時間依存密度汎関数法で探る原子核ダイナミクス:
原子核反応から超流動現象，中性子星まで

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Brief personal history


Cherry blossoms
in Satte City

1988: Born in Tokyo, grew up in Satte City in Saitama

2003-2006: Inagakuen Public High School


2006-2010: Tokyo University of Science (BSc)

2010-2015: University of Tsukuba (MSc-PhD)

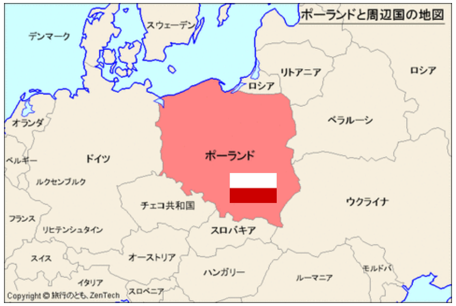
Apr. 2015-Aug. 2017: Warsaw University of Technology, Poland (Postdoc)

Sep. 2017-Dec. 2017: University of Washington, USA (Postdoc)

Jan. 2018-Mar. 2021: Niigata University (Assistant Professor, tenure track)

Apr. 2021-Present: Tokyo Institute of Technology (Associate Professor)

Main research field: Nuclear Theory





Lecture Plan

Theory (8/7 10:00-11:30)

#1. An introduction to microscopic mean-field approaches and (TD)DFT

Nuclear reactions (8/7 13:00-14:30)

#2. Recent advances in microscopic approaches for heavy-ion reactions

Superheavy element synthesis & deep-inelastic collisions

Neutron stars (8/8 10:00-11:30)

#3. Neutron-star “glitch” and neutron superfluid

Dynamics of quantized vortices in the inner crust of neutron stars

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From **quarks** to atomic nuclei

Standard model of the elementary particles

- ✓ Elementary particles: fundamental particles **without structure**
- ✓ Four forces: **strong, weak, electromagnetic**, and gravitational forces
- ✓ Particle physics explores an **ultimate theory** of the Universe

Higgs boson

Fermions

	1st gen.	2nd gen.	3rd gen.	Charge
Quarks	u up	c charm	t top	$+\frac{2}{3}$
	d down	s strange	b bottom	$-\frac{1}{3}$
Leptons	e electron	μ muon	τ tau	-1
	ν_e electron neutrino	ν_μ muon neutrino	ν_τ tau neutrino	0

Gauge bosons

Strong force

Gluons

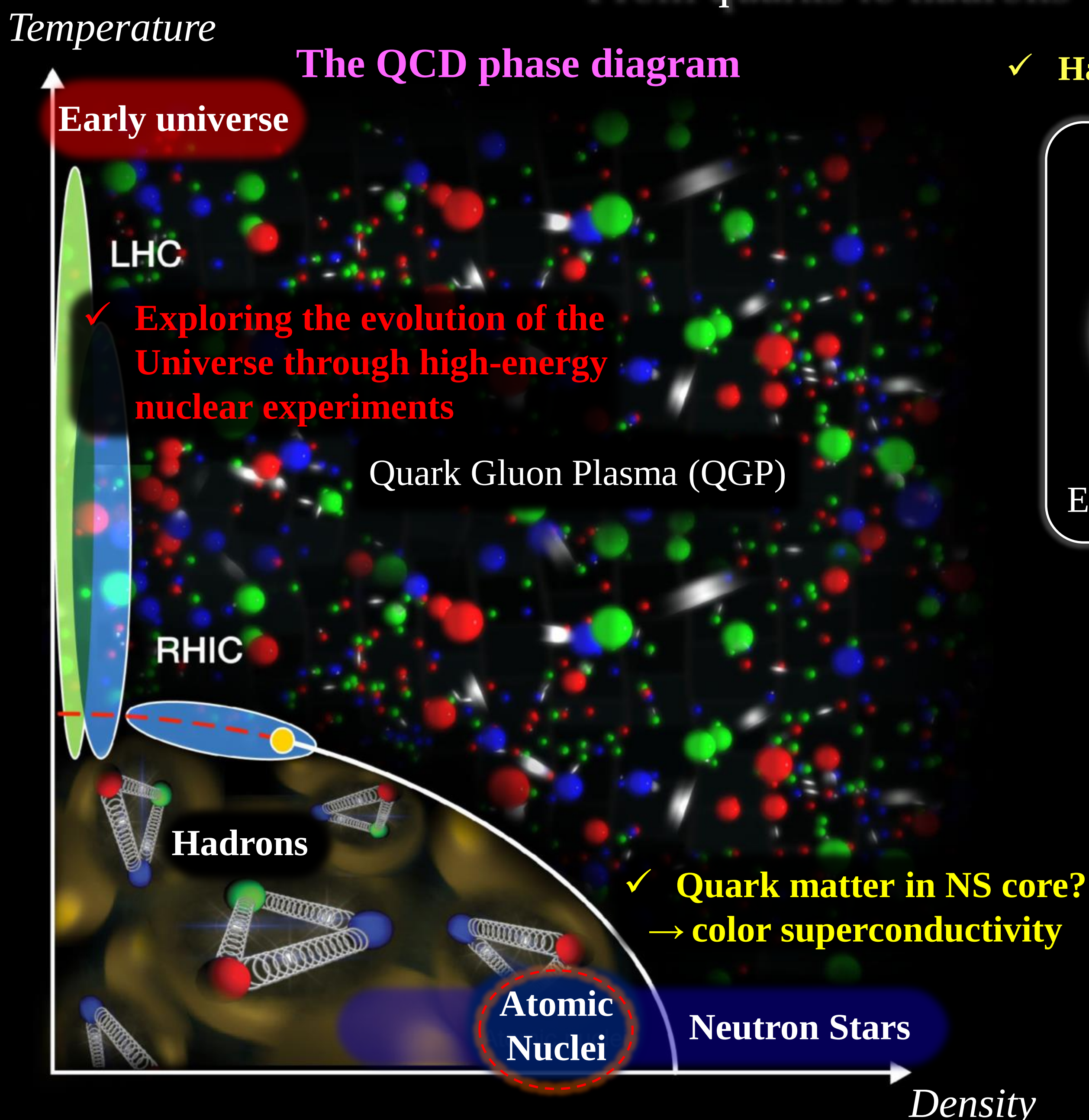
EM force

Photons

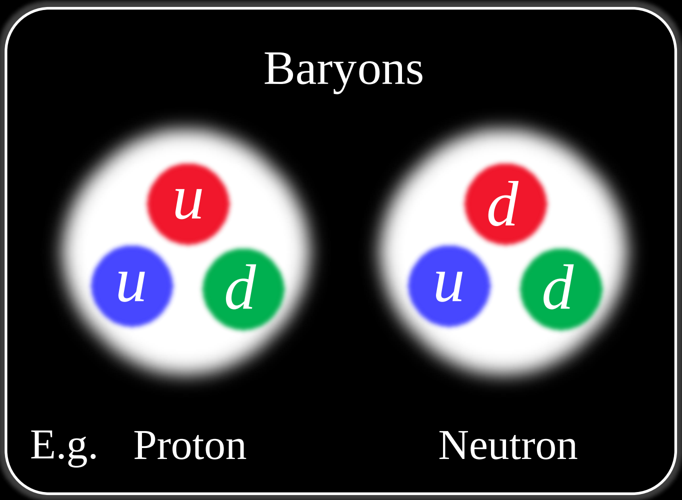
Weak force

$W^{\pm}$, Z^0 bosons

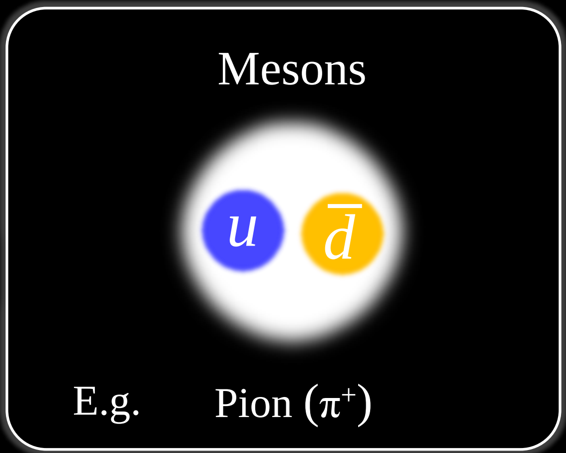
From quarks to hadrons



✓ **Hadrons:** composite particles of quarks



➢ A nucleon (proton or neutron) is a baryon.



Left figure: https://www.bnl.gov/newsroom/news.php?a=24281

Energy scales and degrees of freedom

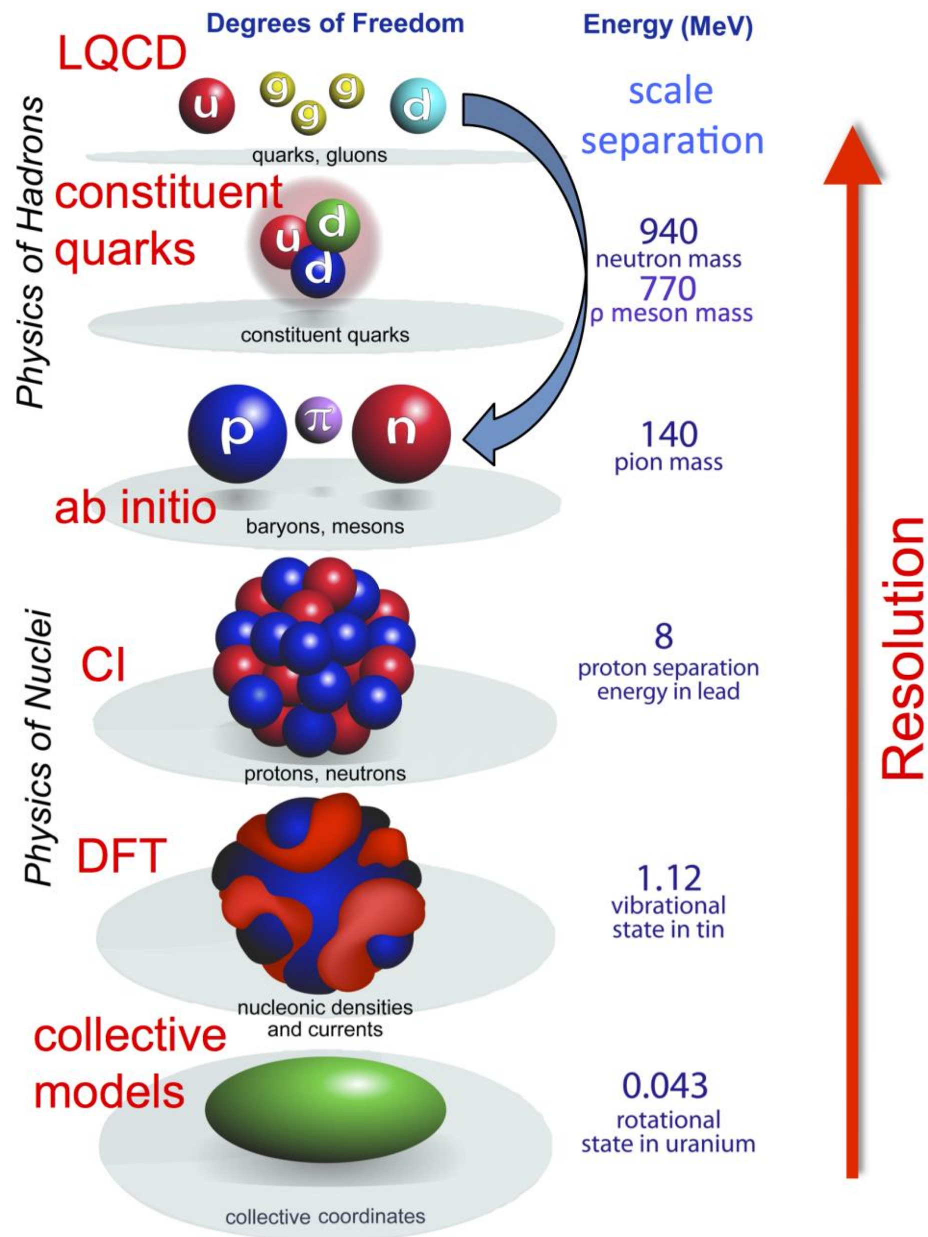


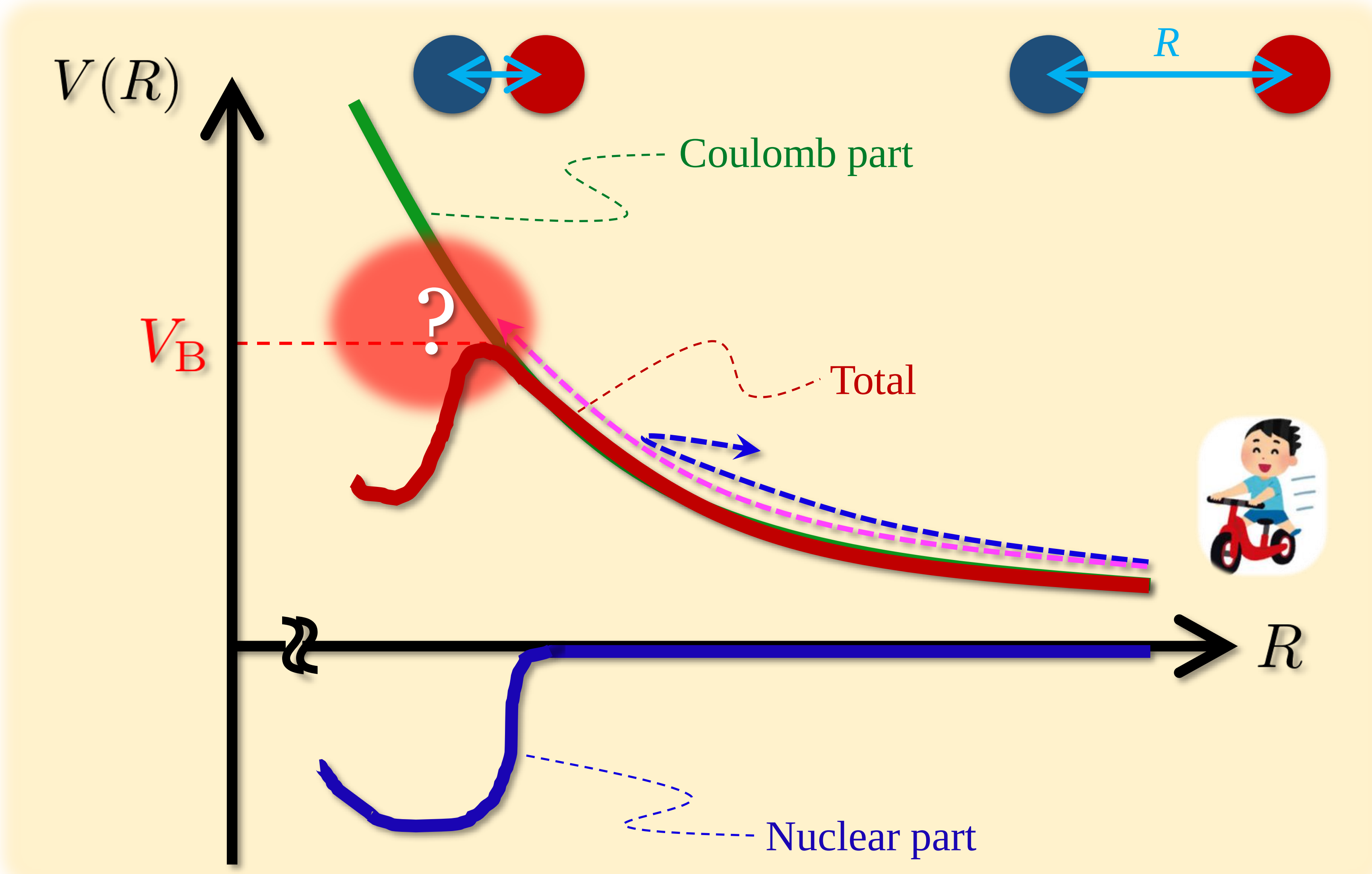
Figure: https://www.asc.ohio-state.edu/physics/ntg/6805/slides/6805_overview_slides.php#Dofs

Not this "high energy" !!

Animation: Brookhaven National Laboratory (http://www.bnl.gov/rhic/); https://youtu.be/Vyq_AYWctSo

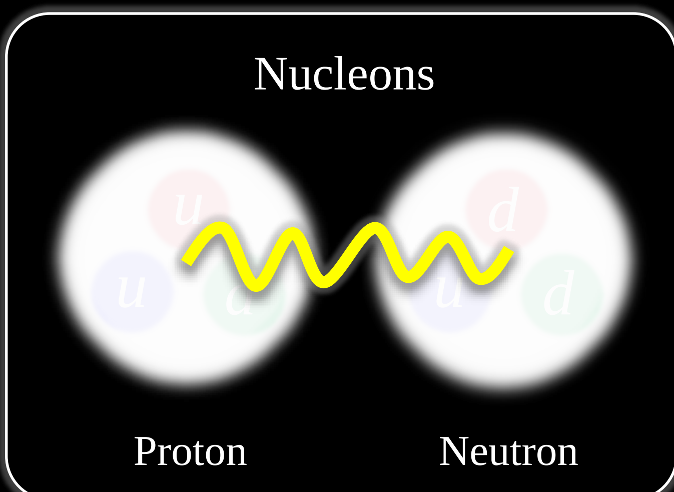
We collide two nuclei “gently”

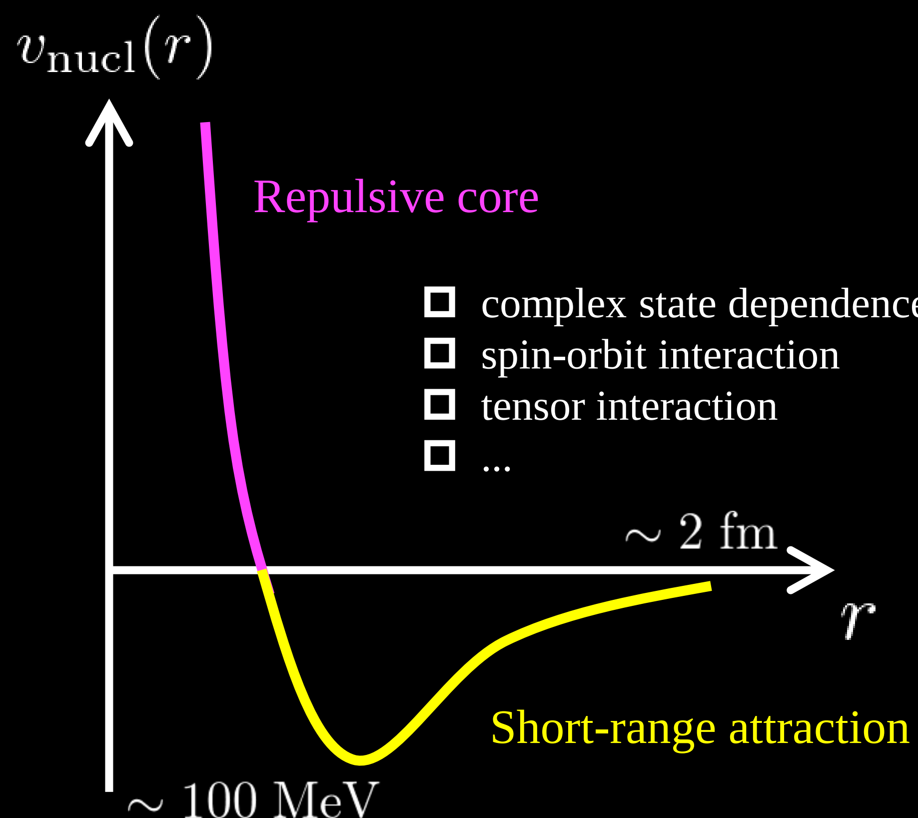
and study quantum many-body dynamics of neutrons and protons



In "low-energy" nuclear physics,
we treat neutrons and protons as building blocks

What we study is:
A quantum many-body problem of <u>fermions</u> interacting through the <u>nuclear force</u>





Mean-field theories in nuclear physics

Single-particle vs. collective pictures

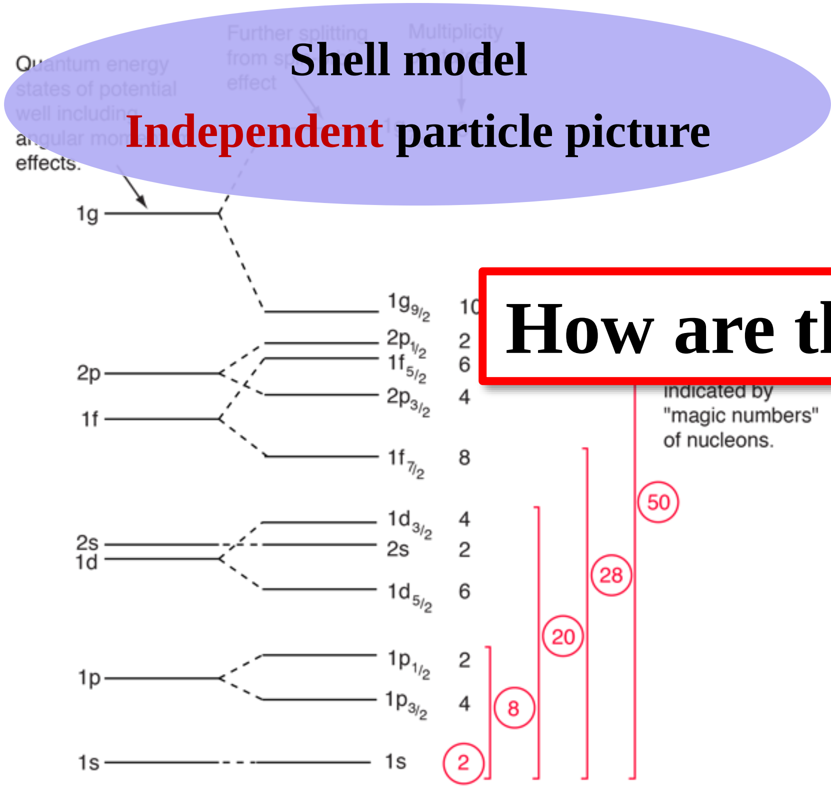
The Nobel Prize in Physics 1963

M.G. Mayer

J.H.D. Jensen

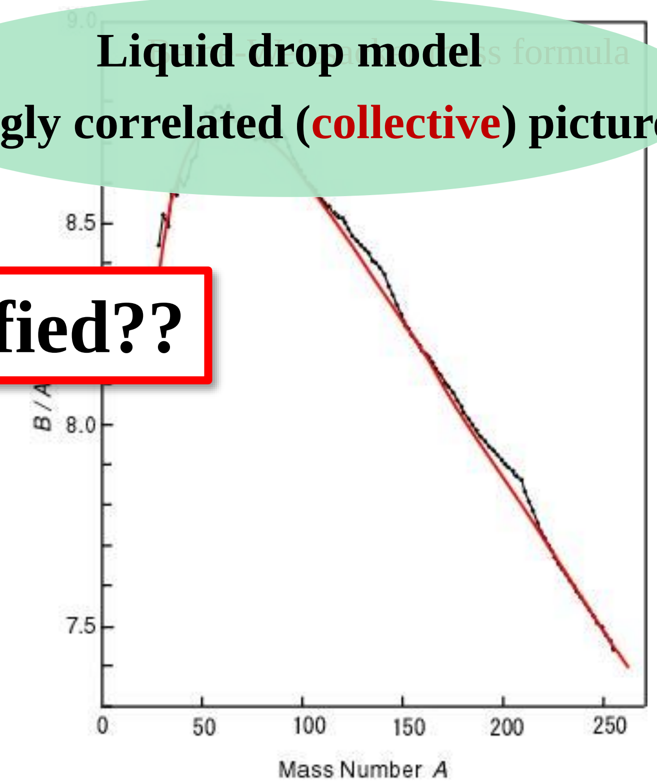
Shell model

Independent particle picture



Liquid drop model

strongly correlated (collective) picture



How are they unified??

Photos: https://www.nobelprize.org; B/A (九州大学名誉教授 高田健次郎氏ウェブサイトより)

Many-body wave function is <u>approximated</u> by a single Slater determinant

$$E = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Unrestricted variation

$$\frac{\delta E}{\delta \langle \Psi |} = 0$$

Schrödinger equation:

$$\hat{H} | \Psi \rangle = E | \Psi \rangle$$

HF approximation

$$\Psi \approx \Phi(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det\{\phi_i(x_j)\}$$

$$\frac{\delta}{\delta \phi_i^*} \left[E - \sum_{ij} \varepsilon_{ij} \langle \phi_i | \phi_j \rangle \right] = 0$$

Hartree-Fock equation:

$$\int \hat{h}_{\mathrm{HF}}(\boldsymbol{r}, \boldsymbol{r}') \phi_i(\boldsymbol{r}') d\boldsymbol{r}' = \varepsilon_i \phi_i(\boldsymbol{r})$$

where

Single-particle Hamiltonian:

$$\hat{h}_{\mathrm{HF}}(\boldsymbol{r}, \boldsymbol{r}') = \left[-\frac{\hbar^2}{2m} \nabla^2 + \Gamma_{\mathrm{H}}(\boldsymbol{r}) \right] \delta(\boldsymbol{r} - \boldsymbol{r}') - \Gamma_{\mathrm{F}}(\boldsymbol{r}, \boldsymbol{r}')$$

Hartree potential (direct term):

$$\Gamma_{\mathrm{H}}(\boldsymbol{r}) = \int \hat{v}(\boldsymbol{r}, \boldsymbol{r}') \rho(\boldsymbol{r}') d\boldsymbol{r}'$$

$$\rho(\boldsymbol{r}, \boldsymbol{r}') = \sum_{i=1}^{N} \phi_i(\boldsymbol{r}) \phi_i^*(\boldsymbol{r}')$$

Fock potential (exchange term):

$$\rho(\boldsymbol{r}) = \rho(\boldsymbol{r}, \boldsymbol{r})$$

$$\Gamma_{\mathrm{F}}(\boldsymbol{r}) = \hat{v}(\boldsymbol{r}, \boldsymbol{r}') \rho(\boldsymbol{r}, \boldsymbol{r}')$$

How can we describe the pairing properties?

→ One may build the BCS theory on top of the Hartree-Fock

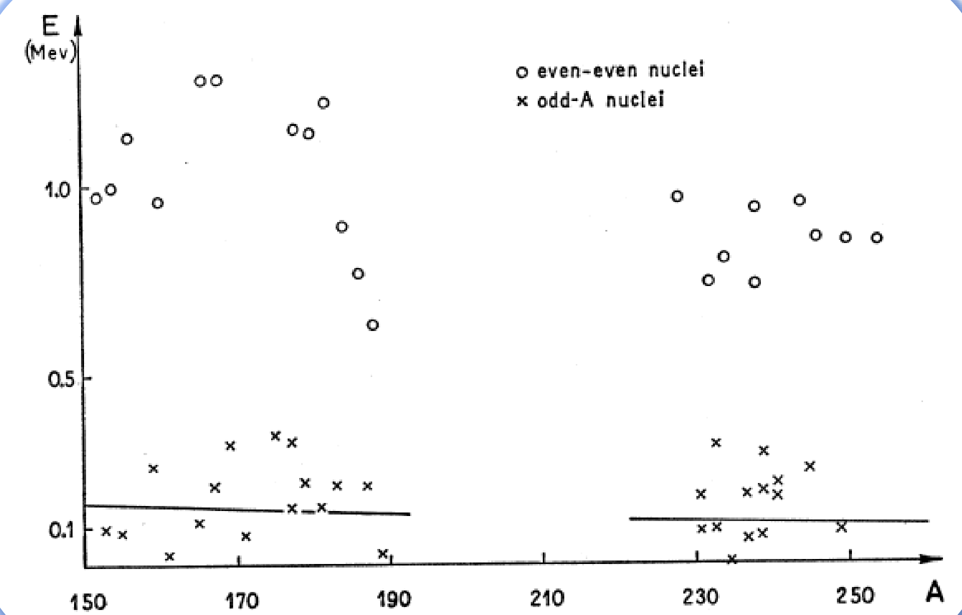
— the HF+BCS approach —

Necessity of pairing

✓ **Soon after the establishment of the BCS theory, pairing was recognized in nuclear physics**

The BCS wave function:

$$|\mathrm{BCS}\rangle = \prod_{k>0}^{\infty} (u_k + v_k \hat{a}_k^\dagger \hat{a}_{-k}^\dagger)|0\rangle$$



Phys. Rev. **108**, 1175 (1957)

Theory of Superconductivity*

J. Bardeen, L. N. Cooper,† and J. R. Schrieffer‡
Department of Physics, University of Illinois, Urbana, Illinois

(Received July 8, 1957)

Phys. Rev. **110**, 936 (1958)

Possible Analogy between the Excitation Spectra of Nuclei and Those of the Superconducting Metallic State

A. Bohr, B. R. Mottelson, and D. Pines*
Institute for Theoretical Physics, University of Copenhagen, Copenhagen, Denmark, and Nordisk Institut for Teoretisk Atomfysik, Copenhagen, Denmark

(Received January 7, 1958)

We will just use:

$$\{\hat{a}_k^\dagger, \hat{a}_l\} = \hat{a}_k^\dagger \hat{a}_l + \hat{a}_l \hat{a}_k^\dagger = \delta_{kl}$$

$$\{\hat{a}_k, \hat{a}_l\} = \{\hat{a}_k^\dagger, \hat{a}_l^\dagger\} = 0$$

$$\hat{a}_k|0\rangle = 0 \qquad \langle 0|\hat{a}_k^\dagger = 0$$

Norm

$$\langle \mathrm{BCS}|\mathrm{BCS}\rangle = \langle 0|\prod_{k>0}^{\infty}(u_k + v_k\hat{a}_{-k}\hat{a}_k)\prod_{l>0}^{\infty}(u_l + v_l\hat{a}_{-l}^\dagger\hat{a}_l^\dagger)|0\rangle$$

$$= \langle 0|(u_1 + v_1\hat{a}_{-1}\hat{a}_1)\cdots(u_\infty + v_\infty\hat{a}_{-\infty}\hat{a}_\infty)\boxed{(u_1 + v_1\hat{a}_1^\dagger\hat{a}_{-1}^\dagger)}\cdots(u_\infty + v_\infty\hat{a}_\infty^\dagger\hat{a}_{-\infty}^\dagger)|0\rangle$$

We can reorder the $a^\dagger$ as there are 0 or even numbers of a

$$= \langle 0|\prod_{k>0}^{\infty}(u_k + v_k\hat{a}_{-k}\hat{a}_k)(u_k + v_k\hat{a}_k^\dagger\hat{a}_{-k}^\dagger)|0\rangle$$

$$= \langle 0|\prod_{k>0}^{\infty}\left[u_k^2 + u_k v_k(\cancel{\hat{a}_k^\dagger\hat{a}_{-k}^\dagger} + \cancel{\hat{a}_{-k}\hat{a}_k}) + v_k^2\,\underline{\hat{a}_{-k}\hat{a}_k\hat{a}_k^\dagger\hat{a}_{-k}^\dagger}\right]|0\rangle$$

vanish by acting on the bra/ket

$$= \hat{a}_{-k}(1 - \hat{a}_k^\dagger\hat{a}_k)\hat{a}_{-k}^\dagger = 1 \cancel{- \hat{a}_{-k}^\dagger\hat{a}_{-k} + \hat{a}_{-k}\hat{a}_k^\dagger\hat{a}_{-k}^\dagger\hat{a}_k}$$

vanish by acting on the ket

$$= \prod_{k>0}^{\infty}(u_k^2 + v_k^2)$$

✓ Norm of the BCS wave function:

$$\langle \mathrm{BCS}|\mathrm{BCS}\rangle = \prod_{k>0}^{\infty}(u_k^2 + v_k^2)$$

➢ $u_k^2 + v_k^2 = 1$ must be fulfilled for all k to normalize the BCS wave function!

Particle number operator:

$$\hat{N} = \sum_{k>0} (\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k})$$

Particle-number expectation value

$$\langle \mathrm{BCS}|\hat{N}|\mathrm{BCS}\rangle = \langle 0|(u_1 + v_1 \hat{a}_{-1}\hat{a}_1)\cdots(u_\infty + v_\infty \hat{a}_{-\infty}\hat{a}_\infty)\hat{N}(u_1 + v_1 \hat{a}_1^\dagger \hat{a}_{-1}^\dagger)\cdots(u_\infty + v_\infty \hat{a}_\infty^\dagger \hat{a}_{-\infty}^\dagger)|0\rangle$$

index = k index = k

$$= \sum_{k>0}^{\infty} \langle 0|(\cancel{u_k} + v_k \hat{a}_{-k}\hat{a}_k)(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k})(\cancel{u_k} + v_k \hat{a}_k^\dagger \hat{a}_{-k}^\dagger) \underbrace{\prod_{l(\neq k)>0}^{\infty} (u_l + v_l \hat{a}_{-l}\hat{a}_l)(u_l + v_l \hat{a}_l^\dagger \hat{a}_{-l}^\dagger)}_{=1} |0\rangle$$

$a^\dagger$ acts on the bra a acts on the ket

$$\to u_l^2 + u_l v_l (\cancel{\hat{a}_l^\dagger \hat{a}_{-l}^\dagger} + \cancel{\hat{a}_{-l}\hat{a}_l}) + v_l^2 \underbrace{\hat{a}_{-l}\hat{a}_l \hat{a}_l^\dagger \hat{a}_{-l}^\dagger}_{\to 1}$$

vanish by acting on the bra/ket

$$\to \prod_{l(\neq k)>0}^{\infty} (u_l^2 + v_l^2) = 1$$

$$= \sum_{k>0}^{\infty} v_k^2 \langle 0|\underline{\hat{a}_{-k}\hat{a}_k(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k})\hat{a}_k^\dagger \hat{a}_{-k}^\dagger}|0\rangle$$

From each of two terms, one finds a unity
(others vanish acting on the bra/ket)

$$= 2\sum_{k>0}^{\infty} v_k^2$$

✓ Expectation value of the particle-number operator:

$$\langle \mathrm{BCS}|\hat{N}|\mathrm{BCS}\rangle = 2\sum_{k>0}^{\infty} v_k^2$$

➢ v_k^2 can be interpreted as a probability for a pair $(k, -k)$ being occupied.
(u_k^2 is the probability being unoccupied.)

Particle number operator:

$$\hat{N} = \sum_{k>0} (\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k})$$

Particle-number dispersion

The **dispersion** of the particle-number expectation value is defined by:

$$(\Delta N)^2 = \langle \text{BCS} | \hat{N}^2 | \text{BCS} \rangle - \langle \text{BCS} | \hat{N} | \text{BCS} \rangle^2$$

In a very similar manner, one can calculate (try it!):

$$\langle \text{BCS} | \hat{N}^2 | \text{BCS} \rangle = 4 \sum_{k>0}^{\infty} v_k^2 + 4 \sum_{\substack{k,l(>0) \\ (k \neq l)}}^{\infty} v_k^2 v_l^2$$

Since we have

$$\langle \text{BCS} | \hat{N} | \text{BCS} \rangle^2 = 4 \sum_{k>0}^{\infty} v_k^4 + 4 \sum_{\substack{k,l(>0) \\ (k \neq l)}}^{\infty} v_k^2 v_l^2$$

one finds:

✓ Particle-number dispersion in the BCS state:

$$(\Delta N)^2 = 4 \sum_{k>0}^{\infty} (1 - v_k^2) v_k^2 = 4 \sum_{k>0}^{\infty} u_k^2 v_k^2$$

➢ Particle-number fluctuation originates from the fractionally-occupied states around the Fermi level. (where $u_k^2 \neq 1, v_k^2 \neq 1$)

Energy expectation value and its variation

Let us consider a simple Hamiltonian with a constant pairing interaction:

$$\hat{H} = \sum_{k,l(\gtrless 0)} t_{kl}\, \hat{a}_k^\dagger \hat{a}_l - G \sum_{k,l(>0)} \hat{a}_k^\dagger \hat{a}_{-k}^\dagger \hat{a}_{-l} \hat{a}_l$$

The energy expectation value reads (try it!):

$$\langle \mathrm{BCS}|\hat{H} - \lambda \hat{N}|\mathrm{BCS}\rangle = 2\sum_{l>0} v_l^2\,(t_{ll} - \lambda) - G\left(\sum_{l>0} u_l v_l\right)^2 - G\sum_{l>0} v_l^4$$

Taking a variation with respect to v_k , one obtains:

$$\delta\langle \mathrm{BCS}|\hat{H} - \lambda \hat{N}|\mathrm{BCS}\rangle = \left(\frac{\partial}{\partial v_k} + \underbrace{\frac{\partial u_k}{\partial v_k}}_{= -v_k/u_k \quad \because\, u_k = \sqrt{1 - v_k^2}} \frac{\partial}{\partial u_k}\right)\langle \mathrm{BCS}|\hat{H} - \lambda \hat{N}|\mathrm{BCS}\rangle$$

$$= 4(t_{kk} - \lambda)v_k - 4Gv_k^3 - 2G\left(\sum_{l>0} u_l v_l\right)u_k + 2G\frac{v_k}{u_k}\left(\sum_{l>0} u_l v_l\right)v_k$$

$$= 4(t_{kk} - \lambda - Gv_k^2)v_k + 2\Delta\left(\frac{v_k^2}{u_k} - u_k\right) = 0$$

$$\Leftrightarrow \boxed{2(\varepsilon_k - \lambda)u_k v_k + \Delta(v_k^2 - u_k^2) = 0}$$ $\cdots$ *The BCS condition*

$$\Delta \equiv G\sum_{k>0} u_k v_k$$

$$\varepsilon_k \equiv t_{kk} - Gv_k^2$$

✓ As a result of the variation, $\delta E = 0$, we got the BCS condition:

$$\boxed{2(\varepsilon_k - \lambda)u_k v_k + \Delta(v_k^2 - u_k^2) = 0}$$

Single-particle energy:

$$\varepsilon_k \equiv t_{kk} - G v_k^2$$

Pairing gap:

$$\Delta \equiv G \sum_{k>0} u_k v_k$$

One can analytically solve it for v_k^2 and u_k^2, leading to:

$$v_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k - \lambda}{\sqrt{(\varepsilon_k - \lambda)^2 + \Delta^2}}\right)$$

$$u_k^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_k - \lambda}{\sqrt{(\varepsilon_k - \lambda)^2 + \Delta^2}}\right)$$

• • • ★

✓ These amplitudes satisfy the BCS condition (i.e., $\delta E = 0$)

Since we have

$$v_k^2 u_k^2 = \frac{1}{4}\left(1 - \frac{(\varepsilon_k - \lambda)^2}{(\varepsilon_k - \lambda)^2 + \Delta^2}\right) = \frac{1}{4}\frac{\Delta^2}{(\varepsilon_k - \lambda)^2 + \Delta^2}$$

one obtains:

➢ **The gap equation:**

$$\Delta = \frac{G}{2}\sum_{k>0}\frac{\Delta}{\sqrt{(\varepsilon_k - \lambda)^2 + \Delta^2}}$$

where λ can be determined by

$$N = 2\sum_{k>0} v_k = \sum_{k>0}\left(1 - \frac{\varepsilon_k - \lambda}{\sqrt{(\varepsilon_k - \lambda)^2 + \Delta^2}}\right)$$

: Particle-number condition

➢ Since the above set of equations sustains the relation "★", *which is equivalent to the BCS condition*, it offers a practical way of determining Δ, λ, and v_k, for a given set of ε_k.

More sophisticated approach to include pairing

→ the Hartree-Fock-Bogoliubov theory

(a.k.a. the Bogoliubov-de Gennes theory)

- The BCS wave function can be interpreted as a vacuum of *quasi-particles*, *i.e.*:

$$\hat{\alpha}_k|\mathrm{BCS}\rangle = 0 \quad \textit{i.e.} \quad |\mathrm{BCS}\rangle = \prod_k \hat{\alpha}_k|0\rangle$$

where

$$\hat{\alpha}_k = u_k\hat{a}_k - v_k\hat{a}^\dagger_{-k} \qquad \hat{\alpha}_{-k} = u_k\hat{a}_{-k} + v_k\hat{a}^\dagger_k$$

Annihilation of a quasiparticle in a state *k*

Creation of a quasiparticle in a state *-k*

- A quasiparticle is a mixture of particle and hole states

- The HFB wave function would be the most generalized mixture of particle and hole states:

$$\hat{\beta}_\mu|\mathrm{HFB}\rangle = 0 \quad \textit{i.e.} \quad |\mathrm{HFB}\rangle = \prod_\mu \hat{\beta}_\mu|0\rangle$$

✓ The "generalized" Bogoliubov transformation is given by:

$$\hat{\beta}_\mu = \sum_{k=1}^{M}\left(U^*_{k\mu}\hat{a}_k + V^*_{k\mu}\hat{a}^\dagger_k\right) \qquad \hat{\beta}^\dagger_\mu = \sum_{k=1}^{M}\left(U_{k\mu}\hat{a}^\dagger_k + V_{k\mu}\hat{a}_k\right)$$

or in a matrix form:

$$\begin{pmatrix}\hat{\boldsymbol{\beta}}\\ \hat{\boldsymbol{\beta}}^\dagger\end{pmatrix} = \begin{pmatrix}U^\dagger & V^\dagger\\ V^{\mathrm{T}} & U^{\mathrm{T}}\end{pmatrix}\begin{pmatrix}\hat{\boldsymbol{a}}\\ \hat{\boldsymbol{a}}^\dagger\end{pmatrix} = \mathcal{W}^\dagger\begin{pmatrix}\hat{\boldsymbol{a}}\\ \hat{\boldsymbol{a}}^\dagger\end{pmatrix}$$

where there hold

$$\{\hat{\beta}^\dagger_\mu, \hat{\beta}_\nu\} = \delta_{\mu\nu} \qquad \{\hat{\beta}_\mu, \hat{\beta}_\nu\} = \{\hat{\beta}^\dagger_\mu, \hat{\beta}^\dagger_\nu\} = 0$$

$$\mathcal{W}^\dagger\mathcal{W} = \mathcal{W}\mathcal{W}^\dagger = I$$

The HFB theory

Energy expectation value

$$\hat{H} = \sum_{kl} \varepsilon_{kl} \hat{a}_k^\dagger \hat{a}_l + \frac{1}{4} \sum_{klmn} \bar{v}_{klmn}\, \hat{a}_k^\dagger \hat{a}_l^\dagger \hat{a}_n \hat{a}_m$$

$$\boxed{\langle \mathrm{HFB} | \hat{H} | \mathrm{HFB} \rangle = \mathrm{Tr}[\varepsilon\rho] + \frac{1}{2}\mathrm{Tr}[\Gamma\rho] + \frac{1}{2}\mathrm{Tr}[\Delta\kappa^\dagger]}$$

$\rho_{kl} = \langle \hat{a}_l^\dagger \hat{a}_k \rangle = (V^* V^{\mathrm{T}})_{kl}$: Density matrix

$\kappa_{kl} = \langle \hat{a}_l \hat{a}_k \rangle = (V^* U^{\mathrm{T}})_{kl}$: Pairing tensor

$h = \varepsilon + \Gamma$: Single-particle Hamiltonian

$\Gamma_{kl} = \sum_{mn} \bar{v}_{kmln}\, \rho_{nm}$: Mean field

$\Delta_{kl} = \frac{1}{2} \sum_{mn} \bar{v}_{klmn}\, \kappa_{mn}$: Pairing field

$\rho^\dagger = \rho \qquad \Gamma^\dagger = \Gamma$

$\kappa^{\mathrm{T}} = -\kappa \qquad \Delta^{\mathrm{T}} = -\Delta$

$h^\dagger = h$

Result of a variation

$$\boxed{[\mathcal{H}, \mathcal{R}] = 0} \quad \cdots \textit{The HFB condition}$$

HFB matrix:

$$\mathcal{H} = \begin{pmatrix} h - \lambda I & \Delta \\ -\Delta^* & -h^* + \lambda I \end{pmatrix}$$

Generalized density matrix:

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & I - \rho^* \end{pmatrix}$$

or equivalently

$$\begin{pmatrix} h - \lambda I & \Delta \\ -\Delta^* & -h^* + \lambda I \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} U \\ V \end{pmatrix} \begin{pmatrix} E_1 & & 0 \\ & E_2 & \\ 0 & & \ddots \end{pmatrix}$$

➢ By diagonalizing the HFB matrix, one can determine U and V, which fulfill the HFB condition!

(TD)DFT in a tiny nutshell

What is DFT?

A theory which gives us access to the *exact* solution

Equivalent!
(for a special EDF)

$$\hat{H}\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N) = E\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)$$

Kohn-Sham equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\mathrm{KS}}[\rho(\boldsymbol{r})]\right]\phi_i(\boldsymbol{r}) = \varepsilon_i\,\phi_i(\boldsymbol{r})$$

EDF

This is the key!

$$v_{\mathrm{KS}}[\rho(\boldsymbol{r})] = \frac{\delta\mathcal{E}[\rho]}{\delta\rho} \qquad \rho(\boldsymbol{r}) = \sum_{i=1}^{N}|\phi_i(\boldsymbol{r})|^2$$

Energy can also be written as a functional of density

$$E[\rho] = \langle\underline{\Psi[\rho]}|\hat{H}|\underline{\Psi[\rho]}\rangle$$

w.f. is a functional of density

P. Hohenberg and W. Kohn, Phys. Rev. B **136**, 864 (1964)

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Kohn-Sham equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\rm KS}[\rho(\boldsymbol{r})]\right]\phi_i(\boldsymbol{r}) = \varepsilon_i\,\phi_i(\boldsymbol{r})$$

EDF

This is the key!

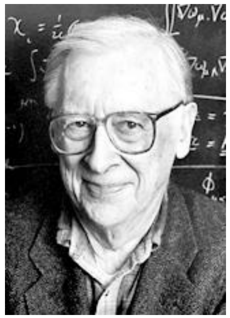
$$v_{\rm KS}[\rho(\boldsymbol{r})] = \frac{\delta\mathcal{E}[\rho]}{\delta\rho} \qquad \rho(\boldsymbol{r}) = \sum_{i=1}^{N}|\phi_i(\boldsymbol{r})|^2$$

<u>**Existence was proven, but "shape" is unknown**</u> **:(**

Great Success of the Density Functional Theory

The Nobel Prize in Chemistry 1998

Walter Kohn



John Pople

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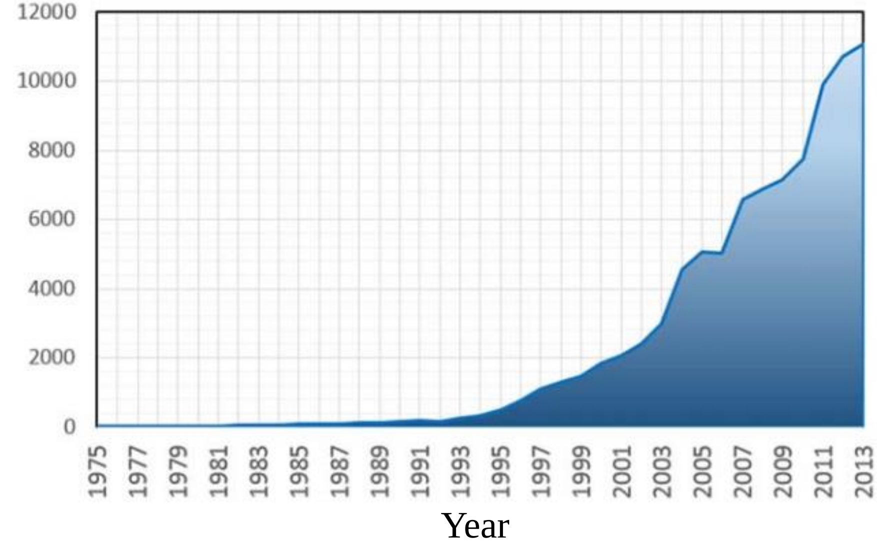
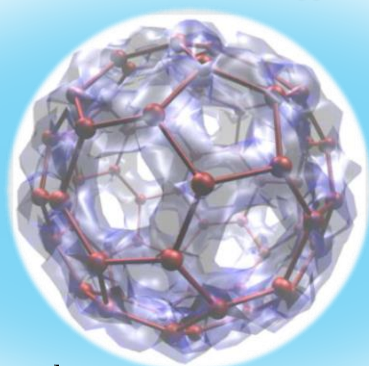
Number of publications with “DFT” (till 2013)



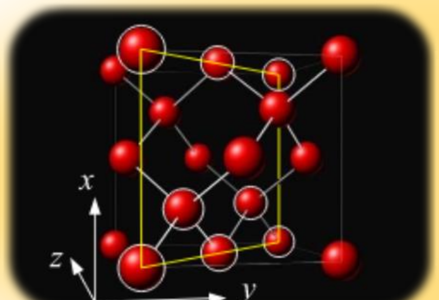
A. Galano and J.R. Alvarez-Idadoy, J. Compt. Chem. **35**, 2019 (2014)

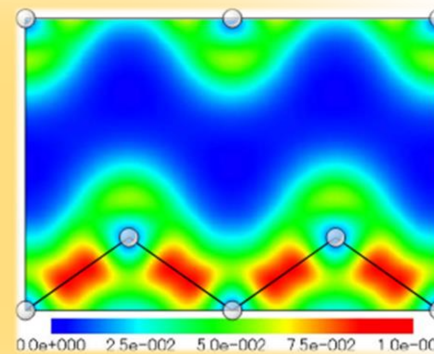
Fullerene: C_{60}



C-Z. Gao et al.,
J. Phys. B: At. Mol. Opt. Phys. **48**, 105102 (2015)

Si crystal





Y. Shinohara, K. Yabana, Y. Kawashita, J.-I. Iwata, T. Otobe, and G. F. Bertsch,
Phys. Rev. B **82**, 155110 (2010)

The seminal papers on DFT
- P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964) ➡ **19,015 citations!**
- W. Kohn and L.J. Sham, Phys. Rev. **140**, A1133 (1965) ➡ **24,384 citations!**

What's behind the wonder of DFT?

→ Hohenberg-Kohn theorem & Kohn-Sham scheme

DFT in a tiny nutshell (1/2) - Hohenberg-Kohn theorem

Assumption:

Two different wave functions Ψ and Ψ' provide the same one-body density $\rho(\boldsymbol{r})$

$$\hat{H} = \hat{T} + \hat{V} + \hat{V}_{\mathrm{ext}} \qquad \hat{H}' = \hat{T} + \hat{V} + \hat{V}'_{\mathrm{ext}}$$

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \qquad \hat{H}'|\Psi'\rangle = E'|\Psi'\rangle$$

Now, one finds:

$$\begin{aligned} E &= \langle\Psi|\hat{H}|\Psi\rangle < \langle\Psi'|\hat{H}|\Psi'\rangle \\ &= \langle\Psi'|\hat{H}'|\Psi'\rangle + \langle\Psi'|\hat{V}_{\mathrm{ext}} - \hat{V}'_{\mathrm{ext}}|\Psi'\rangle \\ &= E' + \int \rho(\boldsymbol{r})[v_{\mathrm{ext}}(\boldsymbol{r}) - v'_{\mathrm{ext}}(\boldsymbol{r})]d\boldsymbol{r} \qquad \cdots \text{(a)} \end{aligned}$$

However, one also gets:

$$\begin{aligned} E' &= \langle\Psi'|\hat{H}'|\Psi'\rangle < \langle\Psi|\hat{H}'|\Psi\rangle \\ &= E + \int \rho(\boldsymbol{r})[v'_{\mathrm{ext}}(\boldsymbol{r}) - v_{\mathrm{ext}}(\boldsymbol{r})]d\boldsymbol{r} \qquad \cdots \text{(b)} \end{aligned}$$

(a) + (b) $\quad E + E' < E + E' \quad ?$

P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964)

Assumption:

Two different wave functions Ψ and Ψ' provide the same one-body density $\rho(\boldsymbol{r})$

$$\hat{H} = \hat{T} + \hat{V} + \hat{V}_{\rm ext} \qquad \hat{H}' = \hat{T} + \hat{V} + \hat{V}'_{\rm ext}$$

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \qquad \hat{H}'|\Psi'\rangle = E'|\Psi'\rangle$$

Our assumption was wrong!

Now, one finds:

"reductio ad absurdum"

$$\begin{aligned} E &= \langle\Psi|\hat{H}|\Psi\rangle < \langle\Psi'|\hat{H}|\Psi'\rangle \\ &= \langle\Psi'|\hat{H}'|\Psi'\rangle + \langle\Psi'|\hat{V}_{\rm ext} - \hat{V}'_{\rm ext}|\Psi'\rangle \\ &= E' + \int \rho(\boldsymbol{r})[v_{\rm ext}(\boldsymbol{r}) - v'_{\rm ext}(\boldsymbol{r})]d\boldsymbol{r} \qquad \cdots \text{(a)} \end{aligned}$$

However, one also gets:

$$\begin{aligned} E' &= \langle\Psi'|\hat{H}'|\Psi'\rangle < \langle\Psi|\hat{H}'|\Psi\rangle \\ &= E + \int \rho(\boldsymbol{r})[v'_{\rm ext}(\boldsymbol{r}) - v_{\rm ext}(\boldsymbol{r})]d\boldsymbol{r} \qquad \cdots \text{(b)} \end{aligned}$$

(a) + (b) $\quad E + E' < E + E' \quad$?

P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964)

The 1st HK theorem:

There is a one-to-one correspondence between Ψ and ρ $\quad \Psi \leftrightarrow \rho(\boldsymbol{r})$

Now, one finds:

"reductio ad absurdum"

$$\begin{aligned} E &= \langle\Psi|\hat{H}|\Psi\rangle < \langle\Psi'|\hat{H}|\Psi'\rangle \\ &= \langle\Psi'|\hat{H}'|\Psi'\rangle + \langle\Psi'|\hat{V}_{\text{ext}} - \hat{V}'_{\text{ext}}|\Psi'\rangle \\ &= E' + \int \rho(\boldsymbol{r})[v_{\text{ext}}(\boldsymbol{r}) - v'_{\text{ext}}(\boldsymbol{r})]d\boldsymbol{r} \qquad \cdots \text{(a)} \end{aligned}$$

However, one also gets:

$$\begin{aligned} E' &= \langle\Psi'|\hat{H}'|\Psi'\rangle < \langle\Psi|\hat{H}'|\Psi\rangle \\ &= E + \int \rho(\boldsymbol{r})[v'_{\text{ext}}(\boldsymbol{r}) - v_{\text{ext}}(\boldsymbol{r})]d\boldsymbol{r} \qquad \cdots \text{(b)} \end{aligned}$$

(a) + (b) $\quad E + E' < E + E' \quad ?$

P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964)

The 1st HK theorem:

There is a one-to-one correspondence between Ψ and ρ $\quad \Psi \leftrightarrow \rho(\boldsymbol{r})$

The one-body density can be the fundamental degree of freedom!

The 2nd HK theorem:

$$\hat{H} \overset{\text{SE}}{\longleftrightarrow} \Psi \overset{\text{HK}}{\longleftrightarrow} \rho(\boldsymbol{r})$$

- Ψ can be written as a functional of ρ: $\quad \Psi = \Psi[\rho]$
- Any observable can be written as a functional of ρ: $\quad \mathcal{O}[\rho] = \langle \Psi[\rho] | \hat{\mathcal{O}} | \Psi[\rho] \rangle$
- **Minimization of EDF with respect to ρ will provide $E_{\text{g.s.}}$ and $\rho_{\text{g.s.}}$:**

$$E[\rho] = \langle \Psi[\rho] | \hat{H} | \Psi[\rho] \rangle$$ **: Energy Density Functional (EDF)**

$$E_{\text{g.s.}} = E[\rho_{\text{g.s.}}] = \min_{\rho} \left[\min_{\Psi \to \rho} E[\rho] \right]$$

Kohn-Sham scheme makes DFT computationally solvable

Kohn-Sham scheme:

W. Kohn and L.J. Sham, Phys. Rev. **140**, A1133 (1965)

- ✓ The EDF of the many-body system:

$$E[\rho] = \langle \Psi[\rho] | \hat{H} | \Psi[\rho] \rangle$$

This contains all necessary info to get the many-body ground state

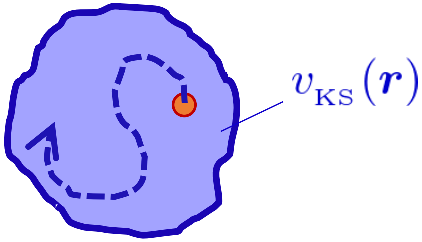
- ✓ Let us rewrite it as:

$$E[\rho] = \int d\boldsymbol{r}\, \frac{\hbar^2}{2m} \sum_{i=1}^{N} |\nabla \phi_i(\boldsymbol{r})|^2 + E'[\rho]$$

E' is the rest of EDF except the one-body kinetic term

- ✓ Taking the variation w.r.t. single-particle orbitals,

$$\frac{\delta}{\delta \phi_i^*} \Big[E[\rho] - \sum_{kl} \varepsilon_{kl} \Big(\langle \phi_k | \phi_l \rangle - \delta_{kl} \Big) \Big] = 0$$



one finds:

$$\Big[-\frac{\hbar^2}{2m} \nabla^2 + v_{\rm KS}[\rho(\boldsymbol{r})] \Big] \phi_i(\boldsymbol{r}) = \varepsilon_i \phi_i(\boldsymbol{r})$$

: Kohn-Sham equation

Kohn-Sham potential:

$$v_{\rm KS}[\rho(\boldsymbol{r})] = \frac{\delta E'[\rho]}{\delta \rho}$$

One-body density:

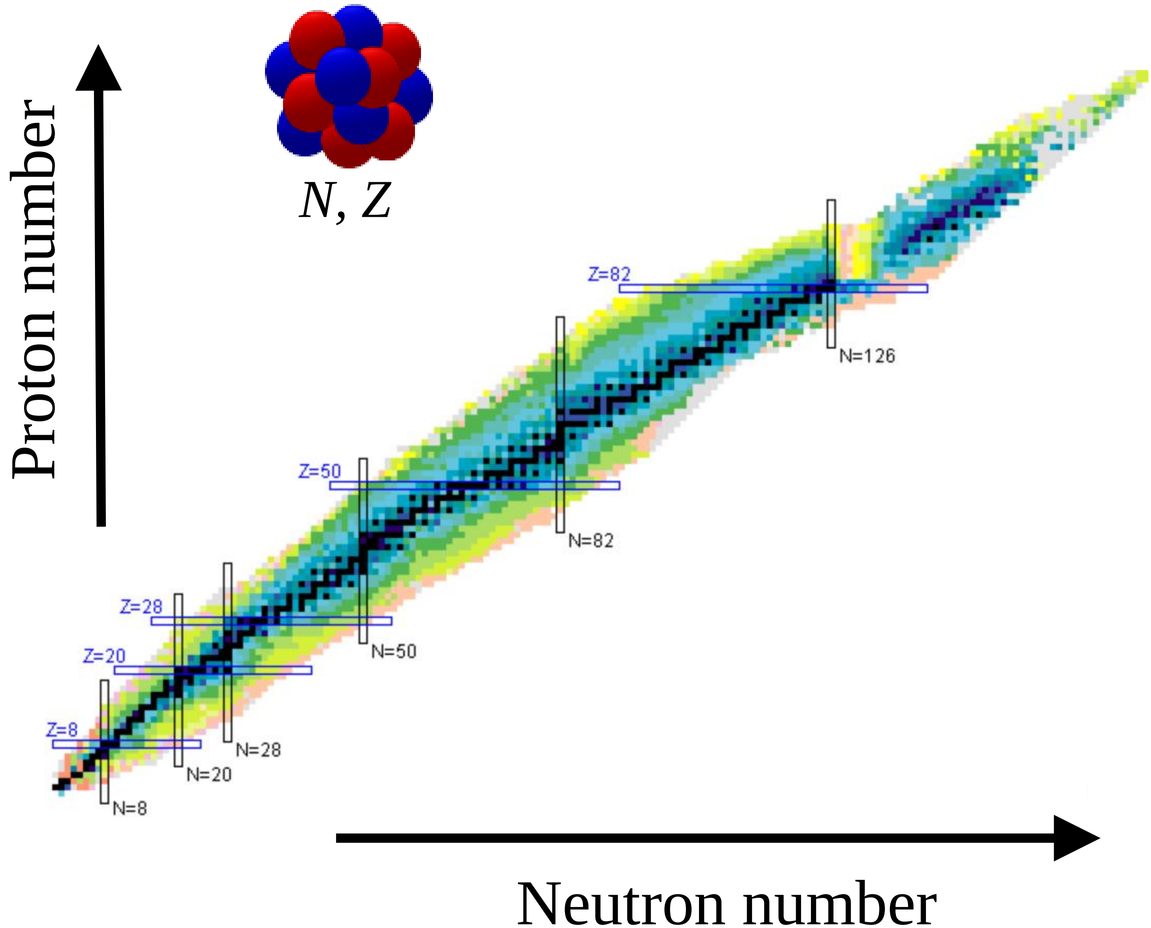
$$\rho(\boldsymbol{r}) = \sum_{i=1}^{N} |\phi_i(\boldsymbol{r})|^2$$

Kohn-Sham orbitals:

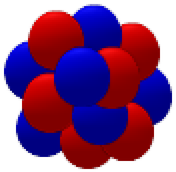
$$\phi_i(\boldsymbol{r}) \quad (i = 1, \ldots, N)$$

Then, how it works?

All nuclei can be described with a *single* EDF

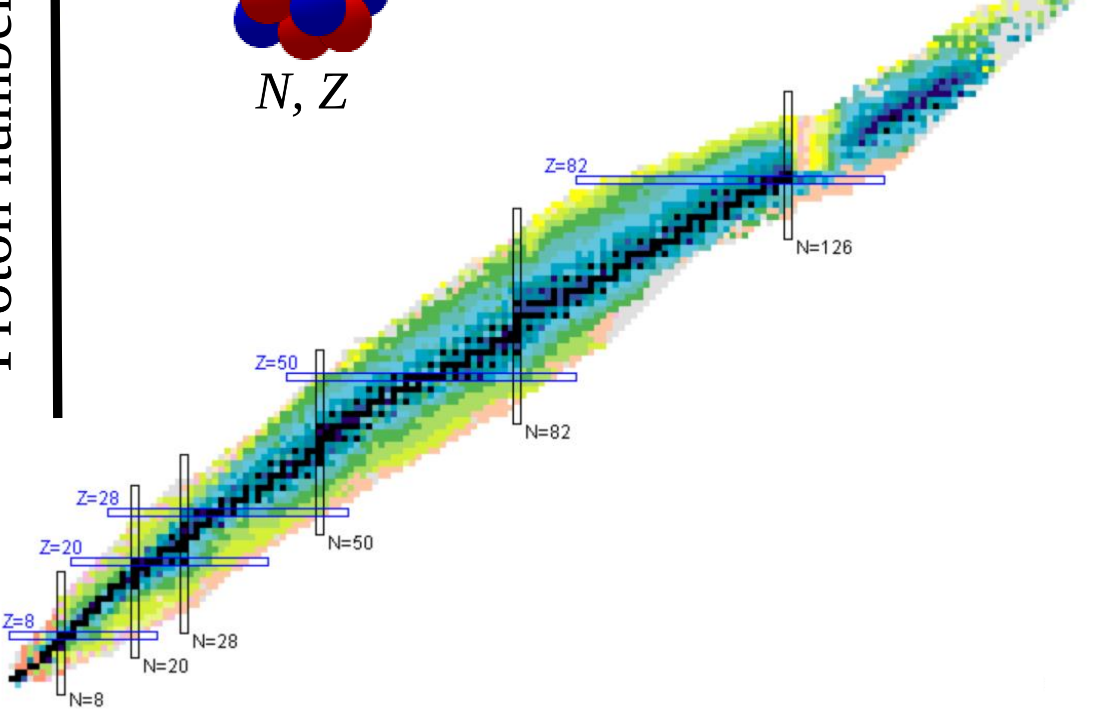


All nuclei can be described with a *single* EDF

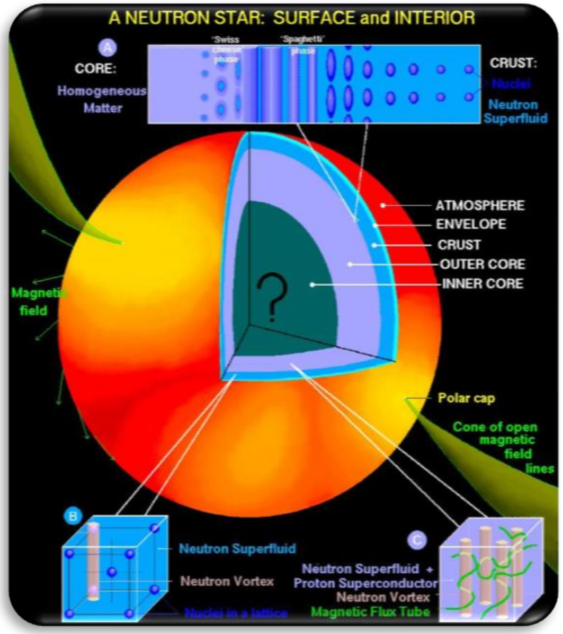


N, Z

Proton number



Neutron star

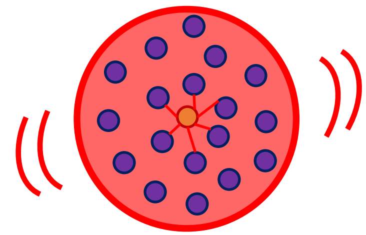


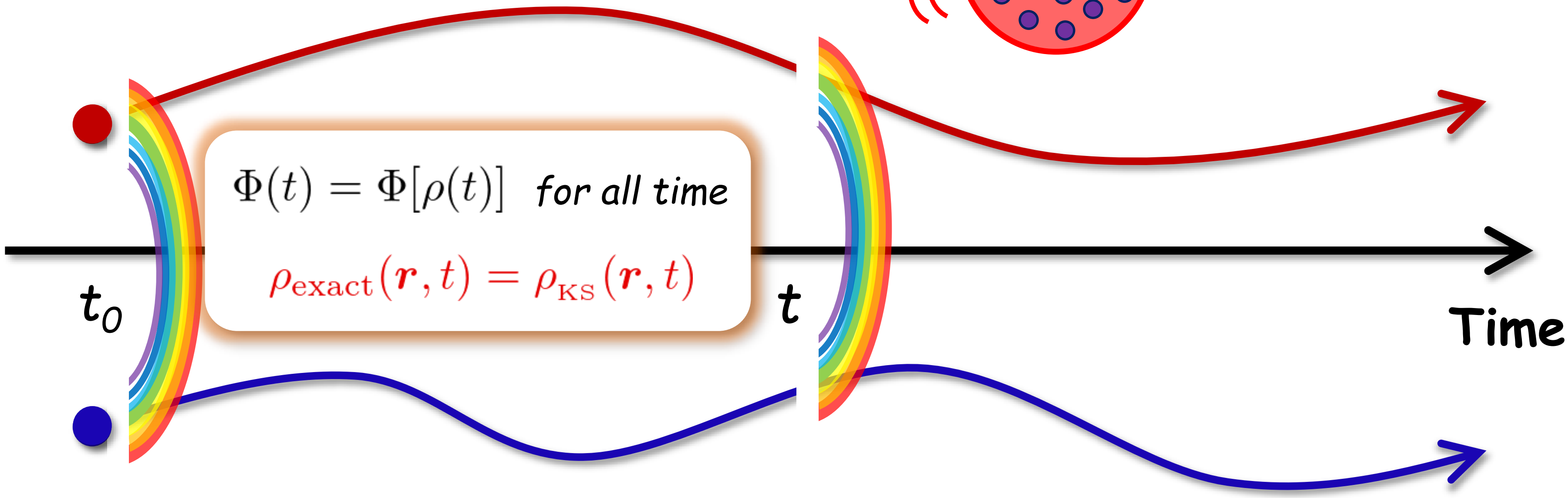
Neutron number

TDDFT is a time-dependent extension of DFT

TDSE for an *N*-body system

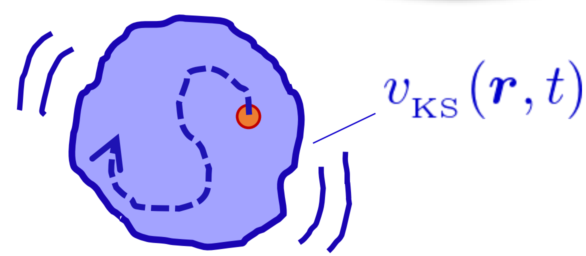
$$i\hbar\frac{\partial}{\partial t}\Phi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_N,t)=\hat{H}\Phi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_N,t)$$





TDKS eq. in TDDFT

$$i\hbar\frac{\partial\phi_i(\boldsymbol{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+v_{\rm KS}[\rho(\boldsymbol{r},t)]\right]\phi_i(\boldsymbol{r},t)$$



E. Runge and E.K.U. Gross, Phys. Rev. Lett. **52**, 997 (1984); R. van Leeuwen, Phys. Rev. Lett. **82**, 3863 (1999).

TDDFT in a tiny nutshell - Runge-Gross theorem

E. Runge and E.K.U. Gross, Phys. Rev. Lett. **52**, 997 (1984)

One-body density:

$$\rho(\boldsymbol{r},t) = N\int d\boldsymbol{r}_2 \cdots \int d\boldsymbol{r}_N |\Psi(t)|^2$$

One-body current density:

$$\boldsymbol{j}(\boldsymbol{r},t) = \frac{\hbar N}{2im}\int d\boldsymbol{r}_2 \cdots \int d\boldsymbol{r}_N \left[\Psi^*(t)\nabla\Psi(t) - \Psi(t)\nabla\Psi^*(t)\right]$$

TDSE:

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$$

$$\Psi = \Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N, t)$$

The rate of change of the current density reads:

$$\frac{\partial \boldsymbol{j}}{\partial t} = \frac{N}{2m}\int d\boldsymbol{r}_2 \cdots \int d\boldsymbol{r}_N \left[(H\Psi)^*\nabla\Psi - \Psi^*\nabla(H\Psi) + (H\Psi)\nabla\Psi^* - \Psi\nabla(H\Psi)^*\right] \quad \cdots \text{(a)}$$

$$\frac{\partial \boldsymbol{j}'}{\partial t} = \frac{N}{2m}\int d\boldsymbol{r}_2 \cdots \int d\boldsymbol{r}_N \left[(H'\Psi')^*\nabla\Psi' - \Psi'^*\nabla(H'\Psi') + (H'\Psi')\Psi'^* - \Psi'\nabla(H'\Psi')^*\right] \quad \cdots \text{(b)}$$

(a) − (b)

$$\boxed{\frac{\partial}{\partial t}\left[\boldsymbol{j}(\boldsymbol{r},t) - \boldsymbol{j}'(\boldsymbol{r},t)\right] = -\frac{1}{m}\rho(\boldsymbol{r},t)\nabla\underbrace{\left[v_{\text{ext}}(\boldsymbol{r},t) - v'_{\text{ext}}(\boldsymbol{r},t)\right]}_{\neq c(t)}} \quad \cdots (\bigstar)$$

*One can obtain equations for higher-order derivatives in the same manner

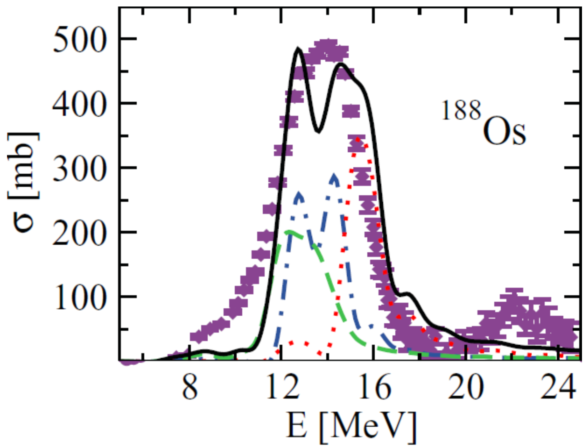
As in the case of static DFT, we have a TDKS scheme according to the following one-to-one correspondences:

$$\hat{H}(t) \overset{\text{TDSE}}{\Leftrightarrow} \Psi(t) \overset{\text{RG}}{\Leftrightarrow} \boldsymbol{j}(\boldsymbol{r},t)\ \&\ \rho(\boldsymbol{r},t)$$

*Taking divergence of Eq.(★) and using the continuity equation, one can obtain equations for the density. $\frac{\partial\rho}{\partial t} + \nabla\cdot\boldsymbol{j} = 0$

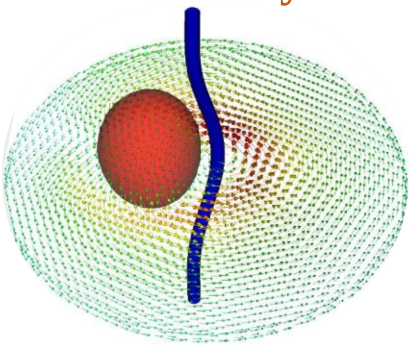
TDDFT is a versatile tool!!

IVGDR



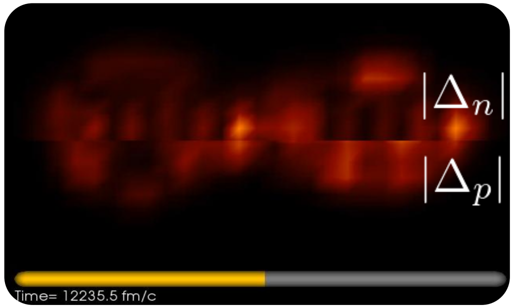
Phys. Rev. C **84**, 051309(R) (2011)
I. Stetcu, A. Bulgac, P. Magierski, and K.J. Roche

Vortex-nucleus dynamics



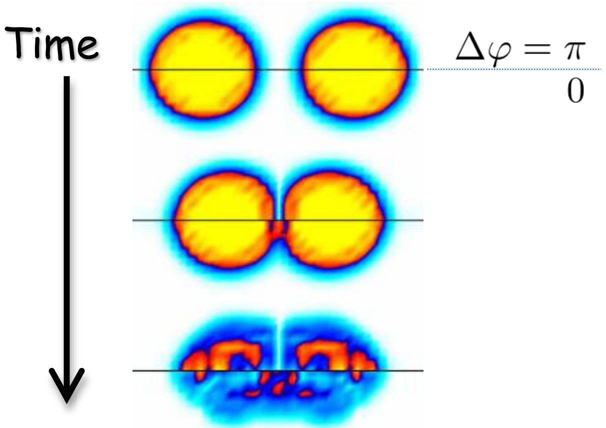
Phys. Rev. Lett. **117**, 232701 (2016)
G. Wlazłowski, K.S., P. Magierski, A. Bulgac, and M.M. Forbes

Induced fission of ^{240}Pu



Phys. Rev. Lett. **116**, 122504 (2016)
A. Bulgac, P. Magierski, K.J. Roche, and I. Stetcu

Low-energy heavy-ion reactions



Phys. Rev. Lett. **119**, 042501 (2017)
P. Magierski, K.S., and G. Wlazłowski

Q. What are difference and relevance between Hartree-Fock theory and DFT?

A. HF $\neq$ DFT, but HF with an “effective interaction” may be regarded as Kohn-Sham DFT

Hartree-Fock theory vs. DFT

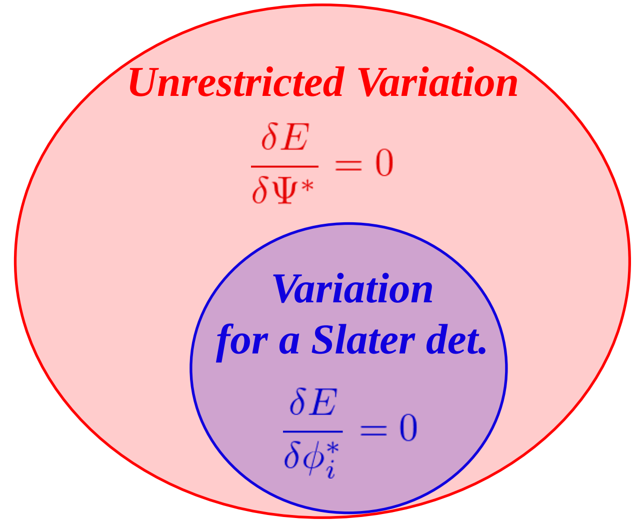
Regarding E_{Skyrme} as an EDF, Skyrme-HF eq. may be regarded as KS eq. in DFT

Unrestricted variation

Schrödinger eq:

$$\hat{H}\big|\Psi\big\rangle = E\big|\Psi\big\rangle$$

so, of course, HF ≠ DFT



Variation for a Slater determinant

Hartree-Fock eq: **Integro-differential eq.*

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \Gamma_{\mathrm{H}}(\boldsymbol{r})\right)\phi_i(\boldsymbol{r}) + \int \Gamma_{\mathrm{F}}(\boldsymbol{r},\boldsymbol{r}')\phi_i(\boldsymbol{r}')d\boldsymbol{r}' = \varepsilon_i\phi_i(\boldsymbol{r})$$

Slater determinant:

$$\Phi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N) = \frac{1}{\sqrt{N!}}\det\{\phi_i(\boldsymbol{r}_j)\}$$

Orthonormal condition:

$$\big\langle\phi_i\big|\phi_j\big\rangle = \delta_{ij}$$

Hartree potential (direct term):

$$\Gamma_{\mathrm{H}}(\boldsymbol{r}) = \int v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

Fock potential (exchange term):

$$\Gamma_{\mathrm{F}}(\boldsymbol{r},\boldsymbol{r}') = v(\boldsymbol{r},\boldsymbol{r}')\sum_i \phi_i(\boldsymbol{r})\phi_i^*(\boldsymbol{r}')$$

$$E = \frac{\big\langle\Psi\big|\hat{H}\big|\Psi\big\rangle}{\big\langle\Psi\big|\Psi\big\rangle}$$

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} v(\boldsymbol{r}_i,\boldsymbol{r}_j)$$

Regarding E_{Skyrme} as an EDF, Skyrme-HF eq. may be regarded as KS eq. in DFT

- One may also regard Skyrme-TDHF as TDKS in TDDFT

Unrestricted variation

Schrödinger eq:

$$\hat{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

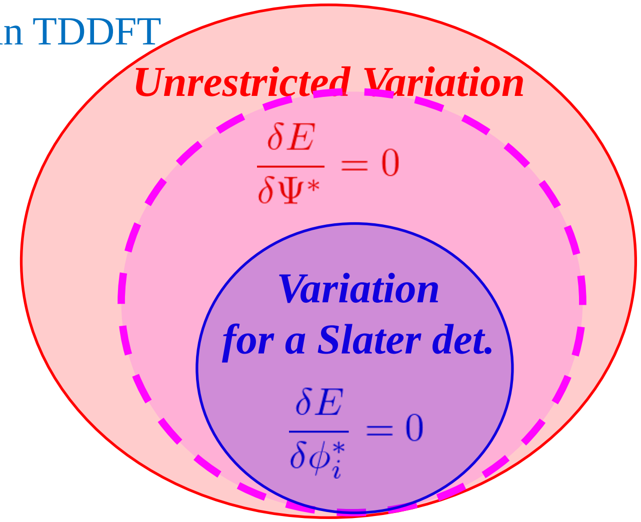
Kohn-Sham equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_{\text{KS}}[\rho(\boldsymbol{r})]\right]\phi_i(\boldsymbol{r}) = \varepsilon_i\,\phi_i(\boldsymbol{r})$$

Variation for a Slater determinant

Hartree-Fock eq: **Integro-differential eq.*

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \Gamma_{\text{H}}(\boldsymbol{r})\right)\phi_i(\boldsymbol{r}) + \int \Gamma_{\text{F}}(\boldsymbol{r},\boldsymbol{r}')\phi_i(\boldsymbol{r}')d\boldsymbol{r}' = \varepsilon_i\phi_i(\boldsymbol{r})$$



Skyrme "effective interaction" **$t_{0\text{-}3}$, $x_{0\text{-}3}$, W_0, and α are the parameters*

T.H.R. Skyrme, Philos. Mag. **1**, 1043 (1956)

$$\hat{v}_{ij} = t_0(1 + x_0\hat{P}_\sigma)\delta(\boldsymbol{r}) + \frac{1}{6}t_3\rho^\alpha(\boldsymbol{R})(1 + x_3\hat{P}_\sigma)\delta(\boldsymbol{r})$$
$$+\frac{1}{2}t_1(1 + x_1\hat{P}_\sigma)\left[\delta(\boldsymbol{r})\hat{\boldsymbol{k}}^2 + \hat{\boldsymbol{k}}'^2\delta(\boldsymbol{r})\right] + t_2(1 + x_2\hat{P}_\sigma)\hat{\boldsymbol{k}}'\cdot\delta(\boldsymbol{r})\hat{\boldsymbol{k}}$$
$$+iW_0(\hat{\boldsymbol{\sigma}}_i + \hat{\boldsymbol{\sigma}}_j)\cdot\left[\hat{\boldsymbol{k}}'\times\delta(\boldsymbol{r})\hat{\boldsymbol{k}}\right]$$

$\boldsymbol{r} = \boldsymbol{r}_i - \boldsymbol{r}_j$: Relative coordinate

$\boldsymbol{R} = (\boldsymbol{r}_i + \boldsymbol{r}_j)/2$: C.M. coordinate

$\hat{\boldsymbol{k}} = (\nabla_i - \nabla_j)/2i$: Relative momentum op.

$\hat{P}_\sigma$: Spin exchange op.

Skyrme-Hartree-Fock eq:

$$-\frac{\hbar^2}{2m}\nabla^2\phi_i(\boldsymbol{r},\sigma) + \sum_{\sigma\sigma'}\Gamma^{\text{HF}}_{\sigma\sigma'}(\boldsymbol{r})\phi_i(\boldsymbol{r},\sigma') = \varepsilon_i\phi_i(\boldsymbol{r},\sigma)$$

$$E_{\text{Skyrme}} = \left\langle\Phi\middle|\hat{H}_{\text{Skyrme}}\middle|\Phi\right\rangle = E[\rho,\tau,\boldsymbol{j},\boldsymbol{s},\boldsymbol{T},J_{\mu\nu}]$$

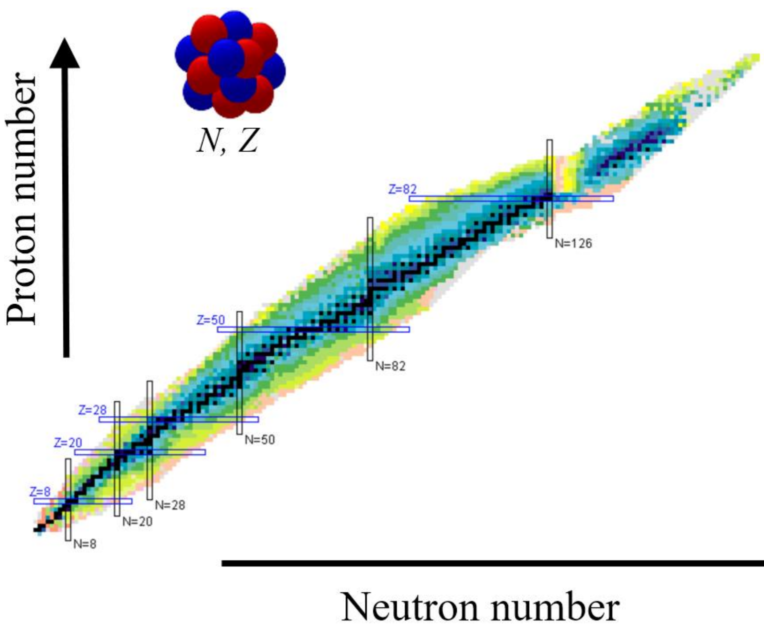
$$\Gamma^{\text{HF}}_{\sigma\sigma'} = \sum_\alpha \frac{\delta E}{\delta \xi_\alpha}$$

*E is a functional of various densities
*ξ_α stands here for various densities

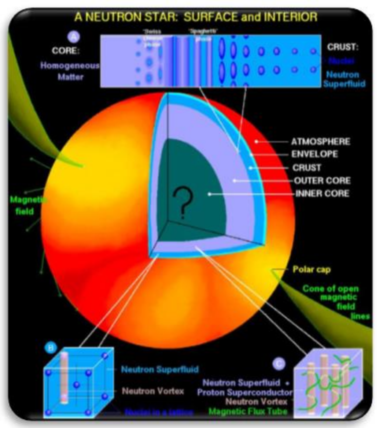
Summary

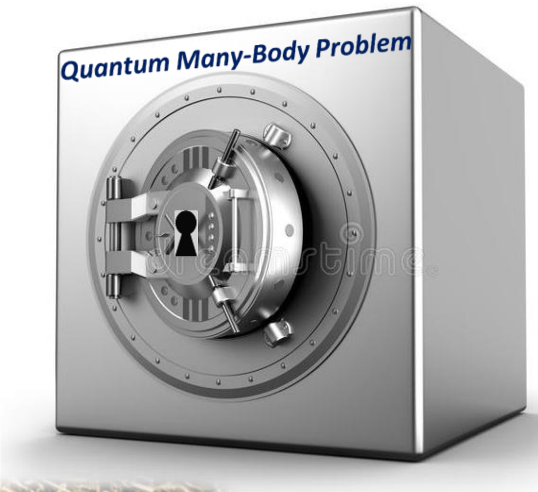
Takeaway message

✓ (TD)DFT is a powerful theoretical framework to study quantum many-body problems of nucleons at low energy from nuclei to neutron stars



Neutron star





Lecture Plan

Theory

#1. An introduction to microscopic mean-field approaches and (TD)DFT

Nuclear reactions

#2. Recent advances in microscopic approaches for heavy-ion reactions

Superheavy element synthesis & deep-inelastic collisions

Neutron stars

#3. Neutron-star “glitch” and neutron superfluid

Dynamics of <u>quantized vortices</u> in the inner crust of neutron stars

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