On the Ginzburg-Landau Free Energy of Charge Density Waves with a Three-Dimensional Order

Masahiko Hayashi\textsuperscript{1,3} and Hideo Yoshioka\textsuperscript{2,3}

\textsuperscript{1}Graduate School of Information Sciences, Tohoku University, Aramaki Aoba-ku, Sendai 980, Japan
\textsuperscript{2}Department of Physics, Kitauoyanishimachi, Nara Women’s University, Nara 630-8506, Japan
\textsuperscript{3}Department of Applied Physics, Delft University of Technology, 2628CJ Delft, The Netherlands

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The effective free energy of a charge density wave (CDW) with a three-dimensional order is derived from a microscopic model (Frölich model) based on the path integral method. Electron hoping and Coulomb interaction between chains are taken into account perturbatively, leading to an elastic interchain coupling of the CDW ordered state.

I. INTRODUCTION

After a pioneering study by Peierls \cite{1}, charge density wave (CDW) has been a subject of continuous interest because of its unique nature as an electronic condensate. Especially, its behavior under an electric field was investigated by Frölich \cite{2} as a possible origin of superconductivity. Although it turned out that the CDW mechanism does not apply to the superconductivity, many interesting behaviors have been found in the electromagnetic response of CDW \cite{3,4}. Even today, experimental developments are adding intriguing new phenomena to the book of CDW. For example, AB effect in CDW’s with columnar defects \cite{5}, field effect \cite{6} and current effect \cite{7} of CDW transport have been discovered although some theoretical developments are needed for the full understanding of these phenomena.

In a preceding paper \cite{8}, we have studied CDW’s in a transverse (perpendicular to the chains) electric field and pointed out a possibility of a state similar to the mixed state of superconductors. Although interchain coupling plays an essential role in this theory, it was only phenomenologically introduced. The aim of the present paper is to give a microscopic foundation of the interchain coupling by deriving it from the electron-phonon model.

Although there have been proposed several origins of the interchain coupling \cite{3,4}, the derivation of the Ginzburg-Landau (GL) type effective free energy taking them into account in a unified framework has not been given until now. We reexamine the effective free energy of the CDW taking account of the electron hopping and the Coulomb interaction between chains as sources of the interchain coupling. These effects are treated perturbatively employing the path integral formulation. It is shown that the free energy previously used by the present authors \cite{8} can be derived from a microscopic model.

For simplicity we limit our discussion to the case without impurity and commensurability pinning.

II. FREE ENERGY OF A CDW SYSTEM

We consider a three-dimensional (3-D) stack of 1-D conducting chains, each of which is described by Frölich model (coupled electron-phonon system). At low temperatures, this system is expected to show a 3-D CDW order due to interchain coupling \cite{3,4}. We treat the Coulomb interaction and the electron hopping between chains as origins of interchain coupling. However the electron hopping is assumed to be small so that it does not break the one-dimensionality of the system \cite{8}.

A. One-dimensional electron-phonon system

The action of the electron-phonon system $S_{\text{e-p}}$ is given by,

\begin{equation}
S_{\text{e-p}} = \int_0^{\hbar \beta} d\tau \sum_i \left[ \int dx \psi_{i\sigma}^*(x) \left( \hbar \partial_\tau - \frac{\hbar^2}{2m} \partial_x^2 - \mu \right) \psi_{i\sigma}(x) + \sum_q b_i^*(q) \left( \hbar \partial_\tau + \hbar \omega_q \right) b_i(q) + \frac{1}{\sqrt{L}} \sum_{k,q} g_q a_{i\sigma}(k+q) a_{i\sigma}(k) \left\{ b_i(q) + b_i^*(-q) \right\} \right],
\end{equation}

where $i$ is the index numbering the chains, $L$ is the length of the chains and, $m$ and $-\epsilon$ are the mass and charge of an electron, respectively. The chemical potential $\mu$ is given by $\mu = \hbar^2 k_F^2/(2m)$ with $k_F$ being the Fermi wave number. We assume that $\mu$ is common to all the chains \cite{1}.

The phonon frequency and electron-phonon coupling constant of wave number $q$ are denoted by $\omega_q$ and $g_q$, respectively. Electron field on the $i$-th chain with spin $\sigma$ is represented by $\psi_{i\sigma}(x,\tau)$ and its Fourier transformation is given by $a_{i\sigma}(k,\tau) = L^{-1/2} \int dx \psi_{i\sigma}(x,\tau) \exp(-ikx)$. Note that the summation over $\sigma$ is suppressed in the present paper. The Fourier component of phonon field of the $i$-th chain is denoted by $b_i(q)$ which is related to the displacement of ions $u_i(x)$ by,

\begin{equation}
u_i(x) = \frac{i}{\sqrt{L}} \sum_q \alpha_q \xi_q \left\{ b_i(q) + b_i^*(-q) \right\} e^{iqx},
\end{equation}
where \( \omega_q = \hbar/\sqrt{2\rho_M\hbar q} \) with \( \rho_M \) being the average mass density of ions and \( \epsilon_q = q/|q| \). Here we have considered only the phonons corresponding to the displacement of ions parallel to the chains.

We consider the Peierls instability at the wave number \( Q \equiv \pm 2k_F \) and treat only the phonons with wave number close to \( \pm 2k_F \). It is convenient to divide \( \psi_{\sigma} \) into two parts as \( \psi_{\sigma} = e^{i k_F x} R_\sigma + e^{-i k_F x} L_\sigma \), where \( R_\sigma \) and \( L_\sigma \) stand for right and left moving electrons, respectively, and are assumed to be slowly varying fields.

The complex order parameter (or energy gap) of CDW is introduced by

\[
\Delta_i(x) = \frac{q}{\sqrt{L}} \sum_q \langle b_i^\dagger (-Q - q) + b_i(Q + q) \rangle e^{i q x},
\]

where \( \langle \cdots \rangle \) denotes the statistical average and we neglect the \( q \)-dependence of \( g_{Q+q} \), writing it as \( g \). Here we have assumed that the phonon field and the order parameter are classical fields which do not depend on imaginary time \( \tau \). Then the action can be rewritten as,

\[
S_{\text{el}} = \int_0^\beta dt \sum_i \int_0^L dx \left[ \Psi_{\sigma} \cdot \mathbf{K}_i \cdot \Psi_{\sigma} + \frac{\hbar \omega_Q}{2g^2} |\Delta_i|^2 \right],
\]

where

\[
\mathbf{K}_i(x, \tau) = \begin{pmatrix} \hat{k}_i^{(+)} & \Delta_i(x) \\ \Delta_i^*(x) & \hat{k}_i^{(-)} \end{pmatrix},
\]

\[
\hat{k}_i^{(\pm)} = \hbar \partial_x - \frac{\hbar^2}{2m} (\pm ik_F + \partial_x)^2 - \mu.
\]

Here \( q \)-dependence of \( \omega_{Q+q} \) is ignored as \( \omega_{Q+q} \rightarrow \omega_Q \). By applying the variation with respect to \( \Delta_i^*(x) \) we obtain self-consistent equation,

\[
\Delta_i(x) = -\frac{2g^2}{\hbar \omega_Q} \langle R_\sigma(x, \tau) R_\sigma(x, \tau) \rangle.
\]

**B. Interchain Coupling**

1. **Coulomb Interaction**

As a source of the interchain coupling we first consider the Coulomb interaction. The Coulomb interaction is introduced by adding the following action,

\[
S_{\text{el}} = -i \int dt \int dz \sum_i \varphi_i(x, \tau) \rho_i(x, \tau) + \int dt \int dr \frac{1}{8\pi} |\nabla \varphi(r, \tau)|^2,
\]

where \( \varphi_i(x, \tau) \) is the value of the scalar potential \( \varphi(r, \tau) \) on the \( i \)-th chain and \( \rho_i(x, \tau) \) is the total charge density on the \( i \)-th chain. We write \( \rho_i(x, \tau) = \rho_i^{\text{el}}(x, \tau) + \rho_i^{\text{ion}}(x, \tau) \), where \( \rho_i^{\text{el}}(x, \tau) \) and \( \rho_i^{\text{ion}}(x, \tau) \) are the electronic and the ionic contribution to the charge density, respectively.

The electronic contribution \( \rho_i^{\text{el}} \) has two characteristic parts, the long range (\( q \sim 0 \)) and the short range (\( q \sim 2k_F \)) charge modulation, which we denote by \( \rho_0^{\text{el}} \) and \( \rho_{Q_i}^{\text{el}} \), respectively. These quantities are written as,

\[
\rho_i^{\text{el}} = \rho_0^{\text{el}} + \rho_{Q_i}^{\text{el}},
\]

\[
\rho_0^{\text{el}} = -e \left( R_\sigma R_\sigma + L_\sigma L_\sigma \right),
\]

\[
\rho_{Q_i}^{\text{el}} = -e \left( L_\sigma^* R_\sigma e^{iQx} + R_\sigma^* L_\sigma e^{-iQx} \right).
\]

The ionic contribution \( \rho_i^{\text{ion}} \) also has two contributions \( \rho_0^{\text{ion}} \) and \( \rho_{Q_i}^{\text{ion}} \). For ions \( \rho_0^{\text{ion}} \) is a constant, since we take account of the phonons with wave numbers close to \( \pm 2k_F \) only. Noting that the displacement of ions \( u_i(x) \) is given from Eqs. (2.2) and (2.3) by,

\[
u_i(x) = \frac{i\alpha}{g} \left\{ \Delta_i(x)e^{iQx} - \Delta_i^*(x)e^{-iQx} \right\},
\]

we obtain the ionic contribution to the charge density modulation as,

\[
\rho_i^{\text{ion}} = \bar{\rho},
\]

\[
\rho_{Q_i}^{\text{ion}} = -\bar{\rho} \frac{\partial u_i}{\partial x},
\]

\[
= \frac{\rho_0 Q}{g} \left\{ \Delta_i(x)e^{iQx} + \Delta_i^*(x)e^{-iQx} \right\},
\]

where \( \bar{\rho} \) is the average ion charge density. Note that we neglected the derivative \( \partial_x \Delta(x) \) in Eq. (2.12), since its effect is negligible as compared to \( Q \Delta_i \).

As a whole, the total charge density \( \rho_0 \) and \( \rho_{Q_i} \) are given by the summation of the electronic and the ionic contributions as,

\[
\rho_0(x) = \bar{\rho} - e \left( R_\sigma R_\sigma + L_\sigma L_\sigma \right),
\]

\[
\rho_{Q_i} = A_i^*(x)e^{iQx} + A_i(x)e^{-iQx},
\]

where

\[
A_i(x) = \eta \Delta_i(x) - eL_\sigma^* R_\sigma,
\]

with \( \eta \) being \( \bar{\rho}\alpha Q/g \).

In order to clarify the nature of the Coulomb interaction, first we trace out \( \varphi(x, \tau) \). One can easily see that the following term is generated,

\[
S_C = \frac{1}{2} \int_0^\beta dt \sum_{ij} \int_0^L dx \int_0^L dx' \frac{\rho_i(x)\rho_j(x')}{\sqrt{(x - x')^2 + d_{ij}^2}},
\]

where \( d_{ij} \) is the distance between the \( i \)-th and the \( j \)-th chain and the summation over \( i \) and \( j \) should be taken.
over all the chains. This expression can be rewritten using Fourier transformation as,

\[ S_C = \frac{1}{2} \int_0^{\beta \hbar} d\tau \sum_{i,j} \sum_q \tilde{v}_{ij}(q) \tilde{\rho}_i(q) \tilde{\rho}_j(-q), \]  

(2.17)

\[ \tilde{\rho}_i(q) = \int_0^L dx \rho_i(x) e^{-i q x}, \]  

(2.18)

\[ \tilde{v}_{ij}(q) = \int_0^L dx \frac{e^{-i q x}}{\sqrt{x^2 + d_{ij}^2}}, \]  

(2.19)

where \( K_0(x) \) is the modified Bessel function. We assume that \( d_i \equiv d_0 \neq 0 \) in order to avoid divergence which occurs when \( i = j \) in Eq. (2.13). The divergence arises from the fact that we considered the purely one-dimensional case, i.e., infinitely thin chains. In reality, \( d_0 \) corresponds to the actual thickness of the chains, which may be given by the size of ions (or, more precisely, the extension of the electronic wave function on an ion).

By substituting \( \rho_i(x) = \rho_0i(x) + \rho_{Q_i}(x) \) into Eqs. (2.17) and (2.18), we obtain,

\[ S_C = \frac{1}{2} \int_0^{\beta \hbar} d\tau \sum_{i,j} \sum_q [\tilde{v}_{ij}(q) \tilde{\rho}_0i(q) \tilde{\rho}_0j(q)] + 2 \tilde{v}_{ij}(Q + q) \tilde{A}_i(q) \tilde{A}_j(q)], \]  

(2.20)

where \( \tilde{\rho}_0i(q) \) and \( \tilde{A}_i(q) \) are the Fourier components of \( \rho_0i(x) \) and \( A_i(x) \), respectively. We have neglected the cross term between \( \rho_0i(x) \) and \( \rho_{Q_i}(x) \), since \( R_{i\sigma} \) and \( L_{i\sigma} \) are slowly varying.

Note that the interactions in \( S_C^{(1)} \) and \( S_C^{(2)} \) have different range in \( d_{ij} \). As is shown in Eq. (2.19), \( \tilde{v}_{ij}(q) \) is given by \( 2K_0(d_{ij}|q|) \) which decays exponentially for \( d_{ij}|q| \geq 1 \). Since the wave number \( q \) in \( S_C^{(1)} \) can take the value \( q \approx 0 \), \( K_0(d_{ij}|q|) \) is not negligible even for large \( d_{ij} \). In \( S_C^{(2)} \), on the other hand, \( \tilde{v}_{ij}(Q + q) \) equals approximately to \( 2K_0(Qd_{ij}) \) and this is negligible for \( d_{ij} \gtrsim 1/Q = 1/(2K_F) \). The Fermi wavelength is usually the order of the lattice constant and we can limit the summation with respect to \( i \) and \( j \) in \( S_C^{(2)} \) to adjacent chains only.

We rewrite the long range part \( S_C^{(1)} \), restoring the scalar potential, as

\[ S_C^{(1)} = \int_0^{\beta \hbar} d\tau \sum_i \int_0^L dx \left[ -i \phi_i \{ \tilde{\rho} - e (R_{i\sigma}^* R_{i\sigma} + L_{i\sigma}^* L_{i\sigma}) \} + \frac{1}{8\pi} \left\{ (\partial_x \phi_i)^2 + \sum_\alpha \frac{(\phi_{i+\alpha} - \phi_i)^2}{d_{i\alpha}^2} \right\} \right], \]  

(2.21)

where \( \alpha = \{ \bar{y}, \bar{z} \} \) and \( i + \bar{y} \) and \( i + \bar{z} \) symbolically denote the chains shifted by one lattice vector in positive \( y \)- and \( z \)-direction from the \( i \)-th chain, respectively. Note that only the slowly varying part of the scalar potential with a wave vector much smaller than \( K_F \) should be taken into account here.

The short range part \( S_C^{(2)} \) can be divided into two kinds of terms: \( \text{intrachain} \) term \((j = i)\) and the \( \text{nearest-neighbor} \) term \((j = i + \alpha)\). The \( \text{intrachain} \) term has three parts: ion-ion interaction, electron-ion interaction and electron-electron interaction. The first and the second one are absorbed into the phonon energy \( \hbar \omega_Q \) and the electron-phonon coupling constant \( q \), respectively. In this paper we assume that the electron-electron interaction is small and negligible. Hence we suppress the intrachain term in the following.

The \( \text{nearest-neighbor} \) term \((j = i + \alpha)\) can be written, using the approximation, \( \tilde{v}_{ii+\alpha}(Q + q) \rightarrow \tilde{v}_{ii+\alpha}(Q) \equiv \tilde{v}_\alpha \), as,

\[ S_C^{(2)} = \int_0^{\beta \hbar} d\tau \sum_{i,\alpha} \int_0^L dx \left\{ \tilde{A}_i(x) \tilde{A}_{i+\alpha}(x) - A^*_i(x) A_{i+\alpha}(x) \right\}. \]  

(2.22)

2. Electron hopping

Next we discuss the effect of electron hopping between chains. We consider only the hopping between adjacent chains and introduce the following term,

\[ S_{\text{hop}} = \int_0^{\beta \hbar} d\tau \sum_{i,\alpha} \int_0^L dx \left\{ t_\alpha \left( R_{i+\alpha}^* R_{i\sigma} + L_{i+\alpha}^* L_{i\sigma} \right) + \text{c.c.} \right\}, \]  

(2.23)

where \( t_\alpha \) is transfer integral between the \( i \)-th and the \((i + \alpha)\)-th chains and c.c. stands for the complex conjugate.

C. Chiral Transformation

In integrating out the electronic degree of freedom, it is convenient to employ chiral transformation so that the phase \( \theta(x) \) is eliminated from \( \Delta_i(x) \). In this paper we study the temperature region not too close to \( T_c \). Hence the amplitude of the order parameter can be treated as a constant. We write \( \Delta_i(x) = \Delta \ e^{i \theta_i(x)} \) in the following. The chiral transformation is introduced as follows:

\[ R_{i\sigma} \rightarrow \exp(i \theta_i/2) R_{i\sigma}, \quad L_{i\sigma} \rightarrow \exp(-i \theta_i/2) L_{i\sigma}. \]  

(2.24)

By this transformation \( S_{\text{e-p}} \) is changed to,

\[ S_{\text{e-p}} = \int_0^{\beta \hbar} d\tau \sum_i \int_0^L dx \left\{ \Psi_i^\dagger \cdot K_i \cdot \Psi_i - \frac{\hbar \omega_Q}{2g_F} \chi_i^2 \right\}, \]  

(2.25)
where
\[ K_i(x, \tau) = \left( \frac{\hat{k}_i^{(+)} + \hat{k}_i^{(-)}}{\Delta_i} \right), \]
and \( v_F = \hbar k_F / m \) is the Fermi velocity.

In Eq. (2.27) we have neglected the term proportional to \( \partial_\tau^2 \). As pointed out by Ishikawa and Takayama [13], this term is necessary to obtain the free energy which describes electromagnetic response of the system correctly. On the other hand, if one neglects this term and approximates the dispersion by a linear one, so-called chiral anomaly term must be taken into account [14]. In this paper, we take the latter way and add the following term to our action,
\[ S_{\text{ch}} = \int_0^\beta d\tau \sum_i \int_0^L dx \frac{i e}{\pi} \partial_\tau \theta_i(x) \varphi_i(x). \tag{2.29} \]

The terms \( S_C^{(2)} \) and \( S_{\text{hop}} \) are transformed as,
\[ S_C^{(2)} \rightarrow \int_0^\beta d\tau \sum_{i, \alpha} \overline{\nu}_\alpha \int_0^L dx \left[ 2 \eta^2 \Delta_i \Delta_{i+\alpha} \cos(\theta_{i+\alpha} - \theta_i) - \eta e \left( \Delta_i \left( \frac{R_{i+\alpha} \varphi_{i+\alpha} e^{-i(\theta_{i+\alpha} - \theta_i)} + \text{c.c.}}{\Delta_i} \right) + (i \leftrightarrow i + \alpha) \right) + \epsilon^2 \left( \frac{R_{i+\alpha} \varphi_{i+\alpha} e^{-i(\theta_{i+\alpha} - \theta_i)}}{\Delta_i} + \text{c.c.} \right) \right], \tag{2.30} \]
\[ S_{\text{hop}} \rightarrow \int_0^\beta d\tau \sum_{i, \alpha} \int_0^L dx \left\{ t\alpha \left( e^{-\theta_{i+\alpha} + \theta_i} R_{i+\alpha} \varphi_i + e^{\theta_{i+\alpha} - \theta_i} L_{i+\alpha} \varphi_i + \text{c.c.} \right) \right\}. \tag{2.31} \]

III. DERIVATION OF THE GL FREE ENERGY

The effective free energy of the condensate can be obtained by integrating out the electronic degree of freedom in the following way,
\[ F[\theta_i, \varphi_i, \varDelta_i] = -\frac{1}{\beta} \ln \int \mathcal{D}[\Psi_{i\sigma}], \Psi_{i\sigma}] e^{-S_{\text{tot}}/\hbar}, \tag{3.1} \]
where \( S_{\text{tot}} \) is the total action. In performing this path integral, the following perturbative treatment is available,
\[ Z(\beta) = \int \mathcal{D}[\Psi_{i\sigma}], \Psi_{i\sigma}] \exp \left[ \{-S_0 + \delta S\}/\hbar \right], \]
\[ = \int \mathcal{D}[\Psi_{i\sigma}], \Psi_{i\sigma}] \sum_{n=0}^\infty \frac{(-1)^n \delta S^n}{n!} e^{-S_0/\hbar}, \]
\[ = Z_0(\beta) \times \sum_{n=0}^\infty \frac{(-1)^n \langle \delta S^n \rangle_c}{n!}, \]
\[ = Z_0(\beta) \times \exp \left[ -\sum_{n=0}^\infty \frac{\langle \delta S^n \rangle_c}{n!} \right], \]
\[ = Z_0(\beta) \times \exp \left[ W\{\theta_i, \varphi_i, \varDelta_i\} \right], \tag{3.2} \]
where \( S_0 \) and \( \delta S \) are the unperturbed and perturbed part, respectively. The bracket \( \langle \cdots \rangle_c \) indicates that only the “connected diagrams” should be taken into account and \( Z_0(\beta) \) is the unperturbed partition function. From this formula, the effective free energy \( F \) is given by \( F = F_0 - W/\beta \) where \( F_0 = -\ln(Z_0(\beta)/\beta) \). From now on we assume that the amplitude of the order parameter \( \Delta_i \) does not depend on the chain index and write \( \Delta = \Delta_i \).

Based on the above mentioned method, the effective free energy can be derived. Here, for simplicity, we discuss only the resulting free energy, leaving the details of the calculations for Appendix A. The free energy consists of two parts, the intrachain part \( F_{\text{intr}} \) and the interchain part \( F_{\text{inter}} \). The intrachain part is given by,
\[ F_{\text{intr}} = \sum_i \int_0^L dx \left[ \frac{\hbar v_F}{4\pi} f_s (\theta_i \varphi_i)^2 + \frac{c^2(1 - f_s)}{\pi \hbar v_F} \varphi_i^2 + \frac{ie f_s}{\pi} \partial_\tau \theta_i \varphi_i \right], \tag{3.3} \]
where the condensate fraction \( f_s \) behaves as,
\[ f_s = \left\{ \begin{array}{ll} \frac{1}{\varpi_\alpha} \beta^2 \varDelta^2 \zeta(3, 1/2) & \text{for } \varDelta \ll 0 \\ 1 - \sqrt{2\pi \beta \varDelta} \exp (-\beta \varDelta) & \text{for } \varDelta \gg 0 \end{array} \right. \tag{3.4} \]
with \( \zeta(3, 1/2) \) being the zeta function. (See Appendix B for details.) The interchain part \( F_{\text{inter}} \) is given by,
\[ F_{\text{inter}} = \text{const.} + \sum_{i, \alpha} \int dx \hbar \Gamma_\alpha \cos(\theta_{i+\alpha} - \theta_i), \tag{3.5} \]
where \( \Gamma_\alpha \) is the interchain coupling constant given by,
\[ \Gamma_\alpha = \frac{2 \hbar}{\varpi^2} \left( \frac{\rho c Q Q}{g} + \frac{e \hbar \omega Q}{2g^2} \right)^2 + \frac{|f_s|^2}{\pi \hbar^2 v_F} f_s. \tag{3.6} \]
As one can see from Eqs. (3.3) and (3.6), the CDW prefers the phase difference of the neighboring chains to be \( \pi \) since \( \Gamma_\alpha \) is positive. In this paper we assume that the chains form a bipartite crystal and shift the phase of the chains on one sublattice by \( \pi \). In this new notation \( \Gamma_\alpha \) is changed to \( -\Gamma_\alpha \), leading to the following expression for \( F_{\text{inter}} \).
\[ F_{\text{inter}} = \text{const.} - \sum_{i,\alpha} \int dx \hbar \Gamma_{\alpha} \cos(\theta_{i+\alpha} - \theta_i), \]

\[ \approx F_{\text{inter}}^{(0)} + \sum_{i,\alpha} \int dx \frac{\hbar \Gamma_{\alpha}}{2} (\theta_{i+\alpha} - \theta_i)^2. \]  

(3.7)

where \( F_{\text{inter}}^{(0)} \) is the change of the condensation energy due to interchain coupling.

Next we take the continuum limit with respect to the chain index \( i \) by writing \( \theta(\mathbf{r}) \) instead of \( \theta_i(x) \). The total free energy becomes,

\[ F = F^{(0)} + \int d\mathbf{r} \left[ \frac{K}{2} \left( (\partial_x \theta)^2 + \gamma_y^2 (\partial_y \theta)^2 + \gamma_z^2 (\partial_z \theta)^2 \right) + i e J \varphi \partial_x \theta + \frac{1}{8\pi} \left\{ |\nabla \varphi|^2 + (\lambda_0^2 - \lambda_{\text{res}}^2) \varphi^2 \right\} + i e \varphi \rho_{\text{ext}}(\mathbf{r}) \right]. \]

(3.8)

where \( K = \hbar v_F N_{\perp} f_s / (2\pi) \) and \( J = N_{\perp} f_s / \pi \) with \( N_{\perp} \) being the cross sectional density of the chains. The anisotropy parameters \( \gamma_y \) and \( \gamma_z \) are given by \( K \gamma^2_{\alpha} = \hbar \Gamma_{\alpha} \alpha^2_\alpha (\alpha = y, z) \). Here we have included the energy of electric field, i.e., the last two terms of Eq. (2.21) and also introduced the external charge \( \rho_{\text{ext}}(\mathbf{r}) \) which is a source of the external electric field.

The first and the second term of \( \Gamma_{\alpha} \) in Eq. (3.4) are proportional to \( \Delta^2 \) and \( f_s \), respectively. As is known for the case of superconductivity, these quantities, namely the square of the gap and the superfluid density, have different temperature dependence at \( T \ll T_c \), although the relation \( f_s \propto \Delta^2 \) holds near \( T_c \). Therefore \( \gamma^2_{\alpha} \), which is proportional to \( \Gamma_{\alpha} / f_s \), has a weak temperature dependence at \( T \ll T_c \) arising from the difference between \( \Delta^2 \) and \( f_s \). This temperature dependence, however, is almost negligible because the temperature dependence of \( \Delta^2 \) and \( f_s \) are both exponentially suppressed at low temperatures.

In Eq. (3.8) \( \lambda_0 \) is the electrostatic screening length by the quasiparticles, which is given by \( \lambda_0^{-2} = \lambda_{\text{TF}}^{-2}(1 - f_s) \) where \( \lambda_{\text{TF}}^{-2} = 8e^2 N_{\perp} / (\hbar v_F) \) is the Thomas-Fermi screening length of the individual 1-D chain. At \( T = 0, f_s \) tends to 1 and \( \lambda_0 \) diverges. This is because we have assumed the complete nesting in our calculation. In actual CDW’s, there exists residual carriers which does not contribute to CDW ordering even at 0K. Such materials are called “metallic” CDW’s. In this case, the divergence of \( \lambda_0 \) is suppressed. We have introduced \( \lambda_{\text{res}} \) to incorporate the contribution of these carriers.

The amplitude fluctuation of the order parameter can be treated in a similar way as we have treated the phase fluctuation in this paper. For purely one-dimensional systems this was carried out by Brazovskii and Dzyaloshinskii [18]. The extension of the present calculation to the case with the amplitude mode may be straightforward.

IV. SUMMARY

In this paper we have derived the effective free energy of the phase of CDW employing the path integral method. Especially, a careful treatment of the interchain coupling, i.e., Coulomb interaction and electron hopping, was presented. We have clarified the followings:

1. The Coulomb interaction is divided into two parts, which correspond to slow modulation \( (q \sim 0) \) and fast oscillation \( (q \sim 2k_F) \) of charge density. The former determines the large scale electromagnetic response of the CDW’s and the latter plays an important role in the elastic coupling between CDW’s on adjacent chains.

2. The electron hopping between neighboring chains also contributes to the elastic interchain coupling of CDW.

3. The contribution of the Coulomb interaction and the electron hopping to the interchain coupling have slightly different temperature dependence at low temperatures. As a result the anisotropy parameters also become weakly temperature dependent at low temperatures, although its dependence is negligibly small.

4. The quasiparticles give a finite electrostatic screening length. The length is given by the Thomas-Fermi length above \( T_c \) but is enhanced in lower temperatures due to the suppression of the density of states by the energy gap of CDW. In “semiconducting” CDW’s, the quasiparticle screening length is divergent at \( T = 0 \) but it remains finite in “metallic” ones.

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APPENDIX A: INTEGRATION OVER ELECTRONIC FIELD

From Eqs. (2.21), (2.25), (2.29), (2.30) and (2.31), we obtain the total action of the system. For simplicity we set \( \Delta_i \rightarrow \Delta \) in the following. We divide the total action into two parts, unperturbed part \( S_0 \) and perturbed part \( \delta S \). Here we assign \( S_0 \) the part of \( S_{\text{e-p}} \) in Eq. (2.25).
which does not include \( \theta_i \). The rest of the terms are assigned to \( \delta S \).

The unperturbed action is given as follows,

\[
\frac{S_0}{\hbar} = \int_0^{\beta \hbar} d\tau d\tau' \sum_i \int_0^L dx \ dx' \Psi_{i\sigma}^\dagger (x, \tau) \cdot \{-\mathcal{G}(x - x', \tau - \tau')\}^{-1} \cdot \Psi_{i\sigma}(x', \tau'),
\]

\[
\Psi_{i\sigma}^\dagger (k, i\varepsilon_n) \cdot \{-\tilde{\mathcal{G}}(k, i\varepsilon_n)\}^{-1} \cdot \tilde{\Psi}_{i\sigma}(k, i\varepsilon_n),
\]

where,

\[
\tilde{\mathcal{G}}(k, i\varepsilon_n) = \begin{pmatrix} \tilde{\mathcal{G}}^R(k, i\varepsilon_n) & \tilde{\mathcal{F}}(k, i\varepsilon_n) \\ \tilde{\mathcal{F}}^\dagger(k, i\varepsilon_n) & \tilde{\mathcal{G}}^L(k, i\varepsilon_n) \end{pmatrix},
\]

and the Green functions are given by

\[
\tilde{\mathcal{G}}^R(k, i\varepsilon_n) = -\frac{\hbar}{(i\hbar \varepsilon_n + \xi)} \frac{E_i(k)^2}{(E_i(k)^2 + \xi^2)},
\]

\[
\tilde{\mathcal{G}}^L(k, i\varepsilon_n) = -\frac{\hbar}{(i\hbar \varepsilon_n - \xi)} \frac{E_i(k)^2}{(E_i(k)^2 + \xi^2)},
\]

\[
\tilde{\mathcal{F}}(k, i\varepsilon_n) = -\frac{\hbar \Delta}{(i\hbar \varepsilon_n)^2 + (E(k))^2},
\]

with \( E(k) = \sqrt{\xi^2 + \Delta^2}, \xi = \hbar v_F k \) and \( \varepsilon_n = (2n - 1)\pi/(\beta \hbar) \).

The perturbed term \( \delta S \) is given as follows,

\[
\delta S = S_1 + S_2 + S_C^{(2)} + S_{\text{hop}},
\]

\[
S_1 = \int d\tau \sum_i \int dx \chi_i(x) \left( R_{\sigma\sigma} R_{\sigma\sigma} + L_{\sigma\sigma} L_{\sigma\sigma} \right),
\]

\[
S_2 = -i \int d\tau \sum_i \int dx \varphi_i \left\{ \tilde{\rho} - \frac{\epsilon}{\pi} \partial_x \chi_i \right\},
\]

where \( \chi_i(x) \) is defined by

\[
\chi_i(x) \equiv \frac{i e}{\hbar} \varphi_i + \frac{1}{2} v_F \partial_x \chi_i + \frac{\hbar}{8m} (\partial_x \chi_i)^2.
\]

\( S_C^{(2)} \) and \( S_{\text{hop}} \) are given by Eq. (2.33) and Eq. (2.34), respectively. The energy of the electric field, i.e., the last two terms of Eq. (2.21) is not included here.

After the integration with respect to the electronic degree of freedom we obtain the following results:

\[
\langle S_1 \rangle_c = \int d\tau \sum_i \int dx n_e \chi_i(x),
\]

where \( n_e \) is the equilibrium electron density on a chain which is assumed to be a constant independent of \( i \) and given by \( 2k_F/\pi \). In Eq. (A8), the first term of \( \chi_i(x) \) should be cancelled by the ionic background charge, i.e., the first term of Eq. (A7) for charge neutrality. In the present calculations, the cancellation of second term of \( \chi_i(x) \), which is proportional to \( \partial_x \chi_i \), is not complete. This term should vanish in order to maintain the stability of CDW with a wave number \( 2k_F \). We consider that this cancellation is fulfilled if we take into account the \( \partial^2 \)-term which we have neglected in Eq. (2.20).

The second order term with respect to \( S_1 \) is given as follows,

\[
\langle \{ S_1 \}^2 \rangle_c = \sum_i \int dx \ dx' \chi_i(x) \chi_i(x') \times 2 \left\{ -G^R(X - X')G^R(X' - X) \right. \\
- G^L(X - X')G^L(X' - X) \\
- 2 F(X - X') F(X' - X) \right\},
\]

where we have introduced \( X \equiv (x, \tau) \) for simplicity. Since \( \chi_i(x) \) is slowly varying as compared to \( G^R, G^L \) or \( F \), we can use the following treatment,

\[

\text{This treatment corresponds to GL expansion. As we see in the next section, the following quantities are rewritten in terms of the the condensate fraction} f_s \text{ as,}
\]

\[
\frac{1}{\beta \hbar L} \sum_{k, i\varepsilon_n} \left\{ \tilde{G}^R(k, i\varepsilon_n)^2 + \tilde{G}^L(k, i\varepsilon_n)^2 \right\}
- \frac{1}{\pi v_F} \left(1 - \frac{f_s}{2}\right),
\]

\[
\frac{1}{\beta \hbar L} \sum_{k, i\varepsilon_n} \tilde{F}(k, i\varepsilon_n)^2 = \frac{1}{4\pi v_F} f_s,
\]

which yields the following expression,

\[

\text{The terms which includes two chains are given as follows,}
\]

\[

\text{where} \tilde{W}_1 = \cdots.
\]
where we have used the relation, Eq. \((2.7)\). We also obtain for the hopping term,

\[
\langle \{ S_{\text{hop}} \}^2 \rangle_c = 4 \int \text{d}X \text{d}X' \sum_{i,\alpha} |t_{\alpha}|^2 \left\{ -G^R(X - X')G^R(X' - X) - G^L(X - X')G^L(X' - X) - F^*(X - X')F(X' - X)e^{-i(\theta_{i+\alpha} - \theta_i)} - F_i(X - X')F_i^*(X' - X)e^{i(\theta_{i+\alpha} - \theta_i)} \right\},
\]

\[
= 4 \int \text{d}X \sum_{i,\alpha} |t_{\alpha}|^2 \left\{ \frac{1}{\pi v_F} \left( 1 - \frac{f_s}{2} \right) - \frac{f_s}{2\pi v_F} \cos(\theta_{i+\alpha} - \theta_i) \right\}. \tag{A16}
\]

Collecting these terms we obtain the interchain terms as,

\[
- \frac{1}{h} \left\langle \frac{G^R(\theta^2)}{2 \pi^2} \right\rangle_c + \frac{1}{2h^2} \langle \{ S_{\text{hop}} \}^2 \rangle_c
= \int \text{d}r \sum_{i,\alpha} \int \text{d}x \left\{ \frac{2|t_{\alpha}|^2}{h^2 \pi v_F} \left( 1 - \frac{f_s}{2} \right) - \Gamma_{\alpha} \cos(\theta_{i+\alpha} - \theta_i) \right\},
\]

\[
\equiv W_2. \tag{A17}
\]

where

\[
\Gamma_{\alpha} = \frac{2}{h} \bar{\nu}_\alpha \Delta^2 \left( \frac{\bar{\nu}_\alpha Q}{g} + \frac{2\epsilon\omega Q}{2g^2} \right)^2 + \frac{|t_{\alpha}|^2}{\pi^2 v_F} f_s. \tag{A18}
\]

Here we assumed \(\theta_i\) and \(\varphi_i\) to be classical variables and neglected their \(\tau\)-dependence.

The intrachain part \(F_{\text{intra}}\) and the interchain part \(F_{\text{inter}}\) of the free energy are given, respectively, by \(F_{\text{intra}} = -W_1 / \beta\) and \(F_{\text{inter}} = -W_2 / \beta\).

**APPENDIX B: CALCULATION OF THE GL COEFFICIENTS**

In this section we derive Eq. \((A12)\) and \((A13)\). We introduce a cut off energy, \(\hbar v_F |k| \sim \Lambda\), which should be set to \(\infty\) in the end of the calculation.

Eq. \((A12)\) can be obtained in the following way,

\[
\frac{1}{\beta h L} \sum_{k,\omega_n} \left\{ \bar{G}^R(k, \epsilon_n)^2 + G^L(k, \epsilon_n)^2 \right\}
= \frac{2}{\beta h} \sum_{\epsilon_n} \frac{\hbar}{\pi v_F} \int_0^\Lambda \text{d} \xi \frac{-(\hbar \epsilon_n)^2 + \xi^2}{(\hbar \epsilon_n)^2 + E(k)^2},
\]

\[
= \frac{2}{\beta h} \sum_{\epsilon_n} \frac{\hbar}{\pi v_F} \int_0^\Lambda \text{d} \xi \left[ \frac{\xi^2 - (\hbar \epsilon_n)^2 - \Delta^2}{(\hbar \epsilon_n)^2 + E(k)^2} \right] + \frac{\Delta^2}{(\hbar \epsilon_n)^2 + E(k)^2}.
\]

\[
\equiv I_1 + I_2. \tag{B1}
\]

\(I_1\) is calculated as,

\[
I_1 = \frac{1}{\beta h} \sum_{\epsilon_n} \frac{\hbar}{\pi v_F} \left( \frac{-\Lambda}{2\pi^2 + (\hbar \epsilon_n)^2 + \Delta^2} \right),
\]

\[
= -\frac{1}{\pi v_F} \frac{\Lambda}{\sqrt{\Lambda^2 + \Delta^2}} \tanh \frac{\beta \Lambda^2 + \Delta^2}{2},
\]

\[
\rightarrow -\frac{1}{\pi v_F} \frac{\Lambda}{\Lambda} \ (\Lambda \rightarrow \infty), \tag{B2}
\]

using the identity,

\[
\tanh z = z \sum_{n=\infty} \frac{1}{(2n-1)^2 + z^2}. \tag{B3}
\]

\(I_2\) is also calculated in a similar way as,

\[
I_2 = \frac{\Delta^2}{\pi v_F} \sum_{\epsilon_n} \frac{2\hbar}{\beta} \frac{1}{\frac{1}{2}(\hbar \epsilon_n)^2 + \Delta^2} \left\{ \frac{1}{2\sqrt{(\hbar \epsilon_n)^2 + \Delta^2}} \arctan \frac{\Lambda}{\sqrt{(\hbar \epsilon_n)^2 + \Delta^2}} \right\},
\]

\[
= \frac{\Delta^2}{\pi v_F} \sum_{\epsilon_n} \frac{1}{\beta} \frac{1}{\frac{1}{2}(\hbar \epsilon_n)^2 + \Delta^2} \left\{ \frac{1}{\sqrt{\Lambda^2 + \Delta^2}} \tanh \frac{\beta \Lambda^2 + \Delta^2}{2} \right\}
- \frac{1}{\pi v_F} \frac{\Lambda}{\sqrt{(\hbar \epsilon_n)^2 + \Delta^2}}.
\]

\[
\times \arctan \frac{\Lambda}{\sqrt{(\hbar \epsilon_n)^2 + \Delta^2}}, \tag{B4}
\]

We define the condensate fraction \(f_s\) by

\[
f_s = 2\pi v_F I_2
\]

\[
= \frac{4}{\beta} \sum_{\epsilon_n} \int_0^\Lambda \text{d} \xi \frac{\Delta^2}{\left\{ \xi^2 + (\hbar \epsilon_n)^2 + \Delta^2 \right\}^2},
\]

\[
= \frac{2\Delta^2}{\pi \beta} \sum_{\epsilon_n} \left\{ (\hbar \epsilon_n)^2 + \Delta^2 \right\}^{-\frac{3}{2}} \times \arctan \frac{\Lambda}{\sqrt{(\hbar \epsilon_n)^2 + \Delta^2}}. \tag{B5}
\]

Then from Eq. \((B2)\) and \((B4)\) we obtain Eq. \((A12)\).

In a similar way we obtain,

\[
\frac{1}{\beta h L} \sum_{k,\omega_n} F(k, \epsilon_n)^2 = \frac{I_2}{2}, \tag{B6}
\]
which reduces to Eq. (A13).

Next we examine the behavior of \( f_s \) in two limiting cases, \( \beta \Delta \ll 1 \) and \( \beta \Delta \gg 1 \).

1. **The case of \( \beta \Delta \ll 1 \)**

In this case, we can simply expand Eq. (B5) with respect to \( \Delta \) and obtain,

\[
\begin{align*}
\frac{1}{\beta} \sum_{\epsilon_n} \frac{\Delta^2}{(\hbar \epsilon_n)^2} &= \frac{1}{4 \pi^2} \sum_{n=1}^{\infty} \frac{1}{(n - \frac{1}{2})^2} \\
&= \frac{(\beta \Delta)^2}{4 \pi^2} \xi(3, \frac{1}{2}).
\end{align*}
\]

(B7)

2. **The case of \( \beta \Delta \gg 1 \)**

In this case the following method is more useful [19]. From Eq. (B7), we obtain,

\[
\begin{align*}
f_s &= \frac{4}{\beta} \sum_{\epsilon_n} \int_0^\Lambda d\xi \left[ \frac{\Delta^2}{(\xi^2 + (\hbar \epsilon_n)^2 + \Delta^2)^2} \right] \\
&= 2\beta \Delta \int_0^\Lambda d\xi \frac{\partial}{\partial \Delta} \sum_{\epsilon_n} \frac{-1}{(2n-1)^2 \pi^2 + \beta^2 (\xi^2 + \Delta^2)^2} \\
&= -\frac{\partial}{\partial \Delta} \int_0^\Lambda d\xi \frac{1}{E} \tanh \frac{\beta E}{2}, \\
&= -\frac{\partial}{\partial \Delta} \left[ \log \left( \frac{\Lambda + \sqrt{\Lambda^2 + \Delta^2}}{\Delta} \right) \right] \\
&+ 2 \sum_{m=1}^{\infty} (-1)^m \int_1^{\sqrt{\Lambda^2 + \Delta^2} / \Delta} \frac{1}{e \sqrt{\epsilon^2 - 1}} e^{-\Delta \epsilon m}, \\
&\to 1 + 2\beta \Delta \sum_{m=1}^{\infty} (-1)^m m K_1(\beta \Delta m) \quad (\Lambda \to \infty), \\
&\approx 1 - \sqrt{2 \pi \beta \Delta} e^{-\beta \Delta}, \quad (B8)
\end{align*}
\]

where \( E = \sqrt{\xi^2 + \Delta^2} \) and \( \epsilon = E / \Delta \). \( K_1(\epsilon) \) is the modified Bessel function given by,

\[
\begin{align*}
K_1(\epsilon) &= -\frac{d}{dz} K_0(\epsilon) \\
&= -\frac{d}{dz} \int_1^{\infty} dy \frac{1}{y^2 - 1} e^{-yz}.
\end{align*}
\]

(B9)

In the last line of Eq. (B8), we have employed the asymptotic form of \( K_1(\epsilon) \).