}c_1 + H_{22}c_2 = E c_2$$
$$H_{12} = H_{21}, \quad H_{11} = H_{22}$$
$$E = H_{11} \pm H_{12} \qquad c_1 = \pm c_2$$

$\psi_s \chi_a$
$\psi_a \chi_s$

Second Approximation:

2^3S, 2^1S. $\longrightarrow$ (1S)(2S).

$$u_0(r) = \sqrt{\frac{Z_1^3}{\pi a_0^3}}\, e^{-Z_1 r/a_0}$$

$$v_0(r) = \sqrt{\frac{Z_2^3}{2\pi a_0^3}}\left(1 - \frac{Z_2 r}{2a_0}\right) e^{-Z_2 r/2a_0}$$

$\left(\frac{Z}{2a_0}\right)^{3/2}\frac{1}{\pi}$

2, Z_a ... parameters.

Such a procedure does not give good results.

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$$\psi_{nlm} = N_{nlm} e^{-\frac{r}{r_0}} \left(\frac{2r}{r_0}\right)^l L_{n+l}^{2l+1}\left(\frac{2r}{r_0}\right) P_l^m(\cos\theta)$$

$$\times e^{im\varphi}$$

$n=2$: $r_0 = \frac{2a_0}{Z}$ $x = \frac{2r}{r_0} = \frac{Zr}{a_0}$

$l=0$; $L_2^1(x) = \frac{d}{dx}\left(e^x \frac{d^2}{dx^2}(x^2 e^{-x})\right)$

$= \frac{d}{dx}\left(e^x \frac{d}{dx}(2x - x^2)e^{-x}\right) = \frac{d}{dx}(2 - 2x - 2x + x^2)$

$= -4\left(1 - \frac{x}{2}\right) = -4\left(1 - \frac{2r}{2a_0}\right)$

$$N_{200} = N_{\substack{n=2\\l=0\\m=0}} = \sqrt{\left(\frac{Z}{a_0}\right)^3 \cdot \frac{1}{4\cdot 8} \cdot \frac{1}{4\pi}}$$

$$= \sqrt{\left(\frac{Z}{2a_0}\right)^3 \cdot \frac{1}{\pi} \cdot \frac{1}{4}}.$$

$$\psi_{200} = \sqrt{\left(\frac{Z}{2a_0}\right)^3 \frac{1}{\pi}}\, e^{-\frac{Zr}{2a_0}}\left(1 - \frac{Zr}{2a_0}\right)$$

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l (x^2-1)^l}{dx^l}$$

$l=0$: $P_0(x) = 1$

$l=1$: $P_1(x) = \frac{1}{2} 2x = x$.

$P_1^0(x) = x$ $\quad P_1^1(x) = (1-x^2)^{\frac{1}{2}}$.

$(\sin\theta\, e^{-i\varphi},\ \cos\theta,\ e^{i\varphi})$

$$N_{210} = \sqrt{\left(\frac{Z}{a_0}\right)^3 \frac{1}{4\cdot(6)^3} \cdot \frac{3}{4\pi}} \cdot =$$

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$h_3^3(x) = -6.$

$$\psi_{210} = \sqrt{\left(\frac{Z}{a_0}\right)^3 \frac{1}{2\pi}} \cdot \left(\frac{Zr}{4a_0}\right) e^{-\frac{Zr}{2a_0}} \cos\theta$$

$$\psi_{21,\pm1} = \sqrt{\left(\frac{Z}{a_0}\right)^3 \frac{1}{2\pi}} \cdot \left(\frac{Zr}{4a_0}\right) e^{-\frac{Zr}{2a_0}} \frac{\sin\theta}{\sqrt{2}} e^{\pm i\varphi}$$

$$\psi_{21\,\pm1} = \sqrt{\left(\frac{Z}{a_0}\right)^3 \frac{1}{2\pi}} \left(\frac{Zr}{4a_0}\right) e^{-\frac{Zr}{2a_0}} \frac{\sin\theta}{\sqrt{2}} e^{i\varphi}$$

$v_{210} =$ 〃 $\cos\theta$

$v_{21,-1} =$ 〃 $\frac{\sin\theta}{\sqrt{2}} e^{-i\varphi}$

$v_{211} = v_1(r) \frac{\sin\theta}{\sqrt{2}} e^{i\varphi}$

$v_{210} = v_1(r) \cos\theta$

$v_{21,-1} = v_1(r) \frac{\sin\theta}{\sqrt{2}} e^{-i\varphi}$

$$\begin{cases} U_{+1} = v_0(r_1) v_1(r_2) \frac{\sin\theta_2}{\sqrt{2}} e^{i\varphi_2} \pm v_0(r_2) v_1(r_1) \frac{\sin\theta_1}{\sqrt{2}} e^{i\varphi_1} \\ U_0 = v_0(r_1) v_1(r_2) \cos\theta_2 \pm v_0(r_2) v_1(r_1) \cos\theta_1 \\ U_{-1} = v_0(r_1) v_1(r_2) \frac{\sin\theta_2}{\sqrt{2}} e^{-i\varphi_2} \pm v_0(r_2) v_1(r_1) \frac{\sin\theta_1}{\sqrt{2}} e^{-i\varphi_1} \end{cases}$$

$Z \to Z_1, Z_2$

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Hartree Approximation
(Method of Self-Consistent Field
for many electron system)

$$H = H_0 + H'$$

$$H_0 = -\frac{\hbar^2}{2m}\sum_{k=1}^{n}\Delta_k + V(r_k)$$

$$V(r_k) = -\frac{Ze^2}{r_k}$$

$$H' = \sum_{k<l}\frac{e^2}{r_{kl}}$$

ground state:

$$\overline{H} = \int\cdots\int \tilde{\psi} H \psi \, dv_1 \cdots dv_n$$

$$\delta \int\cdots\int \tilde{\psi}(H-E)\psi \, dv_1 \cdots dv_n = 0$$

~~$\overline{H} =$~~ $\psi = u_1(r_1)u_2(r_2)\cdots u_n(r_n)$

conditions $\int \tilde{u}_k(r_k) u_k(r_k) dv_k = 1 \qquad k = 1, 2, \cdots n$

$$\overline{H} = \sum_k \int \tilde{u}_k\left(-\frac{\hbar^2}{2m}\Delta_k - \frac{Ze^2}{r_k}\right)u_k \, dv_k + \sum_{k<l}\int\int \tilde{u}_k(r_k)\tilde{u}_l(r_l)\frac{e^2}{r_{kl}}u_k(r_k)u_l(r_l) \times dv_k\, dv_l$$

$$\delta\overline{H} - \sum_k W_k \delta\left(\int \tilde{u}_k u_k dv_k\right) = 0$$

$$\left(-\frac{\hbar^2}{2m}\Delta_k - \frac{Ze^2}{r_k}\right)u_k + \sum_{l\neq k}\left(\int \tilde{u}_l(r_l)u_l(r_l)\frac{e^2}{r_{kl}}dv_l\right)\cdot u_k = W_k u_k$$

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Thus, the minimum value of $\overline{H}$ under the condition that ~~$\psi = u$~~ $\psi = u_1 u_2 \cdots u_n$ with u_k normalized is obtained by solving the set of equations ~~with~~ each for one electron on which ~~the~~ ~~all the~~ electrostatic repulsion of all ~~other~~ electron is exerted as if the charge distribution of the k-th electron is given by $\tilde{u}_k u_k$. In other words, the effect ~~of the~~ on one electron of the rest is approximated by the self-consistent field.

Now, we start from a set of trial functions $u_1^{(0)} \cdots u_n^{(0)}$, and insert them in the electronic term and solve the eq. The solutions $u_1^{(1)} \cdots u_n^{(1)}$ is, in general, different from $u_1^{(0)} \cdots u_n^{(0)}$. Then, start all over again from $u_1^{(1)} \cdots u_n^{(1)}$. If the trial functions are suitable, the difference between $u_k^{(n)}$ and $u_k^{(n-1)}$ will be smaller and smaller and we finally arrive at a set of self-consistent solutions.

We may take advantage of the shell structure of the atom and assume the same central field for all electrons in the same shell in order to find the trial functions.

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Remark: Notice that

$$\sum_{k=1}^{n} W_k = \sum_k \int \tilde{u}_k \left(-\frac{\hbar^2}{2m}\Delta_k - \frac{Ze^2}{r_k}\right) u_k \, dv_k$$
$$+ 2\sum_{k<l} \iint \tilde{u}_k(r_k) u_k(r_k) \frac{e^2}{r_{kl}} \tilde{u}_l(r_l) u_l(r_l) \times dv_k \, dv_l$$

Total energy

$$E = \sum_{k=1}^{n} W_k - \sum_{k<l} \iint \tilde{u}_k(r_k) u_k(r_k) \frac{e^2}{r_{kl}} \times \tilde{u}_l(r_l) u_l(r_l) \, dv_k \, dv_l$$

Example:

Ground state of helium atom

0-th approximation

$u \simeq u_0$: hydrogen-like eigenfn

$$\left(-\frac{\hbar^2}{2m}\Delta_1 - E_0 - \frac{2e^2}{r_1}\right) u_0(r_1) = 0$$

1st approximation

$$\left(-\frac{\hbar^2}{2m}\Delta_1 - E_1 - \frac{2e^2}{r_1} + \int \frac{e^2}{r_{12}} u_0^2(r_2)\, dv_2\right)$$
$$\times u_1(r_1) = 0$$

. . . .

$$\left(-\frac{\hbar^2}{2m}\Delta_1 - E_{co} - \frac{2e^2}{r_1} + \int \frac{e^2}{r_{12}} u_{co}^2(r_2)\, dv_2\right)$$
$$u_{co}(r_1) = 0$$

Ionization potential

$$-J_{theor.} = 2E_{co} - \int u^2(r_1) \frac{e^2}{r_{12}} u^2(r_2)\, dv_1 dv_2 - E_0$$
$$= \left\{2 \times 4(-1.835) - 2.064 + 4\right\}\left(\frac{e^2}{2a_0}\right)$$

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$$= -1.734\left(\frac{e^2}{2a_0}\right)$$

$$J_{exp} = 1.810\left(\frac{e^2}{2a_0}\right)$$

$$(\sim 24.4\ eV)$$

Problem: Show that

$$-J_{theor.} = E_{\infty} + \int \frac{e^2}{r_{12}} u^2(r_2)\, dv_1 dv_2 \times \left(\frac{u_0(r_1)\, u_1(r_1)}{\int u_0(r_1)\, u_1(r_1)\, dv_1} - \frac{u_1^2(r_1)}{\int u^2(r_1)\, dv_1} \right)$$

or

$$-J_{theor.} \geq E_{\infty}$$

Actually

$$-E_{\infty} - J_{theor.} = 1.835 - 1.734$$

$$= 0.101\left(\frac{e^2}{2a_0}\right)$$

(about 5% of E_{∞})

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Remark: Notice that

$$\sum_{k=1}^{n} W_k = \sum_k \int \tilde{u}_k \left(-\frac{\hbar^2}{2m}\Delta_k - \frac{Ze^2}{r_k}\right) u_k \, dv_k + 2\sum_{k<l} \iint \tilde{u}_l(r_l)\, u_l(r_l)\, \frac{e^2}{r_{kl}}\, \tilde{u}_k(r_k)\, u_k(r_k)\, dv_k\, dv_l$$

is not equal to the total energy E, because the electronic repulsion is counted twice.

$$E = \sum_{k=1}^{n} W_k - \sum_{k<l} \iint \tilde{u}_l(r_l)\, u_l(r_l)\, \frac{e^2}{r_{kl}}\, \tilde{u}_k(r_k)\, u_k(r_k)\, dv_k\, dv_l$$

ground state of Helium atom

$$\left(-\frac{\hbar^2}{2m}\Delta_1 - E_0 - \frac{Ze^2}{r_1} + \int \frac{e^2}{r_{12}} u_1^2(r_2)\, dv_2\right) u(r_1) = 0$$

0-th appr. $E = 2E_0 - \int u^2(r_1)\frac{e^2}{r_{12}} u^2(r_2)\, dv_1\, dv_2$

$u = u_0$: hydrogen like eigenfunction

u_0: 1st. appr.

$$\left(-\frac{\hbar^2}{2m}\Delta_1 - E_1 - \frac{Ze^2}{r_1} + \int \frac{e^2}{r_{12}} u_0^2(r_2)\, dv_2\right) u_1(r_1) = 0$$

$$(E_1 - E_0) = \int \frac{e^2}{r_{12}} u_0^2(r_2)\, u_0(r_1)\, u_1(r_1)\, dv_1 dv_2$$

$\int u_0(r_1) u_1(r_1)\, dv_1$

Ionisation potential J.

$$-J = E - E_0 = E_1 + (E_1 - E_0) - \int u_1^2(r_1)\frac{e^2}{r_{12}} u_1^2(r_2)\, dv_1 dv_2$$

$$\approx E_1 + \int \frac{e^2}{r_{12}} dv_2 \left\{ u_1(r_1) \left[\frac{\int u_0^2(r_2)\, dv_2}{\int u_0 u_1\, dv_2} u_0(r_1) - \frac{\int u_1^2(r_2)\, dv_2}{\int u_1^2\, dv_2} u_1(r_1) \right] \right.$$

$$\approx E_1 + \int \frac{e^2}{r_{12}} dv_1\, u_1^2(r_1) \left\{ \frac{\int u_0 u_1\, dv}{\int u_0 u}\right.$$

(continued)

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Hartree-Fock Approximation

(Slater, P.R. 81 (1951), 385

$$\Psi = \frac{1}{\sqrt{n!}} \begin{vmatrix} u_1(x_1) & \cdots & u_1(x_n) \\ \vdots & & \vdots \\ u_n(x_1) & \cdots & u_n(x_n) \end{vmatrix}$$

$u_i(x_k)$ are normalized and ~~$u_i(x_k)$ can be assumed to be~~ orthogonal. This assumption does not mean essential any restriction other than that Ψ has a determinant form. x_k: coordinates, spin in z-direction.

Reason: $u_1(x_1)$: normalized

$$\begin{vmatrix} u_1(x_1) & \cdots & u_1(x_n) \\ u_2(x_2) - \int \tilde{u}_1 u_2 u_1(x_1) & & u_2(x_n) - \int \tilde{u}_1 u_2 u_1(x_n) \\ u_3(x_1) & & u_3(x_n) \\ \vdots & & \vdots \\ u_n(x_1) & & u_n(x_n) \end{vmatrix}$$

$$\propto \begin{vmatrix} u_1(x_1) & \cdots & u_1(x_n) \\ u_2'(x_1) & \cdots & u_2'(x_n) \\ u_3 - (\tilde{u}_1 u_3) u_1 - (\tilde{u}_2' u_3) u_2' & \cdots & \cdots \\ \vdots & & \vdots \end{vmatrix}$$

u_2': orthogonal to u_1 and normalized

u_3': orthogonal and normalized

etc.

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$$\overline{H} = \int \tilde{\Psi} H \Psi \, dx_1 \cdots dx_n$$

$\sigma_z, x_k p_k z_k, \sigma_x \sigma_y, p_{kx} p_{ky} p_{kz}$

$$H = \sum_{k=1}^{n} H(x_k, p_k) + \sum_{k<l} V(x_k, x_l)$$

$$= \sum_{k=1}^{n} H_k + \sum_{k<l} V_{kl} \qquad V_{kl} = \frac{e^2}{r_{kl}}$$

$$\overline{H_k} = \int \tilde{\Psi} H_k \Psi \, dx_1 \cdots dx_n$$

$$= \frac{1}{n!} \sum_{k} \int \tilde{u}_1(x_k) H_k u_1(x_k) \, dx_k \cdot (n-1)!$$

$$+ \frac{1}{n!} \int \tilde{u}_2(x_k) H_k u_2(x_k) \, dx_k \, (n-1)!$$

$$+ \cdots$$

$$= \frac{1}{n} \sum_{r=1}^{n} \tilde{u}_r(x_k) H_k u_r(x_k) \, dx_k$$

$$\sum_{k=1}^{n} \overline{H_k} = \frac{1}{n} \sum_{k=1}^{n} \sum_{r=1}^{n} \tilde{u}_r(x_k) H_k u_r(x_k) dx_k$$

$$\overline{V_{kl}} = \frac{1}{n!} \iint \tilde{u}_1(x_k) \tilde{u}_2(x_l) V_{kl} u_1(x_k) u_2(x_l)$$
$$dx_k \, dx_l \, (n-2)!$$
$$+ \frac{1}{n!} \iint \tilde{u}_1(x_k) \tilde{u}_3(x_l) V_{kl} u_1(x_k) u_3(x_l)$$
$$dx_k \, dx_l \, (n-2)!$$
$$+ \cdots$$
$$- \frac{1}{n!} \iint \tilde{u}_2(x_k) \tilde{u}_2(x_l) V_{kl} u_2(x_k) u_1(x_l)$$
$$dx_k \, dx_l \, (n-2)!$$
$$- \cdots$$

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$$\overline{V_{kl}} = \frac{1}{n(n-1)} \sum_{r \neq s} \iint \tilde{u}_r(x_k) \tilde{u}_s(x_l) V_{kl} u_r(x_k) \times u_s(x_l)\, dx_k\, dx_l$$

$$- \frac{1}{n(n-1)} \sum_{r \neq s} \iint \tilde{u}_r(x_k) \tilde{u}_s(x_l) V_{kl} \times u_s(x_k) u_r(x_l)\, dx_k\, dx_l$$

$$\sum_{kl} \overline{V_{kl}} = \frac{1}{2} \sum_{r \neq s} \cdots \qquad \sim \frac{1}{2} \sum_{r \neq s} \cdots$$

$$\overline{H} = \sum_k H_k + \sum_{k<l} \overline{V_{kl}}$$

$$\delta \overline{H} = 0 \qquad \delta \int \tilde{u}_{k_r}(x_k) u_{k_s}(x_k)\, dx_k = 0$$

$$\delta \overline{H} - \delta \sum W_{k;r} \int \tilde{u}_r(x_k) u_s(x_k)\, dx_k = 0$$

$$\delta u_r(x_k): \quad \frac{1}{n} H_k u_r(x_k) + \frac{1}{n(n-1)} \sum_{l \neq k} \sum_{r<s} \int \tilde{u}_s(x_l) V_{kl} u_s(x_l)\, dx_l \cdot u_r(x_k)$$

$$- \frac{1}{n(n-1)} \sum_{l \neq k} \sum_{r<s} \int \tilde{u}_s(x_k) V_{kl} u_r(x_k)\, dx_l \cdot u_s(x_k) = W_{k,r} u_r(x_k)$$

$$= \frac{1}{n} W_{k,r} u_r(x_k) = \frac{1}{n} W_{k;r} u_r(x_k)$$

because the form of $u_r(x_k)$ is the same for all $x_1, x_2, \cdots x_n$.

$$\int \tilde{u}_r(x_k) u_s(x_k)\, dx_k = \delta_{rs}$$

$$\Sigma = \overline{H} - \frac{1}{n} W_{k;r,s} \int \tilde{u}_r(x_k) u_s(x_k)\, dx_k$$

$$W_{k,r} u_r(x_k) \to \sum_s W_{k_s} u_s(x_k)$$

$$W_{k,r} = \int \tilde{u}_r(x_k) H_k u_r(x_k)\, dx_k + \sum_{s \neq r} \int \tilde{u}_s(x_l) V_{kl} u_s(x_l)\, dx_l \cdot u_r(x_k) \equiv W^{(0)}_{k,r}$$

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$$H_k u_r(x_k^1) + \Big(\sum_{s\neq r}\int \tilde{u}_s(x_k^2) V_{kk}^{12} u_s(x_k^2)\,dx_k^2\Big)\cdot u_r(x_k^1)$$
$$- \Big(\sum_{s\neq r}\int \tilde{u}_s(x_k^2) V_{kk}^{12} u_r(x_k^2)\,dx_k^2\Big)\cdot u_s(x_k^1)$$
$$= W_{r,r}\, u_r(x_k^1) + \sum_{s\neq r} W_{r,s}\, u_s(x_k^1)$$

$$u_r(x_k) = a_r{}^\rho v_\rho(x_k)$$
$$v_\rho(x_k) = b_\rho{}^r u_r(x_k)$$
} orthogonal transf.

$$\sum_{r,s} \tilde{b}_\rho{}^r b_\sigma{}^s \delta_{rs} = \delta_{\rho\sigma}$$
$$\sum_r \tilde{b}_\rho{}^r b_\sigma{}^r = \delta_{\rho\sigma}$$
$$\sum_\rho \tilde{a}_r{}^\rho a_s{}^\rho = \delta_{rs}$$
$$\sum_\rho b_\rho{}^r a_r{}^\sigma = \delta_{\rho\sigma}$$
$$\sum a_r^\rho b_\rho{}^s = \delta_{rs}$$
$\Big\}\rightarrow b_\sigma{}^r = \tilde{a}_r{}^\sigma$

$$W_{k,rs} = \int \tilde{u}_s(x_k) H_k u_r(x_k)\,dx_k$$
$$= \int \tilde{u}_s(x_k) \Big[\int \tilde{u}_t(x_l) V_{kl} u_r(x_l)\,dx_l\Big] dx_k \qquad (s\neq r)$$
$$= W_{rs}^{(0)} - W_{rs}$$

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$$b_\rho^{\ r} \quad H_k a_r^{\ \sigma} v_{\rho\sigma}(x_k) + \sum_s \int \hat{a}_s^{\ \sigma} \tilde{v}_\sigma(x_l) V_{kl} a_s^{\ \tau} v_\tau(x_l) dx_l$$

$$\times a_r^{\ \omega} v_\omega - \sum_s \int \tilde{a}_s^{\ \sigma} \tilde{v}_\sigma(x_l) V_{kl} a_r^{\ \tau} v_\tau(x_l) dx_l$$

$$\times a_s^{\ \omega} v_\omega = W_{rs} a_s^{\ \sigma} v_\sigma$$

$$H_k v_\rho(x_k) + \sum_\sigma \int \tilde{v}_\sigma(x_l) V_{kl} v_\sigma(x_l) dx_l \cdot v_\rho(x_k)$$

$$- \sum_\sigma \int \tilde{v}_\sigma(x) V_{kl} v_\rho(x_l) dx_l \cdot v_\sigma(x_k)$$

$$= W_\rho v_\rho(x_k)$$

$$b_\rho^{\ r} W_{rs} a_s^{\ \sigma} = W_\rho \delta_{\rho\sigma}$$

$$\text{or} \quad \underline{W_{rs} a_s^{\ \sigma} = W_\rho a_r^{\ \rho\sigma}}$$

$$\| W_{rs} - W \delta_{\rho\sigma} \| = 0$$

$$W = W_1, W_2, \ldots W_n$$

$$\text{or} \quad \Psi = \| u_r(x_k) \| = \| a_r \rho \| \cdot \| v_\rho(x_k) \|$$

$$= e^{i\gamma} \| v_\rho(x_k) \| \quad \because \| a_r \rho \| = e^{i\gamma}$$

$$\| a_r \rho \| \cdot \| \tilde{a}_r \rho \| = 1 .$$

$$H_k(x_1, p_1) u_r(x_1) + V(x_1) u_r(x_1)$$

$$- \sum_s U_{rs}(x_1) u_s(x_1) = W_r u_r(x_1)$$

$$V(x_1) = \sum_s \int \tilde{u}_s(x_2) V_{12} u_s(x_2) dx_2$$

$$U_{rs}(x_1) = \int \tilde{u}_s(x_2) V_{12} u_r(x_2) dx_2$$

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$$U_r(x_1)\,u_s(x_1) = \sum_s \frac{\int \tilde{u}_s(x_2)\tilde{u}_r(x_1) V_{12} u_r(x_2) u_s(x_1)\,dx_2}{\tilde{u}_r(x_1) u_r(x_1)}\, u_s(x_1)$$

$$= U_r(x_1, x_2)\, u_r(x_1)$$

$$U_r(x_1, x_2) = \sum_s \frac{\int \tilde{u}_s(x_2)\tilde{u}_r(x_1) V_{12} u_r(x_2) u_s(x_1)\,dx_2}{\tilde{u}_r(x_1) u_r(x_1)}$$

Exchange charge density

$$\rho_r(x_2; x_1) = \sum_s \frac{\tilde{u}_s(x_2)\,\tilde{u}_r(x_1)\, u_r(x_2) u_s(x_1)}{\tilde{u}_r(x_1) u_r(x_1)}$$

(if V_{12} is independent of spin)
comes only from the particle with parallel spin (parallel to particle 2)

$$\int \rho_r(x_2; x_1)\,dx_2 = 1$$

$$U_r(x_1, x_2) \simeq \int \rho_r(x_2; x_1) V_{12}\,dx_2$$

$u_r(x_1)$

$\rho_r(x_2; x_1)$

x_2

$V(x_1)$: charge density including the particle 1 itself.

$$u_r(x_1) \simeq \delta(x_1) \longrightarrow$$

$$\rho_r(x_2, x_1) \simeq \sum_s \tilde{u}_s(x_2) \cdot \delta(x_2)\, u_s(x_1)/\delta(x_1)$$

$= 0$ x_1 in V, x_2 not in V

$= \infty$ x_1 not in V, x_2 in V

$= \sum_s \tilde{u}_s(x_2) u_s(x_1)$ x_1, x_2 not in V

$= \sum_s \tilde{u}_s(x_2) u_s(x_1)$ x_1, x_2 in V

Correlation

x_1

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$$W_r = \int \tilde{u}_r(x_1) H(x_1, p_1) u_r(x_1)\, dx_1$$
$$+ \int \tilde{u}_r V(x_1) u_r\, dx_1 - \sum_s \int \tilde{u}_r(x_1) U_{rs}(x_1) u_s(x_1)\, dx_1$$
$$\int \tilde{u}_s(x_1) H(x_1, p_1) u_r(x_1)\, dx_1$$
$$+ \int \tilde{u}_s V(x_1) u_r\, dx_1 - \sum_t \int \tilde{u}_s(x_1) U_{rt}(x_1) u_t(x_1)\, dx_1$$
$$= W_r \int \tilde{u}_s u_r\, dx_1$$

$\int u_t(x_2) u_r(x_2)$ → V_{12}

$$\int \tilde{u}_s H(x_1, p_1) u_r(x_1)\, dx_1$$
$$+ \int \tilde{u}_s V(x_1) u_r\, dx_1 - \sum_\tau \int \tilde{u}_t(x_1) U_{ts} u_r(x_1)\, dx_1$$

$\int \tilde{u}_s(x_2) V_{12} u_t(x_2)$

$$= W_s \int \tilde{u}_s u_r\, dx_1$$

or $\int \tilde{u}_s u_r\, dx_1 = \delta_{rs}$.

(consistency)

$$H = \sum_{r=1}^{n} \int \tilde{u}_r(x_1) H(x_1, p_1) u_r(x_1)\, dx_1$$
$$+ \sum_{(r<s)}^{n} \iint \tilde{u}_r(x_1) \tilde{u}_s(x_2) V_{12} u_r(x_1) u_s(x_2)\, dx_1 dx_2$$
$$- \sum_{r<s}^{r,s=1,n} \iint \tilde{u}_r(x_1) \tilde{u}_s(x_2) V_{12} u_s(x_1) u_r(x_2)\, dx_1 dx_2$$

$$\sum_{r=1}^{n} W_r = \sum_{r,s=1}^{n} \int \tilde{u}_r(x_1) H(x_1, p_1) u_r(x_1)\, dx_1$$
$$+ \sum_{r,s=1}^{n} \tilde{u}_r(x_1) \tilde{u}_s(x_2) V_{12} u_r(x_1) u_s(x_2)\, dx_1 dx_2$$
$$- \sum_{r,s=1}^{n} \tilde{u}_r(x_1) \tilde{u}_s(x_2) V_{12} u_s(x_1) u_r(x_2)\, dx_1 dx_2$$

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$$\bar{H} = \sum_{r=1}^{n} W_r - \sum_{r<s} \iint \tilde{u}_r(x_1)\tilde{u}_s(x_2) \times V_{12}\, u_r(x_1) u_s(x_2)\, dx_1 dx_2 + \sum_{r<s} \iint \tilde{u}_r(x_1)\tilde{u}_s(x_2)\, V_{12} \times u_s(x_1) u_r(x_2)\, dx_1 dx_2$$

$\bar{H}$: expectation value of the energy.

or the minimum value of $\bar{H}$ under the above conditions, but $\bar{H}$ is larger than the true energy value E.

$\bar{H} > E$.

$\bar{H} = E$ only if

$H\Psi = E\Psi$.

or Ψ is the true solution of Schrödinger equation.

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Hartree-Fock Model (1)

$$\begin{vmatrix} u_1(x_1) & u_1(x_2) & \cdots & u_{N-1}(x_N) \\ u_2(x_1) & u_2(x_2) & \cdots & u_2(x_N) \\ \vdots & \vdots & & \vdots \\ u_N(x_1) & u_N(x_2) & \cdots & u_N(x_N) \end{vmatrix}$$

$$= \begin{vmatrix} u_1(x_1) & , & , \\ u_2(x_1) - (\tilde{u}_1 u_2) u_1(x_1) & , & , \\ \vdots & , & , \end{vmatrix}$$

$$\ast\quad u_2' = u_2 - (\tilde{u}_1 u_2) u_1$$

$$(\tilde{u}_1, u_2') = (\tilde{u}_1, u_2) - (\tilde{u}_1, u_2)\,\tilde{u}_1, u_1$$

$$= 0 \qquad \text{if } (\tilde{u}_1, u_1) = 1.$$

One can always assume that $u_1, u_2, \cdots u_N$ are orthogonal and normalized.

$$u_n = \sum_{\nu=1}^{N} C_{n\nu} v_\nu \qquad n = 1, 2, \cdots N$$

$C_{n\nu}$: unitary transformation.

$$\| u_n(x_k) \| = \| C_{n\nu} \| \, \| v_\nu(x_k) \|$$

One can choose any set of N functions which can be obtained from the original set by an arbitrary unitary transformation.

ortho-normal

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Example. ~~Fermi~~ Equivalence of Fermi gas model and liquid drop model: Consider N neutrons with parallel spin

$$\psi_\nu = \frac{1}{\sqrt{L}} e^{2\pi i \nu x/L}$$

$$u_n = \sum_{\nu=0}^{N-1} c_{n\nu}^* \frac{e^{2\pi i \nu x/L}}{\sqrt{L}}$$

$$c_{n\nu} = \frac{1}{\sqrt{N}} e^{-2\pi i n\nu/N}$$

$n = 0, 1, 2, \cdots N-1$

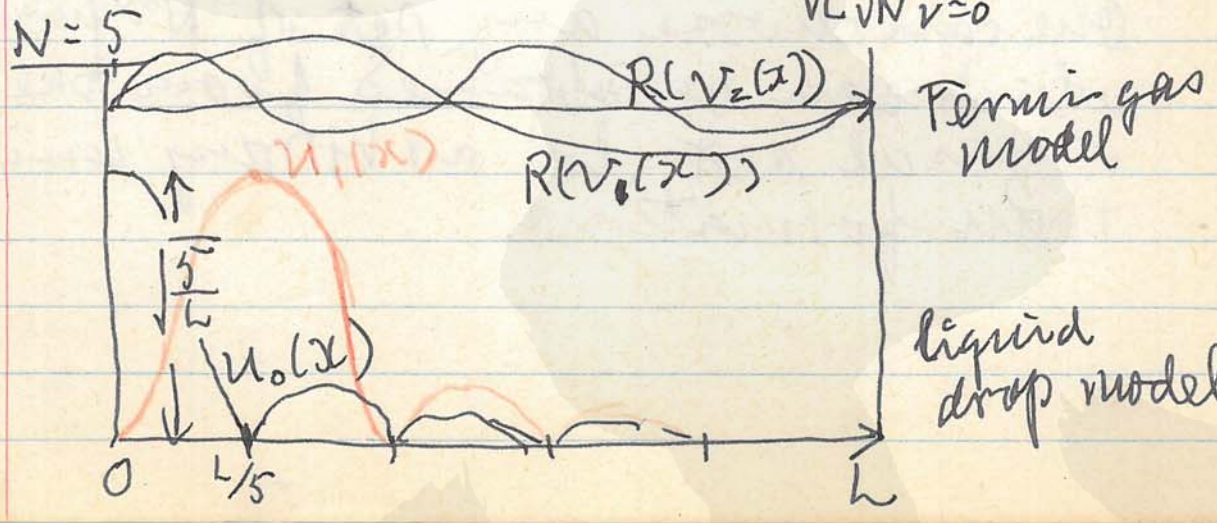
(or $n = 1/2, 3/2, \cdots N-1/2$)

$$\sum_{\nu=0}^{N-1} c_{m\nu}^* c_{n\nu} = \frac{1}{N} \sum_{\nu=0}^{N-1} e^{2\pi i \nu(n-m)/N} = \delta_{mn}$$

$$u_0(x) = \sum_{\nu=0}^{N-1} \frac{e^{2\pi i \nu x/L}}{\sqrt{L}\sqrt{N}}.$$

$x = 0$: $u_0(0) = \frac{\sqrt{N}}{\sqrt{L}}$

$x = L/N$: $u_0(L/N) = \frac{1}{\sqrt{L}\sqrt{N}} \sum_{\nu=0}^{N-1} e^{2\pi i \nu/N} = 0.$



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$$u_n(x) \approx \sum_{\nu=0}^{N-1} e^{\frac{2\pi i \nu n}{L}(x - nL/N)} / \sqrt{L}\sqrt{N}$$

$$u_n(nL/N) = \frac{\sqrt{N}}{\sqrt{L}}$$

$$u_n((n\pm1)L/N) \approx 0$$

Remark:

$$x^{N-1} = \prod_{n=0}^{N-1}(x - \omega_n)$$

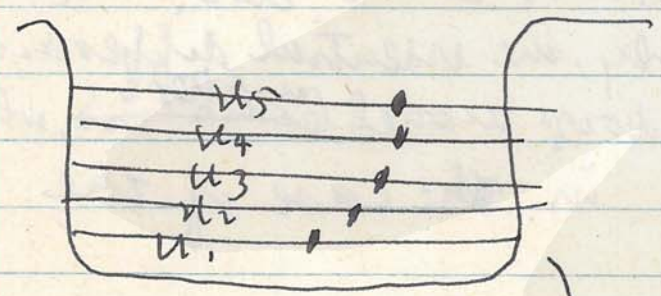
$$N-1\ \omega_n = {}_{N-1}e^{2\pi i n/N}$$

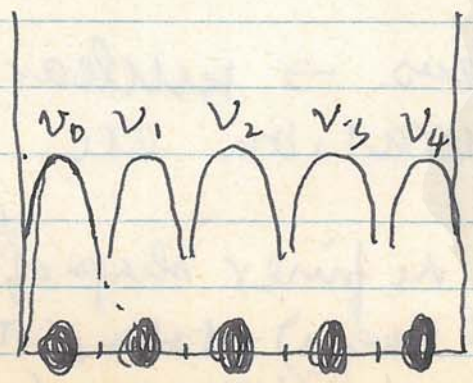
$$\sum_{n=0} \omega_n = \sum_{\nu=0} e^{2\pi i \nu/N} \approx 0$$

$$\sum_{\mu\neq\nu} \omega_\mu \omega_\nu = 0$$

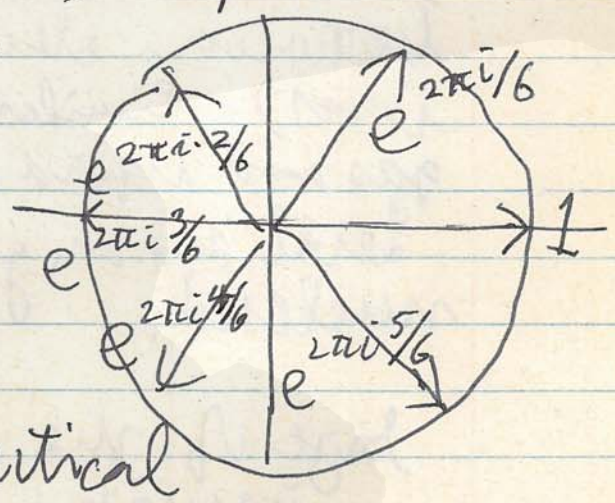
$$\sum_\nu (\omega_\nu^2) = \left(\sum_\nu \omega_\nu\right)^2 - \sum_{\mu\neq\nu} \omega_\mu \omega_\nu = 0$$

$$\sum_\nu (\omega_\nu^3) = \left(\sum_\nu \omega_\nu\right)^3 - 3\sum(\omega_\mu \omega_\nu^2) = 0$$





identical



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Metal ~~Electrons~~ in Metal

The difference between free electron gas ~~pi~~ model and bound electron model is essential, only if we take into account the fine shape of eigenfunction over a distance ~~of the order~~ smaller than the interatomic distance. Conductivity in bound electron model ~~can~~ comes ~~from the overlapping of and other effects~~.

~~eigenfunctions~~

~~If the introduce~~ does not come of the metal ~~cannot~~ from the shape of the eigenfunctions, but due to the band structure of electron levels, which appears only when we take into account the interaction between electrons and atoms (or ions). Similarly, the essential difference between gas and liquid drop model (~~case of~~ interior, when * Level spacing in the case of the nucleus.

Size of the nucleus. → nuclear forces intensity, saturation etc.

* we are interested in the finer shape of each of the eigenfunctions (or over-all wave fn) ~~at~~ at a distance smaller than inter-nucleon (behavior) distances. (~ fm/mc)

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$$\begin{vmatrix} u_1(x_1) & \cdots & u_1(x_{n+1}) \\ \vdots & & \vdots \\ u_{n-1}(x_1) & \cdots & u_{n-1}(x_{n+1}) \\ u_n(x_1) & \cdots & u_n(x_{n+1}) \end{vmatrix} + C_n^{n+1} \begin{vmatrix} u_1(x_1) & \cdots \\ \vdots & \\ u_{n-1}(x_1) & \\ u_{n+1}(x_1) & \end{vmatrix}$$

$$\mp C_{n-1}^{n+1} \begin{vmatrix} u_1(x_1) & \cdots \\ \vdots & \\ u_{n+1}(x_1) & \\ u_n(x_1) & \end{vmatrix} + \cdots$$

$$= \begin{vmatrix} u_1(x_1) & \cdots \\ \vdots & \\ u_{n-1}(x_1) & \\ u_n(x_1) + C_n^{n+1} u_{n+1}(x_1) & \end{vmatrix} + \begin{vmatrix} u_1(x_1) & \cdots \\ \vdots & \\ C_{n-1}^{n+1} u_{n+1}(x_1) & \\ u_n(x_1) + C_n^{n+1} u_{n+1}(x_1) & \end{vmatrix}$$

$$+ \cdots$$

$$= \begin{vmatrix} u_1 & \cdots \\ \vdots & \\ u_{n-1} + C_{n-1}^{n+1} u_{n+1} & \\ u_n + C_n u_{n+1} & \end{vmatrix} + \cdots$$

$$= \begin{vmatrix} u_1 + C_1^{n+1} u_{n+1} & \cdots \\ \vdots & \\ u_{n-1} + C_{n-1}^{n+1} u_{n+1} & \\ u_n + C_n^{n+1} u_{n+1} & \end{vmatrix} + C_n^{n+2} \begin{vmatrix} u_1 & \cdots \\ \vdots & \\ u_{n-1} & \\ u_{n+2} & \end{vmatrix} + \cdots$$

at least two rows are different

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$$= \begin{vmatrix} u_1 + C_1 u_{n-1} \\ u_2 + C_2 u_{n-1} \\ \vdots \\ u_{n-1} + C_{n-1}^{n+1} u_{n+1} \\ u_n + C_n^{n+1} u_{n+1} \end{vmatrix} \begin{vmatrix} \\ \\ \\ \\ + C_n^{n+2} \end{vmatrix} \begin{vmatrix} u_1 + C_1 u_{n-1} \\ u_2 + C_2 u_{n-1} \\ \vdots \\ u_{n-1} \\ u_{n+2} \end{vmatrix}$$

↓ different

~~last two rows are different~~

$$+ \cdots$$

$$= \begin{vmatrix} u_1 + C_1 u_{n-1} & \cdots \\ u_2 + C_2 u_{n-1} & \cdots \\ \vdots & \\ u_{n-1} & \\ u_n + C_n^{n+1} u_{n+1} & \cdots \end{vmatrix} + \begin{vmatrix} u_1 + C_1 u_{n-1} \\ u_2 + C_2 u_{n-1} \\ \vdots \\ C_{n-1}^{n+1} u_{n+1} \\ u_n + C_n^{n+1} u_{n+1} \end{vmatrix}$$

$$+ \begin{vmatrix} u_1 & \\ u_2 & \\ \vdots & \cdots \\ u_{n-1} & \\ C_n^{n+2} u_{n+2} & \end{vmatrix} + \cdots$$

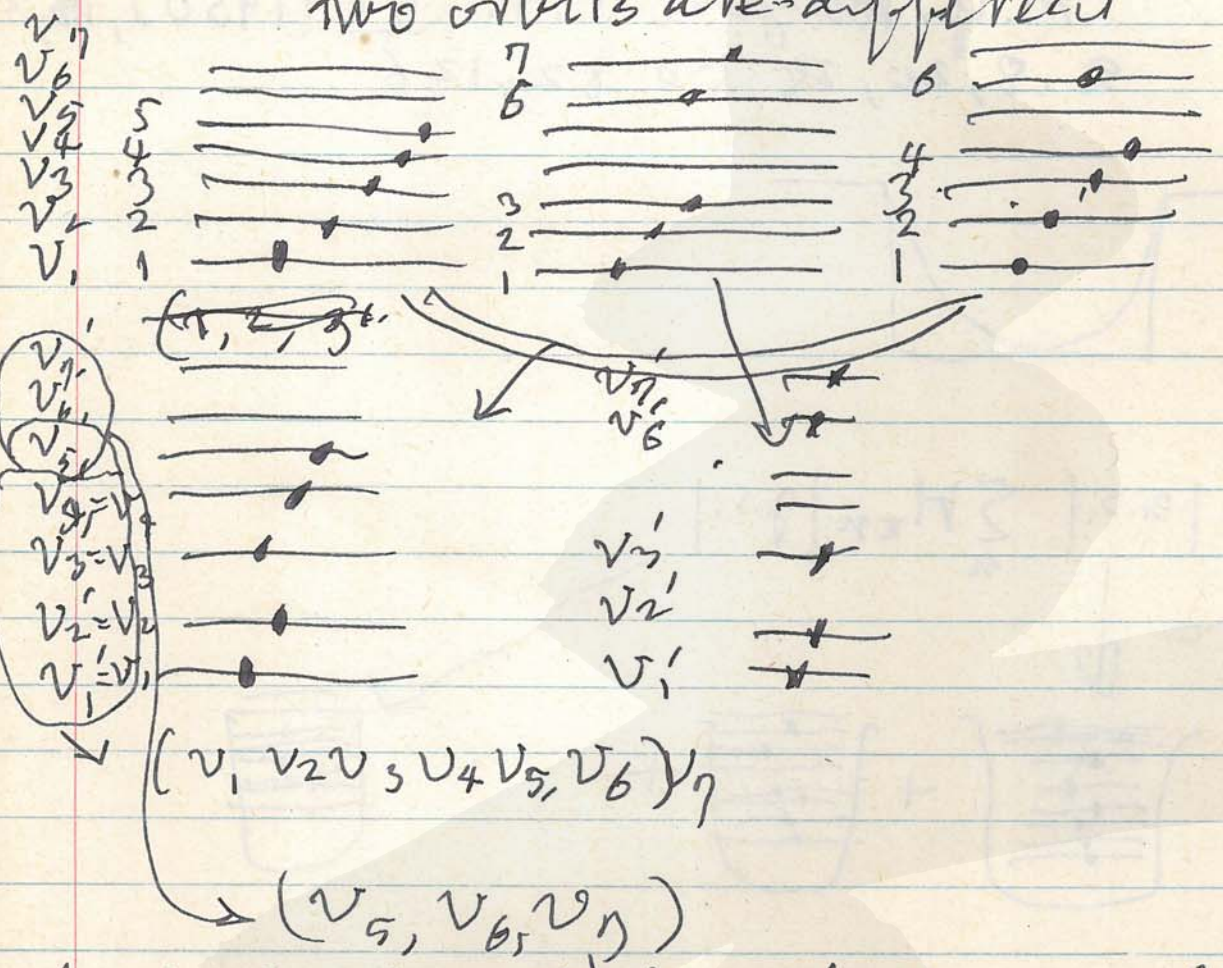
$$= \begin{vmatrix} u_1 + C_1 u_{n-1} \\ u_2 + C_2 u_{n-1} \\ \vdots \\ u_{n-1} \\ u_n + C_n^{n+1} u_{n+1} + C_n^{n+2} u_{n+2} \end{vmatrix} \begin{vmatrix} \\ \\ \\ \\ + \end{vmatrix} \begin{vmatrix} u_1 + C_1 u_{n-1} \\ u_2 + C_2 u_{n-1} \\ \vdots \\ C_{n-1}^{n+1} u_{n+1} \\ u_n + C_n^{n+1} u_{n+1} \end{vmatrix}$$

different

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$$\begin{vmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n-1} \\ v_n \end{vmatrix} + \begin{vmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n+1} \\ v_{n+2} \end{vmatrix} + \cdots$$

two orbits are different



1. Number of particles N is one less than the number of states M in closed shell.
→ individual orbit model

2. Number of particles N is two less than

state A = | | + state B = | | + ⋯
two orbits are changed

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1, Meson - Nucleus.

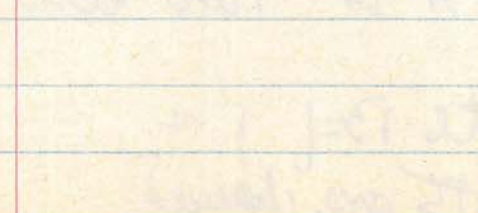
$\pi + A \rightarrow B$

two particle excitation

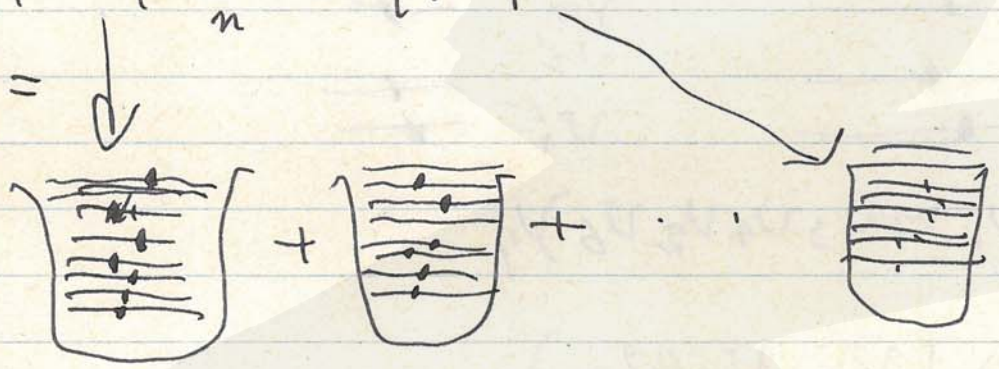
2, Shell structure

M. G. Mayer, P. R. 78 (1950), 16, 22

2, 8, 20, 28, 50, 82, 126



$|e.s.| \sum_n H_{\pi n} |g.s.|$



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Hartree Fock Approximation

Fock. Zs. f. Phys. 61 (1930), 126.

$$H = H_1 + H_2 - \frac{1}{r_{12}}$$

$$\iint \delta\tilde{\Psi}(H - E)\Psi \, dx_1 dx_2 = 0$$

$$\Psi = \psi(x_1)\psi(x_2)$$

$$H_1\psi(x_1) + \int \frac{|\psi(x_2)|^2}{r_{12}} dx_2 \cdot \psi(x_1) - E_0\psi(x_1) = 0$$

$$E_0 = E - \int \tilde{\psi}(x_2) H_2 \psi(x_2) dx_2$$

$$E = 2E_0 - \iint \frac{|\psi(x_2)|^2 |\psi(x_1)|^2}{r_{12}} dx_1 dx_2$$

$$H\psi_q(x) + [V - G_{qq}(x)]\psi_q(x) = W_q'\psi_q(x)$$

$$W_q = E - \sum_{i=1}^{N'} H_{ii} - \sum_{i>k=1}^{N''} W_{ik}$$

$$V = \sum_{k=1}^{N} G_{kkk}(x)$$

$$W_{ik} = \int (ik|G|ik) = \iint \frac{|\psi_i(x)|^2 |\psi_k(x')|^2}{r} \times dx\, dx$$

$$E = \sum_{i=1}^{N} H_{ii} + \sum_{i>k=1}^{N} W_{ik}$$

$$W_q' = H_{qq} + \sum_{i=1}^{N'} W_{iq}$$

$$\sum_{q=1}^{N} W_q' = 2E - \sum_{q=1}^{N} H_{qq}$$

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Dirac, Proc. Camb. Phil. Soc. 27 (1931)

$$\begin{vmatrix} (q_1|1) & \cdots & (q_1|n) \\ (q_2|1) & & \vdots \\ \vdots & & \\ (q_n|1) & & (q_n|n) \end{vmatrix}$$

$$(q'|\rho|q'') = \sum_r (q'|r)(r|q'')$$

invariant with respect to unitary transform

$$\begin{vmatrix} (q'|\rho|q') & (q'|\rho|q'') \\ (q''|\rho|q') & (q''|\rho|q'') \end{vmatrix}$$

probability of finding one el. at q', and one at q''.

$$\begin{vmatrix} (q'|\rho|q') & \cdots & (q'|\rho|q^{(r)}) \\ & & \\ (q^{(r)}|\rho|q') & \cdots & (q^{(r)}|\rho|q^{(r)}) \end{vmatrix}$$

probability of finding electrons at $q', q'', \ldots q^{(r)}$ simultaneously.

$r = 1, 2, \ldots n, n+1, \ldots$

$\rho^2 = \rho$ Hermitian.

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J.C. Slater, Hartree Fock method, P.R. 81 (1951), 385;
E.M. Corson, Perturbation Methods, 1951 (p.143~)

$$\bar{H} = \sum_{r=1}^{n} \int \tilde{u}_r(x_1) H(x_1, p_1) u_r(x_1) dx_1 + \sum_{r<s} \iint \tilde{u}_r(x_1)\tilde{u}_s(x_2) V(1,2) u_r(x_1) u_s(x_2) dx_1 dx_2 - \sum_{r<s} \iint \tilde{u}_r(x_1)\tilde{u}_s(x_2) V_{12} u_s(x_1) u_r(x_2) dx_1 dx_2$$

Supplementary conditions:

$$I_{rs} = \int \tilde{u}_r(x_1) u_s(x_1) dx_1 = \delta_{rs}$$

$$\delta \bar{H} - \sum_{r,s} W_{rs} \delta I_{rs} = 0$$

$\delta \tilde{u}_r(x_1)$:

$\tilde{u}_t(x_1)$: $H(1) u_r(x_1) + C(1) u_r(x_1) - \sum_s A_{rs}(1) u_s(x_1) = \sum_s W_{rs} u_s(x_1)$

$$C(1) = \sum_s \int \tilde{u}_s(2) V(1,2) u_s(2) dx_2$$

$$A_{rs}(1) = \int \tilde{u}_s(2) V(1,2) u_r(2) dx_2$$

$\int \tilde{u}_t(1) H(1) u_r(x_1) + \int \tilde{u}_t(x_1) C(1) u_r(x_1) - \sum_s \int \tilde{u}_t A_{rs} u_s = \sum_s W_{rs} \int \tilde{u}_t u_s$

$\int \tilde{u}_t H u_r + \int \tilde{u}_t C u_r - \sum_s \int \tilde{u}_s A_{st} u_r = \sum_s W_{st} \int \tilde{u}_s u_r$

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$$W_{rs} = W_r \delta_{rs}.$$

$$\sum_s^N \int \tilde{u}_s(x_2)\, V(1,2)\, u_r(x_2)\, dx_2 \cdot u_s(x_1)$$

$$= \sum_{s=1}^{N} \frac{\int \tilde{u}_r(x_1)\tilde{u}_s(x_2)\, V\, u_s(x_1)u_r(x_2)\, dx_1 dx_2}{\tilde{u}_r(x_1)u_r(x_1)} \Big) \cdot u_r(x_1)$$

$$\simeq \frac{\sum_r \sum_s \iint \tilde{u}_r(x_1)\tilde{u}_s(x_2)\, V\, u_s(x_1)u_r(x_2)\, dx_1 dx_2}{\sum_r \tilde{u}_r(x_1)u_r(x_1)} \Big) u_r(x_1)$$

∴ On the average, the probability that an electron at x_1 is in the state u_r is

$$\frac{u_r(x_1)u_r(x_1)}{\sum_s u_s(x_1)u_s(x_1)}$$

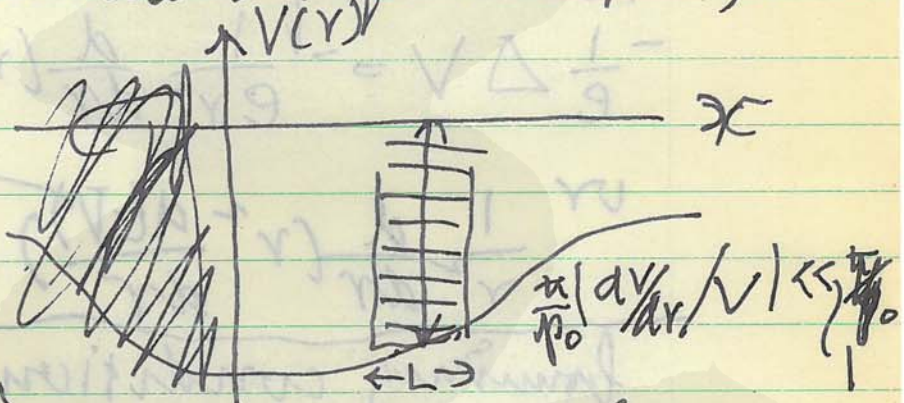
So one can take the weighted mean for as the effective potential acting on the electron at x_1 irrespective of the state $u_r\ (r = 1, 2 \cdots N)$

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Thomas-Fermi approximation

Hartree and H.F. approximations are already too complicated to have the clear insight into the general trend of atoms with large number of electrons. Thomas-Fermi method is less accurate, but much simpler and is a fairly good approxim. for heavier atoms.

According to exclusion principle, the states of the electron with the momentum $p \le p_0$ is occupied, up to a certain maximum value p_0, if the potential $V(r)$ acting on the electron is nearly constant over a region which ~~included~~ is large compared with $\hbar/p_0$.



If we take a cube L^3, the total number of occupied states is

$$2\left(\frac{L}{2\pi}\right)^3 \int_0^{p_0/\hbar} \int_0^{\pi} \int_0^{2\pi} k^2 dk \sin\theta d\theta d\varphi$$

$$= 2\left(\frac{L}{2\pi}\right)^3 4\pi \cdot \frac{1}{3}\left(\frac{p_0}{\hbar}\right)^3 \quad \left(\frac{d}{dr}(\log V) \ll p_0/\hbar\right.$$

$$= \frac{L^3 p_0^3}{\pi^2 \hbar^3}.$$

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Now, the max. energy $\frac{1}{2m}p_0^2$ must be, at most, equal to $-V(r)$, because otherwise the electron will escape from the atom. Thus the charge density at r due to all the bound electrons is

$$\rho(r) = \frac{(-2mV(r))^{3/2}}{3\pi^2\hbar^3}$$

$V(r) = V - V_0$

Poisson eq.:

$$-\frac{1}{e}\Delta V = -\frac{1}{er^2}\frac{d}{dr}\left(r^2\frac{dV}{dr}\right) = +4\pi e\rho$$

or

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d(-V)}{dr}\right) = \frac{4e^2(-2mV)^{3/2}}{3\pi\hbar^3}$$

boundary conditions:

$r \to 0 \quad V(r) \to -\frac{Ze^2}{r}$

$r \to \infty \quad rV(r) \to 0$

(for neutral atom)

T.F. approximation is better, if p_0 is very large, so that the average wave length is very short, whereas the $V(r)$ is finite. This is achieved in the limit $m \to \infty$ by keeping e^4m^3 constant. The electron density will be infinite accordingly, because the spacing of energy levels will be very dense.

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$$V(r) = -\frac{2e^2}{r}\chi(x)$$

$$r = bx$$

$$b = \frac{1}{2}\left(\frac{3\pi}{4}\right)^{2/3}\frac{\hbar^2}{me^2 Z^{1/3}} = \frac{0.885\, a_0}{Z^{1/3}}$$

$U(r)$

$$x^{1/2}\frac{d^2\chi}{dx^2} = \chi^{3/2}$$

$x = 0 : \chi = 1.$
$x = \infty : \chi = 0.$

The radius of the atom is proport. to $Z^{-1/3}$

Problem. Show that the radius of a sphere which encloses a fixed fraction, say $1/2$, of all the electron is proportional to $Z^{-1/3}$.

$$\rho(r) \propto V^{3/2} \propto \frac{Z^{3/2}\chi^{3/2}}{r^{3/2}} \qquad (cZ^{1/3}r)$$

$$\int_0^{r_0} Z^{3/2}\chi^{3/2}\, r^{1/2}\, dr \qquad r = \frac{x}{cZ^{1/3}}$$

$$\propto Z^{3/2}\cdot\frac{1}{Z^{1/2}}\int_0^{x_0}\chi^{3/2}(x)\, x^{1/2}\, dx = \text{const}$$

$$\left(Z\int_0^{\infty}\chi^{3/2}x^2\, dx\right)$$

$$x_0 = \text{const}$$

$$r_0 = x_0/Z^{1/3}.$$

The approximation is better with increasing

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2, because the density is larger.

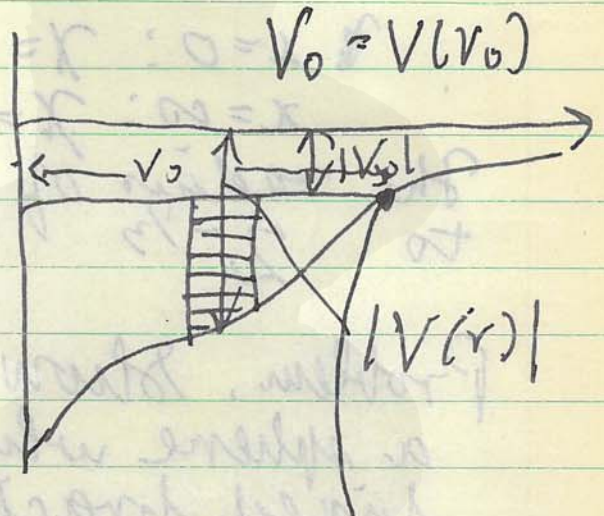
One can start from a slightly more general assumption

$$\frac{1}{2m}p_0^2 = -(V(r) - V_0)$$

$$U = V(r) - V_0$$

$$V_0 = V(r_0)$$

$$= -\frac{2e^2}{r}\chi(x)$$



boundary condition

$$Z' = -\frac{4\pi}{e}\int_0^{r_0}\rho(r)\,r^2 dr$$

Z': number of electrons $\begin{cases} U(r_0)=0 \\ \chi(x_0)=0. \end{cases}$

r_0: boundary of the atom:

$$4\pi\int_0^{r_0}\frac{\sqrt{-2mU(r)}^{3/2}}{3\pi^2\hbar^3}r^2 dr = Z'$$

$$\int_0^{x_0}\frac{2^{3/2}}{3\pi}\chi^{3/2}(x)\frac{x^{1/2}dx}{Z^{1/2}} = Z'$$

$$\int_0^{x_0} x\cdot\frac{d^2\chi}{dx^2}dx = \frac{Z'}{Z}$$

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$$\therefore Z' = 4\pi \int_0^{r_0} \frac{(-2mU)^{3/2}}{3\pi^2\hbar^3} r^2 dr$$

$$= \frac{4(2mZe^2)^{3/2}}{3\pi\hbar^3} \int_0^{r_0} \frac{\chi^{3/2}}{r^{3/2}} r^2 dr$$

$r = bx$. $b = \frac{1}{2}\left(\frac{3\pi}{4}\right)^{2/3} \frac{\hbar^2}{me^2 Z^{1/3}}$

$$Z' = b^{-3/2} \cdot Z \int_0^{x_0} \chi^{3/2} x^{1/2} dx$$

$$= Z \int_0^{x_0} \chi^{3/2} x^{1/2} dx$$

$$\frac{Z'}{Z} = x\frac{d\chi}{dx}\Big|_0^{x_0} - \int_0^{x_0} \frac{d\chi}{dx} dx$$

$$= \left\{x\frac{d\chi}{dx}\right\}_0^{x_0} + \chi(0) - \chi(x_0)$$

$$= 1 + x_0 \frac{d\chi}{dx}\Big|_{x=x_0} \qquad = 1 - \varepsilon + x_0 \frac{d\chi}{dx}\Big|_{x=x_0} < 1.$$

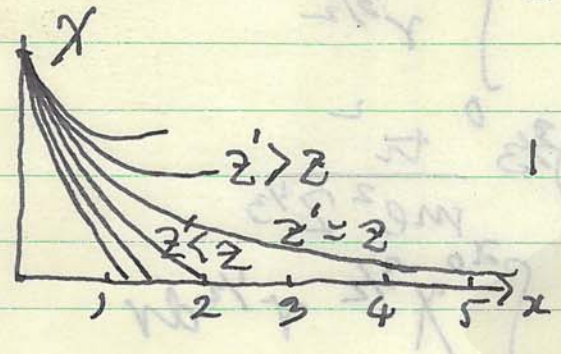
$Z' = Z$ (neutral atom)

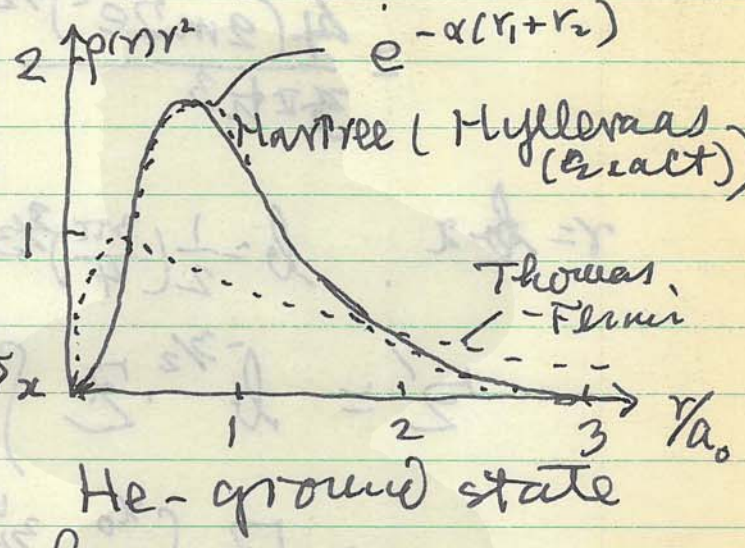
$$\frac{d\chi}{dx}\Big|_{x=x_0} = 0$$

which is true only for $x_0 = \infty$ or $r_0 = \infty$.
Thus the neutral atom has the infinite

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radius. Thus the assumption, just fixed, $V_0 = 0$ is ✓
Positive ions have finite radii, while the method cannot be applied to negative ions





He-ground state

For very large values of x

$$\chi \cong \frac{144}{x^3}$$

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Derivation of Thomas-Fermi model from variation principle.

$$K.E. = 2\int_0^{\infty}\int_0^{p_0(r)} \frac{1}{2m} p^2 \cdot \frac{4\pi p^2 dp}{(2\pi\hbar)^3} \underbrace{4\pi r^2 dr\, d\Omega}_{dv}$$

$$= \frac{8\pi}{2m(2\pi\hbar)^3}\int\int\int \frac{p_0^5(r)}{5} 4\pi r^2 dr d\Omega$$

$$\frac{1}{2\pi^2\hbar^3 m}$$

$$p_0 = (-2mV)^{1/2}$$

$$= \frac{1}{10\pi^2\hbar^3 m}\int_0^{\infty}\int (-2mV)^{5/2} r^2 dr$$

$$\rho(r) = \frac{(-2mV)^{3/2}}{3\pi^2\hbar^3}$$

$$(-2mV)^{5/2} = (3\pi^2\hbar^3\cdot\rho(r))^{5/3}$$

$$= (3\pi^2)^{5/3}\cdot\hbar^5\int \rho^{5/3}$$

$$K.E. = \frac{(3\pi^2)^{5/3}\hbar^2}{10\pi^2 m}\int \rho^{5/3} r^2 dr\, d\Omega$$

$$P.E. = -Ze^2\int^{\infty}\frac{\rho(r)}{r} r^2 dr\, d\Omega$$

$$+ \frac{e^2}{2}\int\int^{\infty}\frac{\rho(r)\rho(r')}{|r-r'|} r^2 dr\cdot r'^2 dr'\, d\Omega \times d\Omega'$$

Normalization

$$\int \rho(r)\, r^2 dr\, d\Omega = Z$$

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$$\delta\{(K.E.)+(P.E)-\lambda\int\rho\, r^2 dr d\Omega\}=0$$

$$\frac{1}{3}\cdot\frac{(3\pi^2)^{5/3}\hbar^2}{2\pi^2 m}\rho^{2/3}-\frac{Ze^2}{r}+e^2\int\frac{\rho(r')dv'}{|r-r'|}$$

$$-\lambda=0$$

$$\rho=\frac{(-2mV)^{3/2}}{3\pi^2\hbar^3}$$

$$\rho^{2/3}=\frac{-2mV}{(3\pi^2)^{2/3}\hbar^2}$$

$$\frac{\hbar^2}{2m}(-V)-\frac{Ze^2}{r}+e^2\int\frac{\rho(r')dv'}{|r-r'|}-\lambda=0$$

$$\Delta(-V)=4\pi e^2\rho$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d(-V)}{dr}\right)=\frac{4e^2(-2mV)^{3/2}}{3\pi\hbar^3}$$

Exchange Effect

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Problem.

Show that, if we ignore the repulsions between electrons completely in the atom and use the hydrogen-like eigenfunctions for the individual electrons, the size of the atom is proportional to $Z^{-1/3}$ instead of $Z^{-1/3}$ for large values of Z.

Hint: Choose the atomic number Z such that the shells are closed up to the principle q.n. n_{max}.

$$\sum_{l=0}^{n-1} (2l+1) = n^2$$

$$2\sum_{n=1}^{n_{max}} n^2 = \frac{1}{3} n_{max}(n_{max}+1)(2n_{max}+1)$$

$$= Z$$

$$n_{max} \approx Z^{-1/3}$$

$$\psi_{nlm} \propto e^{-\frac{Z}{n a_0} r}$$

atomic radius $\propto \frac{n_{max} a_0}{Z} \propto Z^{-2/3}$

Due to the electronic repulsion or screening, the actual radius will be larger than and nearly proportional to $Z^{-1/3}$ (higher values of l are not filled up)

(which is more effective for higher values of l)

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Dirac, P.C.P.S. 26 (1930), 376.

$$i\hbar\frac{\partial}{\partial t}(q'|r) = \int (q'|H_0|q'')\,dq''(q''|r)$$

$$+\sum_s \int (q'|B_{ss}|q'')\,dq''(q''|r)$$

$$-\sum_s \int (q'|B_{sr}|q'')\,dq''(q''|s)$$

$$i\hbar\frac{\partial u_r(x_1)}{\partial t} = H_0 u_r(x_1)$$

$$+\sum_s \int \bar{u}_s(x_2) V_{12} u_s(x_2)\,dx_2 \cdot u_r(x_1)$$

$$-\sum_s \int \bar{u}_s(x_2) V_{12} u_r(x_2)\,dx_2\, u_s(x_1)$$

$$i\hbar\frac{\partial}{\partial t}\int (q|q')\,dq'(q'|r) = 0$$

$$i\hbar\frac{\partial}{\partial t}\int \bar{u}_s(x_1) u_r(x_1)\,dx_1 = 0$$

$$(x'|\rho|x'') = \sum_r u_r(x')\bar{u}_r(x'')$$

$$\rho^2 = \rho.$$

$$i\hbar\dot{\rho} = (H_0 + B - A)\rho - \rho(H_0 + B - A)$$

$$B = \sum_s B_{ss} = \iint (q'q'''|V|q''q^{iv})\,dq'''dq^{iv}\,(q^{iv}|\rho|q'')$$

$$(q'|A|q'') = \iint (q'''q'|V|q''q^{iv})\,dq'''dq^{iv}\,(q^{iv}|\rho|q''')$$

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$$(q'|B|q'') = e^2 \delta(q'-q'') \int \frac{(q'''|\rho|q''')}{r(q'q''')} dq'''$$

$$= e^2 \delta(x'-x'') \int \frac{(x'''|\rho|x''')}{|x'-x'''|} dx'''$$

$$(q'|A|q'') = e^2 \frac{(q'|\rho|q'')}{r(q'q'')}$$

$$= e^2 \frac{(x'|\rho|x'')}{|x'-x''|}$$

Trace $\{\rho(H_0 + \frac{1}{2}B - \frac{1}{2}A)\}$

is a const. of motion.

Reduction to cl. density $f = \alpha\left(\frac{q'+q''}{2}, p\right)$

$$(q'|\alpha|q'') = (2\pi\hbar)^3 \int \alpha(q,p) e^{i(q'-q'')p/\hbar} dp$$

$$\alpha(q,p) = \int (q'|\alpha|q'') e^{-i(q'-q'')p/\hbar} \times \delta(q'-q'')$$

$$B(q,p) = e^2 \int \delta(q'-q'') e^{-i(q'-q'')p/\hbar} \delta(q'-q'') \int \frac{(q'''|\rho|q'')}{r(qq''')} dq'''$$

$$= \frac{e^2}{(2\pi\hbar)^3} \int \frac{dq'}{r(qq')} \int \rho(q'p') dp'$$

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$$A(q,p) = e^2 \int \frac{(q'|\rho|q'')}{r(q'q'')} e^{-i(q'-q'')p/\hbar} \times d(q'-q'')$$

$$= \frac{e^2}{(2\pi\hbar)^3} \int \rho(qp')dp' \int \frac{e^{-i(q'-q'')(p-p')/\hbar}}{r(q'q'')} d(q'-q'')$$

$$= \frac{e^2}{2\pi^2\hbar} \int \frac{\rho(qp')}{|p-p'|^2} dp'$$

$$\rho(qp) = 2 \quad |p| < P$$
$$= 0 \quad |p| > P$$

$$B(q) = \frac{e^2}{3\pi^2\hbar^2} \int \frac{P^3(q')dq'}{r(qq')}$$

$$A(qp) = \frac{e^2}{\pi\hbar}\left[\frac{P^2-|p|^2}{|p|}\log\left|\frac{P+|p|}{P-|p|}\right| + 2P\right)$$

Stationary state: $[P, H] = 0$

$$H(qp) = H_0(qP) + B(q)$$

$$-2e^2/\pi\hbar \cdot P_2$$

$$= -\frac{2e^2}{r} + \frac{P}{2m} - \frac{2e^2P}{\pi\hbar}$$

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$$+\frac{4e^2}{3\pi\hbar^3}\left\{\frac{1}{r}\int_0^r r'^2 p^3(r')dr' + \int_r^\infty r' p^3(r')dr'\right)$$

$$\frac{\partial}{\partial r} = 0: \quad \frac{Ze^2}{r^2} + \frac{d}{dr}\left(\frac{p^2}{2m} - \frac{2e^2 p}{\pi\hbar}\right)$$

$$-\frac{4e^2}{3\pi\hbar^3}\frac{1}{r^2}\int_0^r r'^2 p^3(r')dr'$$

$$\frac{d}{dr}\left\{r^2\frac{d}{dr}\left(\frac{p^2}{2m} - \frac{2e^2}{\pi\hbar}p\right)\right\}$$

$$= \frac{4\hbar^2}{3\pi\hbar^3} r^2 p^3$$

This is only applicable to the interior of Z'd atom.

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Methods of Approximation in ~~Variation~~

C. W. K. B. method *

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \psi + V(r) \psi$$

$$\psi = A e^{i\Phi/\hbar} \qquad A : \text{const.}$$

$$\frac{\partial \Phi}{\partial t} + \frac{1}{2m} (\text{grad}\, \Phi)^2 + V(r) - \frac{i\hbar}{2m} \Delta \Phi = 0$$

(Schiff, p. 178) $\xrightarrow{\hbar \to 0}$ $\frac{\partial W}{\partial t} + H(r, p_{=\text{grad}\, W}) = 0$

Bohm: $\psi = A e^{iS/\hbar}$ A, S: real

$$\frac{\partial A}{\partial t} = -\frac{1}{2m} \{ A \cdot \Delta S + 2 (\text{grad}\, A)(\text{grad}\, S) \}$$

$$\frac{\partial S}{\partial t} = -\left\{ \frac{1}{2m} (\text{grad}\, S)^2 + V(r) - \frac{\hbar^2}{2m} \frac{1}{A} \Delta A \right\}$$

$P = A^2$

$$\frac{\partial P}{\partial t} + \text{div} \left(\frac{P}{m} \text{grad}\, S \right) = 0$$

$$\frac{\partial S}{\partial t} + \frac{1}{2m} (\text{grad}\, S)^2 + V(r) - \frac{\hbar^2}{2m} \left[\frac{1}{P} \Delta P - \frac{1}{2} \frac{1}{P^2} (\text{grad}\, P)^2 \right] = 0$$

$U(r) = V(r) - \frac{\hbar^2}{2m} [\quad]$

quantum mechanical potential.

Wentzel - Kramers - Brillouin

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$$W = S(r) - Et$$

$$\frac{1}{2m}(\mathrm{grad}\, S)^2 - (E - V(r)) - \frac{i\hbar}{2m}\Delta S = 0$$

~~W. K. B. approx. in one dimensional case:~~

~~$$\frac{1}{2m}(\mathrm{grad}\, S)^2 - (E - V(r)) = 0$$~~

$V(r)$: $\psi = \frac{u(r)}{r} Y_{lm}(\theta, \varphi) e^{-iEt/\hbar}$

$$\frac{d^2 u_+}{dr^2} + k_+^2(r) u_+ = 0$$

if where $k_+(r) = \frac{\pm\sqrt{2m(E - V(r))}}{\hbar}$

for $V(r) < E$.

$$\frac{d^2 u_-}{dr^2} - k_-^2(r) u_- = 0$$

$$k_-(r) = \frac{\pm\sqrt{2m(V(r) - E)}}{\hbar}$$

for $V(r) > E$

$$U(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \quad *$$

$u(x) = A e^{iS(x)/\hbar}$

$$i\hbar \frac{d^2 S}{dx^2} - \left(\frac{dS}{dx}\right)^2 \pm \hbar^2 k_\pm^2 = 0$$

$\pm \hbar^2 k_\pm^2 \begin{cases} 2m(E - U) \\ 2m(U - E) \end{cases}$

$S = S_0 + \hbar S_1 + \cdots$

$$\left(\frac{dS_0}{dx}\right)^2 = \pm \hbar^2 k^2$$

---

* one dimensional case

$r \to x$ $\quad u(r) \to \psi(x)$

$k(r) \to k(x)$, $\quad U(r) \to V(x)$,

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$$i\hbar \frac{d^2 S_0}{dr^2} = 2 \cancel{\hbar} \frac{dS_0}{dr} \frac{dS_1}{dr}$$

(+)-region

$$S_0(r) = \pm \hbar \int^r k(r')\,dr'$$

$$\frac{dS_1(r)}{dr} = \cancel{\pm \hbar k(r')} \frac{i}{2} \frac{d}{dr} \log\left(\frac{dS_0}{dr}\right)$$

$$S_1(r) = \frac{i}{2} \log \cdot k(r) + \text{const.}$$

$$u_+(r) = \frac{A}{\sqrt{k_+}} \exp\left(\pm i \int^r k_+(r')\,dr'\right)$$

(−)-region

$$S_0(r) = \pm i \int^r k(r')\,dr'$$

$$u_-(r) = \frac{B}{\sqrt{k_-}} \exp\left(\mp \int^r k_-(r')\,dr\right)$$

Accuracy of solution:

$$\left|\frac{\hbar S_1}{S_0}\right| \ll 1 \qquad \left|\frac{\hbar S_1(r_0) + \hbar \frac{dS_1}{dr}\Big|_{r_0} (r-r_0)}{S_0(r_0) + \frac{dS_0}{dr}\Big|_{r_0} (r-r_0)}\right| \ll 1$$

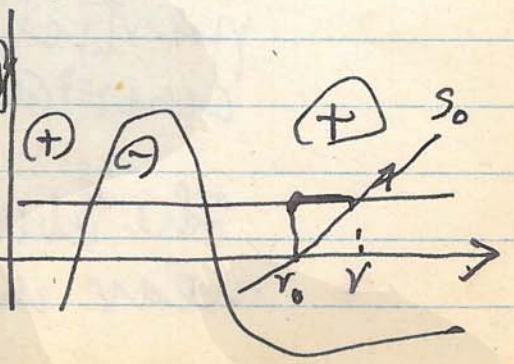
$$S_0(r) = \pm \hbar \int_{r_0}^r k(r')\,dr'$$

where k does not change sign between r_0 and r.

(+)

$$S_1(r) = \frac{i}{2} \left| \log k(r) - \log k(r_0) \right|$$

$$\left|\frac{\hbar \frac{dS_1}{dr}\Big|_{r_0}}{\frac{dS_0}{dr}\Big|_{r_0}}\right| = \left|\frac{k'(r_0)}{2k^2(r_0)}\right| \ll 1.$$



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or $\lambda = 1/k$ ($\Rightarrow \lambda = 2\pi/k$

$\frac{\lambda}{2} \cdot \left|\frac{dk}{dx}\right| \ll k$

or $\frac{\lambda}{2} \cdot \left|\frac{d\lambda}{dx}\right| \ll \frac{\lambda}{2}$

($\because \frac{d\lambda}{dx} = -\frac{1}{k^2}\frac{dk}{dx}$)

$\frac{d\lambda}{dx} = -\frac{1}{k^2}\frac{dk}{dx}$ ($\frac{1}{k}\frac{d}{dx}\log(E-V) \ll 1$)

$\frac{1}{2}\left|\frac{d\lambda}{dx}\right| \ll 1$. or $\frac{\lambda}{4\pi}\left|\frac{d\lambda}{dx}\right| \ll \lambda$

or $\frac{\lambda}{2}\left|\frac{d\lambda}{dx}\right| \ll \lambda$ for $\lambda \to \lambda = 2\pi\lambda$

Thus the (fractional) change in the local wave length over a distance of the wave length λ is small compared with λ. the order of

W.K.B. approximation is valid, only if the change of the potential energy is small that the momentum of the particle stays approximately constant over many wave lengths.

The above condition is violated near the turning point, where classical

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$k = 0$ $\quad$ $k = 0$ at $r = r_0$

(+) $k_+^2(x) = Cx^n$; $\quad (x = 0$ or $x = r - r_0)$

$$u(x) = A \xi^{\frac{1}{2}} k^{-\frac{1}{2}} J_{\pm\nu}(\xi)$$

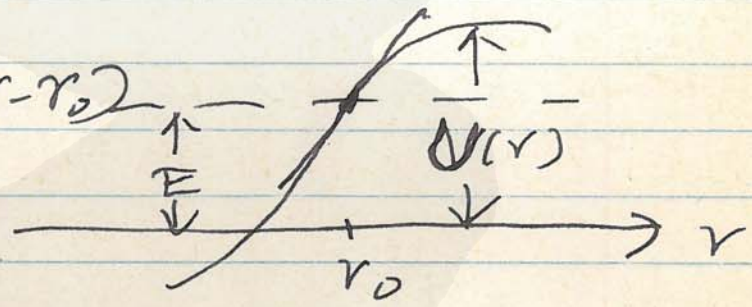
$$\xi = \int_0^x k\,dx$$

$$n = \frac{1}{n+2}$$

Bohm, Chapter 12.

$U(r) \to E = C(r - r_0)$

$$C = \left(\frac{dU}{dr}\right)_{r=r_0}$$



$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + C(x - r_0) = 0$$

$x = r - r_0$:

$$u(x) = A \xi^{1/2} \cdot J$$

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Variation Method as applied to the collision problem (1)

Hulthén
Schwinger
Jackson and Blatt, Phys. Rev. 76 (1949), 18; R. M. P. 22 (1950), 77

Central potential $V(r)$

~~S-wave. $l=0$~~ $\psi \cong e^{ikz} + \frac{e^{ikr} f(\theta)}{r}$

$\psi(r,\theta) = \sum \chi_l(r) P_l(\cos\theta)$

$r \gg R_0$ (outside the range) $l=0$

$\chi_l(r) = r^{-\frac{1}{2}} A_l C_l (J_{l+\frac{1}{2}}(kr) \cos\delta_l + \underbrace{J_{-l-\frac{1}{2}}(kr)}_{(-1)^l} \sin\delta_l)$

$k = \frac{\sqrt{2\mu W}}{\hbar}$ $\quad \underbrace{-\frac{2\mu V(r)}{\hbar^2}}$

$\frac{d^2\chi_l}{dr^2} + \frac{2}{r}\frac{d\chi_l}{dr} + \left(k^2 - \frac{l(l+1)}{r^2}\right)\chi_l = 0$

$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2\delta_l$

Slow particle: S-wave, $l=0$

$r \gg r_0$

$\chi_0(r) = r^{-\frac{1}{2}} \sqrt{\frac{2}{\pi kr}} C_0 (\cos\delta_0 \sin kr + \sin\delta_0 \cos kr)$

$= \frac{u(r)}{r}$

$u(r) = C'(\sin kr + \tan\delta_0 \cos kr)$

~~$\frac{d^2u}{dr^2} + k^2 u = 0$~~ $\quad r=0 : u(r) = 0$

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$$-\left(\frac{d^2}{dr^2}+k^2\right)u = W(r)u$$

$$W(r) = \frac{-2mV(r)}{\hbar^2}$$

Green function

$$-\left(\frac{d^2}{dr^2}+k^2\right)G(r,r') = \delta(r-r')$$

$r<r'$: $G(r,r') = k^{-1}\sin kr\cos kr'$

$r>r'$: $G(r,r') = k^{-1}\cos kr\sin kr'$ }

$\frac{dG}{dr}$ is discontinuous at $r=r'$

$$G(0,r') = 0$$

$$\frac{d^2G}{dr^2}+k^2G = 0 \quad \text{for } r\neq r'$$
$$= \infty \quad \text{for } r=r'$$

$$\int_{r'-\varepsilon}^{r'+\varepsilon}\left(\frac{d^2G}{dr^2}+k^2G\right)dr$$

$$= \left.\frac{dG}{dr}\right|_{r'-\varepsilon}^{r'+\varepsilon} + O(\varepsilon)$$

$$= -\sin k(r'+\varepsilon)\sin kr'$$

$$= \cos k(r'-\varepsilon)\cos kr' + O(\varepsilon)$$

$$= -1 + O(\varepsilon) = -\int_{r'-\varepsilon}^{r'+\varepsilon}\delta(r-r')dr$$

$$\int_0^\infty \left(\frac{d^2G(r,r')}{dr^2}+k^2G\right)f(r)\,dr = -f(r')$$

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$$\int_0^\infty G(r,r')\left(\frac{d^2u}{dr^2}+k^2u\right)dr$$

$$=\lim_{\varepsilon\to 0}\left\{\int_0^{r'-\varepsilon} G\left(\frac{d^2G}{dr^2}+k^2u\right)dr+\int_{r'+\varepsilon}^{\infty} G(\quad)dr\right\}$$

$$= G\frac{du}{dr}\Big|_0^{r'-\varepsilon} - \frac{dG}{dr}u\Big|_0^{r'-\varepsilon} + \int_0^{r'-\varepsilon}\left(\frac{d^2G}{dr^2}+k^2G\right)u\,dr$$

$$+ G\frac{du}{dr}\Big|_{r'+\varepsilon}^{\infty} - \frac{dG}{dr}u\Big|_{r'+\varepsilon}^{\infty} + \int_{r'+\varepsilon}^{\infty}(\quad)u\,dr$$

$$= G\frac{du}{dr}\Big|_0^{\infty} - u(r') - \frac{dG}{dr}u\Big|_0^{\infty}$$

$G(0,r')=0$ $\qquad$ $u(0)=0$

$$\simeq -u(r') + \Big(k^{-1}\cos kr\sin kr'\frac{du}{dr}$$

$$+\sin kr\sin kr'\,u\Big)$$

$$C'(\sin kr+\tan\delta_0\cos kr)$$

$$kC'(+\cos kr+\tan\delta_0\sin kr)$$

$$= -u(r') + C'\sin kr'$$

$$u(r') = C'\sin kr' + \int_0^\infty W(r)u(r)G(r,r')\,dr$$

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or $C' = 0$

$r > R$

$$u(r) = \sin kr + \tan\delta_0 \cos kr$$

$r \gtrless r'$

$$u(r) = \sin kr + \int_0^\infty G(r,r') W(r') u(r') dr'$$

since

$$G(r,r') = G(r,r')$$

$r < r'$ $\quad = k^{-1} \sin kr \cos kr'$

$r \gg r_0$ (range of force)

$$u(r) \triangleq \sin kr + \int_0^\infty k^{-1} \cdot \underbrace{\cos kr}_{\sin kr'} W(r') u(r') dr'$$

because $W(r')$ is different from zero for $r' \lesssim r_0 < r$

$$\tan\delta_0 = k^{-1} \int_0^\infty W(r') u(r') \sin kr' dr'$$

$$\int_0^\infty W(r) u^2(r) dr = \int_0^\infty W(r) u(r) \sin kr\, dr$$

$$+ \int_0^\infty dr \int_0^\infty dr'\, W(r) u(r) G(r,r') W(r') u(r')$$

or $\int_0^\infty W u^2 dr - \int dr \int dr'\, W u G W' u'$

$$= \int W u \sin kr\, dr$$

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$$\text{or} \quad \frac{\int_0^\infty w u^2 dr - \iint_{00}^{\infty\infty} dr dr' w u G w' u'}{\left[k^{-1}\int_0^\infty w u \sin kr\, dr\right]^2}$$

$$= \frac{1}{k^{-1}\left[k^{-1}\int_0^\infty w u \sin kr\, dr\right]^2}$$

$$= \frac{1}{k^{-1} + \tan\delta_0}$$

$$\text{or} \quad k\cot\delta_0 = \frac{\int_0^\infty w u^2 dr - \iint dr dr' w u G w' u'}{\left[k^{-1}\int_0^\infty w u \sin kr\, dr\right]^2} \quad (1)$$

$$\equiv I(u)$$

Variation of u:

$$\left(2\int_0^\infty w u \delta u\, dr - 2\left(\delta u\, dr \int G w' u' dr'\right)\right)$$

$$\times \left(k^{-1}\int_0^\infty w u \sin kr\, dr\right)$$

$$- 2\left[\int_0^\infty w u^2 dr - \iint \cdots\right]$$

$$\times \left(2k^{-1}\int_0^\infty w \delta u \sin kr\, dr\right) = 0$$

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or $Wu - \int_0^\infty G W' u' dr' \cdot u$

$$- \frac{\left[\int_0^\infty W u^2 dr - \iint W u G W' u'\right]}{\left[k^{-1} \int W u \sin kr\, dr\right]}$$

$$\times k^{-1} \int W \sin kr = 0$$

Now this is satisfied by

$$u = \sin kr + \int G W' u' dr'$$

$$\therefore W \sin kr - \frac{\int W u \sin kr\, dr}{\int W u \sin kr\, dr}$$

$$\times W \sin kr \simeq 0$$

Thus, the function $u(r)$ which is the solution of our problem ~~and~~ ~~the~~ makes the above expression (1) extremum and the extremum value of (1) gives the required ~~k~~ k.

This situation ~~can be~~ gives us the new ~~starting~~ point for approximate method in collision theory.

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Namely, take a trial function
$u_0(r)$ $\rightarrow$ $k \cot \delta_0^{(0)}$

$\rightarrow u_1(r) = \sin kr + \int_0^\infty dr' G(r,r') W(r') u_0 dr'$

$\rightarrow k \cot \delta_0^{(1)} \rightarrow \cdots$

with parameters and adjust the parameters such that (1) becomes extremum. Then we obtain $k \cot \delta_0^{(0)}$ in the zeroth approximation.

Since $u(r)$ enters in (1) only in the combination $W(r)u(r)$, the error in $u(r)$ outside the range of forces is unimportant. Also the normalization factor is irrelevant.

Example: Scattering of slow neutrons (not too fast) by protons.
For neutrons of energy up to a few MeV.
Since the nuclear potential is supposed to be very deep (30 ~ 40 MeV) on the average for $r < r_0$ compared with the kinetic energy of the neutron, the behavior of the wave function for $r < r_0$ does

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not dependent much on the energy of the neutron. Thus, we may take as ~~the~~ u_0 the zero approximation function u_0 the wave function for zero energy or $k=0$.

$$-\frac{d^2u_0}{dr^2} = W(r)u_0$$

For $r \gg r_0$,

$$u_0(r) \cong 1 - \alpha r$$

$$\left(\sin kr + \tan\delta \cos kr \right.$$

$$\left. = \tan\delta\,(1 + k\cot\delta \cdot r - \cdots) \right)$$

For small k, $\delta \ll 1$. in order that σ is finite or

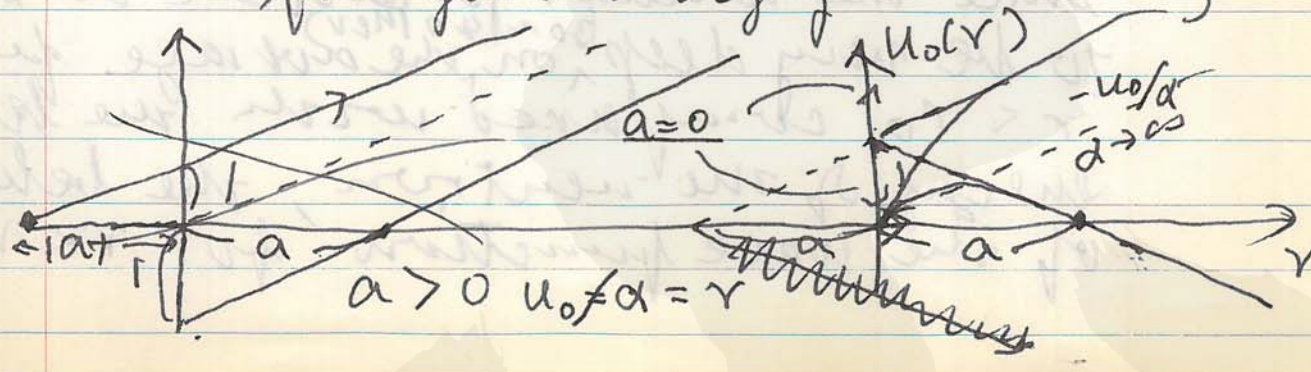
$$u_0(r) \cong 1 + k\cot\delta \cdot r - \cdots$$

where $k\cot\delta$ is, in general, finite, since $\sigma \cong \frac{4\pi}{k^2\cot^2\delta}$

$$\sigma \cong \frac{4\pi}{\alpha^2} = 4\pi a^2$$

$$a = \frac{1}{\alpha} = \frac{1}{k\cot\delta}$$

a: Fermi scattering length for zero energy



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such u_0 is a poor approximation for $r > r_0$, but ~~the only one~~ still it may serve our purpose, since it can be a good approx. for $r < r_0$. The correction $u(r) - u_0(r)$ in/ce the range of nuclear forces is proport. to k^2 (of the order of $k^2/\sqrt{2m\bar{V}/\hbar^2}$, where $\bar{V}$ is the average depth of the nuclear potential) Thus the error in $W(u)$ is $\propto$ to k^2: Now from I (4) we see that the error in k^2 cut δ is ~~$\propto$ to k^4, because in~~

$$\int_0^\infty W(u_0 + k^2 u_1')^2 dr - \iint dr dr' W(u_0 + k^2 u_1) \times G(u_0' + k^2 u_1') \Big/ \left[k^{-1} \int_0^\infty W(u_0 + k^2 u_1) \sin kr \, dr \right]^2,$$

the term which is proportional to $k^2 u_1$ must vanish due to the variation principle. to be proportional to the square of the error in the trial function, because the linear term must vanish on account of the variation principle. Namely

$$\delta I(u) = I(u + \delta u) - I(u) = \int \frac{\partial I}{\partial u} \delta u = 0$$

$u \sim k^2$

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In other words, the error in $k\cot\delta$ must be proportional to k^4. Now if we take $u = u_0$, we obtain in general, the formula

$$k\cot\delta = -\frac{1}{a} + \frac{1}{2}k^2 r_0 (+Pk^4 + \cdots) \quad (2)$$

where the first two terms are correct.* This is a very general conclusion which is largely independent of the detailed shape of the nuclear potential. (Shape indep. approximation.) This is very accurately confirmed by p-p scattering experiment. The nuclear potential must be of such a form that the two constants a and r_0 (effective range) fit with the experiment. r_0 is called an effective range, because it usually falls near the edge of the potential well. It is called effective, because it depends on the depth as well as the width of the potential.

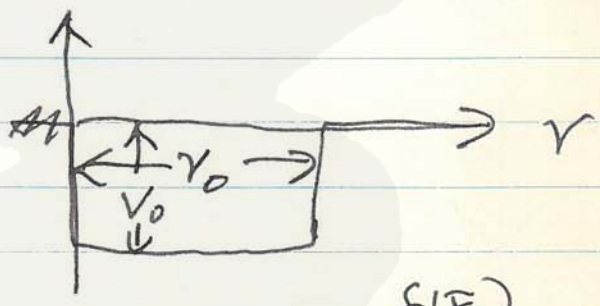
* Although the constants a, r_0 must be calculated by assuming a particular shape for the potential, the relation (2) between $k\cot\delta$ and k^2 does not, its power change.

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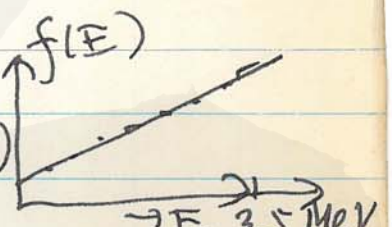
For any ordinary type of nuclear potential, there are two parameters which can be so adjusted as to give the observed values of a and r_0. (for singlet potential and triplet potential separately).

(1) Meson potential
g and x in $g^2 \frac{e^{-\varkappa r}}{r}$

(2) Square well
V_0, r_0



Bethe, P. R. 76 (1949), 38.
p-p-scattering ('S-scattering)



$$f(E) = g(\eta) + \frac{2\pi \cot\delta}{e^{2\pi\eta}-1} \cong D\left[-\alpha' + \tfrac{1}{2}k^2 r_0\right]$$

$$D = 2\pi^2/Me^2 = 5.176\times10^{-12}\ \text{cm}$$

$$\eta = e^2/\hbar v = 1/kD = (25.0\ \text{keV}/E)^{1/2}$$

$$g(\eta) = -2\log\eta + 2\eta^2 \sum_{\nu=1}^{\infty} \nu^{-1}(\nu^2+\eta^2)^{-1}$$

$e \to 0$. $D \to \infty$, $\eta \to 0$, ~~$g(\eta) \cong$~~

$$g(\eta) \cong -2\log(1/kD)/D + 2\frac{1}{(kD)^2 \cdot D}\sum_{\nu=1}^{\infty}\nu^{-3}$$

$\to 0$.

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Physics 237　　Deficiency Examination　　April 24, 1952

1. Discuss the uncertainty principle in the case of the linear harmonic oscillator and show that the relation

$$\Delta q \, \Delta p = \hbar/2$$

holds, only if the oscillator is in the ground state n = 0. Deduce the uncertainty relation for the state n = 1.

2. A particle is scattered by a central potential V(r), which is constant and negative for $r < a$ and zero for $r > a$. What relation between the depth of the potential and the width a must be satisfied in order that the scattering cross-section for a very slow particle becomes very large compared with the geometrical cross-section πa^2?

3. State the reason why the spectral lines of the helium atom are divided into two classes, i.e., parhelium and orthohelium. Draw a qualitative picture of a few low energy levels of the helium atom.

Please return this question sheet with answer books.

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Examination Physics 237

Problem 1.

Discuss the linear uncertainty principle in the case of the harmonic oscillator and show that the relation

$$\Delta q \, \Delta p = \hbar/2$$

hold, only if the oscillator is in the ground state $n = 0$. Deduce the ~~correspon~~ uncertainty relation for the state $n = 1$.

Problem 2.

A particle is scattered by a central potential ~~which~~ $V(r)$, which is constant and negative for $r < a$ and zero for $r > a$. ~~Discuss the ch. For what values of the energy of the particle is the scattering cross-section large compared with the geometrical cross-section πa^2.~~ ~~Find the condition that~~ relation ~~between~~

What relation between the depth of the potential and the width a must be satisfied, in order that the scattering cross-section ~~becom~~ for a very slow particle becomes very large compared with the geometrical cross-section πa^2.

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Problem 3.

State the reason why the spectral lines of the helium atom are divided into two classes, i.e. parhelium and orthohelium. Draw a qualitative picture of a few low energy levels of the helium atom.

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Problem 1.

Show that the differential cross-section of elastic scattering of an electron by an atom is given by

$$d\sigma = \left(\frac{2me^2}{\hbar^2}\right)^2 \frac{(Z - F(\theta))^2}{\left(\frac{2k}{\hbar}\sin\frac{\theta}{2}\right)^2} \sin\theta\, d\theta\, d\varphi,$$

$$= \frac{1}{K^4}$$

~~where Z is the atomic number and with~~ where

$$F(\theta) = 4\pi \int_0^\infty \rho(r) \frac{\sin Kr}{Kr} r^2 dr$$

is the form factor and

$$K = 2k \sin\frac{\theta}{2}.$$

The ~~electrons~~ density of electrons in the atom is assumed to be spherically symmetrical and is denoted by $\rho(r)$.

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Problem 2. (in the stationary state under the attractive force)
An electron is ~~attracted~~ by a fixed centre, the force being proportional to the distance. An external weak and uniform electric field is applied. What is the change in the energy of the stationary state? Compare the results of second order perturbation with those of exact calculation.

$$a(x^2+y^2+z^2)+bx$$
$$= a\left(x^2+\frac{b}{2a}\right)+ay^2+az^2$$
$$-\frac{b^2}{4a}$$

$$-\frac{H_{nn'}H_{n'n}}{E_{n'}-E_n}$$

$$\int H_u \; x \; H_n$$
$$= H_n\left(\frac{1}{2}H_{n+1}+nH_{n-1}\right)$$

$$\frac{1}{2}$$

Remarks: $\psi_n(x) = N_n e^{-\frac{x^2}{2}} H_n(x)$
$N_n = (2^n \cdot n! \sqrt{\pi})^{-\frac{1}{2}}$
$H_{n+1} - 2xH_n + 2nH_{n-1} = 0$
$\frac{d^2\psi_n}{dx^2} - 2x\frac{d\psi_n}{dx} + 2n\psi_n = 0$

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Quantization of Fields

April, 1952

Heisenberg-Pauli's Method

Z.f. Phys. 56 (1929), 1; 59 (1930), 168.

Wentzel, Q. T. of Fields

particles (Classical) field

$q_1, q_2 \cdots q_n$

$\dot{q}_1, \dot{q}_2 \cdots \dot{q}_n$

$\psi_\alpha(x_1, x_2, x_3, x_4)$

$\frac{\partial \psi_\alpha}{\partial t} = c \frac{\partial \psi_\alpha}{\partial x_4}$ $\quad x_4 = ct$

Lagrangian

$L(q_1, q_2 \cdots q_n; \dot{q}_1, \dot{q}_2 \cdots \dot{q}_n)$

Lagrangian density $\mathcal{L}$.

$\bar{L} = \int \mathcal{L}\left(\psi_\alpha, \frac{\partial \psi_\alpha}{\partial x_\mu}\right) \times dx_1 dx_2 dx_3$

$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) = \frac{\partial L}{\partial q_j}$

$j = 1, 2, \cdots n$

$\delta \int_{t_0}^{t_1} L\, dt = 0$

$\delta q_j = 0$ at $t = t_0, t_1$

$\delta \int \bar{L}\, dt = 0$

$\frac{\partial \mathcal{L}}{\partial \psi_\alpha} - \sum_i \frac{\partial}{\partial x_i}\left(\frac{\partial \mathcal{L}}{\partial \frac{\partial \psi_\alpha}{\partial x_i}}\right) - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \frac{\partial \psi_\alpha}{\partial x_4}}\right) = 0$

$\delta \psi_\alpha = 0$ on the boundary surface

$\int \left\{ \delta q_j \left(\frac{\partial L}{\partial q_j}\right) + \delta \dot{q}_j \left(\frac{\partial L}{\partial \dot{q}_j}\right) \right\} dt$

$= \int \delta q_j \left\{ \left(\frac{\partial L}{\partial q_j}\right) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) \right\} dt + \left[\delta q_j \frac{\partial L}{\partial \dot{q}_j} \right]_{t_0}^{t_1} = 0$

or

$\frac{\partial}{\partial x_\mu}\left(\frac{\partial \mathcal{L}}{\partial \frac{\partial \psi_\alpha}{\partial x_\mu}}\right) = \frac{\partial \mathcal{L}}{\partial \psi_\alpha}$

L : invariant.

Left hand side transforms like the right hand side

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L → $\mathcal{L}$

$$\frac{\partial L}{\partial q_j} \longrightarrow \frac{\delta \mathcal{L}}{\delta \psi_\alpha(x_\mu)} = \frac{\partial \mathcal{L}(\partial\psi_\alpha)}{\partial \psi_\alpha(x_\mu)} - \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left(\frac{\partial \mathcal{L}}{\partial \frac{\partial \psi_\alpha(x_\mu)}{\partial x_i}}\right)$$

functional derivative

Canonical conjugate

$$p_j = \frac{\partial L}{\partial \dot{q}_j}$$

Hamiltonian

$$H = \sum_j \dot{q}_j p_j - L$$

$$= H(q_j, p_j)$$

step function → smooth fn

canonical conjugate

$$\Pi_\alpha(x_i, t) = \frac{\delta \mathcal{L}}{\delta \frac{\partial \psi_\alpha(x_i)}{\partial t}}$$

$$= \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi_\alpha}{\partial t}} = \frac{1}{c}\frac{\partial \mathcal{L}}{\partial \frac{\partial \psi_\alpha}{\partial x_4}}$$

Hamiltonian density

$$H = \sum_\alpha \Pi_\alpha \frac{\partial \psi_\alpha}{\partial t} - \mathcal{L}$$

$$= \sum_\alpha \Pi_\alpha \frac{\partial \psi_\alpha}{\partial x_4} - \mathcal{L}$$

$$\Pi_\alpha = \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi_\alpha}{\partial x_4}} = c P_\alpha$$

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Quantum Theory

com. rel.

$[q_j, p_k] = i\hbar\delta_{jk}$

$[q_j, q_k] = [p_j, p_k]$

$= 0$

q. m. eq. of motion

$i\hbar \dot{q}_j = [q_j, H]$

$i\hbar \dot{p}_j = [p_j, H]$

$i\hbar F = [F, H]$

c. r.

$[\psi_\alpha(x,t), P_\beta(x',t)] = i\hbar\delta_{\alpha\beta}\delta(x,x')$

α

$[\psi_\alpha(x,t), \psi_\beta(x',t)]$

$= [P_\alpha(x,t), P_\beta(x',t)]$

$= 0$

or $[\psi_\alpha(x_i, x_4), \Pi_\beta(x_i', x_4')]$

$= i\hbar c\,\delta_{\alpha\beta}\delta(x_i, x_i')$

etc.

field equations

$i\hbar \frac{\partial \psi_\alpha}{\partial t} = [\psi_\alpha, \bar{H}]$

$i\hbar \frac{\partial \Pi_\alpha}{\partial t} = [P_\alpha, \bar{H}]$

$i\hbar \frac{\partial F}{\partial t} = [F, \bar{H}]$

$i\hbar \frac{\partial \bar{F}}{\partial t} = [\bar{F}, \bar{H}]$

or $i\hbar c \frac{\partial F}{\partial x_4} = [F, \bar{H}]$

etc,

$i\hbar c \frac{\partial \Pi_\alpha}{\partial x_4} = [\Pi_\alpha, \bar{H}]$

$i\hbar c \frac{\partial \psi_\alpha}{\partial x_4} = [\psi_\alpha, \bar{H}]$

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Quantization
Real Scalar Field

$$L = -\frac{1}{8\pi}\left(\frac{\partial\varphi}{\partial x_\mu}\frac{\partial\varphi}{\partial x^\mu} + \kappa^2\varphi^2\right)$$

$$= -\frac{1}{8\pi}\left(g_{\mu\nu}\frac{\partial\varphi}{\partial x_\mu}\frac{\partial\varphi}{\partial x_\nu} + \kappa^2\varphi^2\right)$$

$$g_{\mu\nu} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} = g^{\mu\nu}$$

$$x^\mu = g^{\mu\nu}x_\nu, \quad x_\mu = g_{\mu\nu}x^\nu$$

$$\delta\int \bar{L}\,dt = 0$$

$$(\Box - \kappa^2)\varphi = 0$$

or $$g_{\mu\nu}\frac{\partial^2\varphi}{\partial x_\mu \partial x_\nu} - \kappa^2\varphi = 0$$

$$H = \frac{\partial\varphi}{\partial t}\frac{\partial L}{\partial\frac{\partial\varphi}{\partial t}} - L = \frac{\partial\varphi}{\partial x_4}\pi - L$$

$$p = \frac{1}{2\pi c^2}\frac{\partial\varphi}{\partial t} = \frac{1}{4\pi c}\frac{\partial\varphi}{\partial x_4}$$

$$\pi = cp = \frac{1}{4\pi}\frac{\partial\varphi}{\partial x_4}$$

Energy-Momentum Tensor (Density)

$$T_\mu{}^\nu = \frac{\partial\varphi}{\partial x_\nu}\frac{\partial L}{\partial\frac{\partial\varphi}{\partial x_\mu}} - L\delta_{\mu\nu}$$

or $$T_{\mu\nu} = g_{\nu\lambda}T_\mu{}^\lambda = g_{\nu\lambda}\frac{\partial\varphi}{\partial x_\nu}\frac{\partial L}{\partial\frac{\partial\varphi}{\partial x_\lambda}} - g_{\mu\nu}L$$

$$= -\frac{1}{4\pi}\frac{\partial\varphi}{\partial x^\mu}\frac{\partial\varphi}{\partial x^\nu} - g_{\mu\nu}L$$

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symmetric Tensor:

$$T_{\mu\nu} = T_{\nu\mu}$$

$$\frac{\partial T_{\mu\nu}}{\partial x_\mu} = 0 \quad \text{or} \quad \frac{\partial T_{\mu\nu}}{\partial x_\nu} = 0$$

$$\frac{\partial T_{\mu\nu}}{\partial x_\mu} = \frac{\partial T_\mu{}^\nu}{\partial x^\mu}$$

$$= \frac{\partial^2 \varphi}{\partial x^\mu \partial x_\nu} \frac{\partial L}{\partial \frac{\partial \varphi}{\partial x_\mu}} + \frac{\partial \varphi}{\partial x_\nu} \frac{\partial}{\partial x^\mu} \frac{\partial L}{\partial \frac{\partial \varphi}{\partial x_\mu}}$$

$$= \left(\frac{\partial \varphi}{\partial b_\sigma} \frac{\partial}{\partial b_\rho} \gamma^\rho \gamma^\sigma \right) \gamma^\nu \partial_\nu \left(\frac{\partial L}{\partial \frac{\partial \varphi}{\partial b_\sigma}} \right) + \frac{\partial^2 \varphi}{\partial b_\rho^2} \frac{\partial L}{\partial \frac{\partial \varphi}{\partial b_\sigma}} \gamma^\rho \gamma^\sigma \gamma^\nu \partial_\nu$$

$$- \left(\frac{\partial \varphi}{\partial b_\sigma} \gamma^\rho \gamma^\sigma \partial_\rho \right) \left(\frac{\partial L}{\partial \frac{\partial \varphi}{\partial b_\sigma}} \right) \gamma^\nu \partial_\nu + \frac{\partial \varphi}{\partial b_\sigma} \gamma^\rho \gamma^\sigma \gamma^\nu \partial_\nu \frac{\partial L}{\partial \frac{\partial \varphi}{\partial b_\rho}}$$

$$= \gamma^\nu \partial_\nu \left(\frac{\partial \varphi}{\partial b_\sigma} \frac{\partial L}{\partial \frac{\partial \varphi}{\partial b_\sigma}} \right) \gamma^\rho \gamma^\sigma \partial_\rho + \frac{\partial^2 \varphi}{\partial b_\rho^2} \frac{\partial L}{\partial \frac{\partial \varphi}{\partial b_\sigma}} \gamma^\rho \gamma^\sigma \gamma^\nu \partial_\nu$$

$$- \left(\frac{\partial \varphi}{\partial b_\sigma} \gamma^\rho \gamma^\sigma \partial_\rho \right) \left(\frac{\partial L}{\partial \frac{\partial \varphi}{\partial b_\sigma}} \right) \gamma^\nu \partial_\nu + \frac{\partial \varphi}{\partial b_\sigma} \gamma^\rho \gamma^\sigma \gamma^\nu \partial_\nu \frac{\partial L}{\partial \frac{\partial \varphi}{\partial b_\rho}}$$

$$= 0$$

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$$T_{44} = -H.$$

$$\overline{H} = -\int T_{44}\, dv$$

momentum density

$$G_x = -\frac{1}{c} T_{14} \rightarrow \overline{G_x}$$

$$\overline{G_x} = -\frac{1}{c}\int T_{14}\, dv \rightarrow \overline{G_\pi}$$

$$\frac{\partial H}{\partial x_4} + \frac{1}{c}\operatorname{div} G_\pi = 0$$

$$\frac{\partial H}{\partial t} + \operatorname{div} G_\pi = 0$$

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Duality of Wave and Particle

φ : real scalar field
→ spin 0, neutral,

$[\varphi, P] = i\hbar\delta$ → B.E. statistics

free field:

$$\varphi = \sum_k C_{k_0}\left(a_k e^{ikx} + a_k^* e^{-ikx}\right)$$

$$k_0 = \sqrt{k^2 + \kappa^2}$$

$$= \sum_k C_{k_0}\left(a_k e^{i(kx - k_0 ct)} + a_k^* e^{-i(kx - k_0 ct)}\right)$$

$$P \simeq \sum_k \frac{C_{k_0}}{c^2}(-ik_0 c)\left(a_k e^{\cdots} - a_k^* e^{-\cdots}\right)$$

$$\bar{H} = \int\left(\frac{c^2}{2}P^2 + \frac{1}{2}\sum_i\left(\frac{\partial\varphi}{\partial x_i}\right)^2 + \frac{1}{2}\kappa^2\varphi^2\right)dv$$

$$= C_k^2 \cdot L^3 \frac{1}{2}\{ k_0^2 a_{-k} e^{2ik_0 ct}$$

$$\cdots + k_0^2 a_k^* a_k + a_k a_k^* \cdot$$

$$+ k^2 a_k^* a_k + k^2 a_k a_k^* + k^2 a_k a_{-k} e^{\cdots}$$

$$+ \cdots + \kappa^2 a_k^* a_k + \cdots$$

$$+ \kappa^2 a_k a_{-k} e^{\cdots}$$

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$$= \sum_{k} \left(a_k^* a_k + \frac{1}{2} \right) \hbar k_0 c$$

$$C_k^2 = L^{-3} \cdot \frac{\hbar c}{2 k_0} = \frac{\hbar c}{2 V k_0}$$

$$C_k = \sqrt{\frac{\hbar c}{2 V k_0}}$$

$$\varphi = \sum_{\substack{k \\ (k_0 > 0)}} \sqrt{\frac{\hbar c}{2 V k_0}} \left\{ a_k e^{i(kr - k_0 c t)} + a_k^* e^{-i(kr - k_0 ct)} \right\}$$

$$\rho = \sum_{\substack{k \\ (k_0 > 0)}} \sqrt{\frac{\hbar k_0}{2 V \hbar k_0 c}} (-i) \left(a_k e^{i(\cdots)} - a_k^* e^{i(\cdots)} \right)$$

$$[\varphi(r,t), \rho(r';t)]$$

$$= \sum_{k,k'} \frac{-i\hbar}{2 V \hbar k_0} \left\{ [a_k, a_{k'}] e^{i\{(kr + k'r') - (k_0 + k_0')ct\}} - i \cdots \right.$$

$$\left. + [a_k^*, a_{k'}] e^{-i\{\cdots\}} \right\}$$

$$[a_k, a_{k'}] = 0 \quad \text{etc.}$$

$$[a_k, a_{k'}^*] = \delta_{k,k'}$$

$$\sum_{k} e^{ik(r - r')} = \infty \quad \text{for } r = r'$$

$$= 0 \quad \text{for } r \neq r'$$

$$\int \sum_{k} e^{ik(r - r')} f(r')\, dr' =$$

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$$= e^{i\vec{k}\cdot\vec{r}} \int e^{-i\vec{k}\cdot\vec{r}} f(\vec{r})\,d\vec{r}$$

$$\Rightarrow V$$

$$\therefore [\varphi(x,t), P(x',t)] = i\hbar\,\delta(x,x')$$

$N_k = a_k^* a_k$ P.E. statistics

Relativistic Computation Rel.

$$[\varphi(x,t), P(x',t')] =$$

$$[\varphi(x,t), \varphi(x',t')] =$$

Total Momentum

$$G_x = -\frac{1}{c}\int T_{14}\,dV$$

$$= -\int \frac{\partial\varphi}{\partial x_1}\frac{\partial\varphi}{\partial x_4}\,dV$$

$$= \sum_{k,k'} \frac{\hbar\alpha}{2Vk_0} \int (a_k e^{i(\vec{k}\cdot\vec{r} - k_0 ct)} - i k_x a_k^* e^{-i(\,)})$$

$$\times (-ik_0' a_{k'} e^{+i(\,)} + i k_0' a_{k'}^* e^{-i(\,)})\,dV$$

$$= \sum_k \frac{\hbar k_x}{2}(a_k a_k^* + a_k^* a_k)$$

$$= \sum_k \hbar k_x N_k$$

$$\therefore \int e^{i(k-k')x}\,dV = V\delta_{kk'}$$

$$\sum_k k_x (a_k a_{-k}) = \sum_k (-k_x) a_{-k} a_k = 0$$

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Scalar
Complex, field
Conservation of charge
Weinberg

$\mathcal{L}(\varphi_\alpha, \frac{\partial \varphi_\alpha}{\partial x_i}, \frac{\partial \varphi}{\partial t})$ $(\alpha = 1, 2)$

$\varphi = \frac{1}{\sqrt{2}}(\varphi_1 + i\varphi_2)$, $\varphi^* = \frac{1}{\sqrt{2}}(\varphi_1 - i\varphi_2)$

$\mathcal{L}(\varphi; \varphi^*; \frac{\partial \varphi}{\partial x_i}, \frac{\partial \varphi}{\partial t}; \frac{\partial \varphi^*}{\partial x_i}, \frac{\partial \varphi^*}{\partial t})$

$P = \frac{\partial \mathcal{L}}{\partial \frac{\partial \varphi}{\partial t}}$, $P^* = \frac{\partial \mathcal{L}}{\partial \frac{\partial \varphi^*}{\partial t}}$

$P_1 = \frac{\partial \mathcal{L}}{\partial \frac{\partial \varphi_1}{\partial t}} = \frac{\partial \varphi}{\partial \varphi_1}\frac{\partial \mathcal{L}}{\partial \frac{\partial \varphi}{\partial t}} + \frac{\partial \varphi^*}{\partial \varphi_1}\frac{\partial \mathcal{L}}{\partial \frac{\partial \varphi^*}{\partial t}}$

$= \frac{1}{\sqrt{2}}(P + P^*)$ }

$P_2 = \frac{i}{\sqrt{2}}(P - P^*)$

or

$P = \frac{1}{\sqrt{2}}(P_1 - iP_2)$ }

$P^* = \frac{1}{\sqrt{2}}(P_1 + iP_2)$ }

$H = P_1\frac{\partial \varphi_1}{\partial t} + P_2\frac{\partial \varphi_2}{\partial t} - \mathcal{L}$

$= P\frac{\partial \varphi}{\partial t} + P^*\frac{\partial \varphi^*}{\partial t} - \mathcal{L}$

$G_4 = -(P\,\mathrm{grad}\,\varphi + P^*\,\mathrm{grad}\,\varphi)$

$[\varphi(x_i), P(x_i')] = i\hbar\,\delta(x_i, x_i')$

etc.

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$\varphi \to \varphi' = \varphi e^{i\alpha}$, $\psi^* \to \psi'^* = \psi^* e^{-i\alpha}$

$\psi^*\psi \to \varphi^*\varphi$ etc

$L(\varphi) \rightleftharpoons L(\varphi')$

(gage invariance of the ~~first~~ 2nd kind)

charge density

$$\rho = i\left(\varphi \frac{\partial L}{\partial \frac{\partial \varphi}{\partial t}} - \varphi^* \frac{\partial L}{\partial \frac{\partial \varphi^*}{\partial t}}\right)$$

$$\simeq i\left(\frac{\partial L}{\partial \frac{\partial \varphi}{\partial t}}\varphi - \varphi^* \frac{\partial L}{\partial \frac{\partial \varphi^*}{\partial t}}\right)$$

$$= i(P\varphi - \varphi^* P^*)$$

$$I_k = i\left(\frac{\partial L}{\partial \frac{\partial \varphi}{\partial x_k}}\varphi - \varphi^* \frac{\partial L}{\partial \frac{\partial \varphi^*}{\partial x_k}}\right)$$

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\, \mathbf{I} = i\left\{\left(\frac{\partial L}{\partial \varphi}\varphi + \sum_k \frac{\partial L}{\partial \frac{\partial \varphi}{\partial x_k}}\frac{\partial \varphi}{\partial x_k} + \frac{\partial L}{\partial \frac{\partial \varphi}{\partial t}}\frac{\partial \varphi}{\partial t}\right) - \text{h.c.}\right\} = 0$$

$\therefore \varphi \to \varphi(1 + i\alpha)$ $\qquad \varphi^* \to \varphi(1 - i\alpha)$

$$\delta L = i\alpha\left\{\left(\frac{\partial L}{\partial \varphi}\varphi + \cdots\right) - \text{h.c}\right\} = 0$$

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$$\varphi = \sum_k \sqrt{\frac{\hbar c}{2V k_0}} \left(a_k e^{i(kr - k_0 ct)} + b_k^* e^{-i(kr - k_0 ct)} \right)$$

$$\varphi^* = \sum_k \sqrt{\frac{\hbar c}{2V k_0}} \left(b_k e^{i(kr - k_0 ct)} + a_k^* e^{-i(\cdots)} \right)$$

$$\mathcal{L} = -\frac{\partial \varphi^*}{\partial x_\mu} \frac{\partial \varphi}{\partial x^\mu} - \varkappa^2 \varphi^* \varphi$$

$$= \sum_\alpha -\frac{1}{2} \left(\frac{\partial \varphi_\alpha}{\partial x_\mu} \frac{\partial \varphi_\alpha}{\partial x_\mu} + \varkappa^2 \varphi_\alpha \varphi_\alpha \right)$$

$$I = \sum k_0 \hbar c \left(N_k^{(+)} + N_k^{(-)} \right)$$

$$G_\Pi = \sum \hbar \left(N_k^{(+)} + N_k^{(-)} \right)$$

Problem:

Prove that the equation of continuity

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \mathbf{I} = 0$$

$$\left(\rho = -\frac{e}{\hbar} i (\varphi \dot{\varphi}^* - \varphi^* \dot{\varphi}) = \sum e \left(N_k^{(+)} - N_k^{(-)} \right) \right)$$

is satisfied, if the Lagrangian density

$$\mathcal{L}\left(\varphi, \varphi^*, \frac{\partial \varphi}{\partial x_i}, \frac{\partial \varphi^*}{\partial x_i}, \frac{\partial \varphi}{\partial t}, \frac{\partial \varphi^*}{\partial t} \right)$$

is invariant with respect to the gage transformation

$$\varphi \to \varphi e^{i\alpha}$$
$$\varphi^* \to \varphi^* e^{-i\alpha}$$

where α is ~~a constant~~ any real number and ρ, $\mathbf{I}$ are defined by

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ex $\rho = -i\left(\frac{\partial L}{\partial \frac{\partial \varphi}{\partial t}}\varphi - \varphi^* \frac{\partial L}{\partial \frac{\partial \varphi^*}{\partial t}}\right)$

$= -i(P\varphi - \varphi^* p^*)$

ex $I_x = -i\left(\frac{\partial L}{\partial \frac{\partial \varphi}{\partial x}}\varphi - \varphi^* \frac{\partial L}{\partial \frac{\partial \varphi^*}{\partial x}}\right)$

$\left(= i\left(\varphi^* \frac{\partial \varphi}{\partial x} - \varphi \frac{\partial \varphi^*}{\partial x}\right) + \frac{2e}{\hbar c} A_x \varphi^* \varphi\right)$

Interaction with E.M.F.

$L = -\left(\frac{\partial \varphi^*}{\partial x^\mu} + \frac{ie}{\hbar c} A_\mu \varphi^*\right)\left(\frac{\partial \varphi}{\partial x_\mu} - \frac{ie}{\hbar c} A^\mu \varphi\right) - \varkappa^2 \varphi^* \varphi$

$A_1 = A^1 = A_x$ etc, $A_4 = -A^4 = A_0$

$P = \frac{1}{c^2}\left(\frac{\partial \varphi^*}{\partial t} - \frac{ie}{\hbar} A_0 \varphi^*\right)$

$p^* = \frac{1}{c^2}\left(\frac{\partial \varphi}{\partial t} + \frac{ie}{\hbar} A_0 \varphi\right)$

$H = c^2 p^* p + \sum_i \frac{\partial \varphi^*}{\partial x_i}\frac{\partial \varphi}{\partial x_i} + \varkappa^2 \varphi^* \varphi$

$- \frac{ie}{\hbar} A_0 (P\varphi - p^* \varphi^*)$

$+ \frac{ie}{\hbar c} A (\varphi^* \operatorname{grad} \varphi - \varphi \operatorname{grad} \varphi^*) + \frac{e^2}{\hbar c^2} A^2 \varphi^* \varphi$

$\therefore H = P\frac{\partial \varphi}{\partial t} + \frac{\partial \varphi^*}{\partial t} p^* - L$

$= P\left(c^2 p^* - \frac{ie}{\hbar} A_0 \varphi\right) + \left(c^2 P + \frac{ie}{\hbar} A_0 \varphi^*\right) p^*$

$- \varkappa^2 P p^* + \sum_i \left(\frac{\partial \varphi^*}{\partial x_i} + \frac{ie}{\hbar c} A_i \varphi^*\right)$

$\times \left(\frac{\partial \varphi}{\partial x_i} - \frac{ie}{\hbar c} A_i \varphi\right) + \varkappa^2 \varphi^* \varphi$

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Relativistic Commutation Relations for Free Scalar Fields

$$[\varphi(x,t),\varphi(x',t')] = \sum_{k\,(k_0>0)} \frac{\hbar c}{2Vk_0}\{(a_k a_k^* - a_k^* a_k)$$
$$\times (e^{i(kx-k_0ct)} - e^{-i(kx-k_0ct)})\}$$

$$= \frac{i\hbar c}{V}\sum_{k\,(k_0>0)} \frac{1}{2ik_0}(e^{i(kx-k_0ct)} - e^{-i(kx-k_0ct)})$$

$$= i\hbar c\,\Delta(x-x',t-t')$$

$$\Delta(x,t) = \frac{1}{V}\sum_{k\,(k_0>0)} \frac{1}{2ik_0}(e^{i(kx-k_0ct)} - e^{-i(kx-k_0ct)})$$

$$= \frac{1}{(2\pi)^3}\iiint \left(\frac{e^{i(kx-k_0ct)} - e^{-i(kx-k_0ct)}}{2ik_0}\right) \times dk$$

$$\Delta(x,0) = 0$$

$$\frac{1}{c}\frac{\partial\Delta}{\partial t} = \frac{-1}{(2\pi)^3}\iiint e^{ikx}\,dk$$
$$= -\delta(x)$$

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or $\frac{1}{c}\frac{\partial \Delta}{\partial t'} = \delta(r)$

so that

$$[\varphi(r,t), P(r',t)] = [\varphi(r,t), \frac{1}{c^2}\frac{\partial \varphi(r',t)}{\partial t}]$$

$$= i\hbar\, \delta(r)$$

Invariant delta-function for reason:

$$\Delta(r,t) = \frac{1}{8\pi^3} \lim_{K\to\infty} \int_0^K \int_0^{\pi} \int_0^{2\pi} \frac{\sin(kr\cos\theta - k_0 ct)}{k_0}$$

$$\times k^2 dk \sin\theta d\theta d\varphi$$

$$= \frac{1}{4\pi^2 r} \left\{ \int_0^{\infty} \frac{\cos(kr - k_0 ct)}{k_0} k\, dk \right.$$

$$\left. - \int_0^{\infty} \frac{\cos(kr + k_0 ct)}{k_0} k\, dk \right\}$$

$$= \frac{1}{r}\frac{\partial}{\partial r} F(r,t)$$

$$F(r,t) = \frac{1}{4\pi^2} \left\{ \int_0^{\infty} \frac{\sin(kr + k_0 ct)}{k_0} k\, dk \right.$$

$$\left. - \int_0^{\infty} \frac{\sin(kr + k_0 ct)}{k_0} dk \right\}$$

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Region (i) $r > c|t|$

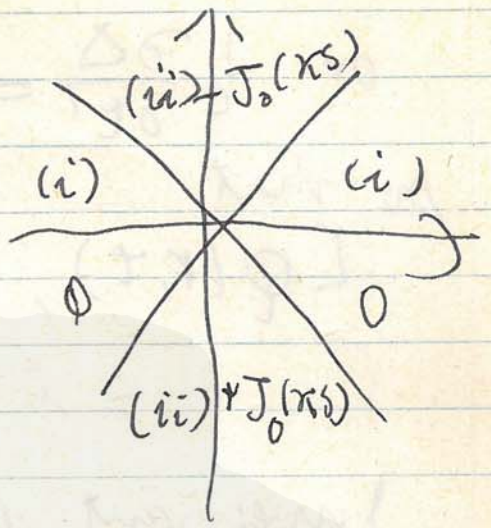
$s = \sqrt{r^2 - c^2t^2}$

$r = s \cosh\varphi$ }

$ct = s \sinh\varphi$ }

$k_0 = \kappa \cosh\chi$ }

$k_R = \kappa \sinh\chi$ }



$$F(r,t) = \frac{1}{4\pi^2}\int_{-\infty}^{+\infty} \sin(\kappa s \sinh(\chi-\varphi))\,d\chi$$

$$= \frac{1}{4\pi^2}\int_{-\infty}^{+\infty} \sin(\kappa s \sinh\chi)\,d\chi$$

$$= 0$$

since the integrand is an odd function of χ.

Region (i.) $r < c|t|$

$s = \sqrt{c^2t^2 - r^2}$ $\quad r = s\cosh\varphi$ }

$ct = \pm s\cosh\varphi$ }

$$F(r,t) = \mp\frac{1}{4\pi}\int_{-\infty}^{\pm\infty} \sin(\kappa s \cosh(\chi+\varphi))\,d\chi$$

$$= \mp\frac{1}{2\pi^2}\int_0^{\infty} (\sin\kappa s \cosh\chi)\,d\chi$$

$\frac{1}{2\pi^2}$ ⟶

$$= \mp\frac{1}{4\pi}J_0(\kappa s)$$

$$J_0(x) = \frac{2}{\pi}\int_0^{\infty} \sin(x\cosh\chi)\,d\chi$$

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$s^2 = \pm(r^2 - c^2t^2)$

$s\,ds = \pm r\,dr$

$\Delta(r,t) = \frac{1}{2\pi}\frac{\partial F(s)}{\partial s}$

$ct > r$ $\quad F = -\frac{1}{4\pi} J_0(\kappa\sqrt{c^2t^2 - r^2})$

$r > ct > -r$ $\quad F = 0$

$-ct < r$ $\quad F = \frac{1}{4\pi} J_0(\kappa\sqrt{c^2t^2 - r^2})$

Thus, $\Delta(r,t)$ is an invariant function which is zero outside the light cone.

There is only one other case

$$\Delta^{(1)}(r, ct) = \frac{1}{8\pi^3}\int \frac{e^{i(kr - k_0 ct)} - e^{i(kr - k_0 ct)}}{2ik_0}$$

which is invariant and satisfies the relativistic equation

$$\left(\Delta - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \kappa^2\right)\Delta^{(a)}(r, ct) = 0$$

But this function is not zero outside the light cone.

The invariance of Δ-function can be shown more directly in the following way;

$$\iiint_{-\infty}^{+\infty} e^{i(kr - k_0 ct)}\,\delta(k^2 - k_0^2 + \kappa^2)\,dk_0\,dk_x\,dk_y\,dk_z$$

$$= \iiint_{-\infty}^{+\infty} e^{i(k'r' - k_0' ct')}\,\delta(k'^2 - k_0'^2 + \kappa^2)\,dk_0'\,dk_x'\,dk_y'\,dk_z'$$

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is obviously invariant with respect to Lorentz transformations.

$$\int f(k, k_0)\,\delta(k^2 - k_0^2 + \kappa^2)\,dk_0 \quad *$$

$$= \int_{-\infty}^{k_0} f(k, k_0 = +\sqrt{k^2+\kappa^2})\frac{dk}{2k_0} + \int_{k_0}^{\infty} f(k, -\sqrt{\;})\frac{dk}{2k_0}$$

where $\kappa = -(k^2 - k_0^2 + \kappa^2)$

$d\kappa = 2k_0\,dk_0$

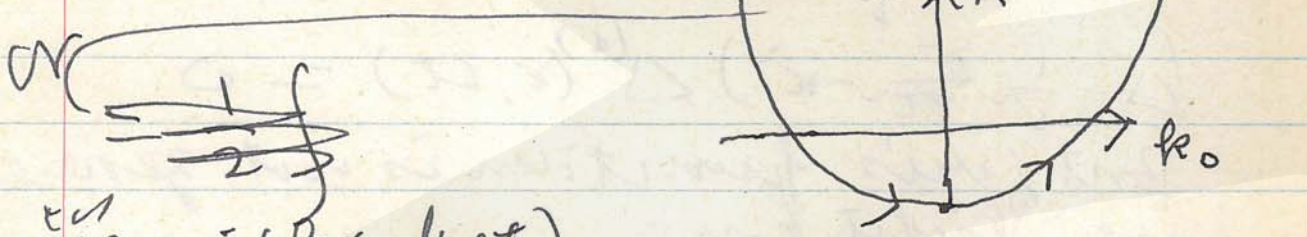
$k_0 = +\sqrt{k^2+\kappa^2} \rightarrow \kappa = 0$

$k_0 = -\sqrt{k^2+\kappa^2} \rightarrow \kappa = 0$

$k_0 = -\infty \Rightarrow \kappa = +\infty$

$k_0 = 0 \Rightarrow \kappa = -k^2$

$k_0 = +\infty \Rightarrow \kappa = +\infty$



$$\iiint_{-\infty}^{t\infty} e^{i(kr - k_0 ct)}\,\delta(k^2 - k_0^2 + \kappa^2)\,dk_0\,dk_x\,dk_y\,dk_z$$

$$= \iiint_{-\infty}^{t\infty} \frac{e^{i(kr - k_0 ct)}\ (k_0 = +\sqrt{\;}) + e^{-i(kr + k_0 ct)}\ (k_0 = -\sqrt{\;})}{2\sqrt{k^2+\kappa^2}}\,dk_x\,dk_y\,dk_z$$

$$= \iiint_{-\infty}^{t\infty} \frac{e^{i(kr - k_0 ct)} + e^{-i(kr - k_0 ct)}}{2\sqrt{k^2+\kappa^2}}\,dk_x\,dk_y\,dk_z$$

$k_0 \gtrless \pm\sqrt{k^2+\kappa^2}$

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$$\iiint_{-\infty}^{+\infty} e^{i(\mathbf{k}\mathbf{r}-k_0 ct)} \frac{k_0}{|k_0|} \delta(\mathbf{k}^2 - k_0^2 + \kappa^2)\, dk_0 \times dk_x dk_y dk_z$$

$$= \iiint_{-\infty}^{+\infty} \frac{e^{i(\mathbf{k}\mathbf{r}-k_0 ct)} - e^{-i(\mathbf{k}\mathbf{r}-k_0 ct)}}{2 \cdot k_0} dk_x dk_y dk_z$$

$$k_0 = +\sqrt{k^2+\kappa^2}$$

$$\Delta(\mathbf{r}, ct) = \frac{1}{(2\pi)^3 i} \iiint_{-\infty}^{+\infty} e^{i(\mathbf{k}\mathbf{r}-k_0 ct)} \times \frac{k_0}{|k_0|} \delta(\mathbf{k}^2 - k_0^2 + \kappa^2)\, dk_0 dk_x dk_y dk_z$$

$$\left.\begin{aligned} \Delta(x_i, x_4) &= \Delta(-x_i, x_4) \\ \Delta(x_i, -x_4) &= -\Delta(x_i, -x_4) \\ \Delta(x_i, x_4) &= -\Delta(-x_i, -x_4) \end{aligned}\right\}$$

$$* \int_{-\infty}^{+\infty} f(\mathbf{k}, k_0)\, \delta(\mathbf{k}^2 - k_0^2 + \kappa^2)\, dk_0$$

$$= \int_{k_0=-\infty}^{k_0=0} f(\mathbf{k}, k_0) \frac{dk_0}{-2k_0} + \int_{k_0=0}^{k_0=+\infty} f(\mathbf{k}, k_0) \frac{dk_0}{2k_0}$$

$$\kappa = -\sqrt{k^2+\kappa^2} \qquad \kappa = +\sqrt{k^2+\kappa^2}$$

$$\delta(k) \qquad \delta(k)$$

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Quantization of the electromagnetic field.

$$L = \frac{1}{2}(E^2 - H^2)$$

$$E_x = \frac{\partial A_1}{\partial x_4} - \frac{\partial A_4}{\partial x^1} = F_{41} = -F^{41}$$

$$H_x = \frac{\partial A_3}{\partial x^2} - \frac{\partial A_2}{\partial x^3} = F_{23}$$

$$L = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \qquad \left(\times \frac{1}{4\pi}\right)$$

$$\delta \int L \, dv dt = 0$$

$$\operatorname{curl} H - \frac{1}{c}\frac{\partial E}{\partial t} = 0 \Big\}$$

$$\operatorname{div} E = 0$$

or

$$\frac{\partial F_{\mu\nu}}{\partial x_\mu} = 0$$

$$P_\mu = \frac{\partial L}{\partial\left(\frac{\partial A_\mu}{\partial t}\right)} = -\frac{1}{c} F_{14} = \frac{1}{c} E_x$$

etc

$$P_4 = 0$$

$$H = \sum_\mu P_\mu \frac{\partial A_\mu}{\partial t} - L$$

$$= \frac{1}{2}(E^2 + H^2) - (E \operatorname{grad} A_0)$$

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Now,

$$\{A_0(x), P_0(x')\} = i\hbar\,\delta(x, x')$$

does not hold.

Fermi's method:

$$L = -\frac{1}{2}\cdot\frac{\partial A_\mu}{\partial x^\nu}\frac{\partial A^\mu}{\partial x_\nu}$$

$$\therefore -\frac{1}{4}\left(\frac{\partial A_\mu}{\partial x^\nu} - \frac{\partial A_\nu}{\partial x^\mu}\right)\left(\frac{\partial A^\mu}{\partial x_\nu} - \frac{\partial A^\nu}{\partial x_\mu}\right)$$

$$L' = -\frac{1}{2}\frac{\partial A_\mu}{\partial x^\nu}\frac{\partial A^\mu}{\partial x_\nu} + \frac{1}{4}\left(\frac{\partial A_\nu}{\partial x^\mu}\frac{\partial A^\mu}{\partial x^\nu} + \frac{\partial A_\mu}{\partial x^\nu}\frac{\partial A^\nu}{\partial x_\mu}\right)$$

$$= -\frac{1}{2}\frac{\partial A_\mu}{\partial x^\nu}\frac{\partial A^\mu}{\partial x_\nu} + \frac{1}{2}\frac{\partial}{\partial x^\mu}\left(A_\nu\frac{\partial A^\mu}{\partial x^\nu}\right)$$

$$\fallingdotseq -\frac{1}{2}A_\nu\frac{\partial}{\partial x^\nu}\left(\frac{\partial A^\mu}{\partial x^\mu}\right)$$

$$\iiint L'\,dx_1 dx_2 dx_3 dx_4$$

$$= \iiint L\,dx_1 dx_2 dx_3 dx_4$$

$$+\frac{1}{2}\iiint\frac{\partial}{\partial x^\mu}\left(A_\nu\frac{\partial A^\mu}{\partial x^\nu}\right)dx_1 dx_2 dx_3 dx_4$$

$$-\frac{1}{2}\iiint A_\nu\frac{\partial}{\partial x_\nu}\left(\frac{\partial A^\mu}{\partial x^\mu}\right)$$

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Thus, if the Lorentz condition

$$\frac{\partial A_\mu}{\partial x_\mu}\Psi = 0$$

is imposed on the wave function Ψ for the whole system, h is equivalent to h', in so far as that

$$P_\mu = \frac{1}{c}\frac{\partial L}{\partial \frac{\partial A_\mu}{\partial x_4}} = -\frac{i}{c}\frac{\partial A^\mu}{\partial x_4}$$

$$= \frac{1}{c^2}\frac{\partial A^\mu}{\partial t}$$

$$P_1 = \frac{1}{c^2}\frac{\partial A_1}{\partial t} \text{ etc}$$

$$P_4 = -\frac{1}{c^2}\frac{\partial A_0}{\partial t}$$

Lorentz condition

$$\left(-\frac{1}{c}P_4 + \operatorname{div} A\right)\Psi = 0.$$

$$[A_\mu(x,t), P_\nu(x',t)] = i\hbar\, \delta(x-x')$$

$$[A_\mu(x,t), A_\nu(x',t')] = i\hbar c\, g_{\mu\nu} \times D(x-x', t-t').$$

$$D(x,t) = \Delta_{r=0}(x,t)$$

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$$\frac{\partial A_\mu}{\partial x_\mu} \Psi = 0$$

$$A_\mu = \sum_{k,\lambda} \sqrt{\frac{\hbar c}{2Vk}} \{ e^{(\lambda)}_\mu a^{(\lambda)}_{k,\lambda} e^{i(kr - kct)} + a^{(\lambda)*}_k e^{-i(kr - kct)} \}$$

$$e^{(\lambda)}_\mu e^{(\lambda')}_\mu = \delta_{\lambda\lambda'}$$

$$[a^{(\lambda)}_k, a^{(\lambda')*}_{k'}] = \delta_{\lambda\lambda'} \delta_{kk'}$$

$$N^{(\lambda)}_k = a^{(\lambda)*}_k a^{(\lambda)}_k \qquad \lambda = 1, 2, 3$$

$$N^{(4)}_k = a^{(4)*}_k a^{(4)}_k - 1 \qquad \lambda = 4$$

$e^{(4)}$, $e^{(2)}$, k : $\perp$ to each other and $e^{(1)}$, $e^{(2)}$ have no time component

$e^{(3)}$ is $\perp$ to k and has no time component.

$e^{(4)}$ is a unit vector in time direction.

Lorentz condition:

$$\left.\begin{aligned} (a^{(3)}_k - a^{(4)}_k) \Psi = 0 \\ (a^{(3)*}_k - a^{(4)*}_k) \Psi = 0 \end{aligned}\right\}$$

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or $\left.\begin{aligned} b_{k}^{(4)*} &= a_{k}^{(4)} \\ b_{k}^{(4)} &= a_{k}^{(4)*} \end{aligned}\right\} N_{k}^{(4)} = b_{k}^{(4)*} b_{k}^{(4)}$

$$[\, b_{k}^{(4)}, b_{k'}^{(4)*} \,] = \delta_{k,k'}$$

$$\left.\begin{aligned} (a_{k}^{(3)} - b_{k}^{(4)*})\,\Psi &= 0 \\ (a_{k}^{(3)*} - b_{k}^{(4)})\,\Psi &= 0 \end{aligned}\right\}$$

$$\Psi(\cdots n_{k}^{(3)}, \cdots n_{k}^{(4)}, \cdots, t):$$

$$\Psi(\cdots, \cdots, \cdots n_{k}^{(3)}+1, \cdots n_{k}^{(4)}, \cdots, t)$$

$$= \Psi(\cdots, \cdots, \cdots n_{k}^{(3)}, n_{k}^{(4)}-1, \cdots, t)$$

$$\Psi(\cdots, \cdots, \cdots n_{k}^{(3)}-1, \cdots n_{k}^{(4)} \cdots, t)$$

$$= \Psi(\cdots, \cdots, n_{k}^{(3)}, \cdots n_{k}^{(4)}+1; t)$$

Thus, if Ψ is different from zero for $n_{k}^{(3)} = n_{k}^{(4)} = 0$, it must also be different from zero for $n_{k}^{(3)} = n_{k}^{(4)} = 1$,

because $a_{k}^{(4)*} b_{k}^{(3)*} \Psi = \Psi$.

Then Ψ must be also differentfrom zero for $n_{k}^{(3)} = n_{k}^{(4)} =$ any positive integer. Thus, the number of longitudinal

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photons and time-like photons ~~are~~ is indefinite, but the numbers must be equal to each other. The total energy of the electromagnetic field is positive definite, as long as the numbers of l. p. and t. lp. are equal to each other.

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Interaction between charged particles and el. mg. field.

$$L = -\frac{1}{2}\frac{\partial A_\mu}{\partial x_\nu}\frac{\partial A^\mu}{\partial x_\nu} + j^\mu A_\mu + (p.l.)$$

$$\frac{\partial A_\mu}{\partial x^\nu \partial x_\nu} = -j_\mu$$

($j_4 = +4\pi\rho$ in absolute ~~coordinate~~ unit system)

(or $j_4 = \sqrt{4\pi}\cdot\rho$ in rational unit system)

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Quantization of Spinor Field

$\frac{i}{\hbar}$

$$\left.\begin{aligned}&\{\gamma^\mu(p_\mu+\tfrac{e}{c}A_\mu)-imc\}\psi=0\\ &\psi^+\{\gamma^\mu(p_\mu+\tfrac{e}{c}A_\mu)-imc\}=0\end{aligned}\right\}$$

$\frac{i}{\hbar}$

$p_\mu = -i\hbar\frac{\partial}{\partial x^\mu}$ charge $-e$

$$\left.\begin{aligned}&\{\gamma^\mu(\tfrac{\partial}{\partial x^\mu}+\tfrac{ie}{\hbar c})+\varkappa\}\psi=0\\ &\{\bar\gamma^\mu(\tfrac{\partial}{\partial x^\mu}+\tfrac{ie}{\hbar c})+\varkappa\}\psi^\dagger=0\end{aligned}\right\}$$

$\bar\gamma$: transposed matrix

$\gamma^\mu\gamma^\nu+\gamma^\nu\gamma^\mu=2g^{\mu\nu}\ (=\delta_{\mu\nu})$

$\bar\psi=\psi^+\gamma^4$ $\quad\psi^+=-\bar\psi\gamma^4=\psi^*(i\beta)$

$(\gamma_1,\gamma_2,\gamma_3)\Rightarrow -i\beta\vec\alpha=\rho_2\vec\sigma$

$(\gamma^1,\gamma^2,\gamma^3)$

$\gamma^4=i\rho=i\rho_3=-\gamma_4$

$$L=+\psi^+\{\gamma^\mu c(p_\mu+\tfrac{e}{c}A_\mu)-imc^2\}\psi$$

is invariant, because

$\psi'=S\psi$, $\quad p'_\mu+\frac{e}{c}A'_\mu=a_\mu^{\ \nu}(p_\nu+\frac{e}{c}A_\nu)$

$\psi'^+=\psi^+S^{-1}$.

$\psi'^+\gamma^\mu(p'_\mu+\frac{e}{c}A'_\mu)\psi'=\psi^+S^{-1}\gamma^\mu S\cdot a_\mu^{\ \nu}(p_\nu+\frac{e}{c}A_\nu)\psi$

$S\gamma^\mu S^{-1}=\gamma^\nu a_\nu^{\ \mu}$ $\quad\gamma^\mu=S^{-1}\gamma^\nu S\,a_\nu^{\ \mu}$

or $S^{-1}\gamma^\mu S\,a_\mu^{\ \nu}=\gamma^\nu$

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$\psi_i(x)\psi_i^*(x') - \psi_i^*(x')\psi_i(x)$

$= \delta(x,x') = \psi_i(x)\psi_i^*(x') - \psi_i^*(x')\psi_i(x)$

$$L = -\psi^*\{(i\rho)\gamma^\mu c(\partial_\mu + \tfrac{e}{c}A_\mu) + \rho mc^2\}\psi$$

$$= -\psi^*\{c\,\alpha(\partial_{\rho\rho} + \tfrac{e}{c}A) - (i\hbar\tfrac{\partial}{\partial t} + eA_0) + \beta mc^2\}\psi$$

$$\frac{\partial L}{\partial \frac{\partial \psi_i}{\partial t}} = i\hbar\psi_i^*$$

$$H = \sum_i i\hbar\psi_i^*\frac{\partial\psi_i}{\partial t} - L$$

$$= -e\psi^* A_0\psi + \psi^*\{\alpha(c\rho + eA) + \beta mc^2\}\psi$$

If we assume

$$[\psi_i(x), \psi_j^*(x')] = \delta_{ij}\delta(x,x')$$
$$[\psi_i(x), \psi_j(x')] = 0$$
$$[\psi_i^*(x), \psi_j^*(x')] = 0 \qquad \}(I)$$

We obtain from

$$i\hbar\frac{\partial\psi_i}{\partial t} = [\psi_i, \overline{H}]$$
$$i\hbar\frac{\partial\psi_i^*}{\partial t} = [\psi_i^*, \overline{H}] \qquad \}(II)$$

Dirac wave equations.

However, this is in direct contradiction with the fact that the electrons obey F.D. statistics!*

Now there is another possibility: Let's introduce the anti-commutators

* Moreover (I) cannot be satisfied by $\psi_i(x)$ and $\psi_i^*(x')$

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$$[A, B]_+ = \{A, B\} = AB + BA$$

and let us assume that, instead of (I)

$$\left.\begin{aligned} &[\psi_i(x), \psi_j^*(x')]_+ = \delta_{ij}\,\delta(x, x') \\ &[\psi_i(x), \psi_j(x')]_+ = 0 \\ &[\psi_i^*(x), \psi_j^*(x')]_+ = 0 \end{aligned}\right\} \text{(I)}'$$

~~In order to~~ see what will come out from these new assumption?

First of all, ~~the (II) gives~~ reduce again to the the equations Dirac wave equations, because

$$[\psi_i(x), \sum_{j,k} \psi_j^*(x')\, \gamma_{jk}\, \psi_k(x')]$$

$$= \sum_{j,k} \{ [\psi_i(x), \psi_j^*(x')]_\mp \gamma_{jk}\, \psi_k(x')$$

$$\pm \psi_j^* \gamma_{jk} [\psi_i(x), \psi_k^*(x')]_\mp \}$$

$$= \sum_{j,k} \delta_{ij}\, \delta(x, x')\, \gamma_{jk}\, \psi_k(x')$$

~~:~~ $[A, BC] = ABC - BCA$

$$= (AB - BA)C + BCAC - CA)$$

$$= (AB + BA)C - BCAC + CA)$$

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$\int \bar{\psi}\psi dx = 1$

$$\left[\psi_i^*(x), \sum_{jk} \psi_j^*(x')\gamma_{jk}\psi_k(x')\right]$$

$$= \sum_{jk}\left\{\left[\psi_i^*(x), \psi_j^*(x')\right]_{\mp}\gamma_{jk}\psi_k(x')\right.$$

$$\left. \pm \psi_j^*(x')\gamma_{jk}\left[\psi_i^*(x), \psi_k(x')\right]_{\mp}\right\}$$

$$= \sum_{jk} \psi_j^*(x)\gamma_{jk}\delta_{ik}\delta(x,x')$$

Secondly, if we take the free field, ~~we can~~ we can expand ψ, ψ^* into Fourier series inside a cube of volume $V = L^3$.

$$\psi_i = \frac{1}{\sqrt{V}}\sum_k \left\{ u_i(k) e^{i(kx - k_0 ct)} + v_i^*(k) e^{-i(kx - k_0 ct)} \right\}$$

$K = k_0 + \kappa$

$$\frac{K^2 - k^2}{K^2 + k^2} = \frac{k_0^2 + 2k_0\kappa + \kappa^2 - k^2}{k_0^2 + 2k_0\kappa + \kappa^2 + k^2} = \frac{2k_0(k_0 + \kappa)}{2k_0(k_0 + \kappa)}$$

$$= \frac{2\kappa K}{2k_0 K} = \frac{\kappa}{k_0}$$

$$\left.\begin{aligned} u_1 &= \frac{K}{\sqrt{K^2 + k^2}} a_k^{(1)} + 0 \cdot a_k^{(2)} \\ u_2 &= 0 + \frac{K}{\sqrt{K^2 + k^2}} a_k^{(2)} \\ u_3 &= \frac{k_z}{\sqrt{K^2 + k^2}} a_k^{(1)} + \frac{k_x - ik_y}{\sqrt{K^2 + k^2}} a_k^{(2)} \\ u_4 &= \frac{k_x + ik_y}{\sqrt{K^2 + k^2}} a_k^{(1)} - \frac{k_z}{\sqrt{K^2 + k^2}} a_k^{(2)} \end{aligned}\right\}$$

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$$v_1^* = \frac{1}{\sqrt{K^2+k^2}}\left(k_z\, b_k^{(1)*} + (k_x - i k_y)\, b_k^{(2)*}\right)$$

$$v_2^* = \frac{1}{\sqrt{K^2+k^2}}\left((k_x + i k_y)\, b_k^{(1)*} - k_z\, b_k^{(2)*}\right)$$

$$v_3^* = \frac{K}{\sqrt{K^2+k^2}}\, b_k^{(1)*}$$

$$v_4^* = \frac{K}{\sqrt{K^2+k^2}}\, b_k^{(2)*}$$

$$K = k_0 + \kappa \qquad k_0 = \sqrt{k^2+\kappa^2}$$

$$\psi_i^* = \frac{1}{\sqrt{V}} \sum_k \left\{ u_{ki}\, e^{i(kx - k_0 ct)} + v_{ki}^*\, e^{-i(kx - k_0 ct)} \right\}$$

$$[\psi_i(x,t),\ \psi_j^*(x',t)]_+ = \delta_{ij}\,\delta(x,x')$$

$$= \sum_k [u_i(k), u_j^*(k)]_+ + [v_i^*(k), v_j(k)]_+ + [u_i(k), v_j(-k)]_+ + [v_i^*(k), u_j^*(-k)]_+$$

$$\left[\int \psi_i(x,t)\, e^{-ikx},\ \int \psi_j^*(x',t)\, e^{ik'x'}\right]_+$$

$$e^{ik_0 ct} \qquad e^{-ik_0 ct} = \delta_{ij} \int e^{-i(k-k')x} = V \delta_{ij}\,\delta_{kk'}$$

$$[u_i(k) + v_i^*(-k),\ v_j(k') + u_j^*(k')]_+ = \delta_{ij}\,\delta_{kk'}$$

$$[u_i(k) + v_i^*(-k),\ \{illegible\}] =$$

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$$[a_k^{(r)}, a_{k'}^{(s)*}]_+ = \delta_{rs}\delta(k,k')$$
$$[b_k^{(r)}, b_{k'}^{(s)*}]_+ = \delta_{rs}\delta(k,k')$$
$$[a_k^{(r)}, b_{k'}^{(s)}]_+ = 0 \quad \text{etc}$$
$$r,s = 1,2.$$

Proof:
$$\psi_i = \frac{1}{\sqrt{V}}\sum_k \varphi_i(k) e^{+ikx}$$
$$\psi_i^* = \frac{1}{\sqrt{V}}\sum \varphi_i^*(k) e^{-ikx}$$
$$[\varphi_i(k), \varphi_j^*(k')]_+ = \delta_{ij}\delta(k,k')$$
$$[\varphi_i(k), \varphi_j(k')]_+ = 0$$
etc
$$\varphi_i = \frac{1}{\sqrt{k^2+k^2}}\{\quad\}$$

Orthogonal transformation

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Relativistic Commutation Relations for Free spinor field

$$[\psi_i(x,t),\ \psi_j^\dagger(x',t')]_+ = \delta_{ij}\,S_{ij}(x,t;x',t')$$

$$\{\gamma^\mu p_\mu - imc\}\psi = 0$$

or $$\{\gamma^\mu \frac{\partial}{\partial x^\mu} + \varkappa\}\psi = 0$$

$$S_{ij}(x,t;x',t') \left(= S_{ij}(x-x', t-t')\right) = -\{\gamma^\mu \frac{\partial}{\partial x^\mu} - \varkappa\}_{ij}\Delta(x-x', t-t')$$

or $$S_{ij}(x,t) \simeq S_{ij}(x_\mu)$$

$$= -\{\gamma^\mu \frac{\partial}{\partial x^\mu} - \varkappa\}_{ij}\Delta(x_\mu)$$

$$\left\{\frac{\partial^2}{\partial x_\mu \partial x^\mu} - \varkappa^2\right\}\Delta \simeq 0$$

$\psi^* = \psi^\dagger \beta^4$ $\qquad \psi^\dagger = -\psi^* \gamma^4 \simeq -\psi^*(i\beta)$

$$[\psi_i(x,t), -\psi^*_k \gamma^4_{kj}]_+$$

$$= -\{\gamma^\mu \frac{\partial}{\partial x^\mu} - \varkappa\}_{ij}\Delta(x-x', t-t')$$

$$- \delta_{ik}\gamma^4_{kj}\,\delta(x-x')$$

$$= + \gamma^4_{ij}\,\frac{1}{c}\frac{\partial \Delta(x,t)}{\partial t}\Big|_{t=0}$$

$$= -\gamma^4_{ij}\,\delta(x-x')$$

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Problem. Prove the C.R., by starting from the Fourier expansion of ψ, ψ^* or $\psi^\dagger$ and making use of the comm. rel.

$$[a_k^{(j)}, a_{k'}^{(j')\dagger}]_+ = \delta_{jj'}\delta_{kk'}$$

etc.

Relation between Spin and Statistics

Pauli, Rev. Mod. Phys. July 1941

or Wentzel page 192.

$$[\varphi(x,t), \varphi(x',t')]_+ = i\hbar c\,\Delta(x-x', t-t')$$
$$[\varphi(x',t'), \varphi(x,t)]_+ = i\hbar c\,\Delta(x'-x, t'-t)$$

$$[\varphi(x,t), \varphi(x',t')]_+ + [\varphi(x',t'), \varphi(x,t)]_+$$
$$= i\hbar c\{\Delta(x-x', t-t') + \Delta(x'-x, t'-t)\}$$

$x \rightleftarrows x'$; $t \rightleftarrows t'$.

left hand side is unchanged
right hand side changes sign, which is impossible unless the both hand side are zero, which implies that. Since left-hand side is positive definite for $x = x'$, $t = t'$, φ is identically zero. (Δ is the only inv. for which sol is infinitesimal and

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which satisfies

$$\Delta = (\Box - \varkappa^2)\Delta = 0$$

In the case of the spinor field, the energy ~~momentum tensor~~ density which was derived from the energy-momentum tensor, is not positive definite whether we ~~take~~ assume B.E. or F.D. statistics ~~to be~~. In the former case, the difficulty of ~~Ehrenfest~~ negative energy particles cannot be avoided by Pauli hypothesis, while it can be in the latter case.

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Generalized Schrödinger Equation in Quantized Field Theory

Field Theory in Heisenberg Representation → Schrödinger Repr.

Particle System

(i) Heisenberg

$$i\hbar \frac{dq^{(H)}}{dt} = [q^{(H)}, H(q^{(H)}, p^{(H)})]$$
$$i\hbar \frac{dp^{(H)}}{dt} = [p^{(H)}, H(q^{(H)}, p^{(H)})]$$

$$\Psi^{(S)}(q, t) = e^{-iHt/\hbar} \Psi^{(H)}(q)$$

$$i\hbar \frac{\partial \Psi^{(H)}}{\partial t} = i\hbar \frac{\partial}{\partial t}\left(e^{iHt/\hbar}\Psi^{(S)}\right) - He^{iHt/\hbar}\Psi^{(S)} = 0$$

(ii) Schrödinger

$$q^{(H)} = e^{iHt/\hbar} q^{(S)} e^{-iHt/\hbar}$$
$$p^{(H)} = e^{iHt/\hbar} p^{(S)} e^{-iHt/\hbar}$$

$$e^{-iHt/\hbar} H(q^{(H)}, p^{(H)}) e^{iHt/\hbar} = H(q^{(S)}, p^{(S)})$$

or

$$H(q^{(H)}, p^{(H)}) = H(q^{(S)}, p^{(S)})$$

$$\frac{dq^{(S)}}{dt} = \frac{dp^{(S)}}{dt} = 0$$

$$i\hbar \frac{d}{dt} q^{(H)} = -H \cdot q^{(H)} + q^{(H)} \cdot H \quad \text{etc.}$$

$$i\hbar \frac{\partial \Psi^{(S)}(q, t)}{\partial t} = H\left(q, -i\hbar \frac{\partial}{\partial q}\right) \times \Psi^{(S)}(q, t)$$

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Field Theory

(i) Heisenberg representation

$$i\hbar \frac{\partial \varphi^{(H)}(x,t)}{\partial t} = [\varphi^{(H)}(x,t), \bar{H}]$$

$$i\hbar \frac{\partial p^{(H)}(x,t)}{\partial t} = [p^{(H)}(x,t), \bar{H}]$$

(field equations with interaction)

$$[\varphi^{(H)}(x,t), p^{(H)}(x',t)] = i\hbar\,\delta(x,x')$$

$$i\hbar \frac{\partial \Psi^{(H)}[\varphi(x),t)}{\partial t} = \bar{H}^{(H)} \Psi$$

(ii) Schrödinger representation

$$\left.\begin{aligned} \varphi^{(S)} &= e^{-i\bar{H}t/\hbar} \varphi^{(H)} e^{i\bar{H}t/\hbar} \\ p^{(S)} &= e^{-i\bar{H}t/\hbar} p^{(H)} e^{i\bar{H}t/\hbar} \end{aligned}\right\}$$

$$i\hbar \frac{\partial \varphi^{(S)}}{\partial t} = 0 \quad \text{etc.}$$

$$i\hbar \frac{\partial \Psi^{(S)}[\varphi(x),t)}{\partial t} = \bar{H} \Psi^{(S)}$$

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(iii') Interaction Representation

$\bar{H} = \int H dv = \bar{H}_0 + \bar{H}'$

$H = H_0 + H'$ $\quad \bar{H}_0 = \int H_0,\ \bar{H}' = \int H dv$

$$\left.\begin{aligned} \varphi^{(I)} &= e^{+i\bar{H}_0 t/\hbar}\, \varphi^{(S)}\, e^{-i\bar{H}_0 t/\hbar} \\ p^{(I)} &= e^{i\bar{H}_0 t/\hbar}\, p^{(S)}\, e^{-i\bar{H}_0 t/\hbar} \end{aligned}\right\}$$

$$i\hbar \frac{\partial \varphi^{(I)}}{\partial t} = [\varphi^{(I)}, \bar{H}_0] \text{ etc}$$

(full form field equations relativistically invariant)

~~$i\hbar \frac{\partial}{\partial t}$~~ $\Psi^{(I)} = e^{i\bar{H}_0 t/\hbar} \Psi^{(S)}$

$$i\hbar \frac{\partial \Psi^{(I)}}{\partial t} = -\bar{H}_0 e^{i\bar{H}_0 t/\hbar} \Psi^{(S)} + e^{i\bar{H}_0 t/\hbar} \bar{H} \Psi^{(S)}$$

$$= -\bar{H}_0 e^{i\bar{H}_0 t/\hbar} \Psi^{(S)} + \bar{H}_0 e^{i\bar{H}_0 t/\hbar} \Psi^{(S)} + e^{i\bar{H}_0 t/\hbar} \bar{H}' e^{-i\bar{H}_0 t/\hbar} \Psi^{(S)}$$

$$i\hbar \frac{\partial \Psi^{(I)}}{\partial t} = \bar{H}'(\varphi^{(I)}, p^{(I)}) \Psi^{(I)}$$

~~Schrödinger repr.~~ Schrödinger repr.

$$\varphi^{(S)}_{(N)} = \sum_k \sqrt{\frac{\hbar c}{2V k_0}} \left(a_k e^{ikr} + a_k^* e^{-ikr} \right)$$

~~(Heisenberg repr.~~

~~$\frac{da_k}{dt}$~~ $\varphi^{(I)}_{(N,t)} = e^{i\bar{H}_0 t/\hbar} \varphi^{(S)} e^{-i\bar{H}_0 t/\hbar}$

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$$\overline{H_0} \simeq \sum_{k} \hbar_0 k c \cdot N_k$$

$$e^{i k_0 c N_k t} a_k e^{-i k_0 c N_k t} \simeq$$

$$a_k a_k^* - a_k^* a_k \simeq 1$$

$$[N_k, a_k] \simeq -a_k$$

$$[N_k^2, a_k] \simeq 2 N_k a_k + a_k N_k$$

$$N_k a_k = a_k (N_k - 1)$$

$$(N_k)^2 a_k = a_k (N_k - 1)^2$$

etc.

$$e^{i k_0 c N_k t} a_k \simeq a_k e^{i k_0 c (N_k - 1) t}$$

$$e^{i k_0 c N_k t} a_k e^{-i k_0 c N_k t} \simeq a_k e^{-i k_0 c t}$$

$$e^{i k_0 c N_k t} a_k^* e^{\cdots} \simeq a_k^* e^{i k_0 c t}$$

$$\varphi^{(+)}(r,t) = \sum_k \sqrt{\frac{\hbar c}{2 V k_0}} \left(a_k e^{i(kr - k_0 c t)} + a_k^* e^{-i(kr - k_0 ct)} \right)$$

$*$ $a_k a_k^* - a_k^* a_k = 1$

$[N_k, a_k] \simeq -a_k$ $\quad [(N_k)^n, a_k] \simeq -n (N_k)^{n-1}$

$$\left[e^{i k_0 c N_k}, a_k \right] = \left[\sum \frac{1}{n!} (i k_0 c N_k)^n, a_k \right]$$

$$= \sum \frac{-1}{(n-1)!} (i k_0 c N_k)^{n-1}$$

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$$[\varphi(x,t), \varphi(x',t')] = i\hbar c \Delta(x-x', t-t')$$

(relativistically invariant)

field equations

$$(\Box - \varkappa^2)\varphi = 0$$

(relativistically invariant)

Schrödinger eq.

$$i\hbar \frac{\partial \Psi}{\partial t} = H'(t)\Psi$$

$$\Psi(\cdots n_R \cdots, t)$$

$$H'(\cdots a_R, \cdots a_R^*, t \cdots)$$

Example: self-interaction

$$H' = \varphi^3 = \left(\sum_R \sqrt{\frac{\hbar c}{2V k_0}} \left(a_R e^{i(kr - k_0 ct)} + a_R^* e^{-i(kr - k_0 ct)} \right) \right)^3$$

This is what we have already used in connection with the radiation theory.

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Example: Interaction between a spinor field and a neutral scalar field (nucleons and neutral mesons)

$$L = L_0 + L_2^{\#} + L_{12}$$

$$L_0 = +\psi^\dagger\{\gamma^\mu(c p_\mu - \cancel{e A_\mu}) - imc^2\}\psi\}$$

$$L_2 = -\frac{1}{2}\left(\frac{\partial\varphi}{\partial x_\mu}\frac{\partial\varphi}{\partial x^\mu} + \varkappa^2\varphi^2\right)$$

$$L_{12} = +g\varphi\psi^\dagger\psi = -g\varphi\psi^*\gamma^4\psi$$

Interaction representation

$$\varphi(r,t) = \sum_k \sqrt{\frac{\hbar c}{2V k_0}}\left(a_k e^{i(kr - k_0 ct)} + a_k^* e^{-i(kr-k_0ct)}\right)$$

$$\psi_i(r,t) = \frac{1}{\sqrt{V}}\sum_{k,r=1,2}\{b_k^{(r)} u_{i,k}^{(r)} e^{i(kr-k_0ct)} + c_k^{(r)*} v_{i,k}^{(r)} e^{-i(kr-k_0ct)}\}$$

$$k_0 = \sqrt{k^2+\lambda^2} \qquad \lambda = \frac{Mc}{\hbar}$$

$$[b_k^{(r)}, b_{k'}^{(s)*}]_+ = \delta_{kk'}\delta_{rs}$$

$$[b_k^{(r)}, c_{k'}^{(s)}]_+ = 0 \quad \text{etc}$$

$$[c_k^{(r)}, c_{k'}^{(s)*}]_+ = \delta_{kk'}\delta_{rs} \quad \text{etc}$$

$$\psi_i^*(r,t) = \frac{1}{\sqrt{V}}\sum_{l,r=1,2}\{b_l^{(r)*} u_{i,l}^{(r)} e^{-i(lr-l_0ct)} + c_l^{(r)} v_{i,l}^{(r)} e^{i(lr-l_0ct)}\}$$

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	$u_\ell^{(1)}$	$u_\ell^{(2)}$	$v_\ell^{(1)}$	$v_\ell^{(2)}$
u_1	$\frac{L}{\sqrt{k^2+l^2}}$	0	$l_z\sqrt{\quad}$	$l_x+il_y\sqrt{\quad}$
u_2	0	$k/\sqrt{k^2+l^2}$	$l_x-il_y\sqrt{\quad}$	$-l_z\sqrt{\quad}$
u_3	$l_z\sqrt{k^2+l^2}$	$l_x-il_y\sqrt{\quad}$	$k/\sqrt{k^2+l^2}$	0
u_4	$l_x+il_y\sqrt{\quad}-l_z\sqrt{\quad}$	0		$k/\sqrt{k^2+l^2}$

$$k = \lambda + l_0$$

$$\begin{cases} \cdot\ i\hbar\frac{\partial\Psi}{\partial t} = \bar{H}'\Psi \\ \Psi(\ldots n_p \ldots; \ldots n_\ell^{(+)(r)} \ldots n_{\ell'}^{(-)(s)} \ldots; t) \end{cases}$$

$$N_p = a_p^* a_p$$

$$N_\ell^{(+)(r)} = b_\ell^{(r)*} b_\ell^{(r)}, \quad N_\ell^{(-)(r)} = c_\ell^{(r)*} c_\ell^{(r)}$$

$$H' = -L_{12} \approx g\,\varphi\,\psi^*\gamma^4\psi$$

$\bar{H}'$ depends explicitly on time, because

$$\bar{H}' \neq a_p^* b_\ell^{(r)*} c_{\ell'}^{(s)*} e^{i(k_0+l_0+l_0')x_4} \times V^{-3/2}\sqrt{\frac{\pi c}{2k_0}}\sum_{ij}\tilde{u}_{i,\ell}^{(r)}\gamma_{ij}^4 v_{j,\ell'}^{(s)}\int e^{-i(p+\ell+\ell')x}\,dv$$

$$V^{-1/2}\,\delta_{p+\ell+\ell',0}$$

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conservation of momentum

$$\Psi = c_0 \Psi_0(\cdots n_{k^0}; \cdots n_{\ell}^{(+)(V)} \cdots; \cdots n_{\ell'}^{(-)(S)} \cdots; 0) \, e^{-i(k_0+\ell_0+\ell_0')t}$$

$$+ \sum c_{0\cdots1\cdots} \Psi_{0\cdots1\cdots;0\cdots1\cdots;0\cdots1\cdots}$$

$$+ \cdots$$

~~$\hbar c (k_0+\ell_0+\ell_0') \Psi_{0\cdots1\cdots;\cdots1\cdots;\cdots1\cdots}$~~

$$\gamma \quad \rho_1(n) = \left(\frac{\partial \varphi_1'^{*}}{\partial t}\right)\varphi_1' + \varphi_1'^{*}\frac{\partial \varphi_1'}{\partial t}$$

$$= 0$$

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Dirac's many time formulation

$q_1 q_2 \cdots q_n$ n-particles

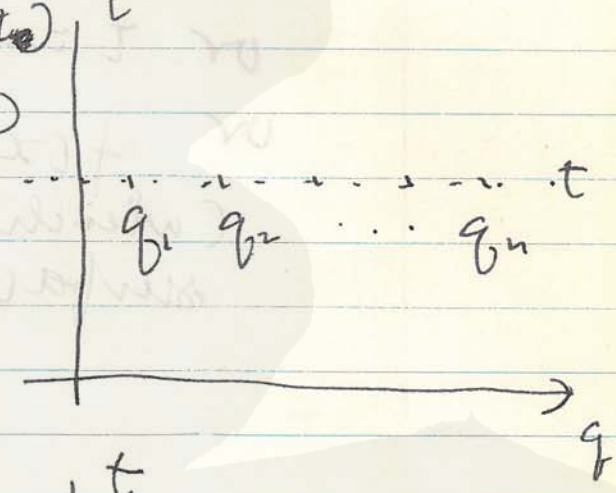
$$i\hbar \frac{\partial \Psi(q_1 q_2 \cdots q_n t)}{\partial t} = H(q_1 \cdots q_n, p_1 \cdots p_n)\Psi$$

$\Psi(q_1 t_1, q_2 t_2, \cdots q_n t_n)$

$(q_1 t_1), (q_2 t_2), \cdots (q_n t_n)$ are all space-like to each other

$$\Psi(q_1 t, q_2 t, \cdots q_n t) = \Psi(q_1 q_2 \cdots q_n, t)$$

$$\frac{\partial \Psi(q_1 t, \cdots q_n t)}{\partial t} = \sum_{i=1}^{n} \frac{\partial \Psi}{\partial t_i}\Big|_{t_i = t}$$



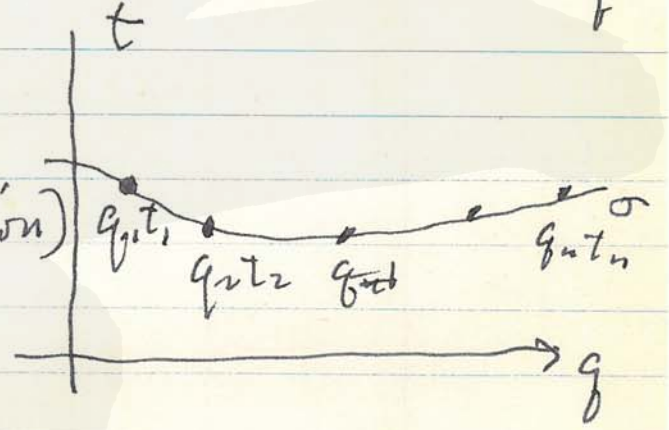
$$i\hbar \frac{\partial \Psi}{\partial t_i} = H_i(q_i, p_i)\Psi$$

(one particle equation)

$t_1, t_2, \cdots t_n \to t$

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$$

with $H = \sum_{i=1}^{n} H_i$



$(q_i t_i) \to \varphi(r_i, t_i)$

$n \to \infty$ $\Psi(\varphi(r_a, t)/\sigma)$ $t(r) = t_{xyz}$

$$i\hbar \frac{\delta \Psi}{\delta \sigma_p} = H_p \Psi$$

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$q, t_1 \cdots q_n t_n$

$\to \rho(q, t_q) \to \rho(x_{yz}, t_{xyz})$

$\to \varphi(x, y, z, t_{xyz})$

$\sigma: \quad t_{xyz} = t(x, y, z)$

or $t = f(x, y, z)$

or $f(x, y, z, t) = 0$

(which defines a space-like surface)

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Tomonaga-Schwinger Eq.

Tomonaga, P. T. P. 1 (1946), 27 etc.
Schwinger, Phys. Rev. 1948 ~ 1949

$[\varphi_1(x,t), \varphi_1(x',t)] = 0$
$[\varphi_2(x,t), \varphi_2(x',t)] = 0$
etc.

74	1439('48)
75	651('49)
76	790('49)

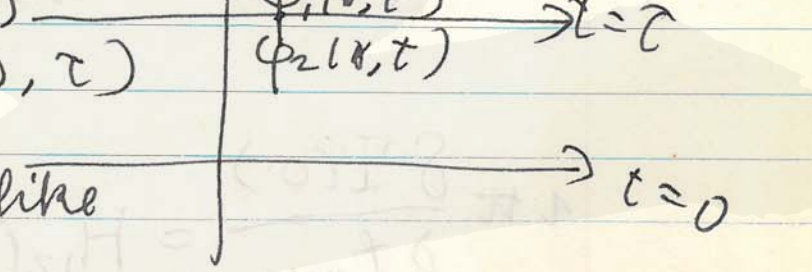
$\Psi(\varphi_1'(x,t); \varphi_2'(x,t); *)$

$$i\hbar \frac{\partial \Psi}{\partial t} = \int H_{12}\left(\varphi_1'(x,t), \varphi_2'(x,t), \frac{\partial \varphi}{\partial x_\mu}, \frac{\partial \varphi_2}{\partial x_\mu}\right) dv \cdot \Psi$$

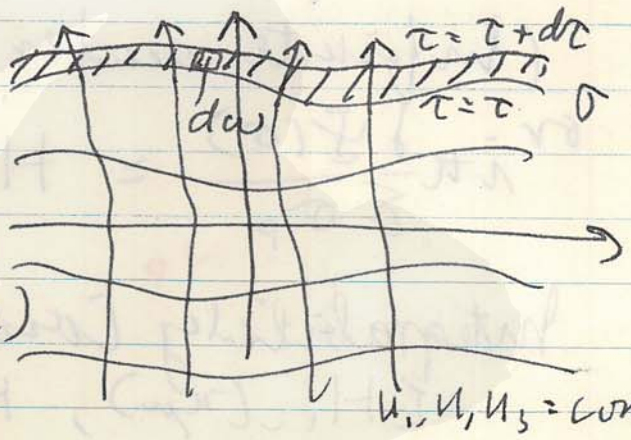
$\Psi(\varphi_1'(x,t+dt); \varphi_2'(x,t+dt)) - \Psi(\varphi_1'(x,t); \varphi_2'(x,t))$
$= -\frac{i}{\hbar} dt \int H_{12}(\,)\, dv \cdot \Psi(\varphi_1'(x,t); \cdots)$

$\Psi(\varphi_1'(x_\mu/\sigma), \varphi_2'(x_\mu/\sigma), \sigma)$

$\Psi(\varphi_1'(u_1,u_2,u_3,\tau), \varphi_2'(u_1,u_2,u_3,\tau), \tau)$



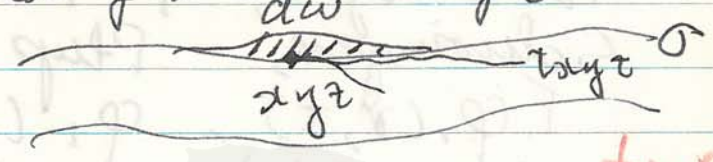
u_1, u_2, u_3 : space-like parameters
τ : time-like parameter



$\Psi(\varphi_1'(u_1,u_2,u_3,\tau+d\tau), \varphi_2'(u_1,u_2,u_3,\tau+d\tau))$
$- \Psi(\varphi_1'(u_1,u_2,u_3,\tau), \varphi_2'(\cdots))$
$= -\frac{i}{\hbar} \int H_{12}(\cdots)\, d\omega \cdot \Psi(\varphi_1'(u_1,u_2,u_3,\tau); \cdots)$

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~~Wilson step~~: super-meeting time



$\Psi(\varphi_1(x,y,z,t_{xyz}),\ldots)$

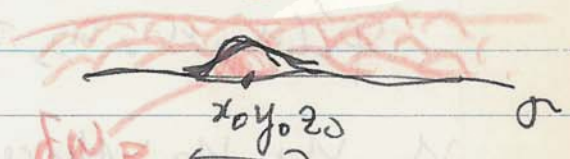
$\Psi(\varphi_1(x,y,z,t_{xyz}+\varepsilon_{xyz}),\ldots)$

$-\Psi(\varphi_1(x,y,z,t_{xyz}),\ldots)$ $\varepsilon\,\delta(x-x_0)$ → $f(x-x_0)$

$= -\frac{i}{\hbar}\iiint H_{12}(\varphi_1(x,y,z,t_{xyz}),\ldots)\,\varepsilon_{xyz}\,dxdydz$

$\delta(x-x_0) \to f(x-x_0)$

or $\dfrac{\delta\Psi}{\delta t_{x_0y_0z_0}} = \lim_{\substack{\varepsilon_{xyz}\to 0 \\ V_0\to 0 \\ (x_0y_0z_0 \text{ in } V_0)}} \dfrac{\Psi(\varphi_1(t+\varepsilon),\ldots)-\Psi(\varphi_1(t),\ldots)}{\iiint_{V_0}\varepsilon_{xyz}\,dxdydz}$



$$i\hbar\frac{\delta\Psi(\sigma)}{\delta t_{xyz}} = H_{12}(\varphi_1(xyz,t_{xyz});\ldots)\Psi(\sigma)$$

(Infinite number of simultaneous equations)

or $$i\hbar\frac{\delta\Psi(\sigma)}{\delta\sigma_P} = H_{12}(P)\Psi(\sigma)$$

δw_P

Integrability condition

$[H_{12}(x_\mu), H_{12}(x'_\mu)] = 0$

for $x_\mu - x'_\mu$: space-like

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Invariance

If H_{12} is invariant, T. S. eq. is invariant, and the motion of space-like surface is relativ. invariant

Feynman 76 (1949), 749; 769
(75, 486; 1736)
(Dyson, P. R. 1949)

Formal integration of T. S. eq.

Formal integration of Schrödinger equation: $H_{12} \to H$

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = \int H'(xyzt)\,dx\,dy\,dz \cdot \Psi(t)$$

1st approximation:

$$\Psi(t) \simeq \Psi(t_0) - \frac{i}{\hbar} \int_{t'=t_0}^{t} \iiint H'(x'y'z't')\,dx'dy'dz'dt' \cdot \Psi(t_0)$$

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = \int H'(x'y'z't')\,dx'dy'dz' \cdot \Psi(t_0)$$

$$- \frac{i}{\hbar} \int H'(xyzt)\,dx\,dy\,dz \times \int_{t'=t_0}^{t} H'(x'y'z't')\,dx'dy'dz'dt' \cdot \Psi(t_0)$$

$$\Psi(t) \simeq \Psi(t_0) - \frac{i}{\hbar} \int_{t'=t_0}^{t} \iiint H'(x'y'z')\,dx'dy'dz'dt' \times \Psi(t_0)$$

$$+ \left(\frac{i}{\hbar}\right)^2 \int_{t'=t_0}^{t} \int_{t''=t_0}^{t'} \iiint H'(x'y'z't') \times H'(x''y''z''t'')\,dx'dy'dz'dt'dx''dy''dz''dt'' \cdot \Psi(t_0)$$

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$$\Psi(t) = U_{(t,t_0)} \Psi(t_0)$$

$$U(t,t_0) = \sum_{n=0} \int\cdots\int \left(\frac{-i}{\hbar}\right)^n H(x'y'z't')\cdots; H(x^{(n)}y^{(n)}z^{(n)}t^{(n)})$$

$$t \geq t' \geq t'' \cdots \geq t^{(n)} \geq t_0 \qquad dx'dy'dz'dt' \cdots dx^{(n)}dy^{(n)}dt^{(n)}dt^{(n)}$$

~~$x_4 = ct$~~, $U(+\infty, -\infty) \equiv S$.

~~$\Psi(x_4) = U(x_4, x_4^{(0)})$~~

$$\Psi(+\infty) = U(+\infty, -\infty)\Psi(-\infty)$$
$$= S\,\Psi(-\infty)$$

$$S = \sum_{n=0}^{\infty} \int\cdots\int \left(\frac{-i}{\hbar}\right)^n H'(x'y'z't')$$
$$(t' \geq t'' \cdots \geq t^{(n)}) \times \cdots H'(x^{(n)}, y^{(n)}, z^{(n)}, t^{(n)})$$
$$\times\, dx'dy'dz'dt' \cdots dx^{(n)} \cdots dt^{(n)}$$

$$S = \sum_{n=0}^{\infty} \int\cdots\int \left(\frac{-i}{\hbar c}\right)^n H'(x'_\mu)\cdots H'(x^{(n)}_\mu)$$
$$x'_4 \geq \cdots x_4^{(n)} \quad \times (dx'_\mu)^4 \cdots (dx^{(n)}_\mu)^4$$

$$\iint_{x'_4 \geq x_4^{(n)}} H'(x'_\mu) H'(x''_\mu)(dx'_\mu)^4 (dx''_\mu)^4$$

$$= \iint H'(x''_\mu) H'(x'_\mu)(dx'_\mu)^4 (dx''_\mu)^4$$

$$x'_4 \leq x_4$$
$$= \frac{1}{2} \iint P\,(H(x'_\mu) H(x''_\mu))(dx'_\mu)^4 (dx''_\mu)^4$$

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$$S = \sum_{n=0}^{\infty} \int \cdots \int \left(\frac{-i}{\hbar c}\right)^n \frac{1}{n!} P\left(H'(x_\mu') \cdots H'(x_\mu^{(n)})\right) (dx_\mu')^4 \cdots (dx_\mu^{(n)})^4$$

~~Relativistic~~ as Generalization:

$$S = \sum_{n=0}^{\infty} \int \cdots \int \left(\frac{-i}{\hbar c}\right)^n \cancel{\theta(x_\mu', x_\mu'')} H'(x_\mu') \theta(x_\mu', x_\mu'') H'(x_\mu'') \theta(x_\mu'', x_\mu''') \cdots H'(x_\mu^{(n-1)}) \theta(x_\mu^{(n-1)}, x_\mu^{(n)}) H'(x_\mu^{(n)}) (dx_\mu')^4 \cdots (dx_\mu^{(n)})^4$$

$$\theta(x_\mu', x_\mu'') = 1 \quad \text{for} \quad \left\{ x_\mu' > x_\mu'' \right.$$

~~future like~~

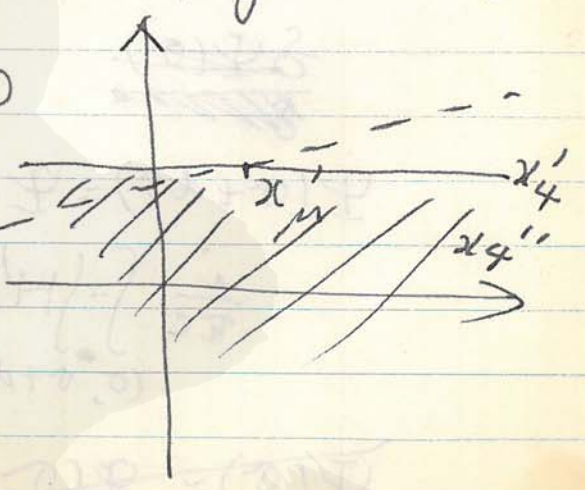
$$\left. x_\mu' - x_\mu'' \right\}$$

$$= 0 \quad \text{for} \quad x_\mu' < x_\mu''$$

S is independent of the choice of ~~for all~~ coordinate system, provided that

$$[H'(x_\mu'), H'(x_\mu'')] = 0$$

for space-like $x_\mu' - x_\mu''$.



Physical Interpretation of S-matrix

$|(m|S|n)|^2$

probability ~ ~ .

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~~Formal Integration of T. S. Equations~~

$$\Psi(-\sigma) = \sum_n C_n(-\sigma)\,\Psi_n$$

$$\Psi(+\sigma) = \sum_n C_n(+\sigma)\,\Psi_n$$

$$\sum_m C_m(\sigma)\Psi_m = \sum_n C_n(+\sigma)\,S\,\Psi_n$$

$$C_m(+\sigma) = \sum_n C_n(+\sigma)\cdot S_{mn}$$

$$S_{mn} = \int \Psi_m^* S\,\Psi_n$$

$C_n(-\sigma) = 1$ for $n = n$

0 otherwise

$$|C_m(+\sigma)|^2 = |S_{mn}|^2$$

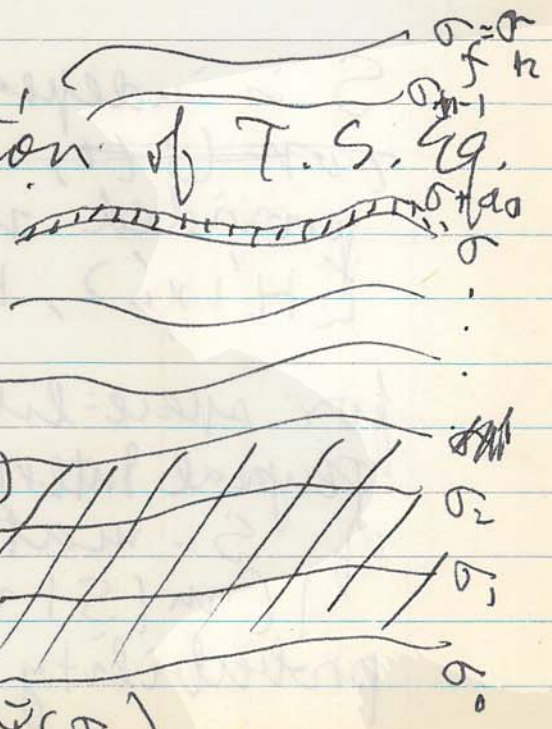
$$\Psi_n \equiv \Psi_{\ldots n_{kl}\ldots}$$

Formal Integration of T. S. Eq.

~~$\delta\Psi(\sigma)$~~

$$\Psi(\sigma+d\sigma) = \Psi(\sigma) - \frac{i}{\hbar c}\int_{(\sigma,\,\sigma+d\sigma)}\cdots\int H'(x_\mu)(dx_\mu)^4\,\Psi(\sigma)$$

~~$\Psi(\sigma) \equiv \Psi(\sigma_0) - \frac{i}{\hbar c}\int_{(\sigma_0,\,\sigma)}\cdots\int H(x_\mu)(dx_\mu)^4\,\Psi(\sigma_0)$~~



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$\sigma_f = \sigma_n$

$$\Psi(\sigma_f) \cong \left(1 - \frac{i}{\hbar c}\int_{\sigma_{f-1}}^{\sigma_f}\cdots\int H(x_\mu)(dx_\mu)^4\right)\Psi(\sigma_{n-1})$$

$$\Psi(\sigma_{n-1}) \cong \left(1 - \frac{i}{\hbar c}\int_{\sigma_{f-2}}^{\sigma_{f-1}}\cdots\int H(x_\mu)(dx_\mu)^4\right)\Psi(\sigma_{n-2})$$

$$\vdots$$

$$\Psi(\sigma_1) \cong \left(1 - \frac{i}{\hbar c}\int_{\sigma_0}^{\sigma_1}\cdots\int H(x_\mu)(dx_\mu)^4\right)\Psi(\sigma_0)$$

$$\Psi(\sigma_f) \cong \prod(1-\cdots)\,\Psi(\sigma_0)$$

$n\to\infty$

$$= \left\{1 - \left(\frac{i}{\hbar c}\right)\int_{\sigma_0}^{\sigma_f}\cdots\int H(x_\mu)(dx_\mu)^4\right.$$

$n\to\infty$

$$+ \left(\frac{-i}{\hbar c}\right)^2\int_{\sigma_0}^{\sigma_f}\cdots\int H(x_\mu)\,H(x'_\mu)(dx_\mu)^4(dx'_\mu)^4$$

$x_\mu \gtrsim x'_\mu$ (x_μ/σ; x'_μ/σ'; σ is later (not earlier) than σ')

$$\cdots$$

$$+ \left(\frac{-i}{\hbar c}\right)^n\int\cdots\int H(x_\mu)\,H(x'_\mu)\cdots H(x_\mu^{(n-1)}) \times (dx_\mu)^4\cdots(dx_\mu^{(n-1)})^4$$

$x_\mu > x'_\mu > \cdots x_\mu^{(n-1)}$

$$\left.+\cdots\right\}\Psi(\sigma_0)$$

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$$\Psi(\sigma_f) = U(\sigma_f, \sigma_0)\Psi(\sigma_0)$$

$$U(\sigma_f, \sigma_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar c}\right)^n \int\cdots\int_{\sigma_0} H'(x_1) \cdots H'(x_n)\, dx_1 \cdots dx_n$$

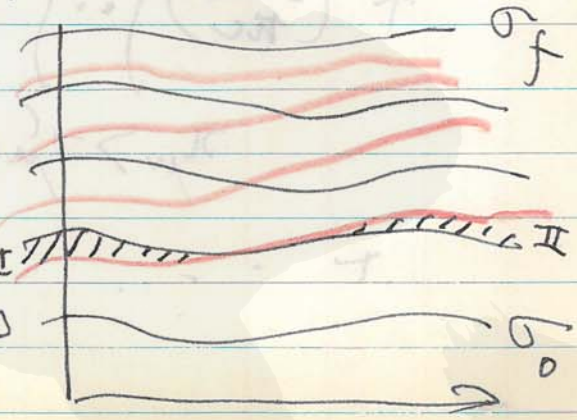
$$x_1 > x_2 > \cdots > x_n$$

$$= \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar c}\right)^n \frac{1}{n!} \int\cdots\int_{\sigma_0}^{\sigma_f} P\left(H'(x_1)\cdots H'(x_n)\right) dx_1 \cdots dx_n$$

Integrability:

$U(\sigma_f, \sigma_0)$ is independent of the choice of the space-like surfaces $\sigma_1, \sigma_2, \cdots \sigma_{n-1}$ ~~between σ_0 and σ_f~~ depends only on σ_f, σ_0, provided field variables, or, that $H'(x_1)$, $H'(x_2)$ are commutative for space-like $x_1 - x_2$.

Proof: the two $P\left(H'(x_1)\cdots H'(x_n)\right)$ in two different families of surfaces $(\sigma_1 \sigma_2 \cdots \sigma_n)$ and



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$(\sigma'_1 \dots \sigma'_{n-1})$ are different, ~~only~~ if, for instance, in the case:

$$P(H'(x_\mu)\, H'(x'_\mu)) = H(x_\mu) H(x'_\mu)$$

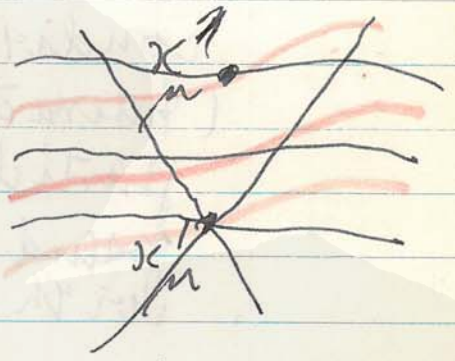
$x_\mu > x'_\mu$ in σ-system

~~Else~~

$$H'(x'_\mu)\, H'(x_\mu)$$

$x_\mu < x'_\mu$ in σ'-system.

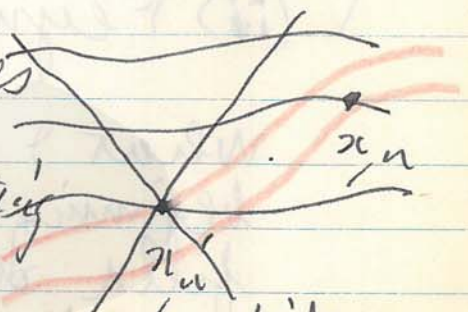
this happens, only if x_μ, x'_μ are space~~-~~like to each other, but in that case the order does not matter, because $H'(x_\mu), H(x'_\mu)$ commute with each other.



time-like
$x_\mu > x'_\mu$ indep of σ-system

$$\Psi(+\infty) = S\, \Psi(-\infty).$$

S-matrix is defined also independ of the choice of the family of space-like surfaces and coincides with the S-matrix obtained by integrating Schrödinger equation.



space-like
$x_\mu > x'_\mu$ (σ)
$x_\mu < x'_\mu$ (σ')

For collision problems, the knowledge of S-matrix is sufficient.

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Remark R: (in ordinary theory)

If the interaction Hamiltonian H_{12} (or H') contains the derivatives of field quantities, the corresponding $H_1(x_4)$ (or $K(x_4)$) in super-many time formalism depends on the surface normal n_μ of σ which passes through x_μ: $H'(x_\mu, n_\mu)$

n_μ: unit vector normal to σ at the point x_μ. The integrability condition is more complicated.

(Interaction between charged scalar particles and el.-mg. field, pseudo-scalar mesons and nucleons with pseudo-vector coupling)

Question of Convergence of S-matrix,

(i) Renormalization,

(ii) Non-local interaction

(iii) Feynman diagram

What I have told is just the beginning of the contemporary relativistic field theories. Further developments of and applications of the general formalism will be discussed in advance q. m. next year.

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May 21, 1952

Physics 238

Professor Yukawa

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Physics 238 Final Examination May 21, 1952

1. What physical interpretation could be given to each of the four components of Dirac wave function? (Discuss in connection with the free electron.)

   What are the relations of Dirac, Pauli, and Schrödinger wave functions to eachother? Draw qualitative diagrams of corresponding energy levels of a hydrogen atom and an alkali atom with a brief explanation.

2. Find by the variation mehod an approximate Schrödinger function for the ground state of the hydrogen atom in the uniform electric field F in z-direction. Take a trial function of the form

$$\psi = Ne^{-r/a}(1 + \mu z)$$

   where N is a normalization constant, and $a = \hbar^2/me^2$, and μ is the parameter to be determined.

   Show that, in this approximation, the energy of the hydrogen atom is given by

$$E = E_0 - 2a^3F^2$$

   where E_0 is the energy of the ground state in the absence of the external field and that the magnitude of the induced electric moment is $4a^3F$.

3. What are the advantages of the method of quantization of fields? Discuss also the problem of positron from the standpoint of the quantized field theory.

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Problem 1.

State the variation principle in non-relativistic quantum mechanics and apply it to the following problem in order to find an approximate solution.

The Hamiltonian for a molecule consisting of N-nuclei and n-electrons be

$$H = +\sum_{\alpha=1}^{N} \frac{\hbar^2}{2M_\alpha} \nabla^2_{\mathbf{P}_\alpha} + \sum_{k=1}^{n} \frac{\hbar^2}{2m} \nabla^2_{\mathbf{r}_k} + V(\mathbf{r}_k, \mathbf{P}_\alpha),$$

and $\psi(\mathbf{r}_k, \mathbf{P}_\alpha)$ be the eigenfunction for an electronic state of the molecule satisfying

$$\left\{ -\frac{\hbar^2}{2m} \Delta_k + V(\mathbf{r}_k, \mathbf{P}_\alpha) \right\} \psi = W(R_{\alpha\beta}) \psi$$

where $R_{\alpha\beta}$ is the distance between α-th nucleus and β-th nucleus.

~~Find the best solution for the whole wave function molecule of the form~~

~~$$\Psi(\mathbf{r}_k, \mathbf{P}_\alpha) = \chi(\mathbf{P}_\alpha) \psi(\mathbf{r}_k, \mathbf{P}_\alpha).$$~~

~~Find~~ What is the differential equation for the nuclear wave function $\chi(\mathbf{P}_\alpha)$, which is so chosen that the whole wave function for the molecule, ~~take~~ of the form

$$\Psi(\mathbf{r}_k, \mathbf{P}_\alpha) = \chi(\mathbf{P}_\alpha) \psi(\mathbf{r}_k, \mathbf{P}_\alpha)$$

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becomes the best solution (in the sense) according of the variation principle.

Remark: $W(R_{\alpha s})$ has a minimum at equilibrium distances R_α between nuclei, and $\nabla_\alpha \psi(r_k, R_\alpha)$ are supposed to be all small for those values of R_α in the neighborhood of the equilibrium ~~distances~~ configuration.

Discuss further, the decomposition of χ into rotational and vibrational functions in the case of diatomic molecule.

Problem 2.

n-identical Fermions (electrons, nucleons, etc) are moving in a common field as given by a ~~certain~~ potential V. If the mutual interaction between these particles is ignored, the ground state of the system is given by

$$\Psi(x_1, \cdots x_n) = \frac{1}{\sqrt{n!}} \begin{vmatrix} \psi_1(x_1) & \cdots & \psi_n(x_n) \\ \vdots & & \\ \psi_n(x_1) & \cdots & \psi_n(x_n) \end{vmatrix}$$

where $\psi_1, \cdots \psi_n$ are ~~mutually~~ normalized orthogonal functions belonging to the lowest energy values of the one-body problem. This will be a good approximation

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~~Now the problem is to show that, if there are only $n-1$ - Fermions instead of n,~~
for the wave function, even when we take into account the interaction between these particles, provided that all other energy ~~levels~~ eigenvalues of the one-body problem are much higher than those which correspond to $\psi_1, \cdots \psi_n$.

Now the problem is to show that, if there are only $n-1$ - Fermions instead of n, the wave function of the form

$$\Psi(x_1 \cdots x_{n-1}) \approx \frac{1}{\sqrt{n!}} \begin{vmatrix} u_1(x_1) & \cdots & u_1(x_{n-1}) \\ \vdots & & \vdots \\ u_{n-1}(x_1) & \cdots & u_{n-1}(x_{n-1}) \end{vmatrix}$$

~~an equal~~ is a good approximation just as in the above case, where $u_1, \cdots u_{n-1}$ are certain linear combinations of $\psi_1, \psi_2 \cdots \psi_m$ ~~and~~ are orthogonal to each other. normalized and are

Problem 3.
What is the ~~pro~~ method of second quantization. Give brief sketch of mathematical formulation of the method in the case of scalar field

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State the variational principle for ~~the~~ Schrödinger equation in n-r-q-m. Show that

Problem: ~~By using~~ Prove that the wave function for a molecule which is given ~~by~~ in the first approximation by

$$\Psi(r_k, R_a) = \sum_q \chi(R_q)\,\psi(r_k, R_a)$$

where ψ is the solution (normalized with respect to r_k)

$$\left(-\sum_{k=1}^{n} \frac{\hbar^2}{2m}\Delta_k + V(r_k, R_a)\right)\psi = W(R_{ab})\,\psi,$$

then $\chi(R_a)$ is the ~~wave~~ function which satisfies

$$\left(-\frac{1}{2M_a}\Delta_a + W(R_{ab}) - E\right)\chi(R_a) = 0$$

where E is the total energy of the molecule. cond

$$\iint \tilde{\Psi} H \Psi \,(dR)^N (dr)^n$$

$$= \int \tilde{\chi}\left\{-\sum \frac{1}{2M_a}\Delta + W(R_{ab})\right\}\chi\,(dR)^N$$

$$-\iint \sum \frac{1}{2M_a}\left\{\tilde{\chi}\chi\,\tilde{\psi}\Delta_a\psi + 2\tilde{\chi}\nabla_a\chi\cdot\tilde{\psi}\nabla_a\psi\right\}(dR)^N \times (dr)^n$$

= min under the cond.

$$\int \tilde{\chi}\chi\, dV = 1$$

$$\iint \sum \frac{1}{2M_a}\nabla_a\tilde{\Psi}\nabla_a\Psi + \iint \tilde{\Psi} H_0 \Psi$$

$$= \int \sum \frac{1}{2M_a}\nabla_a\tilde{\chi}\nabla_a\chi + \int f(\nabla_a\psi, \nabla_a\tilde{\psi}) + \int W(R)\tilde{\chi}\chi\, dV$$

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In the case of the closed shell, the determinant function is a ~~possible~~ solution. Show that it can be ~~extended~~ generalized in the following way:

Remark: We suppose that the electronic function ψ is such that $W(R_{\alpha\beta})$ has a minimum for a set of equilibrium values of distances $R_{\alpha\beta}$.

independently

Problem 2.

~~N~~ - identical Fermions (electrons or nucleons) are supposed to move, in the first approximation, a common ~~co~~ field as given by a certain potential V. Further suppose that the ~~bottom~~ discrete ~~bottom~~ of the eigenvalue of the Hamiltonian

$$H = \sum_{k=1}^{N} \frac{1}{2m} p_k^2 + \cdots$$

$$H_0 = \frac{1}{2m} \sum p^2 + V(r)$$

is so distributed ~~energy~~ that ~~there~~ is a big energy gap between $n+1$ - low energy states and other higher energy states. (for the individual particle) the ground state of the system ~~in the approximation in which only~~ shows that, in the approximation

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so far the wavefunctions of the lowest-lying states can be expressed

can be written in the determinant form

$$\begin{vmatrix} u_1(x_1) & u_1(x_2) & \cdots & u_1(x_n) \\ u_2(x_1) & \cdots & & \\ \vdots & & & \\ u_n(x_1) & & & u_n(x_n) \end{vmatrix}$$

where $u_1, u_2, \ldots u_n$ are n-orthogonal functions which can be ~~constructed~~ each which can be expressed as "linear combinations" of $n+1$ - eigenfunctions for $n+1$ - low energy states.

$$\sum_r C_r v_r(x_1)$$

$$\sum_{k_1,k_2\cdots k_n=1}^{n+1} C_{k_1,k_2\cdots k_n} \underbrace{v_{k_1}(x_1) v_{k_2}(x_2) \cdots v_{k_n}(x_n)}$$

$$= \sum C^{(\text{symm})}_{k_1,k_2\cdots k_n} \sum_{s=1}^{n!} \xi(P_s) P_s\, v_{k_1}(x_1) \cdots v_{k_n}(x_n)$$

$$\| v_1(x_1) \cdots v_n(x_n) \| + \| v_1(x_1) \cdots \overbrace{v_{n+1}(x_{n-1})} \cdots v_n(x_n) \|$$

$$\| v_1(x_1) \cdots v_{n-1}\, v_n'(x_n) \| + \| v_1(x_1) \cdots v_{n+1}\, v_n'(x_n) \| + \cdots$$

$$\| v_1(x_1) \cdots v_{n-2}\, v_{n-1}'\, v_n' \| + \| v_1 \cdots v_{n+1}\, v_{n-1}\, v_n \| = \| v_1 \cdots v_{n+1}\, v_{n+1}'\, v_n' \|$$