Two-cutoff renormalization and quantum versus classical aspects for the one-dimensional electron-phonon system

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We study the $T=0$ K properties of the electron-phonon system with Coulomb interaction using a two-cutoff renormalization procedure. We find that there exist two regimes. The "classical" regime is characterized by a classical amplitude order parameter and exists when the mean-field gap (pseudogap) Δ is larger than the phonon frequencies ω_D. The order parameter for spinless fermions is increased in amplitude by a repulsive nearest-neighbor electron interaction. A repulsive Hubbard interaction in an incommensurate spin-$\frac{1}{2}$ fermion band will increase it at small ω_D and decrease it at finite ω_D/E_F. For half-filled spin-$\frac{1}{2}$ fermion band, however, the molecular crystal (MC) and Su-Schrieffer-Heeger (SSH) models behave in opposite ways, the former having its order parameter decrease with increasing Coulomb interaction. We predict a maximum in the SSH amplitude order parameter as a function of the Hubbard interaction when Δ is equal to the Hubbard gap. This agrees quite well with the result of the simulation of Hirsch. For $\Delta<\omega_D$, we predict a change to a quantum behavior. In this regime long-range molecular order can only exist for a half-filled spin-$\frac{1}{2}$ fermion band whenever the effective electronic interaction is attractive and the umklapp processes are relevant. This quantum order is weakened and can be destroyed by a repulsive Coulomb interaction or a negative forward scattering. We predict the quantum to classical-amplitude crossover to occur when $\Delta\approx\omega_D$. In the case of the MC model with spinless noninteracting fermions, it corresponds to the disappearance of long-range order at values in agreement with the calculation of Hirsch and Fradkin. We analyze the implications of these two regimes on the properties of quasi-one-dimensional solids, more specifically on the effect of interchain potential or hopping ($t_\perp$) couplings. The existence of classical or quantum gaps favors interchain particle-pair tunneling whereas the single-particle interchain hopping is quite pertinent whenever $t_\perp$ is larger than these gaps.

I. INTRODUCTION

One-dimensional (1D) systems are well known for their opposition to long-range order at finite temperature.[1] This is so because of fluctuations, both thermal and quantum, which break up long-range correlations. The interacting 1D electron gas is a good example.[2,3] It is intrinsically a quantum system in which Cooper and zero-sound channels are coupled.[4] The ladder diagrams, which are pertinent to a long-range order parameter, cannot be singled out. One can introduce variants, however, such that this system can develop an amplitude order parameter at $T=0$ K and order in commensurate cases. In the Efetov and Larkin[5] limit of a large number of degenerate conduction bands, the Cooper channel is favored, and the system develops a static superconducting amplitude order parameter. A retarded interaction (electrons interacting with a low-frequency phonon field) can in turn stabilize the zero-sound channel and lead to a charge-density amplitude order parameter.[6,7] These limiting cases possess an amplitude order parameter and can be dealt with by the standard approach.[8,9] What is not so explicit, however, are the intermediate cases.[7] The electron gas can clearly be made to undergo a transition from a quantum state to one with a classical amplitude order parameter by playing on the number of conduction bands or the amount of retardation. These are examples of a quantum-classical-amplitude crossover induced by varying microscopic parameters. A quantum-classical [three-dimensional (3D)] crossover can also occur in quasi-1D systems[10] and may have considerable impact on the understanding of these interesting solids. As a matter of fact, all of quasi-1D physics is strongly tied into the 1D intrachain behavior.[11] It is thus not only interesting but also capital to fully understand the strictly 1D properties.

There has been a lot of interest recently in quantum effects in 1D electron-phonon systems both with and without Coulomb interaction.[7,12–15] Some $T=0$ K simulations for a half-filled band were used to explore the stability of the long-range Peierls order with respect to the phonon frequency and the electron-phonon[7] and Coulomb interaction strengths.[14,15] It is the purpose of this paper to study the 1D electron-phonon system at $T=0$ K, with a two-cutoff scaling model.[16,17] Although one cannot ex-

pect more than a qualitative representation from such a model, and even though it is limited to the weak coupling limit, it will explain the results of Hirsch and Fradkin,[7] Hirsch,[14] and of Mazumdar and Dixit.[15] Moreover, new light will be shed on the role of quantum fluctuations. The model also has the advantage of being easily applied to incommensurate cases.

In Sec. II we relate the model Hamiltonians we shall be studying. In Sec. III we discuss our two-cutoff renormalization procedure and the significance of the quantum-classical-amplitude crossover. In Sec. IV we investigate the pure Peierls case, while we add the Coulomb interaction in Sec. V. In Sec. VI we end with a discussion in which we try to correlate our findings to quasi-1D solids.

II. HAMILTONIANS

Hirsch and Fradkin[7] have explored the electron-phonon problem using two model Hamiltonians defined on a lattice. The first one is the molecular-crystal (MC) Hamiltonian[18]

$$H_{0\mathrm{MC}}=\sum_i\left[\frac{p_i^2}{2M}+\tfrac{1}{2}\kappa q_i^2\right]-t\sum_{i,\alpha}(C_{i\alpha}^\dagger C_{i+1,\alpha}+\mathrm{H.c.})+\lambda\sum_i q_i n_i\ . \tag{1}$$

The first term describes molecules with intramolecular vibrations characterized by a mass M, a harmonic spring constant κ, momentum p_i, and amplitude q_i at site i. The second term describes electrons which can hop from any molecule to a near-neighbor one, through the molecule transfer matrix t. $C_{i\alpha}$ ($C_{i\alpha}^\dagger$) annihilates (creates) an electron of spin α on the ith molecule. The last term describes the electron-phonon coupling on any molecule. It has an interaction strength λ coupling the amplitude q_i and the electron occupancy n_i on the molecule.

The second model was that of Su, Schrieffer, and Heeger (SSH):[19]

$$H_{0\mathrm{SSH}}=\sum_i\left[\frac{p_i^2}{2M}+\tfrac{1}{2}\kappa(q_{i+1}-q_i)^2\right]-\sum_{i,\alpha}[(t-\lambda(q_{i+1}-q_i)](C_{i\alpha}^\dagger C_{i+1,\alpha}+\mathrm{H.c.})\ . \tag{2}$$

The first term describes the acoustic modes of the molecules. These have mass M, momentum p_i, and displacement amplitude q_i. Each one is coupled through a spring constant κ to the nearest neighbors. The second term describes the electron hopping motion. Here, the transfer integral is modulated by the molecular motion. It has an average value t on which the electron-phonon coupling is superimposed.

The Coulomb repulsion can be added on to both models. The extended Hubbard interaction

$$H_H=U\sum_i n_{i+}n_{i-}+V\sum_i n_i n_{i+1} \tag{3}$$

has been used. It describes intramolecular and nearest-neighbor interactions between electrons. Our renormalization procedure requires that one use the continuous limit of these Hamiltonians, the philosophy being that only those electrons lying near the Fermi surface play an important role.[2,3,20] The MC Hamiltonian becomes

$$H_{0\mathrm{MC}}=\sum_q\omega_0(d_q^\dagger d_q+\tfrac{1}{2})+\sum_{k,\alpha}v_F(\,|k|-k_F)C_{k\alpha}^\dagger C_{k\alpha}+gN^{-1/2}\sum_q(d_q+d_{-q}^\dagger)\rho_q\ . \tag{4}$$

The first term describes optical phonons of frequency $\omega_0=(\kappa/M)^{1/2}$ ($\hbar=1$), where d_q ($d_q^\dagger$) annihilates (creates) a phonon of wave number q. The second term is the hopping energy of the electrons linearized around the Fermi wave number, k_F. $C_{k\alpha}$ ($C_{k\alpha}^\dagger$) annihilates (creates) an electron of wave number k and spin α. v_F is the Fermi velocity. There is an energy cutoff $v_F|k|<v_Fk_F=E_F$ at the Fermi energy E_F. The last term corresponds to the electron-phonon coupling with $g=\lambda/(2M\omega_0)^{1/2}$; $\rho_q=\sum_{k,\alpha}C_{k+q,\alpha}^\dagger C_{k\alpha}$ is the electron density operator, and N is the number of molecules in the chain.

The SSH Hamiltonian is written as

$$H_{0\mathrm{SSH}}=\sum_q\omega_q(d_q^\dagger d_q+\tfrac{1}{2})+\sum_{k,\alpha}v_F(\,|k|-k_F)C_{k\alpha}^\dagger C_{k\alpha}+N^{-1/2}\sum_{k,q,\alpha}g(kq)(d_q+d_{-q}^\dagger)C_{k+q,\alpha}^\dagger C_{k\alpha}\ , \tag{5}$$

where the acoustic phonon frequency is $\omega_q=2(\kappa/M)^{1/2}\sin(qa/2)$, the electron-phonon interaction is

$$g(kq)=i4\lambda\sin(qa/2)\cos(ka+qa/2)/(2M\omega_q)^{1/2}\ ,$$

and a is the intermolecular distance.

The Coulomb term, in turn, is to be rewritten in the "g-ology" formulation,[2,3,20]

$$H_H=N^{-1}\sum_{k_1k_2p}\sum_{\alpha,\beta}g_{1H}a_{k_1\alpha}^\dagger b_{k_2\beta}^\dagger a_{k_2+2k_F+p,\beta}b_{k_1-2k_F-p,\alpha}+N^{-1}\sum_{k_1k_2p}\sum_{\alpha,\beta}g_{2H}a_{k_1\alpha}^\dagger b_{k_2\beta}^\dagger b_{k_2+p,\beta}a_{k_1-p,\alpha}+\tfrac{1}{2}N^{-1}\sum_{k_1k_2p}\sum_{\alpha,\beta}g_{3H}(a_{k_1\alpha}^\dagger a_{k_2\beta}^\dagger b_{k_2-2k_F+p,\beta}b_{k_1+2k_F-p-G,\alpha}+\mathrm{H.c.})\ , \tag{6}$$

where $g_{1H}=U-2V$, $g_{2H}=U+2V$, and $g_{3H}=g_{1H}$ are the backward, forward, and umklapp scattering elements, respectively. Note that umklapp processes are important in the half-filled band case and can be present in other commensurate cases. Here, $a_{k\alpha}$ ($b_{k\alpha}$) annihilates an electron with $k>0$ ($k<0$). This last equation assumes that the Fourier transform of the interaction is a slowly varying function of momentum transfer around $k=0$ or $2k_F$. Note that the cutoff in Eq. (6) is also at E_F.

As mentioned previously, the important physics in g-ology occurs at small electron momentum around k_F. The dominant singular diagrams are logarithmic in

$E_F/\max(T,\omega,v_Fq)$ where T, ω, and q are the temperature ($k_B=1$), the frequency, or the momentum transfer, respectively.[20] The renormalization-group approach of Solyom[2,20] selects these logarithmic terms and generates the key, dominant behavior at low (T,ω,v_Fq). It is a very powerful tool, albeit of a qualitative nature, and is strictly technically defendable only for $g_H/(\pi v_F')<1$, where $v_F'=v_F/a$.

III. TWO-CUTOFF RENORMALIZATION

In a $T=0$ K perturbation expansion of the electron-phonon interaction, this interaction appears as a retarded electron-electron interaction $-2g^2(kq)\omega_q/(-\omega^2+\omega_q^2)$. It is attractive for $\omega<\omega_q$. The idea behind the two-cutoff approach[17] is the assumption that the phonon-mediated electron-electron interaction is instantaneous (the $\omega\ll\omega_q$ limit) and equal to $-2g^2(kq)/\omega_q$ for ω less than a typical Debye frequency $\omega_D\sim(\kappa/M)^{1/2}$, and negligible (the $\omega\gg\omega_q$ limit) when $\omega>\omega_D$. It is surely an interesting simplifying approximation. It places all of the retardation effects into the cutoff ω_D. The effective phonon-mediated interaction can be described in terms of the g-ology terminology of backward $[g_{1\,\mathrm{ph}}=-2g^2(k_F,2k_F)/\omega_{2k_F}]$, forward $[g_{2\,\mathrm{ph}}=-2g^2(k_F,0)/\omega_0]$, and umklapp $[g_{3\,\mathrm{ph}}=g_{1\,\mathrm{ph}}]$ scattering (half-filled band case only). In the MC case, one has

$$g_{1\,\mathrm{ph}}=g_{2\,\mathrm{ph}}=g_{3\,\mathrm{ph}}=-\lambda^2/\kappa\ , \tag{7a}$$

while the SSH case gives, for $k_F\sim\pi/2a$,

$$g_{1\,\mathrm{ph}}=g_{3\,\mathrm{ph}}=-4\lambda^2/\kappa\ , \tag{7b}$$

where $g_{2\,\mathrm{ph}}$ is approximately small and negative. The SSH model has an effective interaction which goes to zero at zero momentum transfer. It is not smoothly varying around this value and it is only approximative to describe it within the g-ology framework. The interacting electron-phonon problem is thus reduced to two instantaneous interactions g_{iH} $(i=1,2,3)$ with cutoff E_F and $g_{i\,\mathrm{ph}}$ with cutoff ω_D. If $\omega_D>E_F$, there is but a single effective cutoff E_F which is the natural one for the electron. Our results will be shown to be defective in this case, however.

The idea of the renormalization procedure is to eliminate the degrees of freedom at the high energies starting from E_F down to a new cutoff ω_c. This renormalizes the interactions and the response functions[2,3,20] through the logarithmically dominant contribution. If ω_c is greater than ω_D, the g_{iH} renormalize as in the Solyom multiplicative renormalization theory[2,3,16,17,20] and become $g_{iH}(\omega_c)$. As far as the $g_{i\,\mathrm{ph}}$ are concerned, they are affected selectively.[17] On the one hand, $g_{2\,\mathrm{ph}}$ is unaffected because of its lower-frequency cutoff $\omega_D<\omega_c$. $g_{1\,\mathrm{ph}}$ and $g_{3\,\mathrm{ph}}$, on the other hand, are renormalized through the bubble insertions of Fig. 1, which are always governed by the higher-energy cutoff. One can write the Lie equations corresponding to the terms in Fig. 1:

$$\frac{\partial g'_{1\,\mathrm{ph}}}{\partial X}=-X^{-1}[(g'_{1\,\mathrm{ph}})^2+(g'_{3\,\mathrm{ph}})^2]\bar{N}+\cdots\ , \tag{8a}$$

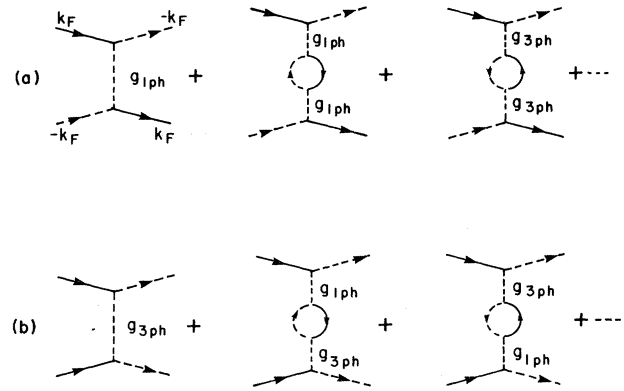

FIG. 1. Bubble insertions which renormalize the phonon-mediated backward (a) $g_{1\,\mathrm{ph}}$ and (b) umklapp $g_{3\,\mathrm{ph}}$ scattering for a cutoff ω_c greater than the Debye frequency.

$$\frac{\partial g'_{3\,\mathrm{ph}}}{\partial X}=-X^{-1}2g'_{1\,\mathrm{ph}}g'_{3\,\mathrm{ph}}\bar{N}+\cdots\ , \tag{8b}$$

where $X=\omega/E_F$, $\bar{N}=\partial N/\partial\ln(\omega/E_F)$, and N is the $2k_F$ charge response of the electron gas, which we define as positive (a dressed bubble substituted for the bare one in Fig. 1). The solution to Eq. (8) at $\omega=\omega_c$ which satisfies the boundary condition $g'_{i\,\mathrm{ph}}(\omega=E_F)=g_{i\,\mathrm{ph}}$ is

$$g'_{1\,\mathrm{ph}}(\omega_c)+g'_{3\,\mathrm{ph}}(\omega_c)=\frac{(g_{1\,\mathrm{ph}}+g_{3\,\mathrm{ph}})}{[1+(g_{1\,\mathrm{ph}}+g_{3\,\mathrm{ph}})N(\omega_c)]}\ , \tag{9a}$$

$$g'_{1\,\mathrm{ph}}(\omega_c)-g'_{3\,\mathrm{ph}}(\omega_c)=\frac{(g_{1\,\mathrm{ph}}-g_{3\,\mathrm{ph}})}{[1+(g_{1\,\mathrm{ph}}-g_{3\,\mathrm{ph}})N(\omega_c)]}\ . \tag{9b}$$

As we observe the half-filled band $(g_{3\,\mathrm{ph}}=g_{1\,\mathrm{ph}})$ and incommensurate $(g_{3\,\mathrm{ph}}=0)$ cases, this reduces to

$$g'_{(\frac{1}{3})\mathrm{ph}}(\omega_c)=g_{(\frac{1}{3})\mathrm{ph}}/[1+(g_{1\,\mathrm{ph}}+g_{3\,\mathrm{ph}})N(\omega_c)]\ . \tag{10}$$

Since $g_{i\,\mathrm{ph}}<0$ and $N>0$, it is obvious that $g'_{i\,\mathrm{ph}}$ increases as the cutoff ω_c is reduced from E_F. It may even diverge if $1+(g_{1\,\mathrm{ph}}+g_{3\,\mathrm{ph}})N(\omega_c)=0$ before ω_c reaches ω_D. This needs to be interpreted. What it means is that the frequencies which have been integrated out between ω_c and E_F renormalize $g_{1\,\mathrm{ph}}$ (and $g_{3\,\mathrm{ph}}$) in such a way that its strength increases. As a consequence, the $2k_F$ phonons, whose frequency is related to $g_{1\,\mathrm{ph}}^{-1}$, become softer and the electrons start to develop a pseudogap Δ. When $g_{1\,\mathrm{ph}}$ becomes very large, the $2k_F$ phonon frequency goes to zero and the pseudogap is fully developed $(\Delta\sim\omega_c)$. A divergence in $g_{1\,\mathrm{ph}}$ points to the occurrence of a mean-field transition to a periodically distorted lattice (a real gap). Our renormalization procedure is, of course, no longer valid in such a situation (the free-electron gas is no longer appropriate as an unpertubed Hamiltonian on which to build the renormalization-group approach). But it does indicate, however, that the system has developed strong lattice correlations and a meaningful *amplitude* order parameter for the $2k_F$ distortion. All the frequencies below this critical cutoff are to be considered as purely static as far as this pseudogap is concerned, although they are surely relevant for the phase fluctuations in the incommensurate case.[12,13] This was the reasoning when it was pro-

posed to replace the cutoff $\max(\omega,T,v_Fq)$ of g-ology (see the end of Sec. II) by $\max(\omega,T,v_Fq,\Delta)$ in the phonon self-energy renormalization and pseudogap calculation of Ref. 21, whenever $\Delta>\omega_D$. All energies less than Δ are irrelevant to the electronic responses. Thermal fluctuations (kinks) must of course be considered in a proper treatment of this static problem. The chain can then be treated by the generalized Ginzburg-Landau method.[8,9] Its quantum version has also been used for the quantum phase fluctuations in the incommensurate cases.[12]

If $g'_{1\,\mathrm{ph}}(\omega_c)$ does not diverge before ω_c reaches ω_D, the chain essentially remains quantum as the amplitude order parameter has no chance to develop. At $\omega_c=\omega_D$, one has the instantaneous interaction g_{it} of Fig. 2 with a single cutoff at ω_D, that is,

$$g_{1t}=\tilde{g}_{1\,\mathrm{ph}}+\tilde{g}_{1\,\mathrm{H}}-2(\tilde{g}_{1\,\mathrm{ph}}\tilde{g}_{1H}+\tilde{g}_{3\,\mathrm{ph}}\tilde{g}_{3H})N(\omega_D)\ , \quad (11a)$$

$$g_{2t}=\tilde{g}_{2\,\mathrm{ph}}+\tilde{g}_{2H}\ , \quad (11b)$$

$$g_{3t}=\tilde{g}_{3\,\mathrm{ph}}+\tilde{g}_{3H}-2(\tilde{g}_{1\,\mathrm{ph}}\tilde{g}_{3H}+\tilde{g}_{3\,\mathrm{ph}}\tilde{g}_{1H})N(\omega_D)\ , \quad (11c)$$

where $\tilde{g}_{i\,\mathrm{ph}}=g_{i\,\mathrm{ph}}(\omega_D)$ and $\tilde{g}_{iH}=g'_{iH}(\omega_D)$. Note that $\tilde{g}_{2\,\mathrm{ph}}=g_{2\,\mathrm{ph}}$. The system has thus been renormalized to a single-cutoff one and can be dealt with as in conventional g-ology.[2,3,20] Note that when $\omega_D>E_F$, the problem becomes that of electrons interacting through $g_{it}=g_{iH}+g_{i\,\mathrm{ph}}$ with the cutoff E_F.

As mentioned in the Introduction, one can foresee the possibility of a quantum-classical-amplitude crossover. It will occur as the mean-field gap Δ or ordering temperature $T_{\mathrm{MF}}\sim\Delta$ determined from

$$1+(g_{1\,\mathrm{ph}}+g_{3\,\mathrm{ph}})N(\Delta)=0 \quad (12)$$

becomes of the order of ω_D. Reducing $|g_{i\,\mathrm{ph}}|$ or N will lower $\Delta(T_{\mathrm{MF}})$ and permit a sweep through the crossover, from a classical amplitude to a quantum regime.

We shall now examine the consequences of our procedure on the various limits of the electron-phonon problem at $T=0$ K (note that our analysis is also valid for temperature by identifying ω_c to T).

IV. PURE PEIERLS

We shall first examine the limit of zero Coulomb interaction for spinless and spin-$\frac{1}{2}$ fermions. In this case, one has for $\omega/E_F\ll 1$

$$N(\omega)=D(0)\ln(E_F/\omega)\ , \quad (13)$$

where $D(0)$ is the density of states at the Fermi level. It is equal to $(2\pi v'_F)^{-1}$ for spinless fermion and $(\pi v'_F)^{-1}$ for spin-$\frac{1}{2}$ fermions.

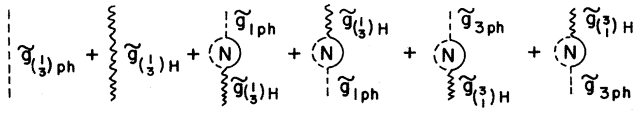

FIG. 2. Diagrams contributing to the renormalized backward g_{1t} and umklapp g_{3t} scattering when the problem has been reduced to a single cutoff. The last four terms are the cross ones between the phonon and Coulomb contributions and involve the $2k_F$ charge response function N at the cutoff.

A. Spinless fermions

The chain develops an amplitude order parameter if Δ [see Eqs. (7), (12), and (13)] is larger than ω_D, that is, for

$$\Delta=E_F\exp(-\mu 2\pi v'_F\kappa/\lambda^2)>\omega_D\ , \quad (14)$$

where $\mu=1$ for an incommensurate MC, $\frac{1}{2}$ for a half-filled band MC, $\frac{1}{4}$ for an incommensurate SSH chain, and $\frac{1}{8}$ for a half-filled band SSH chain. Note this gap is BCS-like. One can then expect a quantum-classical-amplitude crossover when $\Delta=\omega_D$ at a critical value λ_c. In the quantum regime, the problem is reduced to [see Eqs. (10) and (11)]

$$g_{1t}-g_{3t}=g_{1\,\mathrm{ph}}-g_{3\,\mathrm{ph}}\le g_{2t}=g_{2\,\mathrm{ph}}\ .$$

Since this is the spinless-fermion case, g_{3t} is irrelevant (it is cancelled by its own exchange term) and g_{1t} can be absorbed into g_{2t} by the transformation $g_{1t}\to 0$ and $g_{2t}\to g_{2t}-g_{1t}>0$ (the exchange contribution of the backward scattering is equivalent to the direct contribution of the forward scattering and vice versa).[20] This transformation removes a common Hubbard interaction which has no effect on spinless fermions. The problem is thus reduced to that of electrons with positive forward scattering only. The solution of the Luttinger problem is known.[22] The system is indeed highly quantum. It has no fermion quasiparticles, but it does have a power-law singularity for the charge-density response functions. There is no long-range order. The phase diagram for spinless fermions is shown in Fig. 3 and is qualitatively similar to the one obtained by Hirsch and Fradkin[7] for this same problem. Note that for the MC model and with $E_F\sim 2t\sim v_Fk_F$ and $k_F=\pi/2a$, we predict the crossover to occur at $\Delta\sim\omega_D$ that is $t/\omega_D\sim\frac{1}{2}\exp(4t\kappa/\lambda_c^2)$ or $(\kappa t)^{1/2}/\lambda_c\sim 0.4$ if $t/\omega_D\sim 1$. This is indeed quite close to the values of Hirsch and Fradkin (in their Fig. 3).[7] The $\omega_D\to\infty$ limit is correctly described for the molecular crystal, and shows no long-range order. In the same limit for the SSH

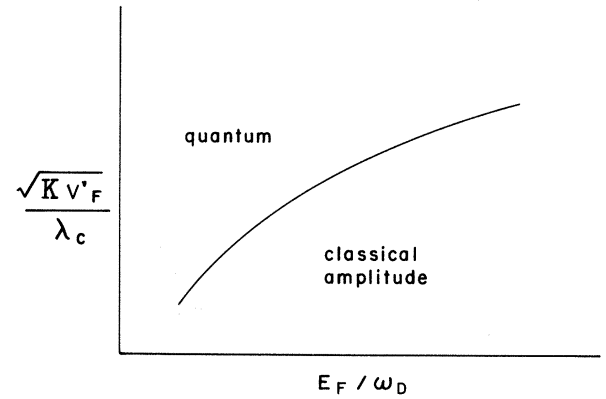

FIG. 3. $T=0$ K phase diagram for the Peierls chain. The classical-amplitude region has a well-defined amplitude order parameter for the $2k_F$ lattice deformation. The quantum region shows a long-range order of a quantum nature (no amplitude parameter) for a half-filled spin-$\frac{1}{2}$ fermion band but no order for the incommensurate spin-$\frac{1}{2}$—fermion or the spinless-fermion cases.

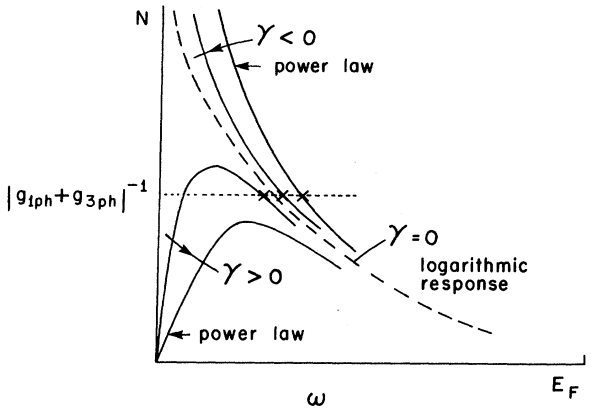

FIG. 4. Qualitative behavior of the charge response function N for spinless fermions as a function of frequency ω and for various values of the power-law exponent γ. The crosses indicate the mean-field solution [Eq. (12)] for $\omega=\Delta\sim T_{\mathrm{MF}}$.

model, however, we predict no long-range order whereas the solution of Hirsch and Fradkin predicts such order when λ is larger than a critical value. The reason is that the dispersion (nonlocality) in the umklapp processes, which we have neglected in our g-ology approach, is quite relevant. As shown by den Nijs[22] it leads to an ordered ground state past a critical coupling strength.

B. Spin-$\frac{1}{2}$ fermions

The quantum-classical-amplitude crossover is qualitatively similar to the one for spinless fermions except for the change in the density of electron states at the Fermi level. One should have $\pi v_F'$ instead of $2\pi v_F'$ in Eq. (14). The quantum regime is different, however.

In the incommensurate case, $g_{3t}=0$ and $g_{1t}<g_{2t}<0$. There is a gap in the spin excitations and a power-law divergence for the charge density and singlet superconductivity (SS) response functions,[3,20] but there is no long-range order.

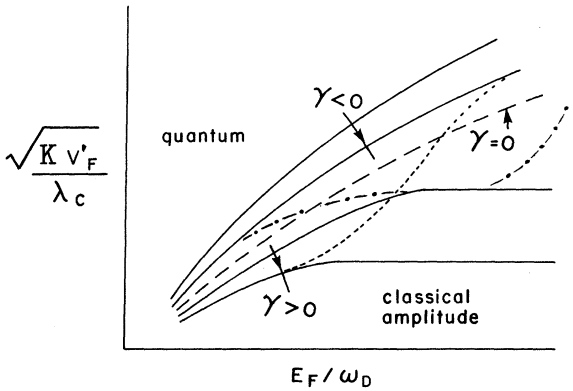

FIG. 5. $T=0$ K phase diagram for the Peierls chain with Coulomb interaction and with spinless fermions. The classical-amplitude region has a non-BCS-like amplitude order parameter for the $2k_F$ lattice distortion. The quantum region has no long-range order. The dotted and dashed-dotted lines refer to the incommensurate spin-$\frac{1}{2}$ fermion cases which show a change in charge response as a function of ω_D.

In the half-filled band case, the umklapp processes are quite relevant. One has $g_{3t}=g_{1t}<g_{2t}<0$, which implies $g_{1t}-2g_{2t}<|g_{3t}|$. There is a gap[3,20] in both charge and spin excitations and thus long-range order. It is of a quantum nature and cannot be associated with an amplitude order parameter in the Landau sense. Thus there is always long-range order in a half-filled spin-$\frac{1}{2}$ fermion band which confirms the results of Hirsch and Fradkin[7] (again the $\omega_D>E_F$ situation should be interpreted cautiously within our scheme since, contrary to what we predict, the $\omega_D\to\infty$ limit is different for the MC and SSH models[7]). However, this long-range order is of a different nature in the classical and quantum cases. The above results are qualitatively shown in Fig. 3.

V. PEIERLS WITH COULOMB INTERACTION

A. Spinless fermions

The Coulomb interaction for the extended Hubbard case and for spinless fermions can be recast as $g_{1H}=g_{3H}=0$ and $g_{2H}=4V$ (see the arguments in Sec. IV A, the Hubbard U interaction has no effect on spinless fermions). The charge-density response of the electron gas for $\omega>\omega_D$ and $(\omega/E_F)\ll 1$ has a power-law behavior[3]

$$N(\omega)=A(\omega/E_F)^{\gamma}\ , \tag{15}$$

where

$$\gamma=2[1-2V/\pi v_F')^{1/2}/(1+2V/\pi v_F')^{1/2}-1]\ , \tag{16}$$

and A is some slowly varying function of ω. Note that $\gamma<0$ if $V>0$ and $\gamma>0$ if $V<0$. This behavior is only valid at small frequencies, and it should join smoothly with the perturbation theory results for the electron-gas response (near logarithm) as $\omega\to E_F$. Perturbation theory predicts an enhancement of $N(\omega)$ for $V>0$ and a reduction for $V<0$ ($\gamma\to -4V/\pi v_F'$) (see Ref. 20 setting $g_{1H}=g_{3H}=0$). The general behavior of $N(\omega)$ is qualitatively shown in Fig. 4.

The chain develops an amplitude order parameter whenever $\Delta>\omega_D$. It is interesting to note that for a small electron-phonon interaction ($g_{i\,\mathrm{ph}}\to 0$) and thus a small mean-field gap Δ, the power-law behavior of $N(\omega)$ leads to the condition that for $V>0$ and thus $\gamma<0$,

$$\Delta=E_F(A^{-1}\mu\kappa/\lambda^2)^{1/\gamma}>\omega_D\ , \tag{17}$$

which is obviously a non-BCS-like relation due to the Coulomb interaction. Generally speaking, the solution to Eq. (12) must be done numerically or graphically, as is shown in Fig. 4. The ensuing quantum-classical-amplitude crossover $\Delta=\omega_D$ is shown in Fig. 5. The interaction V, when positive, strengthens the charge correlations and expands the classical region, the more so the smaller ω_D is and the larger V is [see Eqs. (16) and (17) when ω_D is small; when ω_D is large, $N(\omega)$ is nearly logarithmic]. Obviously, a nearest-neighbor repulsion favors the formation of a charge-density wave (CDW). When V is negative, on the contrary, it weakens the classical regime. The maximum in $N(\omega)$ at a given V results in plateaus at fixed λ_c for small ω_D corresponding to

$N(\omega)_{\max}=(g_{1\,\mathrm{ph}}+g_{3\,\mathrm{ph}})^{-1}$.

In the quantum regime, one recovers the Luttinger model with an effective forward scattering $g_{2_{\mathrm{eff}}}=g_{2t}-g_{1t}$ [see Eq. (11)] which has no long-range order. Depending on the sign of $g_{2_{\mathrm{eff}}}$, the chain can show a power-law divergence of the CDW response function when $g_{2_{\mathrm{eff}}}>0$ or of the superconductivity response function when $g_{2_{\mathrm{eff}}}<0$ (for sufficiently negative V).[3] These effects of the Coulomb interaction on a spinless fermion system are predictions in as much as no simulation has yet been performed.

B. Spin-$\frac{1}{2}$ fermion

1. Incommensurate case

The charge-density response function for the incommensurate cases has a power-law dependence, valid for $(\omega/E_F)\ll 1$, of the form:[3]

$$N(\omega)=\begin{cases}(\omega/E_F)^{\theta_c+\theta_s-2}, & \omega\gg\Delta_1\\ (\omega/E_F)^{\theta_c-2}, & \omega\ll\Delta_1 \text{ and } g_{1H}<0\\ (\omega/E_F)^{\theta_c-1}, & \omega\ll\Delta_1 \text{ and } g_{1H}>0\end{cases} \tag{18a}$$

where

$$\theta_c=\left[\frac{2-(2\bar{g}_{2H}-\bar{g}_{1H})}{2+(2\bar{g}_{2H}-\bar{g}_{1H})}\right]^{1/2}, \tag{18b}$$

$$\theta_s=\left[\frac{2+\bar{g}_{1H}}{2-\bar{g}_{1H}}\right]^{1/2}, \tag{18c}$$

$$\Delta_1\sim E_F\,|\,\bar{g}_{1H}\,|^{\,1/2(1-\theta_s)}, \tag{18d}$$

and

$$\bar{g}_{iH}=g_{iH}/\pi v_F' .$$

If $g_{1H}>0$ (repulsive), $\theta_s>1$ and $\Delta_1\simeq E_F g_{1H}^{(-1/2)|1-\theta_s|^{-1}}\to E_F\bar{g}_{1H}^{-1/\bar{g}_{1H}}\gg E_F$ in the limit $\bar{g}_{1H}\ll 1$. Δ_1 is thus an irrelevant parameter and $N(\omega)\simeq(\omega/E_F)^{\theta_c-1}$ for all the interesting cases ($\bar{g}_{1H}<1$). The situation greatly resembles the spinless-fermion case where θ_c-1 is substituted for γ. θ_c-1 is negative and reinforces the CDW correlations when $2g_{2H}-g_{1H}=g_{1H}+8V=U+6V>0$. A sufficiently negative value of V ($<-U/6$) would then weaken the CDW correlations. These conclusions, however, apply inasmuch as $\omega/E_F\ll 1$. First-order perturbation theory predicts[20] that $N(\omega)$ is reduced by a positive $2g_{1H}-g_{2H}=U-6V$ for small values of $\ln(E_F/\omega)$. Moreover, the simulations of Hirsch and Scalapino[23] confirm that $N(\omega)$ is reduced by a repulsive Hubbard interaction for values of ω/E_F which are not too small. Whenever $\theta_c-1<0$ (for $V>-U/6$) and $U-6V\gtrsim 0$, we expect the result shown by the dotted line in Fig. 5, which is an enhancement of the classical-amplitude region (smaller λ_c) at large E_F/ω_D and a reduction at smaller values. If $U-6V\lesssim 0$, then the $\gamma<0$ curves of Fig. 5 should describe this situation. If $\theta_c-1>0$ (for $V<-U/6$) the solid curves corresponding to $\gamma>0$ in Fig. 5 should prevail. There is no long-range in the quantum regime. The ground state is, however, very different from the spinless-fermion case with the possibility of divergence in all response functions: CDW and SS if $g_{1t}<0$, CDW and spin-density wave (SDW) if $g_{1t}>0$ and $2g_{2t}-g_{1t}>0$, and SS and triplet superconductivity if $g_{1t}>0$ and $2g_{2t}-g_{1t}<0$.

If $g_{1H}<0$ (attractive), $\theta_s<1$ and $\Delta_1\to E_F\,|\,\bar{g}_{1H}\,|^{\,-1/g_{1H}}\ll E_F$ in the limit $|\,\bar{g}_{1H}\,|\ll 1$. Δ_1 is relevant in this case and is the gap in the spin excitations. When $\omega_D<\Delta\ll E_F$, the power exponent θ_c-2 is always negative when $2\bar{g}_{2H}-\bar{g}_{1H}\geq -1$ for all interesting cases in which the renormalization approach is valid. $N(\omega)$ is then always divergent as $\omega_D\to 0$. When $E_F\gg\omega_D>\Delta_1$, the power exponent is $\theta_c+\theta_s-2$. CDW correlations can only be enhanced if $\theta_c+\theta_s-2<0$, which can only occur if $V>0$ (the attractive Hubbard case $V=0$ favors SS response[20]). As mentioned previously, whenever ω_D/E_F is finite, we expect an enhancement of $N(\omega)$ for $U-6V\lesssim 0$ from first-order perturbation theory. The resulting phase diagram will thus be the following: The cases ($\theta_c+\theta_s-2<0$, $U-6V>0$) and ($\theta_c+\theta_s-2>0$, $U-6V>0$) are illustrated by the dotted line in Fig. 5, the case ($\theta_c+\theta_s-2<0$, $U-6V<0$) corresponds to the solid lines labeled $\gamma<0$, and the case ($\theta_c+\theta_s-2>0$, $U-6V<0$) is described by the dashed-dotted line. The quantum region would behave as discussed in the $g_{1H}>0$ case.

The arguments we have used in the static regime when $\omega_D/E_F\to 0$ are similar to those of Chui *et al.*,[23] except that we have examined a more general situation. They had concluded as we have that a repulsive Coulomb interaction should lead to an enhancement of the mean-field Peierls transition when the power-law exponent for the CDW response is negative. In this respect, a positive V strengthens the CDW correlations while a negative V weakens them.

2. Half-filled band

The half-filled band case is by far the most complicated because of the umklapp processes. In the incommensurate case, the electron gas was not pinned to the lattice and it reacted to a charge excitation in an optimal fashion (maximum possible response so as to minimize the energy). In the half-filled band case, the spin-$\frac{1}{2}$ electron gas is in tune with the lattice, and umklapp processes are highly relevant.[3] Because of this, the charge response functions associated with the MC or SSH models will not be the same. In the repulsive Hubbard case[24] the ground state has gapless homopolar excitations, but its ionic excitations have a gap (the Hubbard gap). The MC phonons couple to the ionic excitations (piling more than one electron on a given molecule), while the SSH phonons couple to the homopolar excitations (the dimerization favors intermolecular hopping, and thus a charge buildup between the molecules of a dimer). One thus expects the CDW response function of the MC to be nondivergent, and that of the SSH crystal to be divergent when $U>0$ and $V=0$ (and vice versa if $U<0$). This can be formulated in the following way. We define, as did Kimura,[25] the CDW

response functions $N^{\pm}=N_{++}\pm N_{+-}$, where $N_{+(\pm)}$ is the $+2k_F=\pi/a$ entrance-momentum to $\pm 2k_F$ exit-momentum response functions. It is quite obvious from this structure that N^+ couples (responds) to a charge density of the form $(e^{i2k_Fx}+e^{-i2k_Fx})\sim\cos(2k_Fx)$, while N^- couples to one of the form $\sin(2k_Fx)$. Therefore, N^+ responds to a charge buildup on the molecules (at $x=0$, for instance), while N^- responds to charge buildup between molecules (at $x=\frac{1}{2}\pi/k_F=\frac{1}{2}a$). Consequently, N^+ is pertinent to the MC case, while N^- is to be used for the SSH crystal. The work of Kimura[25] reveals that for $\omega/E_F\ll 1$, one has

$$N^{\pm}(\omega)\sim B^{\pm}(\omega/E_F)^{\gamma_{\pm}}, \tag{19a}$$

where

$$(\gamma_+,\gamma_-)=\begin{cases}(\frac{5}{2},-\frac{3}{2})g_{1H}=g_{3H}>0,\\(-3,1)g_{1H}=g_{3H}<0.\end{cases} \tag{19b}$$

It is assumed that the condition $2\bar{g}_{2H}-\bar{g}_{1H}>-1$ prevails (weak coupling limit). It is thus confirmed that only N^- diverges (the SSH case) when $g_{1H}>0$ and only N^+ (the MC case) otherwise. Even though the exact value of $\gamma_{\pm}$ is subject to controversy,[20] the qualitative physics remains unchanged. The behavior in Eq. (19) is presumed by some to hold even when ω is less than the Hubbard gap Δ_H.[20,25] This gap is pertinent to CDW excitations when $2\bar{g}_{2H}-\bar{g}_{1H}>-|g_{3H}|$. This has been challenged by Emery[3] and Emery *et al.*,[26] who claim that $N(\omega)$ must be constant (that is nonsingular) when $\omega<\Delta_H$. On the other hand, H. J. Schulz has calculated (private communication) that $N^-(\omega)\alpha(t/U)^2\omega^{-1}$ when $|t/U|\ll 1$. We then propose that the charge response function flattens out somewhat for $\omega\leq\Delta_H$ but has a singular behavior at very small frequencies.

We shall first examine the pure repulsive Hubbard case ($U>0$ and $V=0$) for which there is a correlation gap Δ_H. We speculate that $N^{\pm}$ should then behave qualitatively as shown in Fig. 6. Even though the power law is the same

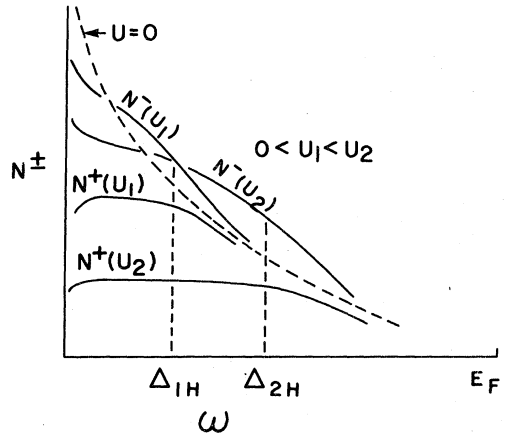

FIG. 6. Qualitative behavior of the charge response functions $N^{\pm}$ as a function of frequency ω and for various values of the Hubbard repulsion U for a half-filled spin-$\frac{1}{2}$ fermion band. Δ_H is the Hubbard gap.

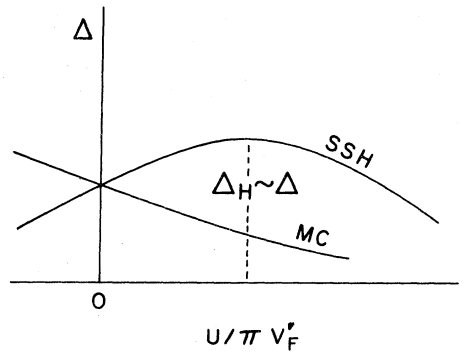

FIG. 7. Qualitative behavior of the mean-field gap Δ as a function of the Hubbard interaction U for the SSH and MC models with a half-filled spin-$\frac{1}{2}$ fermion band.

for all $U\neq 0$ and $\omega>\Delta_H$, one should expect an increase in the amplitude B^- of N^-, which is the strength of the correlations, as U increases and a decrease in the amplitude B^+ of N^+, since the ionic response stiffens (first-order perturbation theory[25] predicts such a decrease in B^+ but leaves B^- unchanged). As mentioned at the end of the last paragraph, $N^+\to 0$ as $U\to\infty$ and N^+ must decrease as U increases for $\omega<\Delta_H$. The Hubbard gap for small U/t is given by[24]

$$\Delta_H\sim 8\pi^{-1}(Ut)^{1/2}\exp(-2\pi t/U). \tag{20}$$

As long as $\omega_D>\Delta_H$, the CDW correlations will be gradually enhanced for the SSH case (N^-) and decreased for the MC case (N^+) as U increases (the enhancement is in the amplitude and not the power-law exponent). As U continues to increase Δ_H will become larger than ω_D [exponentially in Eq. (20)], from which point on N^- decreases, as do the CDW correlations. Thus the mean-field dimerization gap initially increases as U increases and eventually decreases until the quantum crossover is reached (when $\Delta<\omega_D$). This is shown in Fig. 7. This general behavior has been verified by Hirsch[14] (in his Figs. 1 and 4) and Mazumdar and Dixit.[15] The classical-quantum—crossover condition of Fig. 8 appears somewhat similar. We thus predict a maximum in the $\Delta(U)$ curve at $\Delta\sim\Delta_H$. This is quite interesting. If we use the values of Hirsch[14] (in his Fig. 1); $\omega_D=0.066$, $\lambda=0.29$, $\kappa=0.25$,

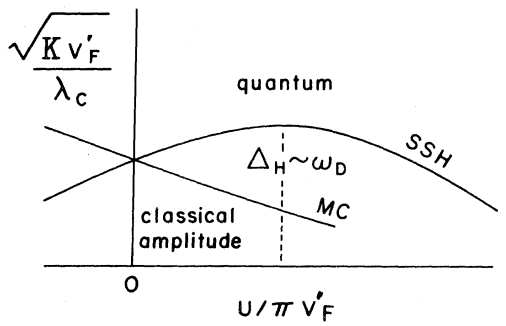

FIG. 8. Qualitative behavior of the critical quantum-classical—crossover condition for fixed ω_D as a function of the Hubbard interaction U for a half-filled spin-$\frac{1}{2}$ fermion band. Δ_H is the Hubbard gap.

$t=1$, and $\Delta=0.3$ at the maximum, we get from Eq. (20) with $\Delta_H=\Delta$ a value of $U\approx 2.5$, which is indeed extremely close to his value of U at the maximum. It would then seem that the criterion $U/\sqrt{2t}\sim 3$ of Mazumdar and Dixit[15] may be slightly inaccurate. In the quantum regime, the situation is the following. The g_{iH} scale towards the values[25] $\bar{g}_{1H}\to 0$, $\bar{g}_{2H}\to 1$, and $\bar{g}_{3H}\to 2$. One can then safely assume that $0<\tilde{g}_{1H}<\tilde{g}_{2H}<\tilde{g}_{3H}$. On the other hand, $\tilde{g}_{1\,\mathrm{ph}}=\tilde{g}_{3\,\mathrm{ph}}<\tilde{g}_{2\,\mathrm{ph}}<0$. Consequently, $g_{it}>\tilde{g}_{i\,\mathrm{ph}}$ and $g_{3t}>g_{1t}$. In the SSH case where $g_{2\,\mathrm{ph}}\sim 0$, one has $g_{2t}>0$. Since $\tilde{g}_{2\,\mathrm{ph}}>\tilde{g}_{1\,\mathrm{ph}}$ in the MC case, one can safely assume that $g_{2t}>g_{1t}$ for small U. The general behavior of g_{it} as a function of U is illustrated in Fig. 9. From the above arguments it is obvious that $g_{1t}-2g_{2t}<|g_{3t}|$ in all cases for the SSH crystal and for most $U/\pi v_F'$ for the MC chain (except when $g_{3t}\sim 0$). The system has long-range order in as much as $g_{1t}<0$ and $g_{1t}-2g_{2t}<|g_{3t}|$. The correlation gap, which occurs in both CDW and SDW excitations, is related to g_{3t}. As U increases, $|g_{3t}|$ decreases from $|g_{3\,\mathrm{ph}}|$. Simultaneously, g_{1t} becomes less and less negative. At a critical value U_c, $g_{1t}=0$, from which point on the chain has no long-range order and dominant SDW divergence.[3,20] This trend is illustrated in Fig. 10. U_c can be estimated from Eq. (11) and the condition

$$g_{1t}\sim\tilde{g}_{1\,\mathrm{ph}}+\tilde{g}_{1H}+2|\tilde{g}_{1\,\mathrm{ph}}|N(\omega_D)(\tilde{g}_{1H}+\tilde{g}_{3H})$$
$$\sim\tilde{g}_{1\,\mathrm{ph}}+\alpha\tilde{g}_{3H}\sim 0\ ,$$

where $\alpha<3$ [indeed, $\tilde{g}_{1H}<\tilde{g}_{3H}$, $\tilde{g}_{1\,\mathrm{ph}}=\tilde{g}_{3\,\mathrm{ph}}$, and $2|\tilde{g}_{1\,\mathrm{ph}}|N(\omega_D)<1$ from Eq. (10), since the chain is in the quantum regime]. Note that $|g_{3t}|\to 0$ before $g_{1t}\to 0$, which would imply some sort of ill-defined region when the long-range order would disappear as U increases and faintly reappear again as U gets closer to U_c (the MC model is even more complex, since $g_{1t}-2g_{2t}$ can become greater than $|g_{3t}|$). Whether this behavior is real or not is uncertain. It may just be an artifice of the method. This regime should be explored by numerical techniques. Aside from this peculiar behavior, which has not been illustrated in Fig. 10, the general trend is as observed by Hirsch (in his Fig. 3). He expected a transition to an undimerized state at $U_c=4\lambda^2/\kappa$ for the SSH model. We get this value if $|g_{1\,\mathrm{ph}}|N(\omega_D)\ll 1$, and thus $|\tilde{g}_{1\,\mathrm{ph}}|\approx|g_{1\,\mathrm{ph}}|=4\lambda^2/\kappa$ for the SSH case, and assuming $\tilde{g}_{1H}\sim g_{1H}=U$ that is for not too much renormalization (large ω_D). In the attractive Hubbard case ($U<0$), the

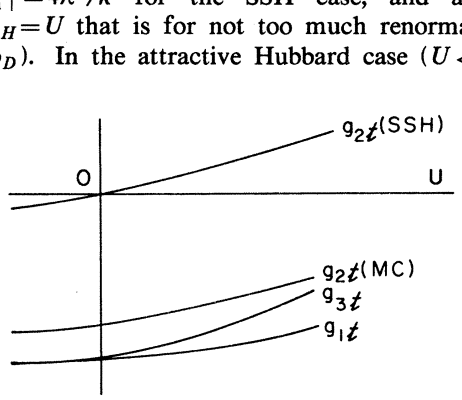

FIG. 9. Qualitative behavior of g_{it} in the quantum region for a half-filled spin-$\frac{1}{2}$ fermion band as a function of the Hubbard interaction U.

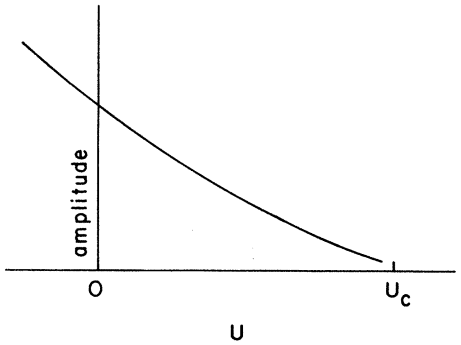

FIG. 10. Qualitative behavior of the amplitude of the long-range order in the quantum regime of a half-filled spin-$\frac{1}{2}$ fermion band. The region close to U_c is uncertain.

Hubbard gap is no longer relevant to the CDW response function of the electron gas. Thus the responses of Eq. (19) are "valid" at all frequencies $\omega/E_F\ll 1$. We then expect the type of behavior illustrated in Fig. 4, N^+ being divergent this time ($\gamma\to u$ in Fig. 4) and N^- going to zero as $\omega\to 0$ ($\gamma\to -U$ in Fig. 4). The smaller U, the larger the coefficient B^+ and the smaller B^- in Eq. (19a). The quantum-classical-amplitude crossover should thus appear qualitatively as in Fig. 5, with $\gamma\to U$ for the MC case and $\gamma\to -U$ for the SSH model. These results are shown in Figs. 7 and 8 and extrapolate from the $U>0$ values. In the quantum regime, $\tilde{g}_{iH}>0$ and thus $g_{it}<0$. From the scaling laws for g_{iH} ($\bar{g}_{1H}\to -2$, $\bar{g}_{2H}\to 0$, and $\bar{g}_{3H}\to -2$),[25] one can conclude that $\tilde{g}_{1H}\sim\tilde{g}_{3H}<\tilde{g}_{2H}<0$. Consequently, $g_{1t}\sim g_{3t}<g_{2t}$ as shown in Fig. 9 (extrapolating from the $U>0$ region). We thus have $g_{1t}-2g_{2t}<|g_{3t}|$ for all values of U and for both the SSH and MC models. The quantum regime thus has long-range order which is stabilized by an attractive interaction (the more so, the more negative U is). This is shown in Fig. 10 and extrapolates from the $U>0$ values.

We shall finally discuss the effect of the nearest-neighbor interaction V. If $U=0$, then $g_{1H}=g_{3H}=-2V$ and $g_{2H}=2V$. A positive V implies an attractive g_{1H} and, as discussed above, a divergent N^+, which in turn favors the MC molecular distortion. On the other hand, a negative V means a divergent N^- and favors the dimerization of the SSH model. Thus, quite generally, when $U\neq 0$ we expect a positive V to decrease N^- and increase N^+ and vice versa for negative V. As a matter of fact, whenever $V\,\mathrm{sign}(U)\geq|U|/2$, g_{1H} changes sign and it can be seen from Eq. (19) that the roles are then reversed for N^+ and N^-. One can thus foresee a dramatic change in the nature of the ground state when this occurs. This is confirmed by Dixit and Mazumdar.[15] In the quantum regime, the fact that $\tilde{g}_{2H}$ is affected differently than $\tilde{g}_{1H}$ or $\tilde{g}_{3H}$ matters only inasmuch as $g_{1t}-2g_{2t}$ can be made larger than $|g_{3t}|$. This requires that $g_{2H}=U+2V<U-2V$ or $V<0$. Whenever this occurs any long-range order disappears, making way for a leading divergence in the SS response function.[3,20]

VI. DISCUSSION

We have studied the low-energy properties of the electron-phonon system with and without Coulomb in-

teraction using a two-cutoff renormalization theory. Within its range of applicability, that is, for weak coupling ($\lambda^2/\kappa\pi v_F$ and $g_{iH}/\pi v_F' \ll 1$) and an appreciable range of phonon frequencies ($0 \leq \omega_D < E_F$), we have been able to reproduce all the results of previously done numerical simulations.

The characteristic feature of the electron-phonon system is surely its two regimes. There is the "static" regime in which there is a well-defined amplitude order parameter for the molecular displacements. This occurs if the mean-field gap (or the pseudogap) is larger than the Debye frequency. This amplitude order parameter is influenced by the Coulomb interaction. A repulsive V increases it for spinless fermions.[22] For spin-$\frac{1}{2}$ fermions, a repulsive Hubbard interaction will also increase it in incommensurate cases when $\omega_D/E_F \to 0$, but decrease it if ω_D/E_F is finite. The half-filled band case is somewhat special. There are different behaviors for the SSH and MC models. The molecules in the MC couple to the ionic charge response of the electrons. It is generally subdued by a repulsive interaction, which means a decrease in the order parameter as g_{1H} increases. The SSH chain couples to the homopolar charge response of the electrons. It is enhanced by increasing the Coulomb interaction until the correlation gap becomes larger than the gap associated with the order parameter. From there on the response function decreases. The amplitude of the order parameter does the same.

There is the quantum behavior in which the electron-phonon coupling appears as an effective attractive interaction between electrons, which is renormalized by any Coulomb interaction, and which add to it. Depending on the value of the net electron interaction, there can be long-range order of a quantum nature in the molecular displacement for the half-filled spin-$\frac{1}{2}$ fermion band case (which could be generalized with some modifications to any commensurate case with umklapp processes, that is $g_{3H} \neq g_{1H}$). This occurs if $g_{1t} < 0$ and $g_{1t} - 2g_{2t} < |g_{3t}|$, since there is then a gap in both spin and charge degrees of freedom. This quantum order is sensitive to the sign of the Coulomb interaction. A positive effective interaction $g_{1H} = U - 2V$ weakens the order and can even destroy it in favor of a divergent spin response function if it gets larger than a critical value (of order of λ^2/κ). A sufficiently negative value of V (or g_{2H}) can also destroy it and favor a singular SS response function.

From our analysis, we are in a position to discuss the limitations of the standard treatments of the 1D low-temperature electron-phonon system. In the case of the pure Peierls system, a classical field (order-parameter) approach in terms of the Ginzburg-Landau (GL) free-energy functional of the order parameter has been extensively used as a starting point for the study of low-temperature fluctuations.[9,27] This approach presupposes the existence of a well-defined static mean-field amplitude order parameter. As mentioned above for fermions with and without spin, this corresponds to the classical regime when $\Delta > \omega_D$, namely that the phonon frequency must be small enough to fulfill the adiabatic condition. It follows that the only relevant correlations come from the zero-sound channel and in principle a Landau-type order parameter can be used. In the half-filled band case, the order parameter is real and corresponds to the static atomic displacement. For this case, the static GL free-energy functional can be obtained in the usual way.[9,27] namely by a mean-field decoupling of the electron-phonon interaction. In the incommensurate case, phase fluctuations are important[27,28] for $T < \Delta$. When $\omega_D \to 0$ the GL free-energy functional for the phase is classical and can be obtained in the same way as for the half-filled band case.[8,9] It also predicts long-range order at $T = 0$. In the case where the phonon frequency ω_D is finite, quantum motion of the phase becomes relevant and a static GL functional is no longer valid at low temperature. At $T = 0$, the zero-point motion of the phase destroys long-range ordering. This is the consequence of the Goldstone mode connected with translational invariance of the incommensurate charge modulation.[12] A quantum generalization of the GL functional for the Peierls quantum phase fluctuations has been proposed phenomenologically by Fukuyama,[12] and its microscopic justification has been obtained by Takano.[13] These approaches are consistent with a small perturbation around the classical mean-field amplitude gap Δ.[28]

In the quantum regime when $\omega_D > \Delta$, nonadiabatic effects are relevant. A Landau order parameter with a well-defined classical amplitude does not exist so that the static GL formulation and its quantum extension become ambiguous. Rigorous functional-integral techniques (FI) have shown[29,30] that if the atomic displacements are quantum, this introduces an additional frequency-dependent classical field which is related to the nonadiabaticity of the electron-phonon system. For example, in the commensurate case the nonadiabatic classical field is purely imaginary, while for the incommensurate case a real and an imaginary component are added. It follows that the interference between the zero sound and the Cooper channels (correlations which occur in the quantum regime $\omega_D > \Delta$) is strongly related to the appearance of supplementary fields in the FI formulation. As far as the quantum long-range ordering at $T = 0$ is concerned for $\omega_D > \Delta$ and a half-filled band, only the interference between the zero sound and the Cooper channels can account for the gaps in both charge and spin degrees of freedom.[3,20] These should be connected in a nontrivial way to both kinds of fields, in contrast to the classical case.[28,29]

It has been shown[30] that the integration of the phonon quantum degrees of freedom can eliminate the supplementary nonordering fields by introducing an effective retarded electron-electron interaction. However, for such functionals, standard approximations which are commonly used in higher dimensions,[31] and for which only one channel of correlations is retained, cannot be trusted[3,4,20] when $\omega_D > \Delta$. In such cases, it is not clear how to recover, by the FI method, the quantum behavior predicted at low temperature by the renormalization-group[3,20] method (see Sec. IV) and confirmed by simulations.[7,14,15] Although a 1D FI formulation can be rigorously constructed in various situations, no controlled approximation exists at the present time for the correlation channel mixing.

In the regime $T < \omega_D > \Delta$, the Peierls system is equivalent to the Fermi-gas model with a single cut-off energy ($\equiv \omega_D$). The difficulties encountered by a FI

method for a Peierls-extended Hubbard model in the quantum regime (see Sec. V) will of course be the same if not worse.[32] For the classical regime when $\omega_D < \Delta$, the absence of channel mixing for $T < \Delta$ indicates adiabaticity and allows one to use tractable approximations for the FI method. However, the mean-field gap expression in Eq. (17) for Δ is obviously not BCS-like when electron-electron interactions are present. The power-law behavior is the signature of quasiparticle confinement for $\Delta < T \ll E_F$ in contrast to the pure Peierls case. For $T < \Delta$ and a half-filled band, a static GL free-energy functional can be constructed with a single real adiabatic order parameter, except that the GL coefficients must be renormalized by Coulomb interactions.[23,33] It follows that the phonon softening will be enhanced compared to the pure Peierls case,[21,23] although long-range order can only occur at $T=0$. For the incommensurate case with $\omega_D \neq 0$, zero-point motion of the phase should destroy the $T=0$ long-range ordering, as in the pure Peierls case.[23]

The repercussion of the above results on the type of long-range ordering at finite temperature in *quasi*-1D systems is of major importance. Among the various mechanisms for interchain coupling which allow the propagation of correlations in the transverse direction, the two most popular are the kinetic and the potential types of coupling.[3,5,10,11,20,27,33]

We shall discuss the kinetic coupling since it is the most interesting and encompasses the potential coupling in limiting cases. It describes the possibility of single electrons hopping from one chain to another. The amplitude for this process is connected to the transverse hopping integral $t_\perp$. Quasi-one-dimensionality is usually characterized by $t_\perp / t_{||} \ll 1$ where $t_{||}$ is the intrachain (1D) hopping integral. A large anisotropy allows us to treat transverse electronic motion as a small perturbation and therefore a large temperature range with 1D electronic properties should exist.[26,27,33] However, at low temperature one can anticipate a dimensionality crossover (1D to 3D).[11,26] The various possibilities of correlation for the electron-phonon system will of course affect the crossover in a variety of ways.[10] Let us survey these possibilities.

In the pure Peierls system the nature of the dimensionality crossover is strongly linked to the existence of a classical regime and the magnitude of Δ [see Eq. (14)] with respect to $t_\perp$. More precisely, if $\Delta > t_\perp$, the dominant transverse motion at low temperature will involve *two*-particle tunneling:[3-5] one electron and one hole which can be considered as bound with an energy 2Δ as in the BCS theory. This mechanism dominates *one*-electron hopping because of the cost in energy to break a bound pair of particles.[3] In such cases the effective transverse coupling $V^\perp$ will be proportional to $t_\perp^2$, and the 1D$\rightarrow$3D crossover will be due to the propagation (tunneling) of $2k_F$ electron-hole pairs in the transverse direction. For $\omega_D \rightarrow 0$ it will be classical. From the scaling argument of Barisic and Uzelac,[34] a mean-field theory for the transverse coupling gives $T_x \simeq (V)^{1/\psi}$ with $\psi = 2$ and also $T_c \propto T_x \sim (V^\perp)^{1/2}$. For $0 < \omega_D < \Delta$ quantum phase fluctuations are present.[12] Because of the adiabaticity, the ratio of the electronic band mass m to the CDW effective mass m^* is very small ($m/m^* \ll 1$), the characteristic energy ω_Q for quantum phase oscillations is small and the effects on the crossover will be weak. Therefore, one still has $T_c \propto T_x \sim (V^\perp)^{1/2}$. When ω_Q is small ($\omega_Q \ll T_x$), the propagation of quantum effects on neighboring chains can be neglected.[10] A static approximation can then be justified for the description of 3D correlations. This can be achieved by 3D GL free-energy functionals.[10,27]

If $t_{||} \gg t_\perp \gg \Delta$ the situation is different. Electron-hole pairs are not stable at $T \sim t_\perp$ and interchain single-particle hopping will dominate. The 1D$\rightarrow$3D crossover is dominated by one-electron processes and is determined when the 3D single-electron motion becomes coherent, namely at $T = T_x \simeq t_\perp$.[11,26] The possibility of a 3D phase transition is now linked to the existence of a nonvanishing 3D potential coupling. If we assume that the phonons are 3D, or if we have interchain backward scattering, the Peierls transition will be anisotropic but BCS-like.[11,26]

In the quantum regime where $\omega_D > \Delta$, effective two-particle processes in the transverse directions are still possible in the presence of a *quantum* gap. As we have seen, this can occur in the following cases. In the incommensurate case and for electrons with spin ($g_{1\,\mathrm{ph}} < 0$ and $g_{2\,\mathrm{ph}} < 0$) we have a gap $\Delta_s < \omega_D$ in the spin degrees of freedom with a power-law divergence in the CDW and possibly for singlet superconductivity.[3,20] In the half-filled band case and for electrons with spin we can have quantum gaps in both charge and spin degrees of freedom ($\Delta_s \neq 0$, $\Delta_\rho \neq 0$). Consequently, if $t_\perp \lesssim \max\{\Delta_s, \Delta_\rho\}$, 3D CDW long-range ordering occurs by electron-hole tunneling ($V^\perp \propto t_\perp^2$). Quantum effects are important for $T < \omega_D$, and the 1D$\rightarrow$3D crossover exponent ψ is no longer classical $\psi \neq 2$. The power-law exponent γ of 1D CDW correlations is highly nonuniversal [see Eqs. (16) and (18)]. By scaling arguments we can show[35] that $T_c \sim T_x \sim (V^\perp)^{1/\gamma}$ with $\psi = \gamma < 2$ in the quantum regime.

The situation changes drastically in the presence of $t_\perp > \{\Delta_s, \Delta_\rho\}$ or with spinless electrons when there is no gap in the quantum regime.[22] The dimensionality crossover will be dominated by *one*-electron transfer. However, in the quantum regime quantum correlations exist in the absence of a gap, and these must affect the one-particle 1D$\rightarrow$3D crossover. As a matter of fact, scaling arguments for the Tomonaga-Luttinger model show[35] that $T_c \propto T_x \sim t_\perp^{1/(1-\alpha)}$, where α is the exponent of the one-particle correlation function (the Green function). The crossover exponent ψ is nonuniversal, $\psi = 1 - \alpha$, since α depends on the interaction.[22] $t_\perp$ acts as the symmetry-breaking parameter. This result for the Tomonaga-Luttinger model can be conjectured for other models.[36] In the quantum regime the characteristic energy for 1D fluctuations ω_Q, which depends on the interactions, is in general not small in this nonadiabatic limit. Consequently, the propagation of *quantum* correlations in the *transverse* direction becomes important whenever $\omega_Q \gg T_x$. Again, this can be achieved by two- or single-particle interchain processes. The 3D long-range order at finite temperature is static, however. So this shows the possibility of a quantum-classical crossover for the quasi-1D correlations. From the work of Ref. 10, for the case where $V^\perp \sim (t_\perp)^2$ we have $\Delta t^* \equiv (T^* - T_c)/T_c \sim (T_c/\omega_Q)^\gamma$, where T^* is the quantum-classical—crossover temperature and the cross-

over exponent becomes $\phi_Q = 1/\gamma$, which is again nonuniversal. It is now the temperature which acts as the symmetry-breaking parameter.[10] The existence of such a crossover puts strong restrictions on the validity of the usual static 3D GL order-parameter functional, namely that the static GL order-parameter description is only valid for $\Delta t < \Delta t^*$, and the GL parameters must be renormalized compared to the usual static description.[10]

The above discussion for the pure Peierls case with arbitrary phonon frequency ($\omega_D \leq E_F$) can be readily extended to the case where Coulomb interactions are added. The limitations of the FI method in 1D vs 3D and the crossover behavior for quasi-1D solids with kinetic and potential interchain couplings follow essentially the same lines. As we have seen, the existence of correlations, their nature (quantum or classical), and their magnitude versus $\{\omega_D, t_\perp\}$ have strong influence on 1D and quasi-1D classical and quantum properties. It must be noted, however, that the presence of 1D Coulomb interactions rules out the possibility of a BCS-type dimerization gap Δ in the classical regime ($\omega_D < \Delta$). This results from the confinement of quasiparticle states which occur for $T < E_F$ and a short-range Coulomb interaction.[3,20,22]

Another interesting feature of the quasi-1D electron-phonon system with strong nonadiabatic effects is the possible competition between two types of long-range ordering.[37] That is particularly true in the presence of Coulomb interaction when $\omega_D > \Delta$, although it can occur to some extent in the pure Peierls case. For example, for electrons with spin and $U \neq 0$, $V \neq 0$ in the incommensurate case, one can have the situation where $g_{1t} - 2g_{2t} \approx 0$, $g_{1t} < 0$, and $g_{2t} < 0$ for $\omega_D > \Delta$. This corresponds to nearly equally divergent 1D CDW and 1D singlet superconductivity response functions.[3,20] In the presence of a kinetic coupling $t_\perp$ with the condition $t_\perp \ll \Delta_s$, $V_\perp \sim (t_\perp)^2$ for both types of instabilities. Then, one can easily find[35] for each type of correlation a 1D$\rightarrow$3D crossover temperature $T_x^{\rm CDW} \sim (V_{\rm CDW}^\perp)^{1/\gamma_{\rm CDW}}$ and $T_x^{\rm SS} \sim (V_{\rm SS}^\perp)^{1/\gamma_{\rm SS}}$ and in principle two quantum-classical—crossover temperatures $\Delta t_{\rm CDW}^* \sim (T_c^{\rm CDW}/\omega_Q)^{\gamma_{\rm CDW}}$ and $\Delta t_{\rm SS}^* \sim (T^{\rm SS}/\omega_Q)^{\gamma_{\rm SS}}$. In practical cases an exact degeneracy is difficult to satisfy. Small additional 1D effects (e.g., Coulomb screening effects[33,38] and impurities[39]) can make $\lambda_{\rm CDW} \neq \lambda_{\rm SS}$ and small interchain potential couplings (backward scattering, 3D phonons, etc.) can easily make $V_{\rm CDW}^{\perp\rm eff} \neq V_{\rm SS}^{\perp\rm eff}$ and induce only one type of long-range ordering. Nevertheless, it is interesting to note that on a smaller 3D scale, quantum nonadiabatic effects allow different types of correlations to coexist.

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