

Mean field theory for emergence of CDW in Holstein model and periodic Anderson model with electron-phonon interactions

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1 Mean-field estimation of CDW transition temperature in Holstein model

Periodic Anderson model with electron-phonon interactions can be seen as a combination of Holstein model and a Kondo model. There are two phases competing with each other, which are the CDW phase and Kondo singlet phase. As a result, there are two characteristic temperatures, that is, CDW transition temperature T_{CDW} and Kondo temperature T_K . The Kondo temperature can be estimated using the expression $T_K = \frac{D}{k_B} e^{-\frac{1}{J\rho_0}}$, where D is the band width, J is the exchange integral between conduction electron and magnetic impurity electron, and ρ_0 is the density of states near the Fermi surface. However, for the CDW transition temperature, there is hitherto no reliable estimation for its value, and in this section we are to develop a mean-field approximation for its evaluation. For sake of clarity and simplicity, we will consider a Holstein Hamiltonian as shown below[1].

$$\hat{H} = \sum_i \left(\frac{P_i^2}{2M} + \frac{1}{2} K q_i^2 \right) - t \sum_{\langle i,j \rangle, \sigma} \left(\hat{c}_{i,\sigma}^\dagger c_{j,\sigma} + H.C. \right) - \lambda \sum_{i,\sigma} q_i n_{i,\sigma} \quad (1)$$

Assume that we have a finite order parameter that corresponds to the phonon displacement, that is, $q_i = (-1)^i m_p$, and that phonon frequency $\omega \rightarrow 0$, then the Holstein Hamiltonian can be simplified into this form:

$$\hat{H} = \sum_i \frac{1}{2} K m_p^2 - t \sum_{\langle i, j \rangle, \sigma} \left(\hat{c}_{i, \sigma}^\dagger c_{j, \sigma} + H.C. \right) - \lambda \sum_{i, \sigma} (-1)^i m_p n_{i, \sigma} \quad (2)$$

With the Fourier transform,

$$\begin{aligned} \hat{c}_i &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} \\ \hat{c}_i^\dagger &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger e^{-i\mathbf{k} \cdot \mathbf{r}_i}, \end{aligned} \quad (3)$$

we can write the simplified Holstein Hamiltonian in momentum space as

$$\begin{aligned} \hat{H} &= \frac{1}{2} N K m_p^2 + 2 \sum_{\mathbf{k}, -\pi < k < \pi} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} - 2\lambda m_p \sum_{\mathbf{k}} \left(\hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}+\pi} + \hat{c}_{\mathbf{k}+\pi}^\dagger \hat{c}_{\mathbf{k}} \right) \\ &= \frac{1}{2} N K m_p^2 + 2 \sum_{\mathbf{k}, -\pi/2 < k < \pi/2} \left(\epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} + \epsilon_{\mathbf{k}+\pi} \hat{c}_{\mathbf{k}+\pi}^\dagger \hat{c}_{\mathbf{k}+\pi} \right) - 2\lambda m_p \sum_{\mathbf{k}} \left(\hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}+\pi} + \hat{c}_{\mathbf{k}+\pi}^\dagger \hat{c}_{\mathbf{k}} \right) \\ &= \frac{1}{2} N K m_p^2 + 2 \sum_{\mathbf{k}} \begin{pmatrix} \hat{c}_{\mathbf{k}}^\dagger & \hat{c}_{\mathbf{k}+\pi}^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{k}} & -\Delta \\ -\Delta & -\epsilon_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}} \\ \hat{c}_{\mathbf{k}+\pi} \end{pmatrix}, \Delta = \lambda m_p \end{aligned} \quad (4)$$

Here, we are using a cubic lattice with lattice constant $a = 1$. The dispersion relation is $\epsilon_{\mathbf{k}} = -2t \sum_{i=1}^D \cos k_i$, and perfect nesting condition $\epsilon_{\mathbf{k}+\pi} = -\epsilon_{\mathbf{k}}$ has been used.

If we define

$$\begin{pmatrix} \hat{d}_{\mathbf{k}} \\ \hat{d}_{\mathbf{k}+\pi} \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}} \\ \hat{c}_{\mathbf{k}+\pi} \end{pmatrix}, \quad (5)$$

and set $\tan 2\theta = \frac{\Delta}{\epsilon}$, then the Hamiltonian can be simplified into the form

$$\hat{H} = \frac{1}{2} N K m_p^2 + 2 \sum_{\mathbf{k}} \begin{pmatrix} \hat{d}_{\mathbf{k}}^\dagger & \hat{d}_{\mathbf{k}+\pi}^\dagger \end{pmatrix} \begin{pmatrix} \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2} & 0 \\ 0 & -\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2} \end{pmatrix} \begin{pmatrix} \hat{d}_{\mathbf{k}} \\ \hat{d}_{\mathbf{k}+\pi} \end{pmatrix} \quad (6)$$

It can be shown that the operators $\hat{d}_{\mathbf{k}}, \hat{d}_{\mathbf{k}+\pi}$ also represent fermions. Therefore the partition function for the Hamiltonian is

$$\begin{aligned} Z &= \text{Tr} e^{-\beta \hat{H}} \\ &= e^{-\frac{1}{2} \beta N K m_p^2} \prod_{\mathbf{k}} \left(1 + e^{2\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \right) \prod_{\mathbf{k}} \left(1 + e^{-2\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \right) \end{aligned} \quad (7)$$

From this, we get the free energy

$$\begin{aligned}
F &= -\frac{1}{\beta} \log Z \\
&= \frac{1}{2} NK m_p^2 - \frac{1}{\beta} \sum_{\mathbf{k}} \log \left(1 + e^{2\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \right) - \frac{1}{\beta} \sum_{\mathbf{k}} \log \left(1 + e^{-2\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \right) \\
&= \frac{1}{2} NK m_p^2 - \frac{1}{\beta} \sum_{\mathbf{k}} \log \left(2 + 2 \cosh 2\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2} \right)
\end{aligned} \tag{8}$$

Take the derivative of free energy with respect to the order parameter m_p and set the derivative equal to 0, we get (remember that $\Delta = \lambda m_p$)

$$\begin{aligned}
\frac{\partial F}{\partial m_p} &= NK m_p - \sum_{\mathbf{k}} \frac{\sinh 2\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}{1 + \cosh 2\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \frac{2\Delta\lambda}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \\
&= NK \frac{\Delta}{\lambda} - 2\lambda\Delta \sum_{\mathbf{k}} \tanh \left(\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2} \right) \frac{1}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \\
&= 0
\end{aligned} \tag{9}$$

From this, we get the self-consistent equation as

$$\begin{aligned}
1 &= \frac{2\lambda^2}{NK} \sum_{\mathbf{k}} \frac{1}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \tanh \left(\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2} \right) \\
&= \frac{2\lambda^2}{K} \int d\epsilon \frac{1}{\sqrt{\epsilon^2 + \Delta^2}} \tanh \left(\beta \sqrt{\epsilon^2 + \Delta^2} \right) \frac{1}{N} \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}) \\
&= \frac{2\lambda^2}{K} \int d\epsilon \frac{1}{\sqrt{\epsilon^2 + \Delta^2}} \tanh \left(\beta \sqrt{\epsilon^2 + \Delta^2} \right) D(\epsilon)
\end{aligned} \tag{10}$$

If we make the assumption that only electrons near the fermi surface participate into this CDW transition, and that only energies up to the Debye frequency is considered, then the above self-consistent equation becomes

$$1 = \frac{2\lambda^2 D_0}{K} \int_0^{\omega_D} d\epsilon \frac{1}{\sqrt{\epsilon^2 + \Delta^2}} \tanh \left(\beta \sqrt{\epsilon^2 + \Delta^2} \right), \tag{11}$$

where D_0 is the DOS near the fermi surface.

This self-consistent equation can be evaluated analytically for two limiting cases, which

are $T = 0$ case and $T = T_c$ case. When temperature $T = 0$, we have

$$\begin{aligned}
1 &= \frac{2\lambda^2 D_0}{K} \int_0^{\omega_D} d\epsilon \frac{1}{\sqrt{\epsilon^2 + \Delta^2}} \\
&= \frac{2\lambda^2 D_0}{K} \log \left(\frac{\omega_D + \sqrt{\omega_D^2 + \Delta^2}}{\Delta} \right) \\
&\approx \frac{2\lambda^2 D_0}{K} \log \frac{2\omega_D}{\Delta}, \text{ assume } \omega_D \gg \Delta
\end{aligned} \tag{12}$$

When $T = T_c$, then energy gap $\Delta = 0$, we have

$$\begin{aligned}
1 &= \frac{2\lambda^2 D_0}{K} \int_0^{\omega_D} d\epsilon \frac{\tanh \beta_c \epsilon}{\epsilon} \\
&= \frac{2\lambda^2 D_0}{K} \int_0^{\frac{\omega_D}{T_c}} dx \frac{\tanh x}{x} \\
&\approx \frac{2\lambda^2 D_0}{K} \log \frac{\omega_D}{T_c}, \text{ assume } \omega_D \gg T_c
\end{aligned} \tag{13}$$

From these two limiting cases, we can get the energy gap at zero temperature and the critical temperature as

$$\begin{aligned}
\Delta(T = 0) &= 2\omega_D \exp \left(-\frac{K}{2\lambda^2 D_0} \right) \\
T_c &= \omega_D \exp \left(-\frac{K}{2\lambda^2 D_0} \right)
\end{aligned} \tag{14}$$

In obtaining these two expressions for energy gap and critical temperature, we have made numerous approximations that need to be justified. In order to test if these two expressions are correct, at least to some extent, we are to evaluate the summation over momentum numerically and see at what temperature the energy gap Δ becomes finite. The temperature at which energy gap becomes finite is then identified as the transition temperature for CDW state, and this transition temperature will undoubtedly depend on the effective electron-phonon interaction strength. It is expected that the CDW state has its origin in the perfect nesting condition which is more manifested in lower dimension than in higher dimension. Thus, we would expect that CDW energy gap would be larger in lower dimension than that in high dimension, and that the transition temperature to CDW state would also be higher in lower dimension than in higher dimension. All of these assertions can be substantiated by numerical evaluation of the summation over momentum space, as will be shown below.

Define a function

$$f(\Delta) = \frac{2\lambda^2}{NK} \sum_{\mathbf{k}} \frac{1}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}} \tanh \left(\beta \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2} \right) - 1, \Delta > 0 \tag{15}$$

The root of this function gives us the energy gap at different temperatures for fixed values of λ and K . We are to find the root of this equation using Newton's method. The summation over momentum depends on the dimension of the system that is being considered, and we will perform this numerical summation for dimensions of 1D, 2D, and 3D. When $\lambda = K = 1$, the energy gap Δ versus temperature T is plotted in Fig. 1.1.

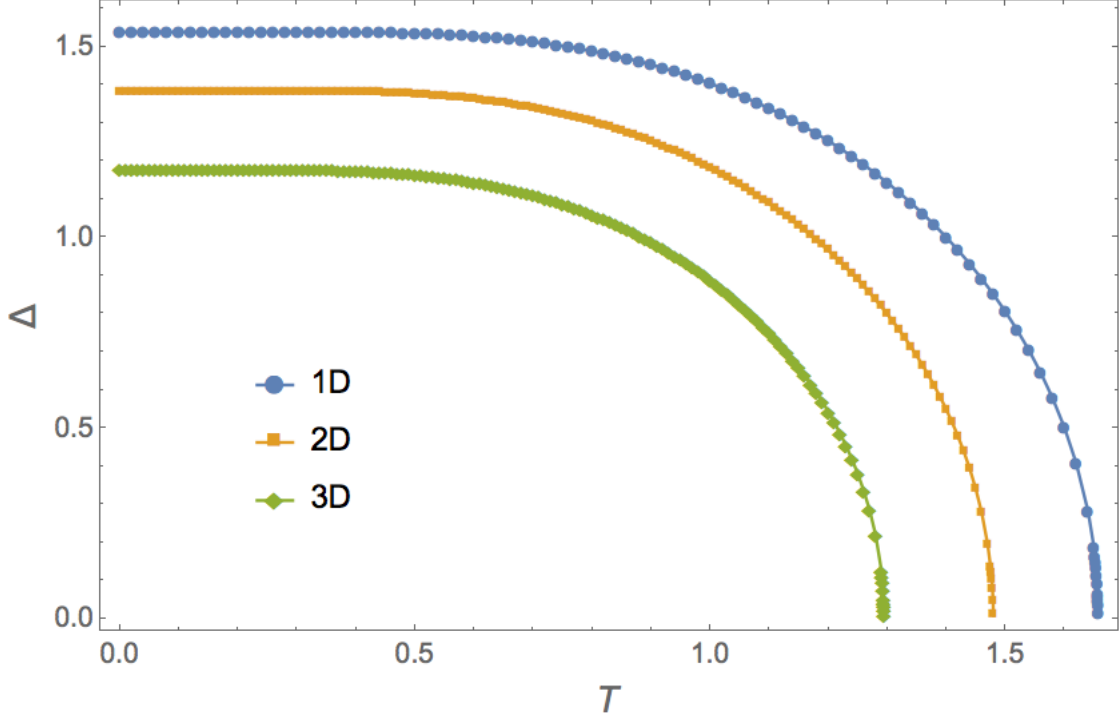


Figure 1.1: CDW energy gap versus temperature for parameters $\lambda = K = 1$ at dimensions of 1D, 2D, and 3D. It can be seen that CDW is more manifested in lower dimension than in higher dimension, just as expected.

The critical temperature T_c for the emergence of CDW state can be identified as the point where energy gap Δ begins to adopt a finite value. The critical temperature, as we would expect, depends on the value of effective electron-phonon interaction strength which is defined as $\frac{\lambda^2}{K}$. We can find the critical temperature T_c for different values of λ while fixing $K = 1$, and plot T_c versus λ in Fig. 1.2.

According to our mean field calculation, CDW critical temperature T_c as a function of electron-phonon coupling constant λ has the form $T_c = \omega_D \exp\left(-\frac{K}{2\lambda^2 D_0}\right)$. In order to test whether this formula holds, and in order to justify the assumptions we have made earlier to derive this formula, we are going to using least square method to fit our data to this formula. That is, we are to fit our data for critical temperature to the curve $T_c = a \exp(-b/\lambda^2)$, and

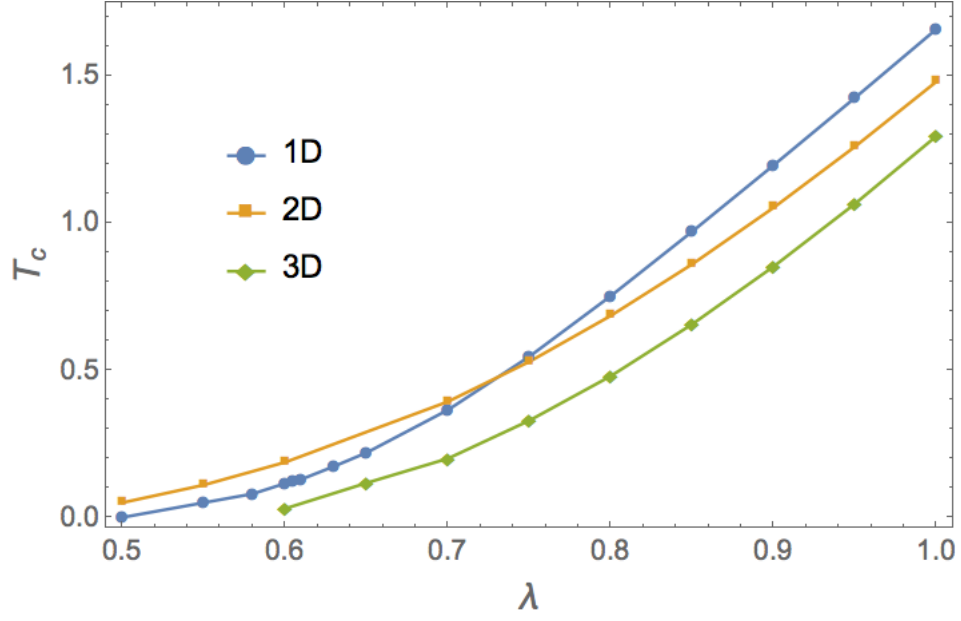


Figure 1.2: CDW transition temperature versus electron-phonon coupling constant λ when $K = 1$ for dimensions 1D, 2D, and 3D.

use the least square method to find the values of a, b and compare the fitted curve to our scatter point diagram.

For dimension $D = 1$, $a = 7.97945, b = 1.52841$; for dimension $D = 2$, $a = 4.06073, b = 1.10541$; for dimension $D = 3$, $a = 10.446, b = 1.99861$. Scattered points and fitted curves are shown together for different dimensions in Fig. 1.3.

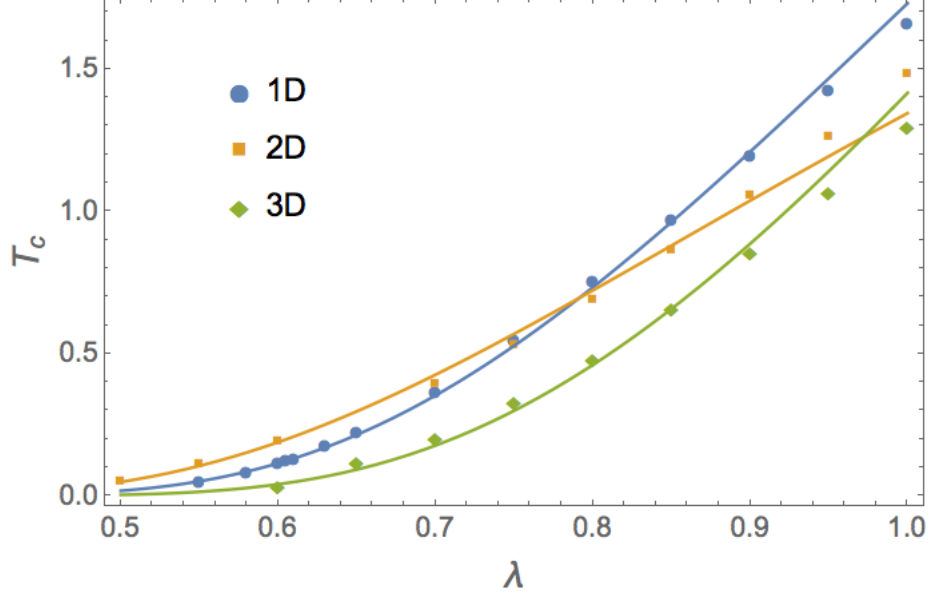


Figure 1.3: CDW transition temperature versus electron-phonon coupling constant λ when $K = 1$ for dimensions 1D, 2D, and 3D. Scatter points and the corresponding fitted curves $T_c = a \exp(-b/\lambda^2)$ are shown together.

2 Mean field method investigation of the competition between hybridization and electron-phonon coupling in the PAM with phonon model

In the previous section, we have investigated the CDW transition temperature as a function of the electron-phonon coupling constant in Holstein model using the mean field solution. Here, in this section, we are to generalize the results of the previous section and apply the mean field method to the PAM with electron-phonon couplings, and study the competition between hybridization term and electron-phonon coupling term in this model. Our model

Hamiltonian in real space is

$$\begin{aligned}
\hat{H} &= \hat{H}_0 + \hat{H}_I \\
\hat{H}_0 &= -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}) + \epsilon_f \sum_{j,\sigma} f_{j,\sigma}^\dagger f_{j,\sigma} \\
&\quad + V \sum_{i,\sigma} (c_{i,\sigma}^\dagger f_{i,\sigma} + f_{i,\sigma}^\dagger c_{i,\sigma}) + \sum_i \left(\frac{p_i^2}{2m} + \frac{1}{2} k X_i^2 \right) \\
\hat{H}_I &= U \sum_i n_{i,\uparrow}^f n_{i,\downarrow}^f + g \sum_{i,\sigma} n_{i,\sigma}^c X_i
\end{aligned} \tag{16}$$

For simplicity, we will now set the Hubbard interaction strength to zero. The effects of finite Hubbard interaction may be studied later on.

Assume that we already have a finite CDW order parameter, then the phonon displacement can be written as $q_i = (-1)^i m_p$. In the limit $\omega \rightarrow 0$, the Hamiltonian in real space is

$$\begin{aligned}
\hat{H} &= -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}) + \epsilon_f \sum_{j,\sigma} f_{j,\sigma}^\dagger f_{j,\sigma} \\
&\quad + V \sum_{i,\sigma} (c_{i,\sigma}^\dagger f_{i,\sigma} + f_{i,\sigma}^\dagger c_{i,\sigma}) + \frac{1}{2} N K m_p^2 + g \sum_{i,\sigma} \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} (-1)^i m_p
\end{aligned} \tag{17}$$

With a Fourier transformation, the Hamiltonian in momentum space is

$$\begin{aligned}
\hat{H} &= \frac{1}{2} N K m_p^2 + 2 \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} + 2 g m_p \sum_{\mathbf{k}} \left(\hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}+\pi} + \hat{c}_{\mathbf{k}+\pi}^\dagger \hat{c}_{\mathbf{k}} \right) \\
&\quad + 2 \epsilon_f \sum_{\mathbf{k}} \hat{f}_{\mathbf{k}}^\dagger \hat{f}_{\mathbf{k}} + 2 V \sum_{\mathbf{k}} \left(\hat{c}_{\mathbf{k}}^\dagger \hat{f}_{\mathbf{k}} + \hat{f}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} \right)
\end{aligned} \tag{18}$$

Using the identity,

$$\begin{aligned}
\sum_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} &= \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}+\pi}^\dagger \hat{c}_{\mathbf{k}+\pi}, \\
\sum_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{f}_{\mathbf{k}} &= \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}+\pi}^\dagger \hat{f}_{\mathbf{k}+\pi},
\end{aligned} \tag{19}$$

the Hamiltonian may be rewritten as

$$\hat{H} = \frac{1}{2} N K m_p^2 + \sum_{\mathbf{k}} \begin{pmatrix} \hat{c}_{\mathbf{k}}^\dagger & \hat{c}_{\mathbf{k}+\pi}^\dagger & \hat{f}_{\mathbf{k}}^\dagger & \hat{f}_{\mathbf{k}+\pi}^\dagger \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{k}} & \Delta & V & 0 \\ \Delta & -\epsilon_{\mathbf{k}} & 0 & V \\ V & 0 & \epsilon_f & 0 \\ 0 & V & 0 & \epsilon_f \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}} \\ \hat{c}_{\mathbf{k}+\pi} \\ \hat{f}_{\mathbf{k}} \\ \hat{f}_{\mathbf{k}+\pi} \end{pmatrix} \tag{20}$$

Here, we have defined a parameter $\Delta = 2gm_p$. With an orthogonal transformation, the Hamiltonian may be diagonalized as

$$\hat{H} = \frac{1}{2}NKm_p^2 + \sum_{\mathbf{k}} \begin{pmatrix} \hat{c}_{\mathbf{k}}^\dagger & \hat{c}_{\mathbf{k}+\pi}^\dagger & \hat{f}_{\mathbf{k}}^\dagger & \hat{f}_{\mathbf{k}+\pi}^\dagger \end{pmatrix} \begin{pmatrix} \lambda_{\mathbf{k}}^{(1)} & 0 & 0 & 0 \\ 0 & \lambda_{\mathbf{k}}^{(2)} & 0 & 0 \\ 0 & 0 & \lambda_{\mathbf{k}}^{(3)} & 0 \\ 0 & 0 & 0 & \lambda_{\mathbf{k}}^{(4)} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}}' \\ \hat{c}_{\mathbf{k}+\pi}' \\ \hat{f}_{\mathbf{k}}' \\ \hat{f}_{\mathbf{k}+\pi}' \end{pmatrix} \quad (21)$$

It can be shown that all the new operators are still Fermion operators, and the eigenvalues are

$$\begin{aligned} \lambda_{\mathbf{k}}^{(1)} &= \frac{\epsilon_f + E_{\mathbf{k}}}{2} - \frac{1}{2}\sqrt{(E_{\mathbf{k}} - \epsilon_f)^2 + 4V^2} \\ \lambda_{\mathbf{k}}^{(2)} &= \frac{\epsilon_f + E_{\mathbf{k}}}{2} + \frac{1}{2}\sqrt{(E_{\mathbf{k}} - \epsilon_f)^2 + 4V^2} \\ \lambda_{\mathbf{k}}^{(3)} &= \frac{\epsilon_f - E_{\mathbf{k}}}{2} - \frac{1}{2}\sqrt{(E_{\mathbf{k}} + \epsilon_f)^2 + 4V^2} \\ \lambda_{\mathbf{k}}^{(4)} &= \frac{\epsilon_f - E_{\mathbf{k}}}{2} + \frac{1}{2}\sqrt{(E_{\mathbf{k}} + \epsilon_f)^2 + 4V^2} \end{aligned} \quad (22)$$

Here, we have defined the energy parameter $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}$.

The partition function for this Hamiltonian is

$$\begin{aligned} Z &= \text{Tre}^{-\beta\hat{H}} \\ &= e^{-\beta NKm_p^2/2} \prod_{\mathbf{k}} (1 + e^{-\beta\lambda_{\mathbf{k}}^{(1)}})(1 + e^{-\beta\lambda_{\mathbf{k}}^{(2)}})(1 + e^{-\beta\lambda_{\mathbf{k}}^{(3)}})(1 + e^{-\beta\lambda_{\mathbf{k}}^{(4)}}), \end{aligned} \quad (23)$$

and the free energy is

$$\begin{aligned} F &= -\frac{1}{\beta} \log Z \\ &= \frac{NK\Delta^2}{8g^2} - \frac{1}{\beta} \sum_{\mathbf{k}} \left(\log(1 + e^{-\beta\lambda_{\mathbf{k}}^{(1)}}) + \log(1 + e^{-\beta\lambda_{\mathbf{k}}^{(2)}}) + \log(1 + e^{-\beta\lambda_{\mathbf{k}}^{(3)}}) + \log(1 + e^{-\beta\lambda_{\mathbf{k}}^{(4)}}) \right) \end{aligned} \quad (24)$$

Take the derivative of the free energy with respect to the order parameter and set the derivative to zero, we can get the self-consistent equation for the order parameter, which is

$$\begin{aligned} 0 &= \frac{\partial F}{\partial \Delta} \\ &= \frac{NK\Delta}{4g^2} \\ &+ \sum_{\mathbf{k}} \left(\frac{e^{-\beta\lambda_{\mathbf{k}}^{(1)}}}{1 + e^{-\beta\lambda_{\mathbf{k}}^{(1)}}} \frac{\partial \lambda_{\mathbf{k}}^{(1)}}{\partial \Delta} + \frac{e^{-\beta\lambda_{\mathbf{k}}^{(2)}}}{1 + e^{-\beta\lambda_{\mathbf{k}}^{(2)}}} \frac{\partial \lambda_{\mathbf{k}}^{(2)}}{\partial \Delta} + \frac{e^{-\beta\lambda_{\mathbf{k}}^{(3)}}}{1 + e^{-\beta\lambda_{\mathbf{k}}^{(3)}}} \frac{\partial \lambda_{\mathbf{k}}^{(3)}}{\partial \Delta} + \frac{e^{-\beta\lambda_{\mathbf{k}}^{(4)}}}{1 + e^{-\beta\lambda_{\mathbf{k}}^{(4)}}} \frac{\partial \lambda_{\mathbf{k}}^{(4)}}{\partial \Delta} \right) \end{aligned} \quad (25)$$

It does not make much difference if we set $\epsilon_f = 0$. When $\epsilon_f = 0$, the above equation may be significantly simplified. In this case, $\lambda_{\mathbf{k}}^{(1)} = -\lambda_{\mathbf{k}}^{(4)}$, $\lambda_{\mathbf{k}}^{(2)} = -\lambda_{\mathbf{k}}^{(3)}$. Therefore, we have

$$\begin{aligned}
\frac{\partial F}{\partial \Delta} &= \frac{NK\Delta}{4g^2} \\
&- \sum_{\mathbf{k}} \left(\frac{\partial \lambda_{\mathbf{k}}^{(1)}}{\partial \Delta} \tanh \frac{\beta \lambda_{\mathbf{k}}^{(1)}}{2} + \frac{\partial \lambda_{\mathbf{k}}^{(2)}}{\partial \Delta} \tanh \frac{\beta \lambda_{\mathbf{k}}^{(2)}}{2} \right) \\
&= \frac{NK\Delta}{4g^2} \\
&- \frac{1}{2} \sum_{\mathbf{k}} \frac{\Delta}{E_{\mathbf{k}}} \left(1 - \frac{E_{\mathbf{k}}}{\sqrt{E_{\mathbf{k}}^2 + 4V^2}} \right) \tanh \frac{\beta \lambda_{\mathbf{k}}^{(1)}}{2} \\
&- \frac{1}{2} \sum_{\mathbf{k}} \frac{\Delta}{E_{\mathbf{k}}} \left(1 + \frac{E_{\mathbf{k}}}{\sqrt{E_{\mathbf{k}}^2 + 4V^2}} \right) \tanh \frac{\beta \lambda_{\mathbf{k}}^{(2)}}{2}
\end{aligned} \tag{26}$$

The self-consistent equation can be finally simplified into the form

$$\begin{aligned}
1 &= \frac{2g^2}{K} \frac{1}{N} \sum_{\mathbf{k}} \left[\frac{1}{E_{\mathbf{k}}} \left(1 - \frac{E_{\mathbf{k}}}{\sqrt{E_{\mathbf{k}}^2 + 4V^2}} \right) \tanh \frac{\beta}{4} \left(E_{\mathbf{k}} - \sqrt{E_{\mathbf{k}}^2 + 4V^2} \right) \right. \\
&\quad \left. + \frac{1}{E_{\mathbf{k}}} \left(1 + \frac{E_{\mathbf{k}}}{\sqrt{E_{\mathbf{k}}^2 + 4V^2}} \right) \tanh \frac{\beta}{4} \left(E_{\mathbf{k}} + \sqrt{E_{\mathbf{k}}^2 + 4V^2} \right) \right]
\end{aligned} \tag{27}$$

Convert the summation over momentum to integral over energy by invoking the density of states, we have the self-consistent equation as

$$\begin{aligned}
1 &= \frac{2g^2}{K} \int d\epsilon D(\epsilon) \left[\left(\frac{1}{\sqrt{\epsilon^2 + \Delta^2}} - \frac{1}{\sqrt{\epsilon^2 + \Delta^2 + 4V^2}} \right) \tanh \frac{\beta}{4} \left(\sqrt{\epsilon^2 + \Delta^2} - \sqrt{\epsilon^2 + \Delta^2 + 4V^2} \right) \right. \\
&\quad \left. + \left(\frac{1}{\sqrt{\epsilon^2 + \Delta^2}} + \frac{1}{\sqrt{\epsilon^2 + \Delta^2 + 4V^2}} \right) \tanh \frac{\beta}{4} \left(\sqrt{\epsilon^2 + \Delta^2} + \sqrt{\epsilon^2 + \Delta^2 + 4V^2} \right) \right]
\end{aligned} \tag{28}$$

2.1 Solution in finite dimensions. $D = 2$.

In the limit $T \rightarrow 0$, we have

$$\begin{aligned}
1 &= \frac{4g^2}{K} \int_0^{\omega_D} d\epsilon D(\epsilon) \frac{1}{\sqrt{\epsilon^2 + \Delta^2 + 4V^2}} \\
&= \frac{4g^2}{K} D(0) \log \frac{\omega_D + \sqrt{\omega_D^2 + \Delta^2 + 4V^2}}{\sqrt{\Delta^2 + 4V^2}}
\end{aligned} \tag{29}$$

Thus, the order parameter at zero temperature is

$$\Delta = 2 \sqrt{\frac{\omega_D^2}{\left(e^{\frac{K}{4g^2D(0)}} - e^{-\frac{K}{4g^2D(0)}}\right)^2} - V^2} \quad (30)$$

From this expression, one can see that the order parameter at zero temperature changes as a function of hybridization value. When the hybridization value increases, the order parameter decreases. For $V > V_c$, the order parameter is zero.

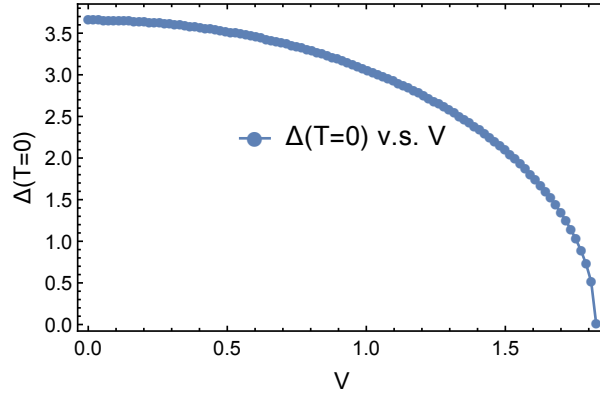


Figure 2.1: Order parameter at zero temperature as a function of hybridization value V . $g = 1, K = 1, t = 1$.

On the other hand, when $T \rightarrow T_c$, $\Delta \rightarrow 0$, then the self-consistent equation becomes

$$1 = \frac{2g^2D(0)}{K} \int_0^{\frac{\omega_D}{T_c}} dx \left[\left(\frac{1}{x} - \frac{1}{\sqrt{x^2 + 4\beta^2V^2}} \right) \tanh \frac{1}{4} \left(x - \sqrt{x^2 + 4\beta^2V^2} \right) + \left(\frac{1}{x} + \frac{1}{\sqrt{x^2 + 4\beta^2V^2}} \right) \tanh \frac{1}{4} \left(x + \sqrt{x^2 + 4\beta^2V^2} \right) \right] \quad (31)$$

If $\omega_D \gg T_c$, then $T_c = \omega_D e^{-\frac{K}{4g^2D(0)}}$. This transition temperature is independent of hybridization value V . In order to study the effect of the hybridization value on the transition temperature, we should NOT adopt this approximation. Instead, we should solve the self-consistent equation numerically.

From the numerical solution, we see that when the effective electron-phonon coupling is fixed, the transition temperature decreases when the hybridization strength increases. There is no longer a CDW transition after the hybridization strength reaches a critical value.

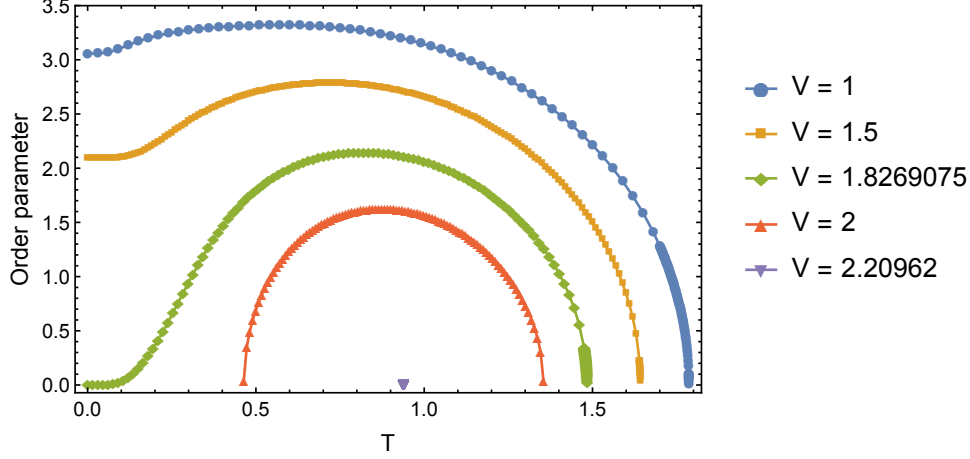


Figure 2.2: Order parameter versus temperature for different hybridization values V . $g = 1$, $K = 1$, $t = 1$.

2.2 Solution in infinite dimension

In the limit $T \rightarrow 0$, we have the equation for the order parameter

$$\begin{aligned}
 1 &= \frac{4g^2}{K} \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} dx \frac{e^{-x^2}}{\sqrt{x^2 + \frac{\Delta^2 + 4V^2}{2t^2}}} \\
 &= \frac{4g^2}{K} \frac{1}{\sqrt{2\pi t}} e^{\frac{\Delta^2 + 4V^2}{4t^2}} K_0\left(\frac{\Delta^2 + 4V^2}{4t^2}\right)
 \end{aligned} \tag{32}$$

Here, $K_0(x)$ is the modified Bessel function of the second kind. Define a function

$$f(\Delta; V) = \frac{4g^2}{K} \frac{1}{\sqrt{2\pi t}} e^{\frac{\Delta^2 + 4V^2}{4t^2}} K_0\left(\frac{\Delta^2 + 4V^2}{4t^2}\right) - 1 \tag{33}$$

The root of this function corresponds to the value of order parameter at zero temperature. If we plot the function $f(\Delta; V)$ for different values of V , we see that the zero temperature order parameter decreases from a finite value to zero as the hybridization value increases. This is consistent with the finite dimensional result. CDW transition temperature can be obtained by plotting the order parameter versus temperature for different values of V . As V increases, the transition temperature decreases. When $V > V_c$, there is no longer a CDW transition. This means that in our model, the hybridization tends to suppress the CDW transition.

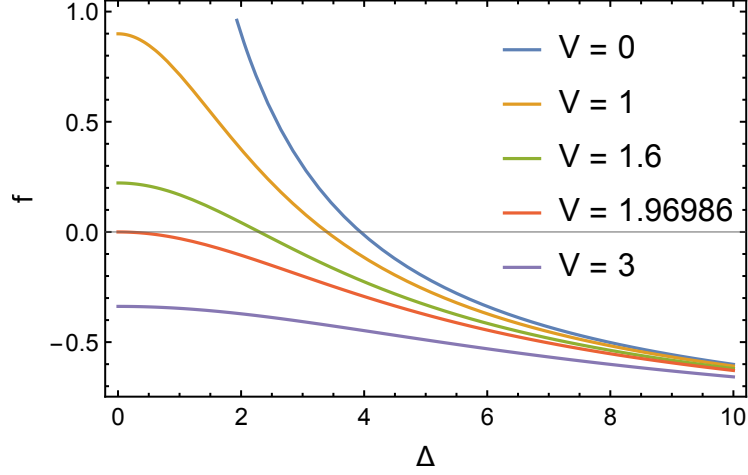


Figure 2.3: $f(\Delta; V)$ versus Δ for different hybridization values V . $g = 1, K = 1, 2t^2 = 1$.

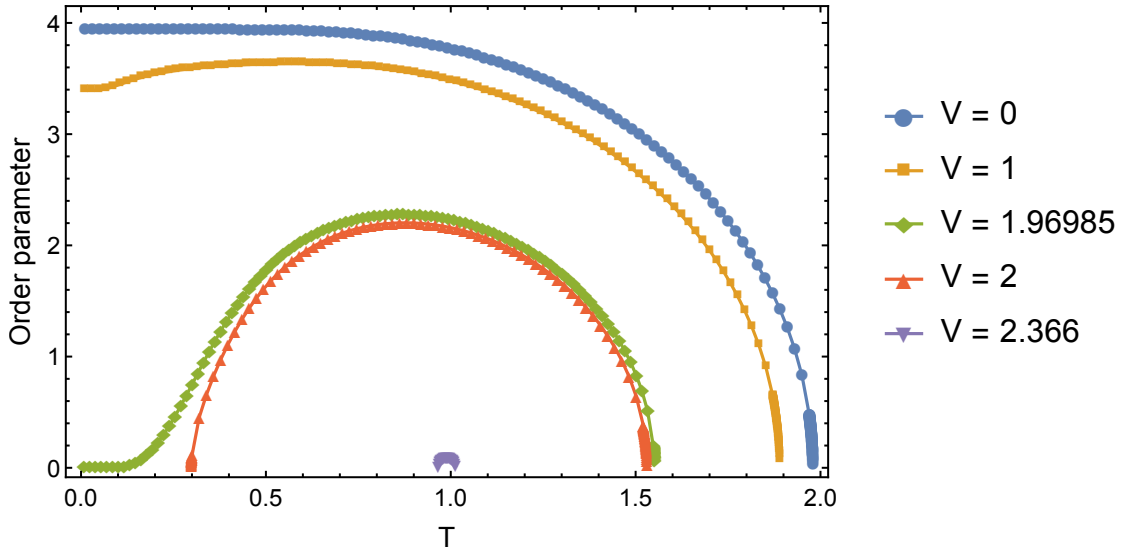


Figure 2.4: Δ versus T for different hybridization values V . $g = 1, K = 1, 2t^2 = 1$.

References

- [1] Jorge E. Hirsch and Eduardo Fradkin. Phase diagram of one-dimensional electron-phonon systems. ii. the molecular-crystal model. *Phys. Rev. B*, 27:4302–4316, Apr 1983.