

2変数の結合のある場合のSCHAの簡単な例

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2変数の結合のある場合のセルフコンシステント調和近似の定式化の例として、位相表示されたハミルトニアンで記述される、鎖間相互作用を考えたトランス・ポリアセチレンの基底状態(結合交替)のエネルギーについて考える^{1), 2)}。2つの鎖について、電荷部分のみ考える。

$$\begin{aligned}
 H = \int dx [& A(\nabla\theta_1)^2 + CP_1^2 - 2gu_1 \cos \theta_1 + B \cos 2\theta_1 \\
 & + A(\nabla\theta_2)^2 + CP_2^2 - 2gu_2 \cos \theta_2 + B \cos 2\theta_2 \\
 & + V_0 \cos(\theta_1 - \theta_2) + \frac{2K}{a}(u_1^2 + u_2^2)]
 \end{aligned} \quad (1)$$

$$g > 0, \quad B < 0, \quad V_0 > 0$$

$$[\theta_1(x), P_1(x')] = [\theta_2(x), P_2(x')] = i\delta(x-x')$$

θ_1, θ_2 の古典的な平衡点 ($i, j = 1, 2$)

$$\theta_{is} = \theta_{js} + \pi = 2n\pi \quad u_i = -u_j = u_0 \quad (2)$$

量子的ゆらぎを考える。 $\theta_i = \theta_{is} + \hat{\theta}_i$

$$\begin{aligned}
 H = \int dx [& A(\nabla\hat{\theta}_1)^2 + CP_1^2 - 2gu_0 \cos \hat{\theta}_1 + B \cos 2\hat{\theta}_1 \\
 & + A(\nabla\hat{\theta}_2)^2 + CP_2^2 - 2gu_0 \cos \hat{\theta}_2 + B \cos 2\hat{\theta}_2 \\
 & - V_0 \cos(\hat{\theta}_1 - \hat{\theta}_2) + \frac{4K}{a}u_0^2]
 \end{aligned} \quad (3)$$

試行ハミルトニアン H_0 として (5) 式を考え、ファインマンの不等式 (4) を用いて、変分パラメータを決める³⁾。

$$F \leq F_0 + \langle H - H_0 \rangle \equiv \widetilde{F} \quad (4)$$

($\langle \dots \rangle$ は H_0 に関する統計平均)

$$\begin{aligned}
 H_0 &= \int dx [A(\nabla \hat{\theta}_1)^2 + CP_1^2 + \widetilde{B}(\hat{\theta}_1^2 - \langle \hat{\theta}_1^2 \rangle) \\
 &\quad + A(\nabla \hat{\theta}_2)^2 + CP_2^2 + \widetilde{B}(\hat{\theta}_2^2 - \langle \hat{\theta}_2^2 \rangle) \\
 &\quad + \widetilde{V}(\hat{\theta}_1 \hat{\theta}_2 - \langle \hat{\theta}_1 \hat{\theta}_2 \rangle) + U_0 + \frac{4K}{a} u_0^2] \\
 &= \sum_k [\widetilde{A}(\hat{\theta}_{1k} \hat{\theta}_{1-k} + \hat{\theta}_{2k} \hat{\theta}_{2-k}) + C(P_{1k} P_{1-k} + P_{2k} P_{2-k}) \\
 &\quad + \widetilde{V} \hat{\theta}_{1k} \hat{\theta}_{2-k}] + \int dx [U_0 + \frac{4K}{a} u_0^2 - \widetilde{B}(\langle \hat{\theta}_1^2 \rangle + \langle \hat{\theta}_2^2 \rangle) - \widetilde{V} \langle \hat{\theta}_1 \hat{\theta}_2 \rangle]
 \end{aligned} \tag{5}$$

$$\begin{aligned}
 \hat{\theta}_i(x) &= \frac{1}{\sqrt{L}} \sum_k \hat{\theta}_{ik} e^{ikx} & P_i(x) &= \frac{1}{\sqrt{L}} \sum_k P_{ik} e^{ikx} \\
 [\hat{\theta}_{ik}, P_{ik'}] &= i\delta_{k,-k'} & \widetilde{A} &= Ak^2 + \widetilde{B}
 \end{aligned} \tag{6}$$

H_0 は線形変換 T により, 2つの独立な調和振動子系のハミルトニアンに変換される。

$$\begin{pmatrix} \hat{\psi}_{1k} \\ \hat{\psi}_{2k} \end{pmatrix} = T \begin{pmatrix} \hat{\theta}_{1k} \\ \hat{\theta}_{2k} \end{pmatrix} \quad \begin{pmatrix} Q_{1k} \\ Q_{2k} \end{pmatrix} = T \begin{pmatrix} P_{1k} \\ P_{2k} \end{pmatrix}$$

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \quad [\hat{\psi}_{ik}, Q_{ik'}] = i\delta_{k,-k'}$$

$$\begin{aligned}
 H_0 &= \sum_k [\widetilde{A}_1 \hat{\psi}_{1k} \hat{\psi}_{1-k} + \widetilde{A}_2 \hat{\psi}_{2k} \hat{\psi}_{2-k} + C(Q_{1k} Q_{1-k} + Q_{2k} Q_{2-k})] \\
 &\quad + \int dx [U_0 + \frac{4K}{a} u_0^2 - \widetilde{B}(\langle \hat{\theta}_1^2 \rangle + \langle \hat{\theta}_2^2 \rangle) - \widetilde{V} \langle \hat{\theta}_1 \hat{\theta}_2 \rangle]
 \end{aligned} \tag{7}$$

$$\widetilde{A}_1 = \widetilde{A} + \frac{\widetilde{V}}{2} \quad \widetilde{A}_2 = \widetilde{A} - \frac{\widetilde{V}}{2} \tag{8}$$

調和振動子系の性質(9)を用いて, $\widetilde{F}$ 及び一組のセルフコンシステント方程式を得る。

$$\begin{aligned}
 \langle \hat{\psi}_{ik} \hat{\psi}_{i-k} \rangle &= \frac{C}{L} \frac{1}{\omega_i(x)} \quad , \quad \omega_i(k) = 2\sqrt{\widetilde{A}_i C} \quad (\text{温度}=0) \\
 \langle \cos(\alpha \hat{\theta}_1 - \beta \hat{\theta}_2) \rangle &= e^{-\frac{1}{2}(\alpha^2 \langle \hat{\theta}_1^2 \rangle + \beta^2 \langle \hat{\theta}_2^2 \rangle)} e^{\alpha\beta \langle \hat{\theta}_1 \hat{\theta}_2 \rangle}
 \end{aligned} \tag{9}$$

$$\begin{aligned}\widetilde{F} = & F_0 - 2gu_0 \left[e^{-\frac{\langle \hat{\theta}_1^2 \rangle}{2}} + e^{-\frac{\langle \hat{\theta}_2^2 \rangle}{2}} \right] + B \left[e^{-2\langle \hat{\theta}_1^2 \rangle} + e^{-2\langle \hat{\theta}_2^2 \rangle} \right] \\ & - V_0 e^{-\frac{1}{2}(\langle \hat{\theta}_1^2 \rangle + \langle \hat{\theta}_2^2 \rangle)} e^{\langle \hat{\theta}_1 \hat{\theta}_2 \rangle} - \widetilde{B} [\langle \hat{\theta}_1^2 \rangle + \langle \hat{\theta}_2^2 \rangle] \\ & - \widetilde{V} \langle \hat{\theta}_1 \hat{\theta}_2 \rangle\end{aligned}\quad (10)$$

$$\begin{aligned}\langle \hat{\theta}_1^2 \rangle = \langle \hat{\theta}_2^2 \rangle & \equiv \langle \hat{\theta}^2 \rangle = \frac{C}{4L} \sum_k \left[\frac{1}{\sqrt{C\widetilde{A}_1}} + \frac{1}{\sqrt{C\widetilde{A}_2}} \right] \\ & = \frac{1}{4\mu} \int dk \left[\frac{1}{\sqrt{k^2 + k_1^2}} + \frac{1}{\sqrt{k^2 + k_2^2}} \right] = \frac{-1}{2\mu} \ln x_1 x_2 \quad (|k| < \frac{\pi}{a})\end{aligned}$$

$$\langle \hat{\theta}_1 \hat{\theta}_2 \rangle = \frac{C}{4L} \sum_k \left[\frac{1}{\sqrt{C\widetilde{A}_1}} - \frac{1}{\sqrt{C\widetilde{A}_2}} \right] = \frac{1}{2\mu} \ln \frac{x_2}{x_1} \quad (11)$$

$$k_1^2 = \frac{1}{A} \left(\widetilde{B} + \frac{\widetilde{V}}{2} \right) \quad k_2^2 = \frac{1}{A} \left(\widetilde{B} - \frac{\widetilde{V}}{2} \right)$$

$$x_1 = \frac{k_1 a}{2\pi} \quad x_2 = \frac{k_2 a}{2\pi} \quad \mu = 2\pi \sqrt{\frac{A}{C}}$$

$$\frac{\partial \widetilde{F}}{\partial \widetilde{B}} = \frac{\partial \widetilde{F}}{\partial \widetilde{V}} = 0, \quad \langle H \rangle = \langle H_0 \rangle \quad \text{より}$$

$$\widetilde{B} = gu_0 e^{-\frac{\langle \hat{\theta}^2 \rangle}{2}} - 2B e^{-2\langle \hat{\theta}^2 \rangle} + \frac{V_0}{2} e^{-\langle \hat{\theta}^2 \rangle} e^{\langle \hat{\theta}_1 \hat{\theta}_2 \rangle}$$

$$\widetilde{V} = -V_0 e^{-\langle \hat{\theta}^2 \rangle} e^{\langle \hat{\theta}_1 \hat{\theta}_2 \rangle} \quad (12)$$

$$U_0^0 = -4gu_0 e^{-\langle \hat{\theta}^2 \rangle/2} + 2B e^{-2\langle \hat{\theta}^2 \rangle} - V_0 e^{-\langle \hat{\theta}^2 \rangle} e^{\langle \hat{\theta}_1 \hat{\theta}_2 \rangle} \quad (13)$$

(11), (12) より

$$x_1^2 = \frac{a^2}{4\pi^2 A} \left[gu_0 (x_1 x_2)^{\frac{1}{4\mu}} - 2B (x_1 x_2)^{\frac{1}{\mu}} \right] \quad (14)$$

$$x_2^2 = \frac{a^2}{4\pi^2 A} \left[gu_0 (x_1 x_2)^{\frac{1}{4\mu}} - 2B (x_1 x_2)^{\frac{1}{\mu}} + V_0 x_2^{\frac{1}{\mu}} \right]$$

(8), (12), (13), (14)より, 系の基底状態のエネルギーは,^{4), 5)}

$$\begin{aligned}
 \frac{E_{gr}}{L} &= \frac{1}{2L} \sum_k [\omega_1(k) + \omega_2(k)] + U_0 + \frac{4K}{a} u_0^2 \\
 &\quad - 2\tilde{B} \langle \hat{\theta}^2 \rangle - \tilde{V} \langle \hat{\theta}_1 \hat{\theta}_2 \rangle \\
 &= 2 \left[\frac{V_F}{4\pi} \left(\frac{\pi}{a} \right)^2 - 2gu_0 \left(1 - \frac{1}{4\mu} \right) (x_1 x_2)^{\frac{1}{4\mu}} \right. \\
 &\quad \left. + B \left(1 - \frac{1}{\mu} \right) (x_1 x_2)^{\frac{1}{\mu}} + \frac{2K}{a} u_0^2 \right] - V_0 \left(1 - \frac{1}{2\mu} \right) x_2^{\frac{1}{\mu}} \quad (15)
 \end{aligned}$$

(5), (13), (14), (15)を用いて

$$u_0 = \frac{ag}{2K} (x_1 x_2)^{\frac{1}{4\mu}} \quad (16)$$

$$\begin{aligned}
 \frac{E_{gr}}{L} &= 2 \left[\frac{V_F}{4\pi} \left(\frac{\pi}{a} \right)^2 - \frac{4Ku_0^2}{a} \left(\frac{1}{2} - \frac{1}{4\mu} \right) + B \left(\frac{2Ku_0^2}{ag} \right)^4 \left(1 - \frac{1}{\mu} \right) \right] \\
 &\quad - V_0 \left(1 - \frac{1}{2\mu} \right) x_2^{\frac{1}{\mu}} \quad (17)
 \end{aligned}$$

簡単のため, $\mu = 1$, $B = 0$ とし, V_0 を摂動 ($\frac{a^2 V_0}{A} \ll 1$) と考え, V_0 の1次をとると

$$\begin{aligned}
 x &= \left(\frac{a^2 g u_0}{4\pi^2 A} \right)^{2/3} \quad u_0 = \frac{ag}{2K} x^{\frac{1}{2}} \\
 \frac{\Delta E_{gr}}{L} &\simeq -\frac{1}{2} V_0 x = -\frac{ag^2}{16\pi^2 K} \frac{a^2 V_0}{A}
 \end{aligned}$$

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