Statistical Mechanics of Davidov-Scott's Protein Model in Thermal Bath

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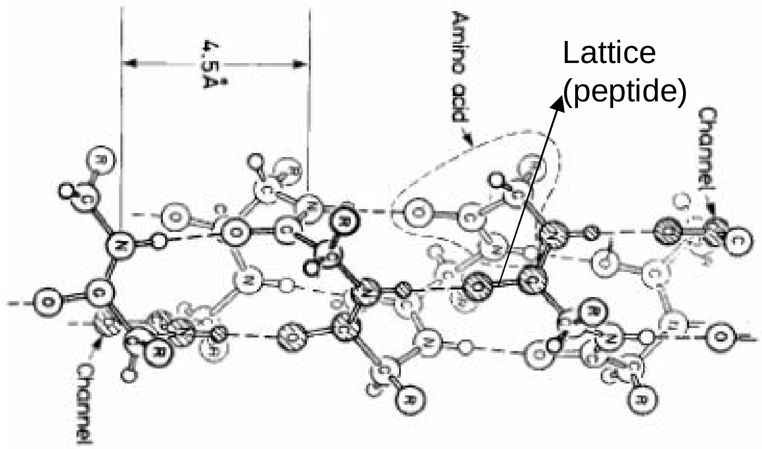
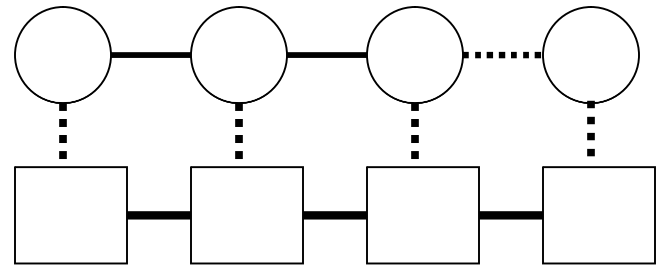
Framework:

- Davydov-Scott: Model of energy transfer mechanism in α helix protein.
- Biological temperature: quantum system contact wih thermal bath.
- Open quantum system: Quantum state diffusion
- Thermal fluctuation: statistical mechanics (specific heat)





Davydov-Scott model: mechanism for the localization and transport of vibrational energy in alpha-helix protein.
the alpha-helix region of a protein is a chain of amino acids held in helical shape by longitudinal hydrogen bonds.

$$\hat{H} = \hat{H}_{\mathrm{ex}} + \hat{H}_{\mathrm{ph}} + \hat{H}_{\mathrm{int}},$$

where

$$\hat{H}_{\mathrm{ex}} = \sum_n \left[E_0 \hat{B}_n^\dagger \hat{B}_n - J\,(\hat{B}_n^\dagger \hat{B}_{n+1} + \hat{B}_n^\dagger \hat{B}_{n-1}) \right],$$

$$\hat{H}_{\mathrm{ph}} = \tfrac{1}{2} \sum_n \left[\hat{p}_n^2 / \tilde{M} + \tilde{w}\,(\hat{u}_{n+1} - \hat{u}_n)^2 \right],$$

$$\hat{H}_{\mathrm{int}} = \chi \sum_n (\hat{u}_{n+1} - \hat{u}_n) \hat{B}_n^\dagger \hat{B}_n.$$

Model:
Vibrational energy of the CO stretching (or Amide-I) is localized through a phonon coupling effect to distort the structure of the helix. The helical distortion reacts again through phonon coupling to trap the Amide-I oscillation energy and prevent its dispersion.
This effect is called *self-trapping (soliton)*

Does the Davidov-Scott's soliton exist at Biological temperature?

Consider The Davidov-Scott monomer, amide-I oscillator expressed by the coordinate (*x*) and momentum (*p*) operators, and the lattice expressed by the displacement and momentum operator *Q* and *P* respectively.

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \frac{P^2}{2M} + \frac{1}{2}\kappa Q^2 + \chi' x Q \ ,$$

Biological temperature: system contact with thermal bath
We have open quantum system. We us Quantum State Diffusion theroy

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H, \rho] + \sum_j (L_j \rho L_j^\dagger - \frac{1}{2} L_j^\dagger L_j \rho - \frac{1}{2}\rho L_j^\dagger L_j)$$

the operator *Lj* is called Lindblad operator. It's may not Hermitian and not unique. We choose

$$L_1 = \sqrt{\gamma(1+\nu)} \left(\sqrt{\frac{M\Omega}{2\hbar}} Q + i\sqrt{\frac{1}{2M\hbar\Omega}} P + \frac{\chi'}{\hbar\Omega}\sqrt{\frac{m\omega}{2\hbar}} x \right)$$

$$L_2 = \sqrt{\gamma\nu} \left(\sqrt{\frac{M\Omega}{2\hbar}} Q - i\sqrt{\frac{1}{2M\hbar\Omega}} P + \frac{\chi'}{\hbar\Omega}\sqrt{\frac{m\omega}{2\hbar}} x \right) \ .$$

The propagator of the master equation

$$K(x,x';Q,Q') = \int\int \mathcal{D}[x]\mathcal{D}[Q]\exp\left[\frac{i}{\hbar}\int \mathrm{d}t\left(\frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\tilde{\omega}^2x^2 + \frac{1}{2}\bar{M}\dot{Q}^2 + \frac{1}{2}\bar{M}\tilde{\Omega}^2Q^2 - \tilde{\chi}xQ\right)\right] , \qquad (6)$$

where $\tilde{\omega}^2 = \omega^2 - i(\delta_3/(m\hbar))$, $\tilde{\Omega}^2 = \Omega^2 - i(\delta_2/(\bar{M}\hbar))$, $\bar{M} = M - (2i\delta_1 M^2)/(\hbar^2)$ and $\tilde{\chi} = \chi - i\delta_4/2$. Making use of the Gaussian approximation, only the classical path of the lattice ($\bar{Q}$) contributes to the interaction term.[8] The propagator become,

$$K(x,x';Q,Q') = K_xK_Q = \int \mathcal{D}[x]\exp\left[-\frac{i}{\hbar}\int \mathrm{d}t\left(\frac{1}{2}m\dot{x}^2 - \frac{1}{2}\tilde{\omega}^2x^2 - \chi x\bar{Q}\right)\right] \times \int \mathcal{D}[Q]\exp\left[-\frac{i}{\hbar}\int \mathrm{d}t\left(\frac{1}{2}\bar{M}\dot{Q}^2 - \frac{1}{2}\bar{M}\tilde{\Omega}^2Q^2\right)\right] . \qquad (7)$$

The result:

$$K(Q,t;Q',0) = \exp\left[-i\frac{\pi}{2}\left(\frac{1}{2} + \|\frac{\tilde{\Omega}t}{\pi}\|\right)\right]\sqrt{\frac{\bar{M}\tilde{\Omega}}{2\pi\hbar|\sin(\tilde{\Omega}t)|}} \times \exp\left\{\frac{\bar{M}\tilde{\Omega}}{2\hbar|\sin(\tilde{\Omega}t)|}\left[(Q'^2+Q^2)\cos(\tilde{\Omega}t) - 2QQ'\right]\right\}$$

$$K(x,t;x',0) = \exp\left[-i\frac{\pi}{2}\left(\frac{1}{2} + \|\frac{\tilde{\omega}t}{\pi}\|\right)\right]\sqrt{\frac{m\tilde{\omega}}{2\pi\hbar|\sin(\tilde{\omega}t)|}}\exp\left\{\frac{i}{\hbar}S_{cl}\right\}$$

$$S_{cl} = \frac{m\tilde{\omega}}{2\sin(\tilde{\omega}t)}\left[(x^2+x'^2)\cos(\tilde{\omega}t) - 2xx'\right] + \frac{\tilde{\chi}\bar{Q}_0x'}{2\sin(\tilde{\omega}t)}\left[\frac{\sin((\tilde{\Omega}-\tilde{\omega})t)}{(\tilde{\Omega}-\tilde{\omega})} - \frac{\sin((\tilde{\Omega}+\tilde{\omega})t)}{(\tilde{\Omega}+\tilde{\omega})}\right] + \frac{\tilde{\chi}\bar{Q}_0\sin(\tilde{\Omega}t)x}{2\sin(\tilde{\omega}t)}\left[\frac{1}{(\tilde{\Omega}+\tilde{\omega})} - \frac{1}{(\tilde{\Omega}-\tilde{\omega})}\right]$$

Thermodynamical Properties

The partition function:

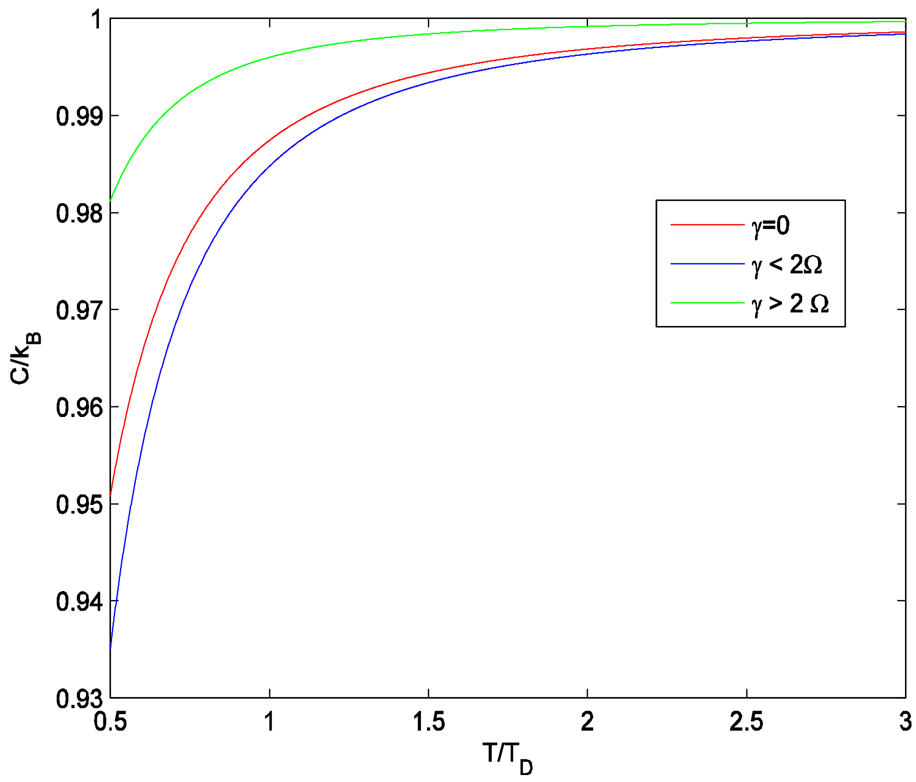
$$Z(\beta) = \frac{\exp\left[-\frac{\pi}{2}\left(i + \|\frac{\tilde{\Omega}\hbar\beta}{\pi}\| + \|\frac{\tilde{\omega}\hbar\beta}{\pi}\|\right)\right]}{4\sinh(\frac{1}{2}\hbar\tilde{\Omega}\beta)\sinh(\frac{1}{2}\hbar\tilde{\omega}\beta)} \times \exp\left[\frac{\tilde{\chi}^2\bar{Q}_0^2}{4m\hbar(\tilde{\Omega}^2-\tilde{\omega}^2)^2}\left\{\sinh(\tilde{\Omega}\hbar\beta) - \cosh(\tilde{\Omega}\hbar\beta)\coth(\frac{1}{2}\tilde{\omega}\hbar\beta)\right\}\right]$$

Specific heat

$$\frac{C}{k_B} = \frac{B^2}{\sinh^2(B)} + \frac{b^2}{\sinh^2(b)} + \bar{\alpha}\frac{\sinh(B)}{\sinh(b)} + \alpha B^2\cosh(B)\coth(b)\left[1 - \frac{c}{\sinh^2(b)}\right]$$

$$C = C_{lattice} + C_{amide-I} + C_{mixing}$$

where $B = (1/2)\tilde{\Omega}\hbar\beta$, $b = (1/2)\tilde{\omega}\hbar\beta$, $\bar{\alpha} = (1/2)\alpha\tilde{\Omega}\tilde{\omega}\hbar\beta^2$, $\alpha = (\tilde{\chi}^2\bar{Q}_0^2)/(4m\hbar^2(\tilde{\Omega}^2 - \tilde{\omega}^2)^2)$ and $c = \tilde{\omega}^2\hbar^2/\tilde{\Omega}^2$.



The temperature dependence of normalized specific heat for various values of γ.

Summary

- The interaction of Davydov-Scott monomer with thermal bath is investigated within the QSD framework.
- The thermodynamic partition function and in particular specific heat are calculated using the path integral methods.
- The specific heat for underdamped condition is lower than no damping condition but higher for overdamped condition.
- It found that for high temperature all condition goes to the same value. It ‘s implies that the Davidov-Scott monomer is exist at biological temperature.