

Electron and phonon correlations in systems of one-dimensional electrons coupled to phonons

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Electron and phonon correlations in systems of one-dimensional electrons coupled to phonons are studied at low temperatures by emphasizing on the effect of electron-phonon backward scattering. It is found that the $2k_F$ -wave components of the electron density and phonon displacement field share the same correlations. Both correlations are quasi-long-ranged for a single conducting chain coupled to one-dimensional or three-dimensional phonons, and they are long-ranged for repulsive electron-electron interactions for a three-dimensional array of parallel one-dimensional conducting chains coupled to three-dimensional phonons.

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I. INTRODUCTION

The physics of one-dimensional (1D) interacting electron systems has attracted a lot of interest. The low-energy long-wavelength excitations of such systems can be described by a Tomonaga-Luttinger liquid (TLL) model.¹ Such systems exhibit a critical-like behavior (power law) of the charge-density correlations at zero temperature. Thus, 1D electron systems are always at the verge of an instability without being able to order.² On the other hand, it was noticed by Peierls³ that due to electron-phonon interactions a charge density wave (CDW) accompanied by a periodic lattice distortion appears in the ground state of a 1D metal, both periods being π/k_F . For an arbitrary band filling the period is incommensurate with the underlying lattice, where the number of electrons per site is not a simple fractional number (e.g., 1/2, 1/3, etc.). Later studies⁴ on incommensurate systems of 1D electrons coupled to 1D phonons (1D1D) show that the tendency to form CDW is increased significantly by electron-phonon coupling. However, true long-range-order CDW is still missing. In reality 1D electron systems are often embedded in three-dimensional (3D) environment, and phonons in such systems are effectively 3D. Therefore, it is interesting to know if the coupling between 1D electrons and 3D phonons could lead to long-range-order CDW.

For simplicity, we limit this paper to spinless incommensurate systems. Our work focuses on the effect of the electron-phonon coupling at large momenta (i.e., backward-scattering process). We show that the $2k_F$ -wave components of the electron density and phonon displacement field share the same correlations at large distance. This result applies to all the systems we consider in this paper. It is *exact* and does not depend on the electron-phonon coupling strength, phonon frequency, and electron-electron interactions. This result implies that phonon correlations are quasi-long-ranged even for arbitrary weak electron-phonon coupling in 1D1D, in which previous studies⁴ showed that electron correlations are quasi-long-ranged.

The first system we consider is a single conducting chain coupled to 3D acoustic phonons (1D3D). We find that electron-phonon coupling in this system does *not* change the qualitative power-law electron correlations, although it does increase the tendency to form CDW significantly (i.e., make electron correlations decay much slower). Surprisingly, our

calculation shows that 1D3D even has less increased tendency to form CDW than 1D1D, given that both the phonon frequency and the electron-phonon coupling strength are the same in these two cases. Furthermore, phonon correlations are also quasi-long-ranged in 1D3D.

The second system we discuss is a 3D array of parallel 1D conducting chains coupled to 3D acoustic phonons (3D3D). For arbitrary weak electron-phonon coupling, the system undergoes a quantum phase transition driven by varying electron-electron interactions. For repulsive electron-electron interactions, electrons on different chains are effectively correlated, which leads to long-ranged-ordered CDW and hence long-ranged phonon correlations. For attractive electron-electron interactions, electron correlations remain 1D, and the system is effectively a simple sum of 1D1D, which leads to quasi-long-ranged electron and phonon correlations. In the limit of strong coupling and/or low phonon frequency, both electron and phonon correlations are long-ranged for repulsive electron-electron interactions, and interestingly, the phase fluctuations of the $2k_F$ -wave components of the electron density and phonon displacement field are *not* independent but locked together. The 3D3D system was also considered recently by Artemenko *et al.*⁵ Their work agrees with ours in the limit of strong coupling and/or low phonon frequency.

It was argued⁶ that the electron-phonon coupling at small momenta (forward-scattering process) is not important since its effect is of the order $c^2/v_F^2 \ll 1$ (v_F is the Fermi velocity and c is the sound velocity). However, it was pointed out⁷ that in strongly correlated systems coupling to small-momentum acoustic phonons can lead to the Wentzel-Bardeen (WB) singularity^{8,9} and hence become important. This singularity is a critical point at which for a critical electron-phonon coupling constant, the attractive electron-phonon interactions cause the system to be unstable. It was shown⁷ that the critical point can be reached as one approaches the half-filling for the Hubbard model.¹⁰ In this paper we assume that the system is far away from the WB singularity for a general filling, and the electron-phonon coupling at small momenta is thus not important. In fact we even find that the WB singularity does *not* exist in 1D3D no matter the filling. This is because the bulk phonon freedom suppresses phonon fluctuations on the chain, thus making the system robust.

This paper is arranged as follows. In Sec. II we introduce the model. In Sec. III we review 1D1D systems. In Secs. IV and V, we discuss 1D3D and 3D3D systems, respectively. Finally some technical details are given in Appendixes A and B.

II. MODEL

In this section we discuss the model for 3D3D, from which the models for 1D1D and 1D3D can be obtained as special cases. Let us start with electrons. Using the TLL description for electrons,^{1,2} the electron density inside the j th chain can be written in the form

$$\rho_e^j = -\frac{1}{\pi} \partial_x \phi_j + \frac{1}{\pi \alpha} \cos(2k_F x + 2\phi_j), \quad (1)$$

where ϕ_j is a slowly varying phase, \hat{x} denotes the direction along the chains, α is the cutoff and of the order of the lattice spacing, and k_F is the Fermi momentum. The first term on the right-hand side of Eq. (1) is the long-wavelength part of the electron density; the second term is the fast oscillating part. The total electron action is a sum of TLL models,

$$S_{el}/\hbar = \frac{1}{2\pi K} \sum_j \int dx d\tau \left[\frac{1}{v} (\partial_\tau \phi_j)^2 + v (\partial_x \phi_j)^2 \right], \quad (2)$$

where v is renormalized Fermi velocity, K is a dimensionless parameter, which is bigger than 1 for attractive electron-electron interactions and less than 1 for repulsive electron-electron interactions, and τ is the imaginary time.

Since electrons are restricted on the chains, an effective phonon action in terms of the on-chain freedom is needed. It can be obtained by starting with the standard lattice version of a 3D phonon action and eliminating the phonon freedom which is not on the chain. This effective action is expected to have the following form:

$$S_{ph}^{3D}[u]/\hbar = \frac{1}{2a\hbar} \sum_j \int dx d\tau \left[m (\partial_\tau u_j)^2 + K_x a^2 (\partial_x u_j)^2 + K_\perp |u_j - u_{j+1}|^2 \right], \quad (3)$$

where \hbar is Planck's constant, a is the lattice spacing, b is the distance between nearest-neighbor chains, m is the atom mass, \perp denotes directions perpendicular to the chains, and K_x and K_\perp are the effective spring constants along \hat{x} and \perp directions, respectively.

In general the action for electron-phonon coupling can be expressed in the form¹¹

$$S_{ep}/\hbar = \frac{\gamma}{\hbar} \sum_j \int dx d\tau (\partial_x u_j) \rho_e^j(x), \quad (4)$$

where γ is the coupling constant. Plugging Eq. (1) into the above action we obtain

$$S_{ep}/\hbar = \frac{\gamma}{\pi\hbar} \sum_j \int dx d\tau \left[-(\partial_x u_j) (\partial_x \phi_j) + \frac{1}{\alpha} (\partial_x u_j) \cos(2k_F x + 2\phi_j) \right]. \quad (5)$$

The first piece on the right-hand side of Eq. (5) corresponds to the electron-phonon coupling at small momenta, which is responsible for the WB singularity. We will discuss it in Sec. IV. The second piece is the coupling at large momenta, which is the main focus of this paper. For this latter type of coupling, only the phonon field with wavelength near $1/2k_F$ is important due to the fast oscillation of the cosine term. We write

$$u_j(x) = \frac{1}{2} [e^{2ik_F x} \tilde{\psi}_j(x) + \text{H.c.}], \quad (6)$$

where $\tilde{\psi}_j$ is a slow varying complex field. Then the action for the coupling at large momenta can be rewritten as

$$S_{ep}^l/\hbar = \frac{\gamma}{4\pi\hbar} \sum_j \int dx d\tau \left[2ik_F \tilde{\psi}_j + \partial_x \tilde{\psi}_j \right] (e^{4ik_F x + 2\phi_j} + e^{-2i\phi_j}) + \text{H.c.}, \quad (7)$$

where the piece which involves $e^{4ik_F x}$ vanishes when integrated over x ; also $\partial_x \tilde{\psi}_j$ is negligible compared to $2k_F \tilde{\psi}_j$ at long wavelength (i.e., $q_x < 2k_F$). The action can be further simplified as

$$S_{ep}^l/\hbar = \frac{i\gamma k_F}{2\pi\hbar\alpha} \sum_j \int dx d\tau \tilde{\psi}_j e^{-2i\phi_j} + \text{H.c.} \quad (8)$$

At this point, it is also convenient to have a phonon action in terms of $\tilde{\psi}_j$. Plugging Eq. (6) into Eq. (3) we obtain

$$S_{ph}^{3D}[\tilde{\psi}_j]/\hbar = \frac{1}{2a\hbar} \sum_j \int dx d\tau \left(\frac{m}{2} |\partial_\tau \tilde{\psi}_j|^2 + 2K_x a^2 k_F^2 |\tilde{\psi}_j|^2 + \frac{K_x}{2} a^2 |\partial_x \tilde{\psi}_j|^2 + \frac{K_\perp}{2} |\tilde{\psi}_j - \tilde{\psi}_{j+1}|^2 \right). \quad (9)$$

For convenience, we rescale the lengths and field such that the actions are fully expressed in terms of dimensionless quantities. An appropriate rescaling is the following:

$$\tau \rightarrow a\tau/(\pi v), \quad x \rightarrow ax/\pi, \quad (10)$$

$$r_\perp \rightarrow br_\perp/\pi, \quad \psi_j = \sqrt{\frac{mv}{2a\hbar}} \tilde{\psi}_j. \quad (11)$$

After rescaling, the actions (2), (9), and (8) become

$$S_{el}/\hbar = \frac{1}{2\pi K} \sum_j \int dx d\tau [(\partial_\tau \phi_j)^2 + (\partial_x \phi_j)^2], \quad (12)$$

$$S_{ph}^{3D}[\psi_j]/\hbar = \frac{1}{2} \sum_j \int dx d\tau \left[|\partial_\tau \psi_j|^2 + g_1^2 \left(\frac{1}{2n_c} \right)^2 |\partial_x \psi_j|^2 + g_1^2 |\psi_j|^2 + \left(\frac{C_\perp}{\pi^2} \right) |\psi_j - \psi_{j+1}|^2 \right], \quad (13)$$

$$S_{\text{ch}}^I/\hbar = ig_2 \sum_j \int dx d\tau \psi_j e^{-2i\phi_j} + \text{H.c.}, \quad (14)$$

where $C_{\perp} \equiv K_{\perp} a^2/mv^2$, the filling factor $n_e = ak_F/\pi$ (i.e., the averaged number of electrons per lattice site) which is of order 1 for a general filling. Both g_1 and g_2 are dimensionless quantities defined as

$$g_1 = 2n_e \left(\frac{c}{v} \right) = (\hbar \omega_{2k_F}) \left(\frac{\hbar \pi v}{a} \right)^{-1}, \quad (15)$$

$$g_2 = \frac{\gamma}{\sqrt{2\pi}} \left(\frac{\hbar^2}{ma^2} \right)^{1/2} \left(\frac{\hbar \pi v}{a} \right)^{-3/2} \left(\frac{an_e}{\alpha} \right), \quad (16)$$

where $c \equiv a\sqrt{K_x/m}$ is the sound velocity along the chains, ω_{2k_F} is the phonon frequency at wave vector $2k_F$, \hbar^2/ma^2 is approximately the ground-state energy of an atom with mass m trapped in an infinite one-dimensional potential well with width a , and $\hbar \pi v/a$ is of the order of the Fermi energy. Typically g_1 is of order 10^{-5} – 10^{-6} . In this paper we assume

$$\frac{g_2}{g_1} \ll 1, \quad (17)$$

which can be fulfilled for a general filling. This condition actually implies that the system is far away from the WB instability, so that the electron-phonon coupling at small momenta is not important. For the Hubbard model near half-filling, since g_1/g_2 which is proportional to $v^{1/2}$ drops rapidly to zero,¹⁰ assumption (17) breaks down. Therefore, the electron-phonon coupling at small momenta could be important. This will be further discussed in Sec. IV.

III. SINGLE CONDUCTING 1D CHAIN COUPLED TO 1D PHONONS

The model for 1D1D can be recovered by restricting the index j to be 1 in the actions (12)–(14) and setting C_{\perp} to be 0. To lighten the notation we drop the index j in this section. First we want to show a very general result which is *exact* and does not depend on the values of K , the electron-phonon coupling strength, and phonon frequency. We introduce a complex field ψ' , which, in Fourier space, is related to ϕ and ψ by

$$\psi'_R(\vec{q}) = \psi_R(\vec{q}) - \frac{2g_2 G_{\text{ph}}(\vec{q})}{\sqrt{V}} \int dx d\tau \sin 2\phi e^{i\vec{q}\cdot\vec{r}}, \quad (18)$$

$$\psi'_I(\vec{q}) = \psi_I(\vec{q}) - \frac{2g_2 G_{\text{ph}}(\vec{q})}{\sqrt{V}} \int dx d\tau \cos 2\phi e^{i\vec{q}\cdot\vec{r}}, \quad (19)$$

where $V \equiv L\hbar v/(k_B T a^2)$, $G_{\text{ph}}^{-1}(\vec{q}) \equiv q_{\tau}^2 + g_1^2(1/2n_e)^2 q_x^2 + g_1^2$, and the subscripts R and I denote the real and imaginary components, respectively. In terms of ψ' and ϕ the total action can be separated into two parts which are completely decoupled from each other:

$$S_{\psi'}/\hbar = \sum_{\vec{q}} G_{\text{ph}}^{-1}(\vec{q}) \psi'(\vec{q}) \psi'(-\vec{q}), \quad (20)$$

$$S_{\text{el}}^{\text{1D}}/\hbar = \frac{1}{2\pi K} \int dx d\tau [\partial_{\tau} \phi]^2 + (\partial_x \phi)^2 - \frac{g_2^2}{g_1} \int dx d\tau d\tau' G_{\text{ph}} \times (\tau - \tau') \cos[2\phi(x, \tau) - 2\phi(x, \tau')], \quad (21)$$

where the phonon correlation function is given by

$$G_{\text{ph}}(\tau) \approx e^{-g_1|\tau|}. \quad (22)$$

To obtain Eq. (21) we have neglected the phonon dispersions $(\partial_x \phi)^2$ since the leading order effect on electron correlations comes from the phonon kinetic energy $(\partial_{\tau} \phi)^2$. Since ψ' and ϕ are decoupled, from Eqs. (18) and (19) the fluctuations of ψ can be calculated as

$$\langle \psi(\vec{q}) \psi(-\vec{q}) \rangle = 16\pi^2 \alpha^2 g_2^2 G_{\text{ph}}^2(\vec{q}) \int dx d\tau [e^{i\vec{q}\cdot\vec{r}} \langle \rho_{2k_F}(\vec{r}) \rho_{2k_F}(\vec{0}) \rangle] + G_{\text{ph}}(\vec{q}), \quad (23)$$

where ρ_{2k_F} is the $2k_F$ -wave component of the electron density. Since $G_{\text{ph}}(\vec{q})$ tends toward a constant for $q \ll g_1$, this result implies that at large distance (i.e., $r \gg g_1^{-1}$) the $2k_F$ -wave component of the phonon displacement field has the same correlations as ρ_{2k_F} .

In the limit of weak coupling and/or high phonon frequency (i.e., $g_2 g_1^{K-2} \ll 1$), the effort is put on the phonon-mediated effective electron action given by Eq. (21). Since the exponentially decaying phonon correlation $G_{\text{ph}}(\tau)$ imposes a cutoff at $\tau \sim 1/g_1$, at the wavelength longer than $1/g_1$ model (21) essentially reduces to the one for free electrons but with renormalized K , which we denote as K' . A Gaussian variational method¹² and a perturbative renormalization group (RG) (Refs. 4 and 12) have been applied to this model. Both find that electron-phonon coupling increases the tendency to form CDW. Specifically, in terms of K' the result is expressed as

$$\left(\frac{K}{K'} \right)^2 - 1 \sim \begin{cases} \left[\left(\frac{g_2}{g_1} \right) g_1^{K-1} \right]^2, & K < \frac{3}{2} \\ -\frac{g_2^2}{g_1} \ln g_1, & K = \frac{3}{2} \\ \frac{g_2^2}{g_1}, & K > \frac{3}{2}. \end{cases} \quad (24)$$

To obtain the above result, it has been assumed that the renormalization of K is small, that is, $(K/K')^2 - 1 \ll 1$, which leads to a self-consistent condition. For $K < 1$, this self-consistent condition is just

$$\frac{g_2}{g_1} \ll g_1^{1-K}, \quad (25)$$

which prohibits the application of the Gaussian variational result in the region above the locus OA in Fig. 2.

When condition (25) is violated, neither the Gaussian variational method nor the perturbative RG can give an analytical result. A different strategy is used. A mean-field theory shows that ψ saturates for $K < 1$. Therefore, it is believed that for $K < 1$ and in the limit of strong coupling and/or low phonon frequency, the important fluctuations of ψ

are its phase fluctuations, and the amplitude fluctuations are massive and hence negligible. Based on this belief we now work on the truncated action,

$$S_{\text{total}}^{\text{1D}}/\hbar = \frac{1}{2} \int dx d\tau \left\{ \frac{1}{\pi K} [(\partial_\tau \phi)^2 + (\partial_x \phi)^2] + \psi_0^2 \left[(\partial_\tau \theta)^2 + g_1^2 \left(\frac{1}{2n_e} \right)^2 (\partial_x \theta)^2 \right] \right\} - 2g_2 \psi_0 \int dx d\tau \cos(2\phi - \theta), \quad (26)$$

where ψ_0 is fixed at the saturated value, and the constant pieces have been neglected. Hereafter we name this strategy as “fixed-amplitude approximation” just for convenience.

We estimate the saturated value of ψ using a mean-field theory. Approximating ψ as uniform both in space and time by doing $\psi \equiv \psi_0$, the total action reduces to

$$S_{\text{total}}^{\text{1D}}/\hbar = \frac{1}{2} \int dx d\tau \frac{1}{\pi K} [(\partial_\tau \phi)^2 + (\partial_x \phi)^2] - 2g_2 \psi_0 \int dx d\tau \cos(2\phi) + \frac{1}{2} \int dx d\tau g_1^2 \psi_0^2, \quad (27)$$

where the electron part of the action is just a Sine-Gordon model. Directly integrating out the field ϕ in favor of ψ_0 using a Gaussian variational method, we get

$$S_{\text{ph}}^{\text{eff}}[\psi_0]/\hbar = \frac{g_1^2}{2} \int dx d\tau \left[(2\pi K g_2 g_1^{K-2} \psi_0)^{2/(2-K)} \frac{(K-2)}{\pi K} + \psi_0^2 \right]. \quad (28)$$

The detailed calculation is shown in Appendix A. The first term in action (28) is negative, which means that a periodic lattice distortion with period π/k_F lowers the electron energy. The second term is the elastic energy for such a lattice distortion and hence positive. To find the ground state, we minimize action (28) with respect to ψ_0 . We find

$$\psi_0 = g_1^{-1} \left[2(\pi K)^{K/2} \left(\frac{g_2}{g_1} \right) \right]^{1/(1-K)} \quad (29)$$

for $K < 1$ and $\psi_0 = 0$ for $K > 1$. This indicates that a periodic lattice distortion with period π/k_F appears in the ground state for repulsive electron-electron interactions. However, ψ is *not* long-range-ordered due to its phase fluctuations. Later in this section we will show that ψ is quasi-long-range-ordered with power-law correlations. For K not very close to 1, the result given in Eq. (29) qualitatively agrees with that in Ref. 4, in which model (27) is mapped to an exactly solvable field-theoretical model (i.e., massive Thirring model). In the limit of $K \rightarrow 1^-$, Eq. (29) gives $\psi_0 \rightarrow 0$, and the classic Peierls theory predicts $\psi_0 \sim \exp(-g_1^2/g_2^2)/g_2$, which is essentially very small.

The above mean-field calculation assumes that the single electron gap opened at the Fermi level is much less than the Fermi energy, that is, $(g_2 \psi_0)^{1/(2-K)} \ll 1$. This assumption combined with Eq. (29) leads to assumption (17), or equivalently

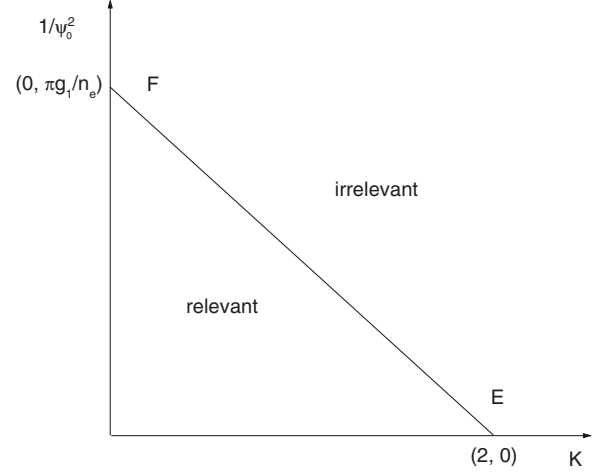


FIG. 1. The line EF is defined by the function given in Eq. (31). The cosine term in action (26) is irrelevant above EF and relevant below it.

$$g_1 \psi_0 \ll 1. \quad (30)$$

Now we discuss the truncated model (26). This model has been studied previously in the context of liquid crystal.¹³ It can be shown that the coupling term in this model is either relevant or irrelevant depending on the values of ψ_0 and K . The critical values of ψ_0 and K satisfy

$$\frac{n_e}{\pi g_1 \psi_0^2} + 2K = 4. \quad (31)$$

The detailed derivation is given in Appendix B. This function defines a critical line in the $\psi_0^2 - K$ plane, which is illustrated in Fig. 1. Thus, for $K < 1$, only for which we can get a non-zero ψ_0 , we have

$$\psi_0^c \sim g_1^{-1/2}. \quad (32)$$

For $\psi_0 < \psi_0^c$, the cosine term becomes irrelevant, and ϕ and θ are decoupled. For $\psi_0 > \psi_0^c$, the cosine term is relevant, and the fluctuations of ϕ and θ are bound together. This implies a self-consistent condition for the fixed-amplitude approximation. The estimated ψ_0 must be bigger than ψ_0^c such that phase fluctuations do not drive the cosine term into irrelevance. This cosine term offsets the positive phonon energy and is necessary for obtaining a nonzero ψ_0 in the first place. In terms of g_1 and g_2 this self-consistent condition is given by

$$\frac{g_2}{g_1} \geq g_1^{(1-K)/2}, \quad (33)$$

which invalidates the fixed-amplitude approximation in the region below the locus OB in Fig. 2.

For the systems satisfying Eq. (33) both the effective actions of ϕ and θ can be obtained by making $2\phi = \theta$ in the truncated model (26), and they are given by

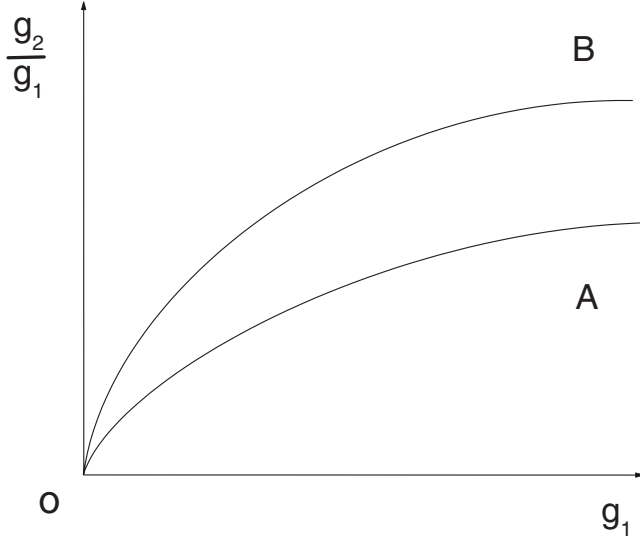


FIG. 2. Limits of the validity of the two approaches. The result of the Gaussian variational method does not apply in the region above OA, while the fixed-amplitude approximation does not apply in the region below OB. The regions below OA and above OB are defined by conditions (25) and (33) in the 1D1D case and by Eqs. (78) and (86) in the 3D3D case, respectively. In the intermediate region between OA and OB neither of the two approaches applies.

$$S[\Xi]/\hbar = \frac{1}{2\pi K} \int dx d\tau [R(\partial_\tau \Xi)^2 + B(\partial_x \Xi)^2], \quad (34)$$

where Ξ can be either ϕ or $\theta/2$, and the parameters R and B are

$$R = (1 + 4\pi K \psi_0^2), \quad (35)$$

$$B = 1 + \pi K g_1^2 \left(\frac{1}{n_e}\right)^2 \psi_0^2. \quad (36)$$

This result is consistent with our earlier conclusion that at large distance the $2k_F$ -wave components of the phonon displacement field and electron density share the same correlations. Note that the correction to B comes from the phonon dispersions along the chains and is much less than 1 according to assumption (30). Also it is of the order of the correction to R multiplied by g_1^2 and hence negligible. Plugging Eq. (29) into Eq. (35) and defining $K' \equiv K/\sqrt{R}$, we get

$$\left(\frac{K}{K'}\right)^2 - 1 \sim g_1^{-2} \left(\frac{g_2}{g_1}\right)^{2/(1-K)}. \quad (37)$$

Now we discuss the validity of the fixed-amplitude approximation. In addition to the self-consistent condition (33) caused by phase fluctuations, there is another one caused by amplitude fluctuations, which is

$$\langle (\delta\psi_0)^2 \rangle \ll \psi_0^2, \quad (38)$$

where $\delta\psi_0$ is the deviation of the amplitude of ψ from the saturated value. For a crude estimation of $\langle (\delta\psi_0)^2 \rangle$, we assume that the effective action for $\delta\psi_0$ (to the quadratic order) has the following form:

$$S[\delta\psi_0]/\hbar = \frac{1}{2\pi^2} \int dx d\tau \left[\frac{2(1-K)g_1^2}{2-K} (\delta\psi_0)^2 + (\partial_\tau \delta\psi_0)^2 + g_1^2 \left(\frac{1}{2n_e}\right)^2 (\partial_x \delta\psi_0)^2 \right], \quad (39)$$

where the mass term is obtained by expanding the mean-field action (28) around its minimum, and the derivative terms come from the free phonon action. Then after a straightforward calculation, condition (38) also leads to Eq. (33) coincidentally.

In both limits the charge-density correlations can be calculated, given by the nonuniversal power laws

$$\langle \rho_{2k_F}(\vec{r}) \rho_{2k_F}(0) \rangle \sim r^{-2K'}, \quad (40)$$

where $\vec{r} = (x, \tau)$. This implies that electron-phonon coupling does *not* change the qualitative TLL behavior, although the tendency to form CDW is increased since K' is smaller than K . Based on the general conclusion given in Eq. (23), at large distance phonon correlations are also governed by the same nonuniversal power laws:

$$\langle \psi(\vec{r}) \psi(0) \rangle \sim r^{-2K'}. \quad (41)$$

Surprisingly, this shows that in 1D1D electron-phonon coupling does change phonon correlations qualitatively. The correlations of the $2k_F$ -wave component of the phonon displacement field, which are short ranged in the absence of electron-phonon coupling, become quasi-long-ranged. According to the self-consistent conditions given by Eqs. (25) and (33), there is an intermediate region in which neither of the two approaches apply, and therefore, no quantitative result is available. This region is illustrated in Fig. 2 as the area between the loci OA and OB. However, in this region we do expect the same qualitative conclusion.

IV. SINGLE CONDUCTING 1D CHAIN COUPLED TO 3D PHONONS

In this section we consider a single 1D conducting chain coupled to 3D phonons. In this case the action for electrons and electron-phonon coupling is the same as that in 1D1D, and the phonon action is given in Eq. (3). For convenience, we transform the phonon action into its continuum version and perform the dimensional rescaling given in Eqs. (10) and (11) and the field rescaling

$$u' = \sqrt{\frac{mv}{2a\hbar}} u. \quad (42)$$

After this procedure, we obtain

$$S_{\text{ph}}^{\text{3D}}[u']/\hbar = \frac{1}{\pi^2} \int d^3 r d\tau \left[(\partial_\tau u')^2 + g_1^2 \left(\frac{1}{2n_e}\right)^2 (\partial_x u')^2 + C_\perp |\vec{\nabla}_\perp u'|^2 \right]. \quad (43)$$

Since electron-phonon coupling only happens on the chain, an effective phonon action for the on-chain freedom is

needed. We integrate out the bulk off-chain phonon freedom in favor of the on-chain one $u'_0(x, \tau) \equiv u'(x, \tau, \vec{r}_\perp = \vec{0})$, where we have assumed that the position of the chain is at $r_\perp = 0$. This leads to an effective 1D phonon action

$$S_{\text{ph}}^{\text{1D}}[u'_0]/\hbar = \frac{1}{2} \sum_{\vec{q}} G^{-1}(\vec{q}) |u'_0(\vec{q})|^2, \quad (44)$$

where

$$G(\vec{q}) = \frac{\pi}{8C_\perp} \ln \frac{q_\tau^2 + \frac{4}{\pi} C_\perp + \left(\frac{g_1}{2n_e}\right)^2 q_x^2}{q_\tau^2 + \left(\frac{g_1}{2n_e}\right)^2 q_x^2}. \quad (45)$$

In the limit $C_\perp \rightarrow 0$, the renormalized 1D phonon propagator given by Eq. (45) reduces to the bare 1D one (i.e., the one which is not renormalized by the bulk phonon freedom) as expected. For $C_\perp \neq 0$, for small \vec{q} s the renormalized one has a logarithmic dependence on \vec{q} , while the bare one has a second-order power-law dependence. This difference has a drastic effect on the electron-phonon coupling at small momenta. We delay this discussion to later on in this section. Now we focus our attention on the electron-phonon coupling at large momenta (i.e., near $2k_F$). Expanding action (44) around $q_x = \pm 2ak_F/\pi, q_\tau = 0$ (the factor a/π is due to the rescaling), we get

$$S_{\text{ph}}^{\text{1D}}[\psi]/\hbar = \frac{1}{4} \sum_{q_x, q_\tau} G^{-1} \left(\frac{2ak_F}{\pi} + q_x, q_\tau \right) |\psi(q_x, q_\tau)|^2, \quad (46)$$

where the complex phonon field ψ is the slow varying part of the $2k_F$ -wave component of the displacement field u'_0 ,

$$u'_0(x) = \frac{1}{2} [e^{2ik_F x} \psi(x) + \text{H.c.}]. \quad (47)$$

The inverse of the propagator in Eq. (46), to the lowest order of q_x, q_τ is given by

$$G^{-1} \left(\frac{2ak_F}{\pi} + q_x, q_y \right) = 2(g_1'^2 + g_3 q_y^2 + g_4 q_x^2) \quad (48)$$

with

$$g_1' \equiv 2 \sqrt{\frac{C_\perp}{\pi} \left(\ln \frac{g_1^2 + 4C_\perp/\pi}{g_1^2} \right)^{-1}}, \quad (49)$$

$$g_3 \equiv \frac{4g_1'^2 C_\perp/\pi}{g_1^2 (g_1^2 + 4C_\perp/\pi)} \left(\ln \frac{g_1^2 + 4C_\perp/\pi}{g_1^2} \right)^{-1}, \quad (50)$$

$$g_4 \equiv \frac{\pi^2 g_1^2 g_3}{4ak_F^2} \left[1 + 4g_1^2 \left(\frac{g_3}{g_1'^2} - \frac{1}{g_1^2 + 4C_\perp/\pi} \right) \right]. \quad (51)$$

To get Eq. (48), we have neglected the term linear in q_x (i.e., $q_x |\psi|^2$), which only leads to boundary effects. Plugging Eq. (48) into Eq. (46) we get

$$S_{\text{ph}}^{\text{1D}}[\psi]/\hbar = \frac{1}{2} \int dx d\tau [\pi g_3 |\partial_\tau \psi|^2 + g_1'^2 |\psi|^2 + g_4 |\partial_x \psi|^2]. \quad (52)$$

Therefore, with respect to the electron-phonon coupling at large momenta, the effective model of phonons in 1D3D is qualitatively the same as that in 1D1D but with modified coefficients. A thoughtful reader might have seen this right from the beginning.¹⁴ Note that g_1' , g_3 , and g_4 are all increasing functions of C_\perp . This is expected since the bulk phonon freedom suppresses phonon fluctuations on the chain.

Since we have shown that the models for 1D3D and 1D1D are essentially the same, the calculations should be also very similar. Repeating the (virtually same) calculation, we obtain, for 1D3D and repulsive electron-electron interactions,

$$\left(\frac{K}{K'} \right)^2 - 1 \sim \frac{g_2^2}{g_1'} \left(\frac{\sqrt{g_3}}{g_1'} \right)^{3-2K} \quad (53)$$

in the limit of weak coupling and/or high phonon frequency and

$$\left(\frac{K}{K'} \right)^2 - 1 \sim g_3 (g_2^2 g_1'^{2K-4})^{1/(1-K)} \quad (54)$$

in the limit of strong coupling and/or low phonon frequency. It can be verified that both K' obtained from the two limits are increasing functions of C_\perp . Therefore, we conclude that a single 1D chain coupled to 3D phonons does not lead to long-range-ordered CDW, instead the increased tendency to form CDW in such systems is even less than that in 1D1D, given that the two dimensionless quantities g_1 and g_2 (or equivalently, the phonon frequency and the coupling strength) are the same in these two cases. This result comes from the combination of two opposite effects. On one hand, the bulk phonon freedom increases the energy cost to form a lattice distortion along the chain, which is manifested in that g_1' is an increasing function of C_\perp . This is a negative effect on the increased tendency to form CDW. On the other hand, both g_3 and g_4 are increasing functions of C_\perp , which enhances the correlations of ψ . This is a positive effect on the increased tendency to form CDW. Only a quantitative calculation can show that the former effect dominates. In principle we could also think about a single 1D chain coupled to 2D phonons. We expect that in such systems long-range-ordered CDW is still missing, and the increased tendency to form CDW is less than that in 1D1D but more than that in 1D3D, given that both g_1 and g_2 are the same in the three cases. In addition, the $2k_F$ -wave components of the phonon displacement field in 1D2D and 1D3D are quasi-long-range-ordered due to electron-phonon coupling.

Now we discuss the electron-phonon coupling at small momenta. According to the action given in Eq. (5), the action for the electron-phonon coupling at small momenta is given by

$$S_{\text{ep}}^s/\hbar = -\frac{\gamma}{\pi\hbar} \int dx d\tau (\partial_x u_0)(\partial_x \phi). \quad (55)$$

After the dimensional and field rescaling which are given in Eqs. (10) and (42), respectively, the above action becomes

$$S_{\text{ep}}^s/\hbar = -\frac{2\pi\alpha g_2}{an_e} \int dx d\tau (\partial_x u'_0)(\partial_x \phi). \quad (56)$$

The effective action for the on-chain phonon field is given by Eq. (44). Since the total action is quadratic in u'_0 , we integrate it out. This leaves us an effective electron action

$$S_{\text{el}}^{\text{total}} = \frac{1}{2\pi K} \sum_{\vec{q}} \left[q_x^2 + q_\tau^2 - 4\pi^3 K \left(\frac{\alpha g_2}{an_e} \right)^2 q_x^4 G(\vec{q}) \right] \times \phi(-\vec{q}) \phi(\vec{q}), \quad (57)$$

where $G(\vec{q})$ is the phonon propagator. The first two terms on the right-hand side of Eq. (57) are from free electrons, and the third term, which is retarded and *negative*, is contributed by phonons. First let us treat phonons as pure 1D. Plugging $G(\vec{q})$ as the bare 1D phonon propagator into Eq. (57), we get

$$S_{\text{el}}^{\text{total}} = \frac{1}{2\pi K} \sum_{\vec{q}} \left[q_x^2 + q_\tau^2 - \frac{2\pi^3 K \alpha^2 g_2^2 q_x^4}{a^2 n_e^2 \left[q_\tau^2 + \left(\frac{g_1}{2n_e} \right)^2 q_x^2 \right]} \right] \times \phi(-\vec{q}) \phi(\vec{q}). \quad (58)$$

In the limit $q_\tau \rightarrow 0$, the retarded part is proportional to q_x^2 and cancels the first term at the point

$$\frac{1}{K} = 8\pi^3 \left(\frac{\alpha g_2}{ag_1} \right)^2, \quad (59)$$

at which the electron density becomes unstable toward long wavelength fluctuations. This singular point is referred to as the Wentzel-Bardeen (WB) singularity. Since K and α/a are both of order 1, as long as assumption (17) is fulfilled, the left-hand side of Eq. (59) is much larger than the right-hand side, and the electron-phonon coupling at small momenta can thus be safely neglected. As we mentioned earlier, for the Hubbard model near half-filling, assumption (17) breaks down, and the WB singularity is reachable. However, in this case the umklapp effect becomes also important, and whether the WB singularity is robust against this additional effect remains an open question. Now we treat phonons as 3D. Plugging Eq. (45) into Eq. (57), we obtain

$$S_{\text{el}}^{\text{total}} = \frac{1}{2\pi K} \sum_{\vec{q}} \left[q_x^2 + q_\tau^2 - \frac{\pi^4 K}{2C_\perp} \left(\frac{\alpha g_2}{an_e} \right)^2 q_x^4 \right. \\ \left. \times \ln \frac{q_\tau^2 + \frac{4}{\pi} C_\perp + \left(\frac{g_1}{2n_e} \right)^2 q_x^2}{q_\tau^2 + \left(\frac{g_1}{2n_e} \right)^2 q_x^2} \right] \phi(-\vec{q}) \phi(\vec{q}). \quad (60)$$

For small \vec{q} s the negative retarded part in Eq. (60) is of the order q_x^4 with a logarithmic correction, which is subdominant

to q_x^2 . This implies that the WB singularity does not exist in 1D3D, since the bulk phonon freedom suppresses phonon fluctuations on the chain and thus stabilizes the system against the attractive electron-phonon coupling. Therefore, in a 1D3D system the electron-phonon coupling at small momenta is not important no matter the filling. A similar discussion for 1D2D leads to the same conclusion.

V. 3D ARRAY OF PARALLEL 1D CONDUCTING CHAINS COUPLED TO 3D PHONONS

In this section we will study a more realistic system: a 3D array of parallel 1D conducting chains coupled to 3D phonons. In 1D1D we derived an exact relation between phonon and electron correlations, which is given in Eq. (23). Performing an almost identical calculation we also find a similar result in 3D3D:

$$\langle \psi(\vec{q}) \psi(-\vec{q}) \rangle = 16\pi^4 \alpha^2 g_2^2 G_{\text{ph}}^2(\vec{q}) \sum_{\vec{r}_\perp} \int dx d\tau e^{i\vec{q}\cdot\vec{r}} \times \langle \rho_{2k_F}(\vec{r}) \rho_{2k_F}(\vec{0}) \rangle + G_{\text{ph}}(\vec{q}), \quad (61)$$

where $G_{\text{ph}}^{-1}(\vec{q}) \equiv [g_1^2 + q_\tau^2 + (g_1/2n_e)^2 q_x^2 + C_\perp q_\perp^2] / \pi^2$. We have replaced the sum over chain index j by the sum over \vec{r}_\perp with $\vec{r}_\perp = n\pi$ [remember that the distance between nearest-neighbor chains is π after the dimensional rescaling given in Eq. (11)], where n is an integer. We will adopt this change hereafter.

For a further understanding of this problem, we follow the logic used in 1D1D and treat this 3D3D problem based on the same two limits. Let us start with the limit of weak coupling and/or high phonon frequency. In this limit we focus on the phonon-mediated effective electron action:

$$S_{\text{eff}}/\hbar = \frac{S_{\text{el}}}{\hbar} - 2g_2^2 \sum_{\vec{r}_\perp, \vec{r}'_\perp} \int d^2 r_\perp d^2 r'_\perp dx d\tau d\tau' \{ \cos[2\phi(x, \tau, \vec{r}_\perp) - 2\phi(x, \tau', \vec{r}'_\perp)] G_{\text{ph}}(\tau - \tau', \vec{r}_\perp - \vec{r}'_\perp) \}, \quad (62)$$

where the phonon propagator is given by

$$G_{\text{ph}}(\tau, \vec{r}_\perp) = \frac{1}{(2\pi)^3} \int d^2 q_\perp dq_\tau \left[\frac{\pi^2}{q_\tau^2 + C_\perp q_\perp^2 + g_1^2} e^{i(\vec{q}_\perp \cdot \vec{r}_\perp + q_\tau \tau)} \right]. \quad (63)$$

We have neglected the phonon dispersions along the chains, which only lead to insignificant correction. The phonon dispersions perpendicular to the chains, although typically very small, are important since they are responsible for the existence of long-range-order CDW. This will be seen later. Now we apply a self-consistent Gaussian variational method² to this model. We approximate action (62) as a quadratic one

$$S_0/\hbar = \frac{1}{2} \sum_{\vec{q}} G_{\text{el}}^{-1}(\vec{q}) \phi(-\vec{q}) \phi(\vec{q}). \quad (64)$$

Then we try to optimize the propagator $G_{\text{el}}^{-1}(\vec{q})$ so as to minimize the variational free energy

$$F_v = F_0 + \langle S - S_0 \rangle_0, \quad (65)$$

where both the free energy F_0 and the average $\langle \rangle_0$ are calculated using the quadratic action S_0 . Performing the procedure we obtain a self-consistent equation,

$$G_{\text{el}}^{-1}(\vec{q}) = \frac{1}{\pi^3 K} (q_x^2 + q_\tau^2) + 16 \left(\frac{g_2}{\pi} \right)^2 \times \sum_{\vec{r}_\perp} \int d\tau e^{-4(\langle \phi^2 \rangle_0 - \langle \phi(0,0,0) \phi(0,\tau,\vec{r}_\perp) \rangle_0)} \times G_{\text{ph}}(\tau, \vec{r}_\perp) [1 - e^{i(\vec{q}_\perp \cdot \vec{r}_\perp + q_\tau \tau)}]. \quad (66)$$

We notice that the right-hand side of the above equation vanishes as $\vec{q} \rightarrow 0$, which implies that the electron excitations are gapless. Furthermore, if we naively expand the cosine in action (62) to the quadratic order of ϕ , we will get corrections to $|\vec{\nabla}_\perp \phi|^2$ and $(\partial_\tau \phi)^2$ and no corrections to $(\partial_x \phi)^2$. Therefore, we assume the following trial solution:

$$G_{\text{el}}^{-1}(\vec{q}) = \frac{1}{\pi^3 K} (q_x^2 + R q_\tau^2 + M q_\perp^2). \quad (67)$$

Hereafter we define K' as the renormalized K , given by

$$K' = K/\sqrt{R}. \quad (68)$$

The self-consistent Eq. (66) can be solved analytically in the limit $M \ll 1$, $(K/K')^2 - 1 \ll 1$. In this limit the system is highly anisotropic. Electron correlations along the chains decay as a power law at length scales shorter than $1/\sqrt{M}$ and tend toward a nonzero constant at longer length scales, while electron correlations along \perp directions decay very rapidly to the same nonzero constant. Specifically, they are given as

$$e^{-\langle \phi^2 \rangle_0 - \langle \phi(0,0,0) \phi(0,\tau,\vec{r}_\perp) \rangle_0} = \begin{cases} \tau^{-K'/2}, & \vec{r}_\perp = \vec{0}, \quad \tau < 1/\sqrt{M} \\ M^{K'/4}, & \vec{r}_\perp \neq \vec{0}, \quad \text{or } \tau > 1/\sqrt{M}, \end{cases} \quad (69)$$

which reduce to the correlations of TLL in the limit $M \rightarrow 0$. Plugging formula (69) into Eq. (66) we obtain two coupled self-consistent equations,

$$\left(\frac{K}{K'} \right)^2 - 1 = 16\pi K g_2^2 \int_{-1/\sqrt{M}}^{1/\sqrt{M}} d\tau \tau^{-2K'} \tau^2 G_{\text{ph}}(\tau, \vec{0}) + 32\pi K g_2^2 \int_{1/\sqrt{M}}^{\infty} d\tau M^{K'} \tau^2 G_{\text{ph}}(\tau, \vec{0}) + 16\pi K M^{K'} g_2^2 g_1^{-4}, \quad (70)$$

$$M = 16\pi K M^{K'} C_\perp g_2^2 g_1^{-4}, \quad (71)$$

where

$$G_{\text{ph}}(\tau, \vec{0}) = \frac{\pi}{4C_\perp \tau} [e^{-g_1 \tau} - e^{-\tau \sqrt{(4C_\perp/\pi) + g_1^2}}]. \quad (72)$$

In the special case $C_\perp = 0$, M vanishes, and the second and the third terms on the right-hand side of Eq. (70) thus vanish, and then Eq. (70) reduces to the result of 1D1D. This is

expected since the 3D3D model with $C_\perp = 0$ corresponds to a simple sum of 1D1D models. For C_\perp being nonzero, M can be easily calculated from Eq. (71) as

$$M = \begin{cases} 0, & K' > 1 \\ (16\pi K C_\perp g_2^2 g_1^{-4})^{1/(1-K')}, & K' < 1. \end{cases} \quad (73)$$

After a more involved, but essentially straightforward calculation, we get, to the lowest order of $(K/K')^2 - 1$,

$$\left(\frac{K}{K'} \right)^2 - 1 \sim g_2^2 g_1^{2K-4} \quad (74)$$

for $C_\perp \ll g_1^2$ and

$$\left(\frac{K}{K'} \right)^2 - 1 \sim \begin{cases} \frac{1}{C_\perp} [M + g_2^2 g_1^{2K-2}], & M \ll g_1^2 \\ M/C_\perp, & M \gg g_1^2 \end{cases} \quad (75)$$

for $C_\perp \gg g_1^2$. The solution of M implies a quantum phase transition at about $K=1$ for arbitrary weak electron-phonon coupling. This critical point can also be obtained by calculating the average of the retarded part of the action for a single chain with respect to the free electron action. This average scales as L^{2-2K} and thus also predicts the critical point $K=1$. For $K < 1$, electrons on different chains are effectively correlated, which leads to long-range-order CDW. The order parameter is the $2k_F$ -wave component of the electron density, whose average is *nonzero* and scales as

$$\langle \rho_{2k_F} \rangle \sim \frac{M^{K'/2}}{2\pi\alpha}. \quad (76)$$

According to the general result given in Eq. (61), the $2k_F$ -wave component of the phonon displacement field also becomes long-range-ordered with its expectation value

$$\langle \psi \rangle \sim \frac{g_2}{g_1} M^{K'/2}. \quad (77)$$

For $K > 1$, electrons on different chains are effectively not correlated, and each chain behaves as an isolated single 1D conducting chain coupled to 3D phonons, which has been discussed in Sec. IV. For self-consistency, solutions (73)–(75) have to satisfy $M \ll 1$ and $(K/K')^2 - 1 \ll 1$, which leads to a restriction on the parameters

$$\begin{cases} \frac{g_2}{g_1} \ll g_1^{1-K}, & C_\perp \ll g_1^2 \\ \frac{g_2}{g_1} \ll \frac{g_1}{\sqrt{C_\perp}}, & C_\perp \gg g_1^2. \end{cases} \quad (78)$$

This condition precludes the application of the Gaussian variational result in the region above OA in Fig. 2.

For stronger coupling and/or lower phonon frequency, the result we get from the Gaussian variational method is not valid since condition (78) is violated. In this case we have to use the fixed-amplitude approximation, which has been discussed in Sec. III. We assume that the important fluctuations of ψ are its phase fluctuations, and the amplitude of ψ can be approximated as fixed at its saturated value ψ_0 . After this approximation we obtain a simplified model,

$$S_{\text{total}}^{\text{3D}}/\hbar = \frac{1}{2\pi^3} \int dx d^2 r_{\perp} d\tau \left\{ \frac{1}{K} [(\partial_{\tau}\phi)^2 + (\partial_x\phi)^2] + \left[(\partial_{\tau}\theta)^2 + g_1^2 \left(\frac{1}{2n_e} \right)^2 (\partial_x\theta)^2 + C_{\perp} |\vec{\nabla}_{\perp}\theta|^2 \right] \pi\psi_0^2 \right\} - \frac{2g_2\psi_0}{\pi^2} \int dx d^2 r_{\perp} d\tau \cos(2\phi - \theta), \quad (79)$$

where we have transformed the action into its continuum version, and the constant pieces have been thrown away. We will calculate the fluctuations of ϕ and θ based on this truncated model.

The locally saturated value of ψ is also estimated by using the mean-field theory, which approximates ψ as uniform both in space and time. Since there are no bare electron correlations between different chains, the mean-field 3D3D model is a simple sum of the mean-field 1D1D models. Therefore, the mean-field calculation is the same as that in 1D1D, and the result is thus also the same. ψ_0 is nonzero and given by formula (29) for $K < 1$, and zero for $K > 1$. However, unlike in 1D1D, ψ is now *truly* long-range-ordered for $K < 1$. In the following we will include the phase fluctuations and calculate the nonzero expectation value of ψ .

Now we discuss the truncated model (79). It can be shown that the cosine term in the model is always relevant no matter the value of ψ_0 , as long as K is less than 2. The proof is given in Appendix B. Therefore, for $K < 1$ the fluctuations of ϕ and θ are always bound together, and both are characterized by the same action

$$S[\Xi]/\hbar = \frac{1}{2\pi^3 K} \int dx d^2 r_{\perp} d\tau \times [R(\partial_{\tau}\Xi)^2 + B(\partial_x\Xi)^2 + M|\vec{\nabla}_{\perp}\Xi|^2], \quad (80)$$

where Ξ can be either ϕ or $\theta/2$, and parameters R , B , and M are given by

$$R = (1 + 4\pi K\psi_0^2), \quad (81)$$

$$B = 1 + 4\pi K g_1^2 \left(\frac{1}{2n_e} \right)^2 \psi_0^2, \quad (82)$$

$$M = C_{\perp} \pi\psi_0^2, \quad (83)$$

respectively. Note that the correction to B is negligible compared to the correction to R , since $g_1 \ll 1$. Plugging the expression of ψ_0 into Eqs. (81) and (83) and writing R in terms of K' using Eq. (68), we get

$$\left(\frac{K}{K'} \right)^2 - 1 \sim (g_2^2 g_1^{2K-4})^{1/(1-K)}, \quad (84)$$

$$M \sim C_{\perp} (g_2^2 g_1^{2K-4})^{1/(1-K)}, \quad (85)$$

which agrees with the result in Ref. 5. This result is consistent with the one obtained by the Gaussian variational method in that both predict long-range-ordered CDW and hence long-range-ordered ψ for $K < 1$. The expectation values of ρ_{2k_F} and ψ are *nonzero* and given by formulae (76)

and (77), respectively. Clearly this fixed-amplitude approximation *cannot* give result for attractive electron-electron interactions since the method relies on the condensation of the phonon field ψ , which is only possible for repulsive electron-electron interactions according to the mean-field theory. Based on the result of weak coupling and/or high phonon frequency, we suspect that for strong coupling and/or low phonon frequency, there also exists a critical K above which both electron and phonon correlations become quasi-long-ranged. However, this critical K could be significantly bigger than 1.

Now let us discuss the validity of the fixed-amplitude approximation. Unlike in 1D1D, based on the above discussions there is no self-consistent condition caused by phase fluctuations in 3D3D. However, the one caused by amplitude fluctuations still exists. After a similar calculation as we did in 1D1D, we find that the fixed-amplitude approximation is self-consistent *only* if

$$\begin{cases} \frac{g_2}{g_1} \gg g_1^{(1-K)/2}, & C_{\perp} \ll g_1^2 \\ \frac{g_2}{g_1} \gg g_1^{(1-K)/2} \left(\frac{g_1}{\sqrt{C_{\perp}}} \right)^{(1-K)/2}, & C_{\perp} \gg g_1^2, \end{cases} \quad (86)$$

which prohibits the application of the fixed-amplitude approximation in the region below OB in Fig. 2.

According to the self-consistent conditions (78) and (86), there is an intermediate region in the parameter space of g_1 and g_2 in which neither of the approaches applies. This region is illustrated in Fig. 2 as the area between the loci OB and OA. In this region, we cannot obtain a quantitatively trustable result. However, we do expect long-ranged electron and phonon correlations for repulsive electron-electron interactions. We also want to point out that for $C_{\perp} \sim g_1^2$, both approaches give the same result:

$$M \sim \left(\frac{g_2}{g_1} \right)^{2/(1-K)}, \quad (87)$$

$$\left(\frac{K}{K'} \right)^2 - 1 \sim (g_2^2 g_1^{2K-4})^{1/(1-K)}. \quad (88)$$

This strongly suggests that in this special case, this quantitative result should also hold in the intermediate region.

So far we have focused on the electron-phonon coupling at large momenta. In Sec. IV we discussed the effect of the electron-phonon coupling at small momenta in 1D1D and 1D3D. Repeating the calculation, we find that the WB singularity also exists in 3D3D and is given by formula (59). Again, for a general filling, according to assumption (17) the system is far away from the WB singularity. Therefore, the electron-phonon coupling at small momenta is not important.

VI. DISCUSSIONS AND CONCLUSIONS

In this paper we have studied electron and phonon correlations in systems of one-dimensional spinless electrons coupled to phonons with incommensurate fillings at low temperatures. The focus is on the effect of backward electron-

phonon scattering. We have been able to obtain quantitative results in the limits of weak coupling and/or high phonon frequency and strong coupling and/or low phonon frequency, which then lead to a qualitative understanding in the intermediate region as well. The whole picture can be summarized as follows. In these incommensurate systems, electron excitations are gapless. This is guaranteed by the symmetry of the systems, that is, no energy should be paid if electron and phonon phases are shifted by any amounts which obey $\theta=2\phi$. This continuous symmetry is broken in the commensurate systems by umklapp process, which results in a gap in electron excitations. In both 1D1D and 1D3D systems, the gapless electron excitations are effectively described by a TLL model with renormalized electron-electron interactions, which implies quasi-long-ranged electron correlations. In 3D3D systems, although the excitations remain gapless, for attractive electron-electron interactions electrons become correlated along transverse directions, which leads to long-ranged electron correlations. In all the three systems phonons share qualitatively the same correlations as electrons. Thus, information about electron correlations can be obtained by examining phonon correlations, which can be measured experimentally by x-ray scattering. Furthermore, the existence of long-rang-ordered CDW in 3D3D systems at low temperature implies a phase transition between ordered and disordered phases at a finite critical temperature.

We notice the similarities between our 3D3D model (62) and the previously studied weakly coupled planar model.¹⁵ In the planar model, vortex-pair excitations have been considered. By analogy, in our calculations we could also take into account the effect of quantum phase slips¹⁶ and treat the electron field ϕ as not single-valued. Since quantum phase slip becomes relevant at $K=1/2$ for a Luttinger liquid in the absence of electron-phonon coupling, we expect that in the limits of weak coupling and/or high phonon frequency, this extra consideration will decrease the critical value of K from 1 to be slightly larger than $1/2$. A rigorous calculation is needed to obtain an accurate result.

The limitation to spinless fermions in our paper has simplified the problem significantly. A full consideration of the real electron-phonon problem has to include spins and is quite involved. However, this does not mean that our work is completely physically irrelevant. Via a Jordan-Wigner transformation, spin-Peierls problems can be mapped to spinless fermions coupled to phonons.¹⁷ Specifically, spin-Peierls systems with (without) magnetic field are related to spinless fermions coupled to phonons with incommensurate (commensurate) filling. The effect of 3D phonons in the zero-field spin-Peierls systems is studied recently in Ref. 18. Our results may have important applications to spin-Peierls systems with finite magnetic field.

It has to be mentioned that our work for the 3D3D case does not take into account the effect of the interchain hopping. It is well known that the interchain hopping can break down the TLL behavior which we have assumed for electrons in our calculations. On the other hand, it is not clear if the effect of the interchain hopping will be suppressed in the presence of electron-phonon coupling. To address these questions, it requires a theory which includes both effects of electron-phonon coupling and the interchain hopping.

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APPENDIX A: CALCULATION OF ψ_0

After the mean-field approximation we get a simplified model,

$$\frac{S_{\text{el}}^{\text{1D}}}{\hbar} + \frac{S_{\text{ep}}^{\text{1D}}}{\hbar} = \frac{1}{2} \int dxd\tau \frac{1}{\pi K} [(\partial_\tau \phi)^2 + (\partial_x \phi)^2] - 2g_2 \psi_0 \int dxd\tau \cos(2\phi), \quad (\text{A1})$$

$$S_{\text{ph}}^{\text{1D}}/\hbar = \frac{1}{2} \int dxd\tau g_1^2 \psi_0^2. \quad (\text{A2})$$

The partition function can be calculated as

$$\begin{aligned} Z &= \int D[\psi_0] D[\phi] e^{-(S_{\text{el}}^{\text{1D}} + S_{\text{ph}}^{\text{1D}} + S_{\text{ep}}^{\text{1D}})/\hbar} \\ &= \int D[\psi_0] e^{-S_{\text{ph}}^{\text{1D}}/\hbar} \int D[\phi] e^{-(S_{\text{el}}^{\text{1D}} + S_{\text{ep}}^{\text{1D}})/\hbar} \\ &\equiv \int D[\psi_0] e^{-(S_{\text{ph}}^{\text{1D}} + F_{\text{el}}[\psi_0])/\hbar}, \end{aligned} \quad (\text{A3})$$

where $F_{\text{el}}[\psi_0]$ is the free energy of electrons for action $S_{\text{el}}^{\text{1D}} + S_{\text{ep}}^{\text{1D}}$ at a fixed ψ_0 . $S_{\text{el}}^{\text{1D}} + S_{\text{ep}}^{\text{1D}}$ is exactly a Sine-Gordon model. Formula (A3) defines an effective action for ψ_0 ,

$$S_{\text{ph}}^{\text{eff}}[\psi_0] = S_{\text{ph}}^{\text{1D}} + F_{\text{el}}[\psi_0]. \quad (\text{A4})$$

To calculate $F_{\text{el}}[\psi_0]$, we use Gaussian variational method.² For any action S_0 , we have

$$F_{\text{el}}[\psi_0]/\hbar = \frac{F_0}{\hbar} - \ln \langle e^{-(S_{\text{el}}^{\text{1D}} + S_{\text{ep}}^{\text{1D}} - S_0)/\hbar} \rangle_0, \quad (\text{A5})$$

where the $\langle \rangle_0$ denotes the average using the action S_0 . Given the convexity of the exponential¹⁹ one has always

$$\langle e^{-(S_{\text{el}}^{\text{1D}} + S_{\text{ep}}^{\text{1D}} - S_0)/\hbar} \rangle > e^{-\langle S_{\text{el}}^{\text{1D}} + S_{\text{ep}}^{\text{1D}} - S_0 \rangle/\hbar} \quad (\text{A6})$$

and thus

$$F_{\text{el}}^{\text{1D}} < F_{\text{var}} = F_0 + \langle S - S_0 \rangle_0. \quad (\text{A7})$$

The basic idea is to optimize S_0 such that F_{var} gets to $F_{\text{el}}^{\text{1D}}$ as close as possible. Assuming that S_0 is Gaussian, and

$$S_0/\hbar = \frac{1}{2} \sum_{\vec{q}} \phi(-\vec{q}) G^{-1}(\vec{q}) \phi(\vec{q}) \quad (\text{A8})$$

with

$$G^{-1}(\vec{q}) = \frac{q^2 + D^2}{\pi K}, \quad (\text{A9})$$

F_{var} can be calculated as

$$F_{\text{var}} = - \sum_{\vec{q}>0} \ln G(\vec{q}) + \frac{1}{2\pi K} \sum_{\vec{q}} q^2 G(\vec{q}) - 2g_2\psi_0 \int dx d\tau e^{-2(\phi^2)_0}. \quad (\text{A10})$$

Minimizing F_{var} with respect to $G(\vec{q})$ by doing $\partial F_{\text{var}}/\partial G(\vec{q})=0$ leads to a self-consistent equation for D ,

$$D^2 = 8\pi K g_2 \phi_0 \left[\frac{D}{1 + \sqrt{1 + D^2}} \right]^K. \quad (\text{A11})$$

Assuming that $g_2\psi_0$ is much less than 1 (i.e., the single electron gap is much less than the Fermi energy), we get

$$D = 2(2\pi K g_2 \psi_0)^{1/(2-K)}. \quad (\text{A12})$$

for $K < 2$ and $D=0$ for $K > 2$. Therefore, $K=2$ is a naive estimation of the critical value of K at which the KBT transition happens for the Sine-Gordon model (A1). Plugging Eq. (A12) into formula (A10), we get the approximated $F_{\text{el}}^{\text{1D}}$,

$$F_{\text{el}}^{\text{1D}}[\psi_0]/\hbar = \frac{1}{2\pi K} \int dx d\tau [-(2-K)(2\pi K g_2 \psi_0)^{2/(2-K)}], \quad (\text{A13})$$

where we have thrown out terms which are independent of ψ_0 . Thus, according to Eq. (A4) the effective action for ψ_0 is given by

$$S_{\text{ph}}^{\text{eff}}[\psi_0]/\hbar = \frac{1}{2\pi K} \int dx d\tau [-(2-K)(2\pi K g_2 \psi_0)^{2/(2-K)} + \pi K g_1^2 \psi_0^2]. \quad (\text{A14})$$

Minimizing it with respect to ψ_0 , we get $\psi_0=0$ for $K > 1$ and

$$\psi_0 = g_1^{-1} \left[2(\pi K)^{K/2} \left(\frac{g_2}{g_1} \right) \right]^{1/(1-K)} \quad (\text{A15})$$

for $K < 1$.

APPENDIX B: CALCULATING PHASE FLUCTUATIONS FROM THE FIXED-AMPLITUDE MODELS

We start with the truncated model (26). For convenience, we rewrite it as

$$S[Y]/\hbar = \frac{1}{2} \sum_{\vec{q}} [G_{\phi}^{-1}(\vec{q}) \phi(\vec{q}) \phi(-\vec{q}) + G_{\theta}^{-1}(\vec{q}) \theta(\vec{q}) \theta(-\vec{q})] - 2g_2\psi_0 \int dx d\tau \cos(2\phi - \theta), \quad (\text{B1})$$

where

$$G_{\phi}^{-1}(\vec{q}) \equiv \frac{1}{\pi K} (q_x^2 + q_{\tau}^2), \quad (\text{B2})$$

$$G_{\theta}^{-1}(\vec{q}) \equiv \left[g_1^2 \left(\frac{1}{2n_e} \right)^2 q_x^2 + q_{\tau}^2 \right] \psi_0^2.$$

Then we define two new variables, so that the action in terms of these two variables is decoupled. That is, the action can be expressed as

$$S[Y, \Sigma]/\hbar = \frac{1}{2} \sum_{\vec{q}} G_{\Sigma}^{-1}(\vec{q}) \Sigma(\vec{q}) \Sigma(-\vec{q}) + \frac{1}{2} \sum_{\vec{q}} G_Y^{-1}(\vec{q}) \times Y(\vec{q}) Y(-\vec{q}) - 2g_2\psi_0 \int dx d\tau \cos Y, \quad (\text{B3})$$

where

$$Y(\vec{q}) \equiv 2\phi(\vec{q}) - \theta(\vec{q}), \quad (\text{B4})$$

$$\Sigma(\vec{q}) \equiv \phi(\vec{q}) - \frac{2Y(\vec{q})G_{\theta}^{-1}(\vec{q})}{G_{\phi}^{-1}(\vec{q}) + 4G_{\theta}^{-1}(\vec{q})}, \quad (\text{B5})$$

$$G_Y^{-1}(\vec{q}) \equiv \frac{G_{\phi}^{-1}(\vec{q})G_{\theta}^{-1}(\vec{q})}{G_{\phi}^{-1}(\vec{q}) + 4G_{\theta}^{-1}(\vec{q})}, \quad (\text{B6})$$

$$G_{\Sigma}^{-1}(\vec{q}) \equiv G_{\phi}^{-1}(\vec{q}) + 4G_{\theta}^{-1}(\vec{q}). \quad (\text{B7})$$

Since Y and Σ are decoupled, using Eqs. (B4) and (B5) the fluctuations of θ and ϕ can be calculated as

$$\langle \phi(\vec{q}) \phi(-\vec{q}) \rangle = G_{\Sigma}(\vec{q}) + \frac{4G_{\theta}^{-2}(\vec{q}) \langle Y(\vec{q}) Y(-\vec{q}) \rangle}{[G_{\phi}^{-1}(\vec{q}) + 4G_{\theta}^{-1}(\vec{q})]^2}, \quad (\text{B8})$$

$$\langle \theta(\vec{q}) \theta(-\vec{q}) \rangle = 4G_{\Sigma}(\vec{q}) + \frac{G_{\phi}^{-2}(\vec{q}) \langle Y(\vec{q}) Y(-\vec{q}) \rangle}{[G_{\phi}^{-1}(\vec{q}) + 4G_{\theta}^{-1}(\vec{q})]^2}. \quad (\text{B9})$$

To calculate $\langle Y(\vec{q}) Y(-\vec{q}) \rangle$, we need to know whether the cosine term is relevant or irrelevant. Thus, we evaluate

$$\int dx d\tau \langle \cos Y \rangle_0 = \int dx d\tau e^{-(Y^2)_0/2}, \quad (\text{B10})$$

where $\langle \rangle_0$ is the average with respect to the harmonic part of action (B3). Let us first calculate

$$\begin{aligned} \langle Y^2 \rangle_0 &= \frac{1}{(2\pi)^2} \int dq_x dq_{\tau} G_Y(\vec{q}) \\ &= \frac{1}{(2\pi)^2} \int dq_x dq_{\tau} \left\{ \frac{1}{\psi_0^2 \left[q_{\tau}^2 + g_1^2 \left(\frac{1}{2n_e} \right)^2 q_x^2 \right]} + \frac{4\pi K}{q_x^2 + q_{\tau}^2} \right\} \\ &= \left(\frac{n_e}{\pi g_1 \psi_0^2} + 2K \right) \ln L. \end{aligned} \quad (\text{B11})$$

Plugging it into Eq. (B10) we obtain

$$\int dx d\tau \langle \cos Y \rangle_0 \sim L^{2-K-(n_e/2\pi g_1 \psi_0^2)}, \quad (\text{B12})$$

which implies a critical line in the ψ_0^2-K plane defined by

$$\frac{n_e}{\pi g_1 \psi_0^2} + 2K = 4. \quad (\text{B13})$$

This critical line is illustrated in Fig. 1. The cosine term in action (B3) is relevant below the critical line and irrelevant above it. In the two limiting cases function (B13) predicts that $\psi_0^2 \rightarrow \infty$ for $K=2$ and $\psi_0^2 \sim g_1^{-1/2}$ for $K=0$. For $K < 1$, it predicts

$$\psi_0^c \sim g_1^{-1/2}. \quad (\text{B14})$$

For $\psi_0 < \psi_0^c$, the cosine term is irrelevant, and we get $\langle Y(\vec{q})Y(-\vec{q}) \rangle = G_Y(\vec{q})$, which combined with Eqs. (B8) and (B9) leads to

$$\langle \phi(\vec{q})\phi(-\vec{q}) \rangle = G_\phi(\vec{q}), \quad (\text{B15})$$

$$\langle \theta(\vec{q})\theta(-\vec{q}) \rangle = G_\theta(\vec{q}). \quad (\text{B16})$$

This implies that θ and ϕ are effectively decoupled. For $\psi_0 > \psi_0^c$, $\langle Y(\vec{q})Y(-\vec{q}) \rangle$ is massive, and we obtain

$$\langle \phi(\vec{q})\phi(-\vec{q}) \rangle = G_\Sigma(\vec{q}), \quad (\text{B17})$$

$$\langle \theta(\vec{q})\theta(-\vec{q}) \rangle = 4G_\Sigma(\vec{q}), \quad (\text{B18})$$

which implies that the fluctuations of θ and ϕ are bound together.

Now we discuss model (79). We follow the same routine as the above. Defining Y and Σ using Eqs. (B4) and (B5), we get a decoupled action:

$$\begin{aligned} S[Y, \Sigma]/\hbar &= \frac{1}{2} \sum_{\vec{q}} G_\Sigma^{-1}(\vec{q}) \Sigma(\vec{q}) \Sigma(-\vec{q}) \\ &+ \frac{1}{2} \sum_{\vec{q}} G_Y^{-1}(\vec{q}) Y(\vec{q}) Y(-\vec{q}) - \frac{2g_2\psi_0}{\pi^2} \\ &\times \int dx d^2r_\perp d\tau \cos Y, \end{aligned} \quad (\text{B19})$$

where $G_Y^{-1}(\vec{q})$ and $G_\Sigma^{-1}(\vec{q})$ are defined in Eqs. (B6) and (B7), respectively. $G_\phi^{-1}(\vec{q})$ and $G_\theta^{-1}(\vec{q})$ are now defined as

$$G_\phi^{-1}(\vec{q}) \equiv \frac{1}{\pi^3 K} (q_x^2 + q_\tau^2), \quad (\text{B20})$$

$$G_\theta^{-1}(\vec{q}) \equiv \left(\frac{\psi_0}{\pi} \right)^2 \left[g_1^2 \left(\frac{1}{2n_e} \right)^2 q_x^2 + q_\tau^2 + C_\perp q_\perp^2 \right]. \quad (\text{B21})$$

To check whether the cosine term is relevant or not, we evaluate the average of the cosine term for a single chain with respect to the harmonic part of the action. After we calculate

$$\begin{aligned} \langle Y^2 \rangle_0 &= \frac{1}{(2\pi)^4} \int dq_x d^2q_\perp dq_\tau G_Y(\vec{q}) \\ &= \frac{1}{(2\pi)^4} \int dq_x d^2q_\perp dq_\tau \left\{ \frac{4\pi^3 K}{q_x^2 + q_\tau^2} \right. \\ &\quad \left. + \frac{\pi^2}{\psi_0^2 \left[q_\tau^2 + g_1^2 \left(\frac{1}{2n_e} \right)^2 q_x^2 + C_\perp q_\perp^2 \right]} \right\} \sim 2K \ln L, \end{aligned} \quad (\text{B22})$$

we obtain

$$\int dx d\tau \langle \cos Y \rangle_0 \sim L^{2-K}. \quad (\text{B23})$$

This implies that for $K < 2$, the cosine term in action (79) is always relevant no matter the value of ψ_0 . Therefore, for $K < 1$ and arbitrary ψ_0 , action (79) predicts that the fluctuations of ϕ and θ are bound together and are given by Eqs. (B17) and (B18), respectively.

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