Quantum Hydrodynamic Modes and Bioenergy Transfer of a Vibrational Polaron in α-helix Protein

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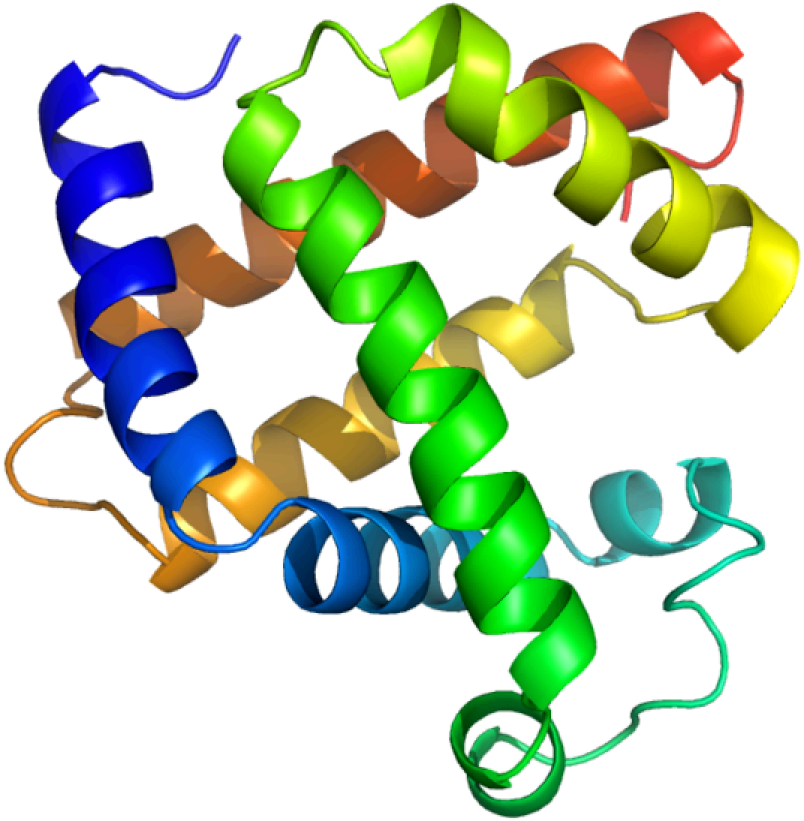
One-dimensional Protein Chain

3D structure of Myoglobyn



S.V.E.Philips, J. Mol. Bio.**142**,531(1980)

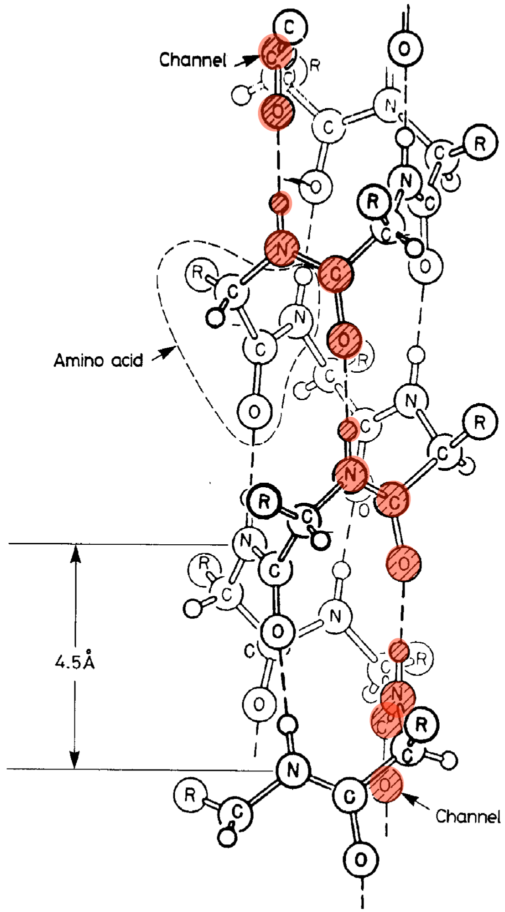
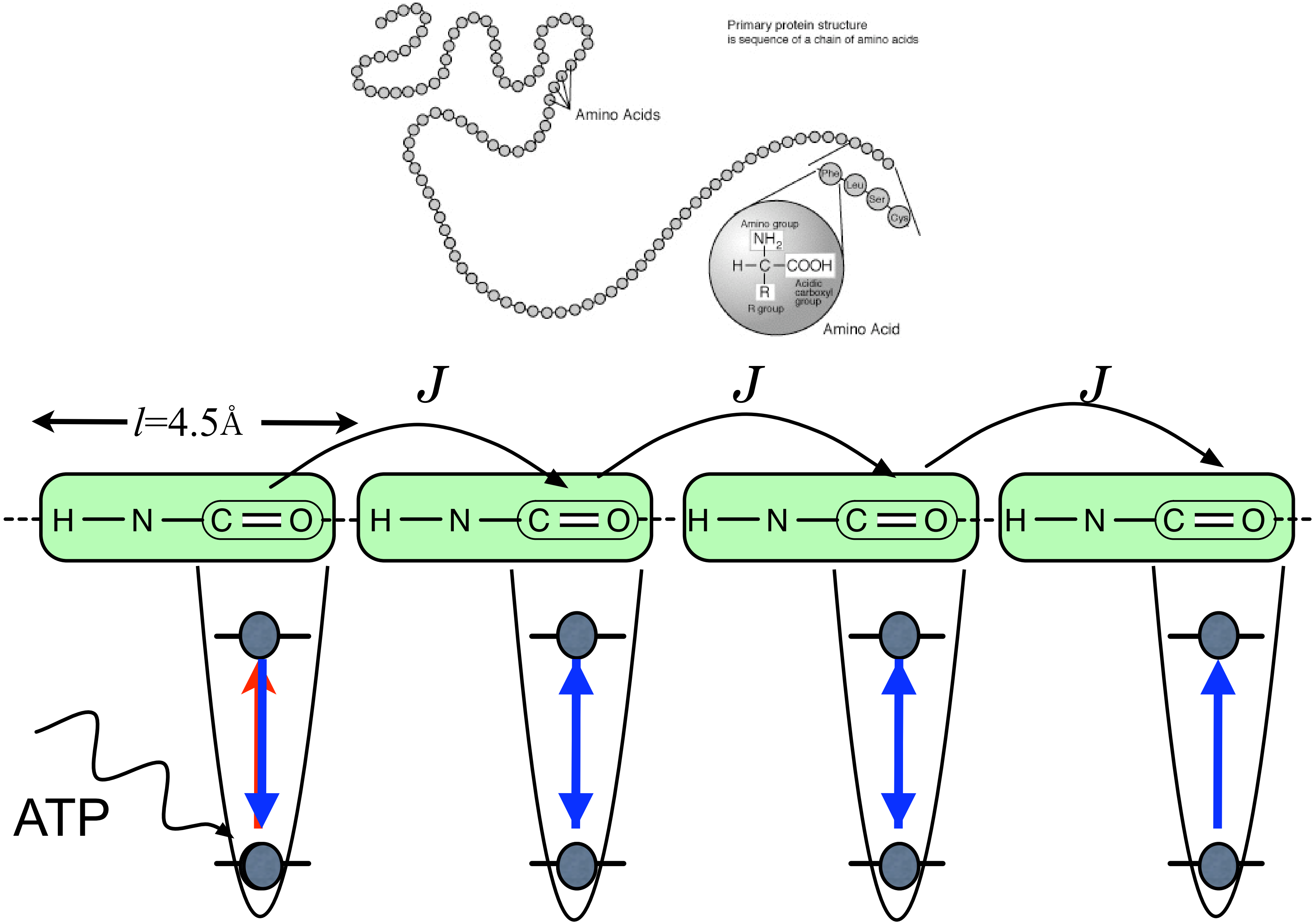


Figure 1. An atomic model of the alpha-helix. One "channel" is cross-hatched.


Primary protein structure
is sequence of a chain of amino acids
Amino Acids
Phe
Leu
Ser
Cys
Amino group
NH2
H—C—COOH
R
R group
Acidic carboxyl group
Amino Acid
J
J
J
l=4.5Å
H—N—C=O
H—N—C=O
H—N—C=O
H—N—C=O
ATP

Davydov's Hamiltonian

$$H = H_{vib} + H_{ph} + H_{vib-ph}$$

$$H_{vib} = \sum_n E_0 B_n^\dagger B_n - J \sum_n (B_{n+1}^\dagger B_n + B_n^\dagger B_{n+1})$$

$$H_{ph} = \frac{1}{2} \sum_n \left[w(u_{n+1} - u_n)^2 + \frac{p_n^2}{M} \right]$$

$$H_{vib-ph} = \chi \sum_n B_n^\dagger B_n (u_{n+1} - u_{n-1})$$

E_0 [cm^{-1}]	J [cm^{-1}]	l [Å]	w [N/m]	M[kg]	χ [pN]
1650	8	4.5	13	1.9 10^{-25}	62

A.S. Davydov, Sov. Phys. JETP 51, 397(1980)

Davydov's soliton

A.S. Davydov (1976)

Trial wave function

$$|\psi(t)\rangle = \sum_n \underline{\phi_n(t)} B_n^\dagger \exp[-i/\hbar \sum_q \underline{\beta_q^n(t)}(a_q - a_q^\dagger)]|vac\rangle$$

Time dependent variational method

$$\delta \int_0^t \langle\psi(\tau)|H|\psi(\tau)\rangle d\tau = 0$$

Non-linear Schrodinger equation => Soliton solution

Bioenergy transport

Problem: At physiological temperature (T=310K)
Soliton is decayed by the thermal fluctuation

P. S. Lomdahl (1985)

1D Polaron Hamiltonian

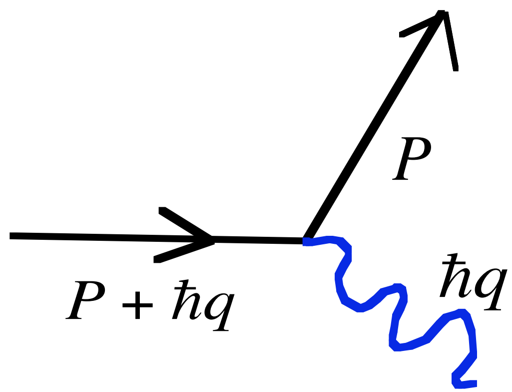
Normal mode representation $$u_n = \sum_q \sqrt{\frac{\hbar}{2L(M/l)\omega_q}}(a_q + a_{-q}^\dagger)e^{iqnl}$$

Momentum representation of a single vibron $$|p\rangle \equiv \frac{1}{\sqrt{N}} \sum_n e^{\frac{i}{\hbar}pnl} B_n^\dagger |vac\rangle$$

$$H_1 = \sum_p \varepsilon_p |p\rangle\langle p| + \sum_q \hbar\omega_q a_q^\dagger a_q + \sqrt{\frac{2\pi}{L}} \sum_{p,q} g_q |p+\hbar q\rangle\langle p|(a_q + a_{-q}^\dagger)$$

$$g_q = 2i\alpha q\sqrt{\frac{\hbar}{4\pi(M/l)\omega_q}} \quad (\alpha \equiv \chi l)$$

$$\varepsilon_p = \frac{p^2}{2m}, \ \omega_q = c|q| \qquad m = \frac{\hbar^2}{2l^2 J}$$



Quantum Liouville eq.

$$i\frac{\partial}{\partial t}\rho(t) = \mathcal{L}\rho(t) \qquad \mathcal{L}\cdot \equiv \frac{1}{\hbar}[H,\cdot]$$

Reduced distribution

$$f(t) \equiv \mathrm{Tr}_{\mathrm{ph}}[\rho(t)]$$

Initial condition: Phonon = thermal equilibrium

$$\rho_{ph} = \frac{1}{Z_{ph}}\exp[-H_{ph}/k_B T] \quad Z_{ph} \equiv \Pi_q \frac{1}{1-\exp[-\hbar\omega_q/k_B T]}$$

Wigner function representation

$$f_k(P;t) \equiv \langle P + \frac{\hbar k}{2} | f(t) | P - \frac{\hbar k}{2} \rangle$$

$$f^W(X, P; t) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} f_k(P;t) e^{ikX} dk$$

- $k=0$: Momentum distribution function

$$f_0(P;t) = < P | f(t) | P > = \int_{-\infty}^{\infty} f^W(X, P; t) dX$$

- $k \neq 0$: Inhomogeneous distribution in space
  => diffusion mode, sound mode

Kinetic equation (k=0 momentum distribution)

$$\frac{\partial}{\partial t} f_0(P;t) = -\hat{\mathcal{K}} f_0(P;t)$$

- Collision operator (weak coupling)

$$\hat{\mathcal{K}} = iP^{(0)}\mathcal{L}_{ep}Q^{(0)}\frac{1}{i0^+ - \mathcal{L}_0}Q^{(0)}\mathcal{L}_{ep}P^{(0)}$$

[$P^{(0)}$ projector onto k=0 space]

$$\begin{aligned}
\hat{\mathcal{K}} \;=\; & \frac{2\pi}{\hbar^2}\int dq|g_q|^2\Big\{\delta(\frac{\varepsilon_P - \varepsilon_{P+\hbar q}}{\hbar} + \omega_q)n_q + \delta(\frac{\varepsilon_{P-\hbar q} - \varepsilon_P}{\hbar} + \omega_q)(n_q+1)\Big\} \\
- & \frac{2\pi}{\hbar^2}\int dq|g_q|^2\Big\{\delta(\frac{\varepsilon_{P-\hbar q} - \varepsilon_P}{\hbar} + \omega_q)n_q \exp[-\hbar q\,\partial/\partial P] \\
& +\delta(\frac{\varepsilon_P - \varepsilon_{P+\hbar q}}{\hbar} + \omega_q)(n_q+1)\exp[\hbar q\,\partial/\partial P]\Big\}
\end{aligned}$$

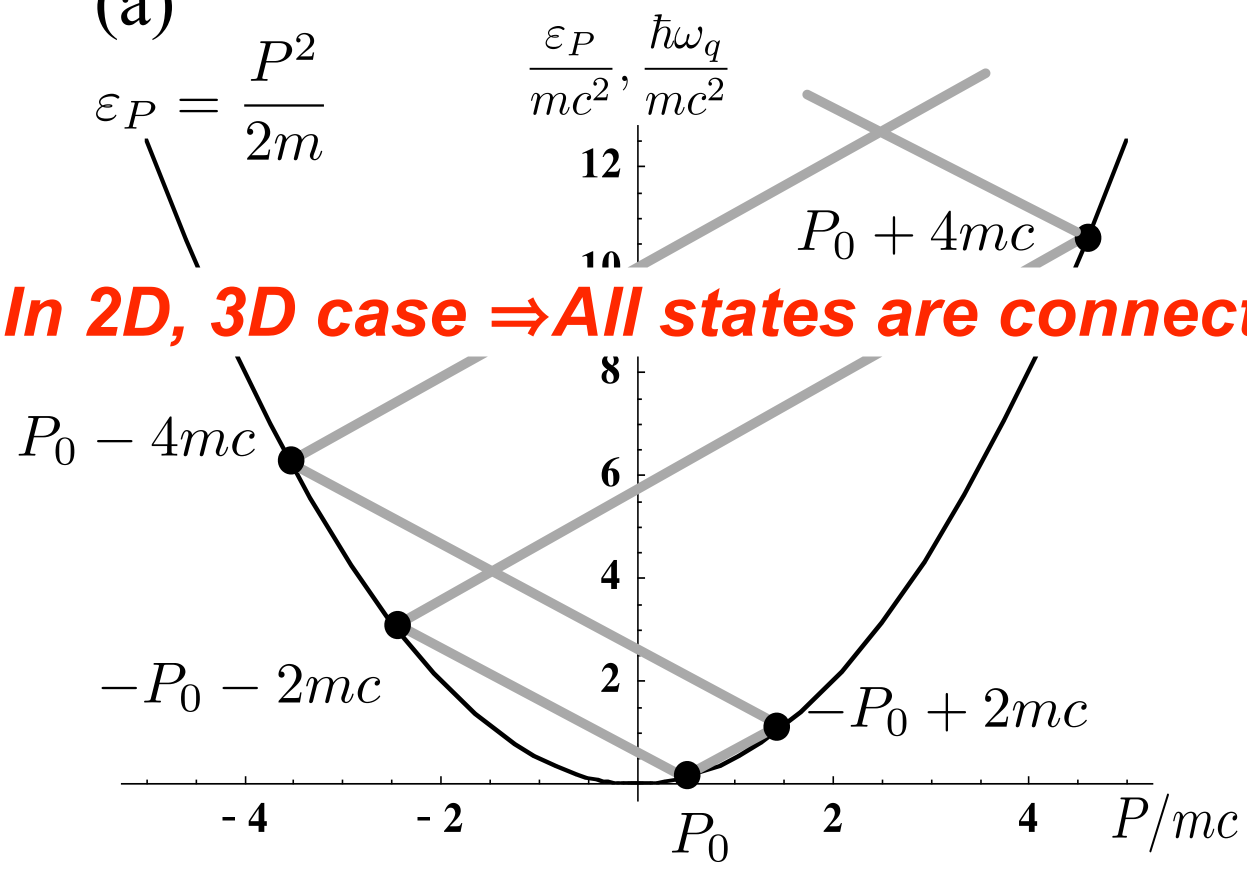
Difference operator:
Quantum effect

$\rightarrow 0 \quad (\hbar \rightarrow 0)$ **No dissipation in Classical limit**

Resonance relation

$$\boxed{\varepsilon_{P\pm\hbar q}-\varepsilon_P=\pm\hbar\omega_q}$$

(a)



In 2D, 3D case ⇒All states are connected

Sequence of the coupled states $|P_{0;n-1}\rangle$, $|P_{0;n}\rangle$, $|P_{0;n+1}\rangle$

$$P_{0;n}\equiv(-1)^n(P_0-2nmc)\quad(n=0,\pm1,\pm2,\cdots)$$

Infinite numbers of disjoint sets of states

Eigenfunctions of $\mathcal{K}$

$$\hat{\mathcal{K}}\phi_j^{(0)}(P) = \lambda_j^{(0)}\phi_j^{(0)}(P)$$

$$f_0(P;t) = \sum_j \exp[-\lambda_j^{(0)}t]\phi_j^{(0)}(P)c_j^{(0)}$$

$$\begin{aligned} \lambda_j^{(0)} &= \frac{2\pi}{\hbar^2}\int dP \int dq |g_q|^2 \varphi_{eq}^{-1}(P) n_q \delta(\underline{\frac{\varepsilon_P - \varepsilon_{P+\hbar q}}{\hbar} + \omega_q)} \\ &\times \underline{\left|\phi_j^{(0)}(P) - e^{\beta\hbar\omega_q}\phi_j^{(0)}(P+\hbar q)\right|}^2 \geq 0 \end{aligned}$$

$\Rightarrow$ H-theorem

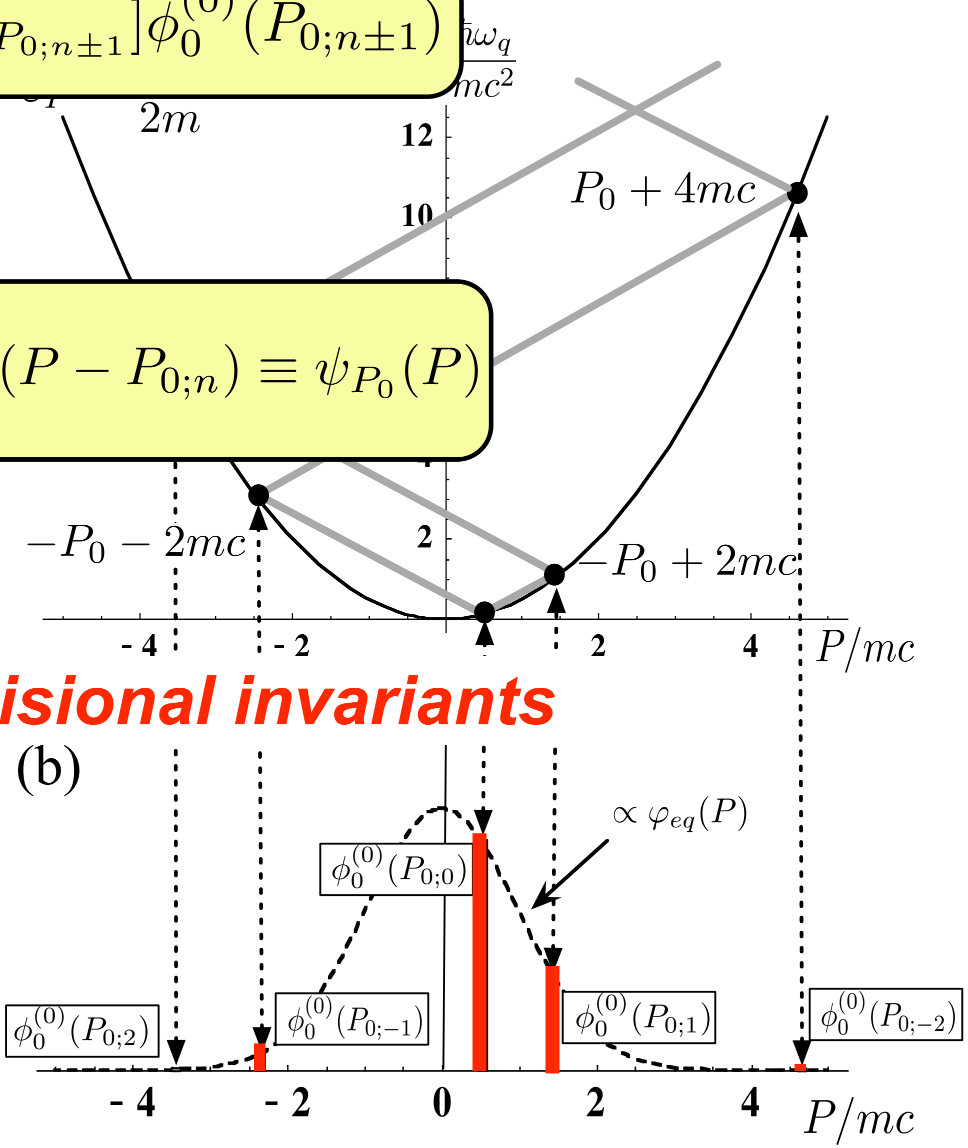
$\boxed{\text{Collision invariant: } \lambda_0^{(0)} = 0}$

Collisional invariants

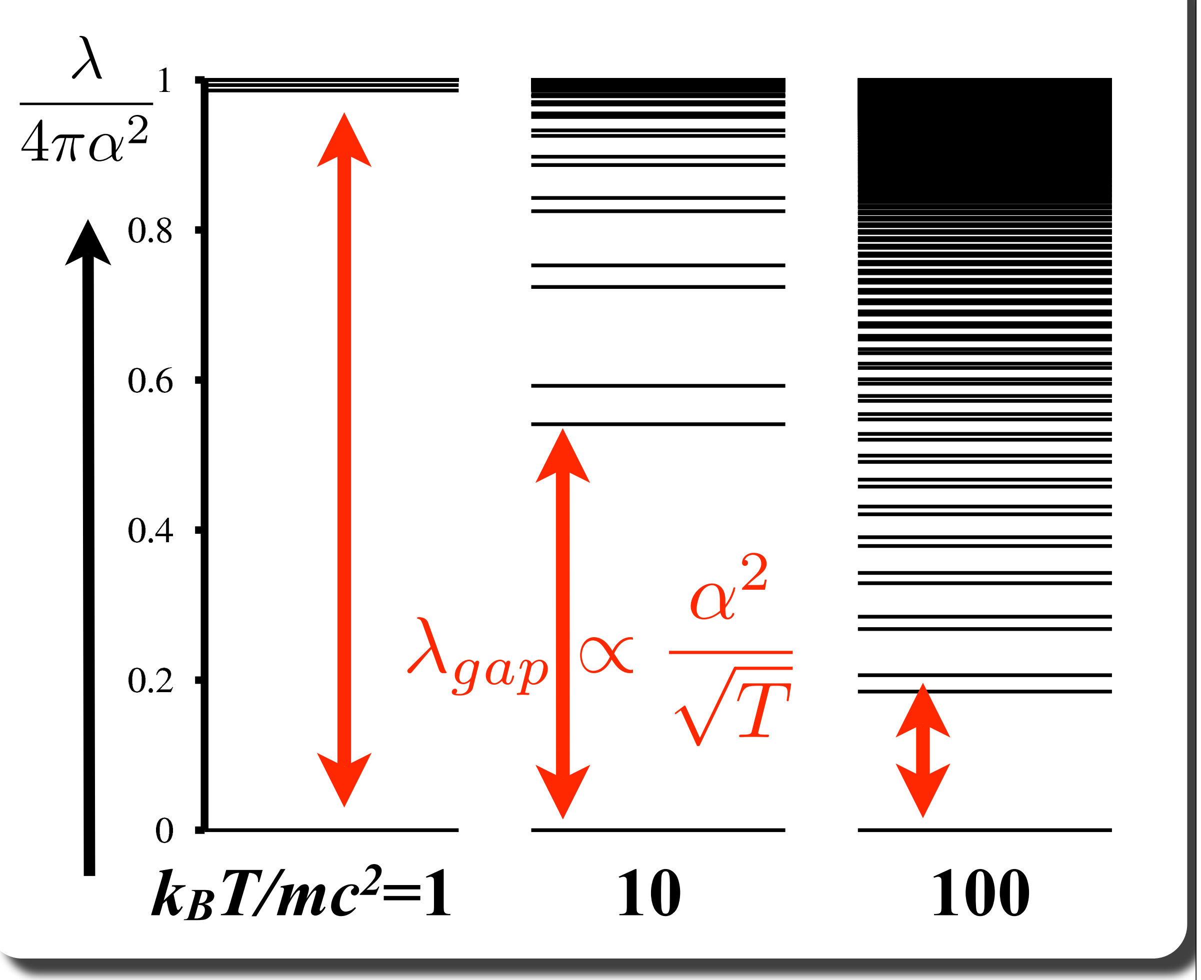
$$\exp[\beta\varepsilon_{P_{0;n}}]\phi_0^{(0)}(P_{0;n}) = \exp[\beta\varepsilon_{P_{0;n\pm1}}]\phi_0^{(0)}(P_{0;n\pm1})$$

$$\phi_0^{(0)}(P) = \mathcal{N}_{P_0}^{-1}\sum_n \exp[-\beta\varepsilon_P]\delta(P - P_{0;n}) \equiv \psi_{P_0}(P)$$

Infinite numbers of collisional invariants



Spectrum of $\mathcal{K}$



Relaxation time $\tau_{rel} \sim 1/\lambda_{gap}$:
relaxation of momentum distribution

Quantum Sound wave

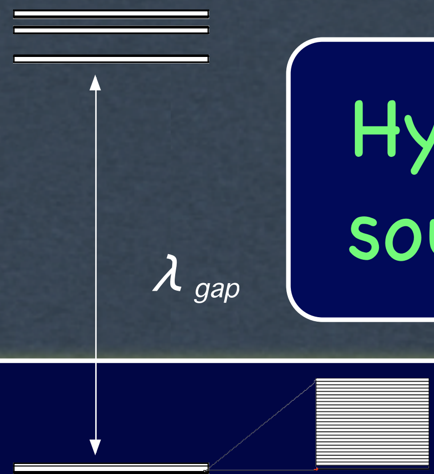
Kinetic equation for spatially inhomogeneous component

$$\frac{\partial}{\partial t} f_k(P,t) = -(\hat{\mathcal{K}} + ikP/m) f_k(P,t)$$

Hydrodynamic condition:

mean free path << inhomogeneity : $|k|c \ll \lambda_1^{(0)}$

(~lattice constant for 310K)

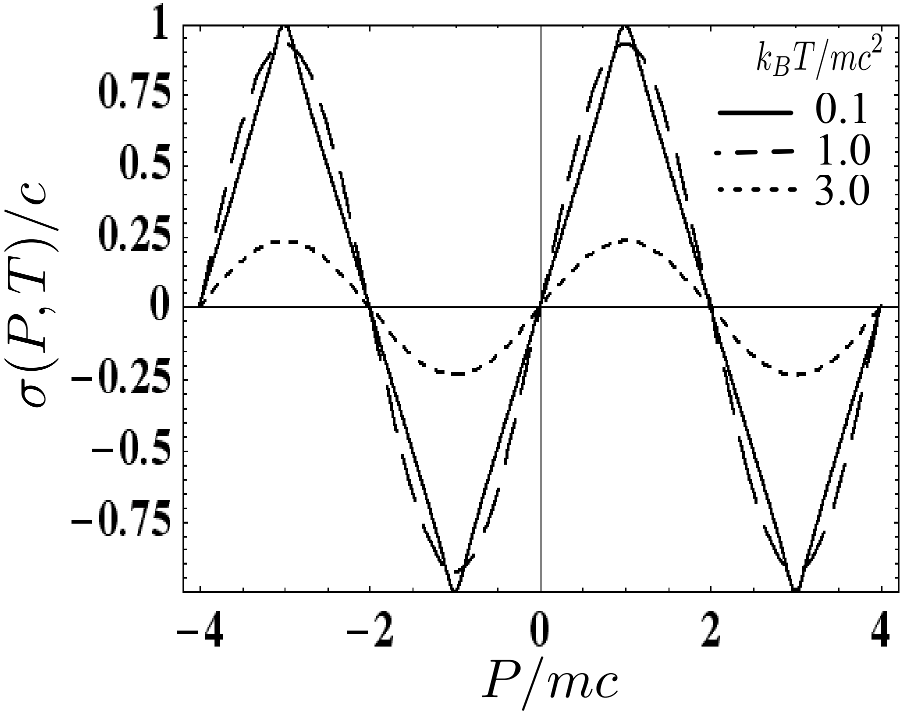


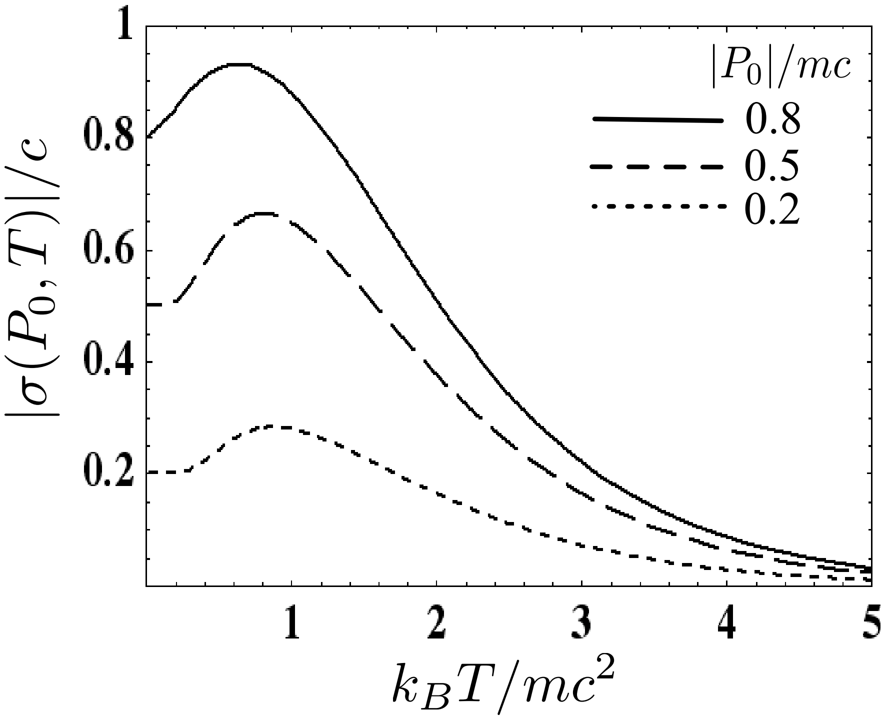
Hydrodynamic modes:
sound mode, diffusion

Collision invariant
infinite degeneracy

Sound velocity : 1st order perturbation

$$\sigma(P_0, T) = \langle\langle \psi_{P_0} | (P/m) | \psi_{P_0} \rangle\rangle = \frac{\sum_{n=-\infty}^{\infty} (P_{0;n}/m) \exp[-\beta \varepsilon_{P_{0;n}}]}{\sum_{n=-\infty}^{\infty} \exp[-\beta \varepsilon_{P_{0;n}}]}$$





Quantum Sound Wave

Initial min ... packet

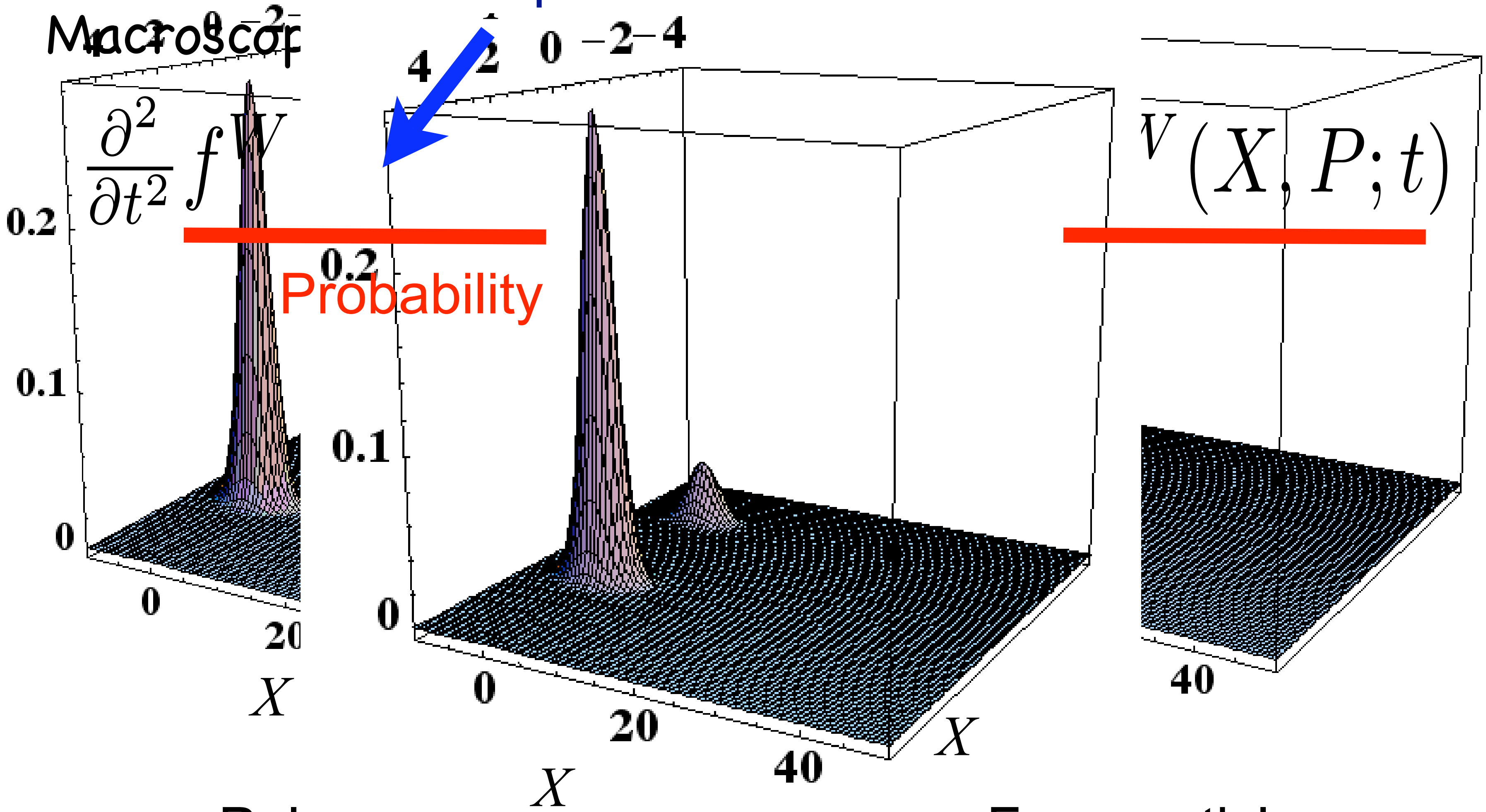
T increases

Wave packet more stable

Macroscop

$$\frac{\partial^2}{\partial t^2} f^W \quad (X, P; t)$$

Probability



Polaron

Free particle

4. Values of Sound Velocity in α-helix

effective mass: $m = \dfrac{\hbar^2}{2l^2 J} = 1.77 \times 10^{-28}\mathrm{kg}$

sound velocity of phonon: $c = l\sqrt{\dfrac{K}{M}} = 3722\mathrm{m/s}$

coupling strength: $\alpha = \chi l = 0.174\mathrm{eV}$

$T_{\mathrm{unit}} \equiv mc^2/k_B$

⇒ Temperature unit: $T_{\mathrm{unit}} = 178\mathrm{K}$

$310\mathrm{K} / T_{\mathrm{unit}} \sim 2$

T= 310K=37℃(Physiological temperature)

relaxation time: $t_r = 42\mathrm{fs}$

maximum quantum sound velocity: $\sigma_{max} = 2400\mathrm{m/s}$

⇒ Time for traveling 100 amino acids: 20 ps

Quantum effect is important even at Physiological temperature

GaAs quantumwire

effective mass: $m = 0.07 m_e = 6.37 \times 10^{-32}\mathrm{kg}$

sound velocity of phonon: $c = 3400\mathrm{m/s}$

coupling strength: $\alpha = 7.2\mathrm{eV}$

$\Rightarrow$ Temperature unit: $T_{\mathrm{unit}} = 0.053\mathrm{K}$

Quantum effect is prominent at very low temperature

9. Summary

- Thermal equilibrium
  Infinite degeneracy of collision invariant
  - Hydrodynamic Quantum Sound mode
  - Macroscopic linear wave equation (probability)
- Dissipation due to purely quantum effect

Optical phonon:

・Collision invariants => even function for P

・No first order perturbation by flow term (kP)

・ No sound mode