Peierls instability in a nearly-free-electron model, including nonlinear screening*†

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We determine the conditions under which a Peierls instability (PI) will occur at $T = 0$°K for a nearly-free-electron model that includes electron-electron interaction. We include nonlinearities in the screening, which are found to be very important, and we do not limit the calculation to $q = 2k_F$. It is found that a PI requires $\gamma > 1$, where γ is a parameter characterizing the electron-phonon interaction. In a special case, $\gamma = \omega_{pl}^2/\omega_q^2$, where ω_{pl} is the (bare) plasma frequency of the *ions*, and ω_q is the *bare* phonon frequency. We find the renormalized phonon frequency generally does *not* have to vanish to have an instability. Furthermore, we find that when $1 < \gamma \lesssim 1$ the instability is likely to occur at $q < 2k_F$ rather than at $q = 2k_F$, thus putting a gap *below* the Fermi level. We find that the size of the instability gap is probably limited by anharmonicities, rather than being limited by minimization of the total energy calculated in the harmonic approximation. It is significant that the most important contributions to the total energy for the screened PI are not present for the unscreened PI. Thus the gap is not expected to have a BCS-type of temperature dependence, contrary to the case of the unscreened PI.

I. INTRODUCTION

In this paper we wish to determine the conditions under which a quasi-one-dimensional (1D) metal undergoes a Peierls instability (PI) at 0 °K, when screening by nearly-free-conduction electrons is included. Many years ago Peierls suggested[1] that a 1D metal would be inherently unstable to a lattice deformation of wave number $q = 2k_F$ (k_F is the Fermi wave number). His suggestion was later justified in more detail in papers by Fröhlich[2] and by Rice and Strässler[3] in which electron-electron interaction, and hence screening, was ignored. The work of these authors was summarized and extended in a different context, by Allender, Bray, and Bardeen.[4] The latter two papers, as well as the present one, were motivated by the observation of what appear to be PI's in such 1D metals as $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$ (KCP),[5-9] and tetrathiafulvalenium-tetracyanoquinodimethanide (TTF-TCNQ).[9-14]

We include here electron-electron interaction in the analysis of the PI. Short-range electron-electron interaction has been included in discussions of the PI that employ a Hubbard model.[15,16] How well the Hubbard model describes the actual electron-electron interaction, which generally is *not* short ranged, is not well understood, especially for bands that are not very narrow.[17] We shall not use a Hubbard model, but rather a nearly-free-electron model. In this case, electron-electron interaction manifests itself as screening by the conduction electrons. It is well known[1] that a given net (i.e., screened) perturbation

$$V' = \sum_{\pm} V_{\pm q} e^{\pm iqz}, \tag{1}$$

due to a lattice deformation, will be most effective in lowering the electronic energy when $q = 2k_F$, thus putting a gap at the Fermi level and depressing all electronic energies. However, the complexity arises when one realizes that the 1D static dielectric function[18] for an electron gas has a singularity at $2k_F$:

$$\epsilon_q = 1 + \frac{\text{const}}{q^3} \ln\left|\frac{q + 2k_F}{q - 2k_F}\right|. \tag{2}$$

Thus it would seem that the electrons would never "see" a lattice distortion—it being perfectly screened—thus giving $V' = 0$, no matter what the unscreened perturbation (i.e., lattice distortion) was. What saves the PI is that in the vicinity of $q = 2k_F$, Eq. (2) holds only for an infinitesimally weak perturbation. In reality the dielectric "constant" depends on the strength of the perturbation. This dependence is usually a weak one *except* in the vicinity of $q = 2k_F$. We will show that when nonlinear effects are included, the singularity disappears and the logarithm in Eq. (2) will have the replacement

$$\ln\left|\frac{q + 2k_F}{q - 2k_F}\right| \xrightarrow[q=2k_F]{} \ln\left(\frac{8E_F}{|V_q|}\right), \tag{3}$$

where E_F is the Fermi energy and V_q refers to a screened potential. The inclusion of this nonlinearity is an essential aspect of the present paper.[19,20]

Thus it is not clear whether or not a PI will be

present in a 1D metal at 0 °K. Furthermore, it is not obvious that it will occur at $q = 2k_F$ when it occurs at all. We will consider here a distortion with a *single* wave number, q, but *not* assume $q = 2k_F$. We will find that a PI is not automatic. Its presence will require for a certain parameter γ, which characterizes the electron-phonon interaction, that

$$\gamma > 1 . \tag{4}$$

We will consider two special cases (Sec. IV C) in which the phonon branch associated with the PI involves only one species of ion that has simply specified interactions with its neighbors. In these cases

$$\gamma = \omega_{pl}^2/\omega_q^2 , \tag{5}$$

where

$$\omega_{pl} = (4\pi NZ^2e^2/M\Omega)^{1/2} \tag{6}$$

is the unscreened plasma frequency of the distorting ions (not electrons), and ω_q is the unscreened frequency for the phonon of wave number q that is associated with the phonon corresponding to the conventional static Peierls distortion. In Eq. (6), N is the number of ions of the species being displaced, M is their mass, Ze is their charge, and the volume of the crystal is Ω. Equations (4)–(6) mean that if an instability is to occur, the *bare* frequency cannot be too large. However, we will find that the Kohn-screened phonon frequency generally does *not* have to vanish to obtain an instability.

Contrary to the results for the unscreened PI of Refs. 1–4, we will find that the gap does *not* go as $e^{-\Lambda^2}$, with Λ being a characteristic parameter inversely proportional to the electron-phonon coupling constant. On the contrary, the gap, if present, will typically be too large to fall within the range of validity of our approximation, and in this case the gap is probably limited by anharmonic interactions with the rest of the lattice. Only when γ is larger than unity but close to it, is the gap corresponding to $q = 2k_F$ determined within our approximation. However, in this region of γ we will find the surprising result that it may well be more favorable energetically to have $q < 2k_F$. Whether or not $q = 2k_F$ in this region will depend on the details of the problem, but in the basic special cases investigated in Sec. IV C we will find the system has a lower energy when $q < 2k_F$. However, when γ is appreciably larger than unity the energy minimum does indeed occur at $q = 2k_F$.

II. HAMILTONIAN

We start with the Hamiltonian for the metallic state

$$H = \sum_i \left(\frac{\vec{p}_i^{\,2}}{2m}\right) + U(\vec{r}_i, \vec{R}_j) + H_{ee} + \sum_{j,\vec{k}} N^{-1/2} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_j}(b_{\vec{k}} + b_{-\vec{k}}^{\dagger}) + \sum_{\vec{k}'} \hbar\omega_{\vec{k}'} b_{\vec{k}'}^{\dagger} b_{\vec{k}'} , \tag{7}$$

and, in the spirit of an effective mass approximation, assume that it can effectively be written, for a 1D conductor,

$$H = \sum_i \frac{-\hbar^2}{2m^*}\frac{d^2}{dz_i^2} + \sum_{j,\vec{k}} N^{-1/2} g_{\vec{k}} e^{i\vec{k}\cdot\vec{r}_j}(b_{\vec{k}} + b_{-\vec{k}}^{\dagger}) + \sum_{\vec{k}'} \hbar\omega_{\vec{k}'} b_{\vec{k}'}^{\dagger} b_{\vec{k}'} . \tag{8}$$

In Eqs. (7) and (8) $\vec{r}_i$ and $\vec{p}_i$ are the position and momentum of the ith electron. The $\vec{R}_j$ are the equilibrium sites of the lattice and $U(\vec{r}_i, \vec{R}_j)$ is the interaction energy of the electrons with the equilibrium lattice sites. H_{ee} is the electron-electron interaction,

$$H_{ee} = \sum_{i<j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} . \tag{9}$$

Furthermore, $g_{\vec{k}}$ is the electron-phonon coupling constant, $b_{\vec{k}}^{\dagger}$ ($b_{\vec{k}}$) are the phonon creation (annihilation) operators, and $\omega_{\vec{k}}$ is the unscreened phonon frequency. We are considering only one phonon branch but do not assume a one-dimensional phonon spectrum. The sums over i and j run over all conduction electrons, and the sum over $\vec{k}$ runs over all wave vectors, where it is understood that for $b_{\vec{k}}$ or $b_{\vec{k}}^{\dagger}$ the reduced $\vec{k}$ is to be used. The sum over $\vec{k}'$ runs over the wave vectors of the first Brillouin zone. We have omitted polarization and spin indices. The 1D direction is taken to be along the z direction. In going from Eqs. (7) to (8) we have assumed that the conduction electrons have energies $E_k^0 = \hbar^2k_z^2/2m^*$ (at least near k_F). In addition, in order to have effectively $\vec{k} \to -i\nabla$, as in the first term of Eq. (8), it is necessary to assume that either the conduction electrons are well described by plane waves or, as can be shown by an extension of effective mass theory that we will not give here, that the period of the Peierls distortion is large compared to the lattice periodicity a; i.e., that $q \ll G$ where $G = 2\pi/a$ is the fundamental reciprocal-lattice vector in the z direction. We do not restrict ourselves to the case of a half-filled band. In fact, our approximations are particularly well applied to the case of a nearly empty or nearly filled band, as in a highly degenerate semiconductor.

Our approach will be to minimize, as well as possible, the expectation value of the energy. To this end we first perform a canonical transformation on H. Let

$$T=\exp\left(\sum_{\pm} i\beta(b_{\pm q}-b_{\pm q}^{\dagger})\right),$$

where β is real and hence T is unitary; $\vec{q}$ is taken to be in the z direction and has a magnitude, q, that is *not* assumed to equal $2k_F$. The transformed Hamiltonian $H'=T^{\dagger}HT$ will have the same eigenvalues as H. One can show that

$$T^{\dagger}b_{\vec{k}}T=b_{\vec{k}}+\beta\delta_{\vec{k},\pm\vec{q}}, \tag{10}$$

and hence that H' is

$$H'=H+2\beta^2\hbar\omega_q+\sum_{j,\pm}2\beta N^{-1/2}g_{\pm q}e^{\pm iqz_j}+\beta\hbar\omega_q\sum_{\pm}(b_{\pm q}+b_{\pm q}^{\dagger}). \tag{11}$$

In Eq. (11) we have not included terms with $g_{\vec{G}',\pm\vec{q}}$, where $\vec{G}'$ is a reciprocal-lattice vector. Such terms arise when one remembers that $\vec{k}$ in Eq. (10) is the reduced $\vec{k}$ while the sum in Eq. (8) is over all $\vec{k}$. These additional terms would not arise if the ions were considered a continuous sea of charge ("jellium") rather than a collection of point charges. We neglect these higher harmonics of the distortion.

For the phonon part of the *metallic* ground state we take the phonon vacuum $|0\rangle$, while for the phonon part of the *Peierls* ground state we take the transformed phonon vacuum $|0'\rangle=T|0\rangle$. From Eq. (10) we see that

$$\langle 0'|b_{\vec{k}}|0'\rangle=\beta\delta_{\vec{k},\pm\vec{q}}. \tag{12}$$

Hence the transformation T with a finite value of β corresponds to a static displacement of the ions, and it is the mathematical expression of the type of deformation one would associate with the PI. We consider β a variational parameter for the determination of the phonon ground state. We will then need to consider the difference in the total system energy that arises according to whether the phonon vacuum is $|0\rangle$ or $|0'\rangle$. Having asserted the phonon ground state, the electronic ground state then needs to be determined. This is done by determining the ground state of the effective Hamiltonian for the metallic state

$$H_{\mathrm{MS}}=\langle 0|H|0\rangle=\sum_i -\frac{\hbar^2}{2m^*}\frac{d^2}{dz_i^2}, \tag{13}$$

from Eq. (8), and by determining the ground state of the effective Hamiltonian for the Peierls state,

$$H_{\mathrm{PS}}=\langle 0'|H|0'\rangle=\langle 0|H'|0\rangle=\sum_i -\frac{\hbar^2}{2m^*}\frac{d^2}{dz_i^2}+V'+2\beta^2\hbar\omega_q, \tag{14}$$

by Eq. (11). Here

$$V'=\sum_i V^{0\prime}(z_i)+\Delta H_{ee}(V'), \tag{15a}$$

$$V^{0\prime}(z_i)=\sum_{\pm}V_{\pm q}^{0}e^{\pm iqz_i}, \tag{15b}$$

and

$$V_q^0=2\beta N^{-1/2}g_q. \tag{15c}$$

In Eq. (15a), ΔH_{ee} is the change in the electron-electron interaction that will be brought on by the perturbation. It is an important term that arises as follows. The initial Hamiltonian of Eq. (7) contains the term H_{ee} that depends on the electronic charge density, and hence on the wave function solutions of the Schrödinger equation. Under the influence of the perturbation, those wave functions change, and the corresponding change in the charge density results in the induced potential ΔH_{ee}. Note that ΔH_{ee} both contributes to and depends on V'. Hence Eq. (15a) represents a self-consistency problem.

III. CALCULATION OF ΔE

We now solve the self-consistent perturbation problem contained in Eq. (15a) in a Hartree approximation (or random-phase approximation). In Sec. V, we will consider the effects of exchange and correlation, where we will argue that they probably do not have a qualitative effect. In the Hartree approximation,[21] in cgs notation, the electron-electron interaction energy is

$$H_{ee}=e^2\sum_{i<j}\int\frac{|\psi_j(\vec{r}_j)|^2|\psi_i(\vec{r}_i)|^2}{|\vec{r}_i-\vec{r}_j|}d\vec{r}_i d\vec{r}_j \tag{16a}$$

$$=\frac{1}{2}\sum_i\langle\psi_i(\vec{r})|V_H(\vec{r})|\psi_i(\vec{r})\rangle=\tfrac{1}{2}\Omega\sum_{\vec{k}}\phi_{\vec{k}}|\rho_{\vec{k}}|^2. \tag{16b}$$

Here ψ_j is the wave function of the jth electron, $\rho_{\vec{k}}=\rho_{-\vec{k}}^{*}$ is the Fourier transform of the electron density,

$$\rho(\vec{r})\equiv\sum_j|\psi_j(\vec{r})|^2=\sum_{\vec{k}}\rho_{\vec{k}}e^{i\vec{k}\cdot\vec{r}}, \tag{17}$$

and $\phi_{\vec{k}}$ is the Fourier transform of the electron-electron interaction

$$\frac{e^2}{|\vec{r}_i-\vec{r}_j|}=\Omega^{-1}\sum_{\vec{k}}\phi_{\vec{k}}e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}, \tag{18a}$$

$$\phi_{\vec{k}}=4\pi e^2/k^2. \tag{18b}$$

In Eq. (16b) we have defined as V_H the potential due to other electrons that an individual electron sees in the Hartree approximation,

$$V_H(\vec{r})=e^2\int\frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}'=\sum_{\vec{k}}\rho_{\vec{k}}\phi_{\vec{k}}e^{i\vec{k}\cdot\vec{r}}. \tag{19}$$

In going from (16a) to (16b) we have dropped an unimportant self-energy term in H_{ee}, which corresponds to the omission of the $i=j$ term in the sum over i and j, and which is relatively smaller by order $1/N_e$, where N_e is the number of electrons.

There are two possible approximations in handling this pseudo-one-dimensional problem: (a) One may consider the crystal as containing $N_\perp$ parallel 1D channels, with the charge-density waves in the different channels to be in phase; or (b) one may take a more one-dimensional approach and consider a single channel ($N_\perp = 1$) and use a modified ϕ_q. We will keep ϕ_q general rather than inserting the specific form (18b). Then both approaches give qualitatively similar results; i.e., in any approximation that uses Eqs. (16b) and (20) (below) with any function ϕ_k, we will obtain the same form [Eq. (37)] for the energy lowering due to a PI and this form will not *explicitly* depend on ϕ_k.

The changes to H_{ee} and V_H due to the Peierls distortion are

$$\Delta H_{ee} = \Omega \phi_q |\rho_q|^2 , \tag{20a}$$

$$\Delta V_H(z) = \sum_{\pm} \rho_{\pm q} \phi_{\pm q} e^{\pm iqz} . \tag{20b}$$

Equations (20) result because in the metallic state nonzero values of $\rho_{\vec{k}}$ will have $\vec{k}$ equal to a reciprocal-lattice vector, so $\vec{k} \neq \vec{q}$, while in the Peierls state there will be a new $\rho_{\vec{k}}$, with, in lowest order, $\vec{k} = \pm\vec{q}$. The Hartree Schrödinger equation[21] is, from Eqs. (14), (15), and (20b):

$$\left(\frac{-\hbar^2}{2m^*} \frac{d^2}{dz^2} + \sum_{\pm} V_{\pm q} e^{\pm iqz} - E_i \right) \psi_i(z) = 0 , \tag{21}$$

where

$$V_q = V_q^0 + \phi_q \rho_q , \tag{22}$$

and E_i is the Peierls state one-electron energy eigenvalue.

V_q is to be considered a perturbation in the solution of Eq. (21). In the rest of this paper we take $k > 0$ to facilitate discussion. Through second order in *non*degenerate perturbation theory, the perturbation couples the state $|k\rangle$ only to the states $|k+q\rangle$ and $|k-q\rangle$. Interaction with other states are of higher order in $V = |V_q|$. However, this is no longer strictly true when second-order *degenerate* perturbation theory must be used, since in this case $|k\rangle$ may also couple to the *one* additional state $|k-2q\rangle$, but then the coupling is of relatively significant order in V only for k near $\frac{1}{2}q$, where $|k\rangle$ and $|k-q\rangle$ are degenerate. We will only be interested in quantities that involve a sum over all electrons, such as total energy or the dielectric function. For such quantities it can be shown that $|k-2q\rangle$ contributes in higher order than $|k \pm q\rangle$. This is because $|k-2q\rangle$ contributes in relatively significant order only for a small range of k near $\frac{1}{2}q$—a range whose width is of higher order in V than $O(1)$. Therefore we will include the interactions of $|k\rangle$ only with $|k+q\rangle$ and $|k-q\rangle$. Of the three states, we treat the interaction between $|k\rangle$ and $|k-q\rangle$ by twofold degenerate perturbation theory, and the interaction with $|k+q\rangle$ by nondegenerate perturbation theory. This will give the change in the total system energy up to and including terms of order V^2.

The results can readily be expressed in terms of the unperturbed electron energy

$$E_k^0 = \hbar^2 k^2 / 2m^* ,$$

the energy shift relative to E_k^0 due to the interaction of $|k\rangle$ and $|k-q\rangle$ alone,

$$\delta(k,q) = \tfrac{1}{2}\{E_{k-q}^0 - E_k^0 + \mathrm{sgn}(k - \tfrac{1}{2}q) \times [(E_{k-q}^0 - E_k^0)^2 + 4V^2]^{1/2}\} , \tag{23}$$

and of the quantity

$$\xi = \hbar^2 q^2 / 2m^* .$$

With

$$\psi_k = a_k |k\rangle + b_k |k-q\rangle + c_k |k+q\rangle , \tag{24a}$$

and

$$|k\rangle = \Omega^{-1/2} e^{ikz} , \tag{24b}$$

one obtains,

$$a_k = \{1 + [\delta(k,q)]^2 / V^2\}^{-1/2} , \tag{24c}$$

$$b_k = \delta(k,q) a_k / V_q , \tag{24d}$$

$$c_k = -V_q a_k / (E_{k+q}^0 - E_k^0) . \tag{24e}$$

One also finds that the energy of an electron in the Peierls state of wave vector $\vec{k} = \vec{k}_z$ is

$$E_k = E_k^0 + \delta(k,q) - V^2 \times (\{1 + [\delta(k,q)]^2 / V^2\}[V^2/\delta(k,q) + 2\xi])^{-1} . \tag{25}$$

For valid results V must be small compared to ξ ($V \ll \xi$) since ξ is the smallest energy distance from $|k\rangle$ to the nearest state other than $|k-q\rangle$, i.e., to states included by nondegenerate perturbation theory.

Using Eqs. (14), (20), and (21) and making the standard correction[21] for overcounting of the Hartree one-particle energies in the ground-state energy, one obtains for the Peierls ground-state energy

$$\langle H_{\mathrm{PS}} \rangle = 2\beta^2 \hbar\omega_q + \sum_i E_i - \Delta H_{ee} = 2\beta^2 \hbar\omega_q + \sum_i E_i - \Omega \phi_q |\rho_q|^2 . \tag{26}$$

The last term, representing an energy lowering, arises from overcounting the interaction energy. It has to be subtracted because the $\sum E_i$ contain the change in the electron-electron interaction energy twice. As we shall see, its contribution is important. Izuyama and Saitoh[22] have taken a qualitative look at the effect of the long-range Coulomb interaction (i.e., ΔH_{ee}). Their conclusions are erroneous because they implicitly use the sum, rather than the difference, of $\sum_i E_i$ and ΔH_{ee}.

The energy difference between the metallic state and the Peierls state is then, in our approximation,

$$\Delta E = \langle H_{\rm PS}\rangle - \langle H_{\rm MS}\rangle = 2\beta^2\hbar\omega_q + \sum_i (E_i - E_i^0) - \Omega\phi_q|\rho_q|^2$$

$$\equiv \Delta E_{\rm ph} + \Delta E_e + \Delta E_{ee}\,, \tag{27}$$

with obvious implicit definitions in the last line.

To evaluate ΔE_{ee} we need to know ρ_q, which, by Eq. (17) can be obtained from a calculation of $\rho(\vec{r})$. In the Appendix we obtain, in a good approximation,

$$\rho_q = (-qV_q/\pi A\xi)\ln|2\xi\delta/V^2+1|\,, \tag{28}$$

where here and below $\delta = \delta(k_F, q)$, and A is the cross-sectional area of a unit cell. We have assumed twofold spin degeneracy.

With Eq. (28), the overcounting contribution to ΔE can be obtained,

$$\Delta E_{ee} = -\Delta H_{ee} = -\Omega\phi_q|\rho_q|^2$$

$$= -\Omega\phi_q^{-1}\alpha(q)^2 V^2 \ln^2|2\xi\delta/V^2+1|\,, \tag{29}$$

where, for later purposes, we have introduced

$$\alpha(q) = 2\phi_q m^*/\pi A\hbar^2 q\,. \tag{30}$$

At $q = 2k_F$ we see that for small V, ΔH_{ee} goes as $+V^2\ln^2 V$, in agreement with the result obtained from a quite different approach (and in a tight-binding approximation) by Izuyama and Saitoh.[22]

The total change in the one-electron energies is obtained in a similar fashion as in the calculation of Eq. (28) in the Appendix:

$$\Delta E_e = \sum_i (E_i - E_i^0) = -N_e\frac{q}{2k_F}\frac{V^2}{\xi} \times\left(\frac{\delta^2}{2V^2} + \ln\left|\frac{2\xi\delta}{V^2}+1\right|\right). \tag{31}$$

Here $N_e = 2N_\perp L k_F/\pi$ is the number of electrons, $N_\perp$ is the number of 1D channels, and L is the length of the crystal.

The phonon contribution to ΔE is

$$\Delta E_{\rm ph} = 2\beta^2\hbar\omega_q\,. \tag{32}$$

But from Eq. (15c) and the self-consistency condition [Eq. (22)], β depends on V and can be eliminated in favor of V. To bring this out let us *define* a static dielectric function

$$\epsilon_q \equiv V_q^0/V_q = 1 - \phi_q\rho_q/V_q\,. \tag{33a}$$

From Eqs. (18), (28), and (33a) we obtain

$$\epsilon_q = 1 + \alpha(q)\ln\left|\frac{2\xi\delta}{V^2}+1\right| \xrightarrow[q=2k_F]{} 1 + \alpha(2k_F)\ln\left|\frac{8E_F}{V}\right|$$

$$\to 1 + \alpha(q)\ln\left|\frac{q+2k_F}{q-2k_F}\right| \quad \text{away from } 2k_F\,. \tag{33b}$$

The form for q away from $2k_F$ is also what nondegenerate perturbation theory gives for all values of q. The 1D static dielectric function is plotted in Fig. 1. Note the nonlinearities at $q = 2k_F$. For comparison, we have also shown in Fig. 1 the Lindhard dielectric function for a 3D electron gas with a spherical Fermi surface [Ziman,[23] Eq. (5.36)]. Equations (15c) and (33a) now relate β and V:

$$\beta = \sqrt{N}V\epsilon_q/2|g_q|\,, \tag{34}$$

and thus Eq. (32) becomes

$$\Delta E_{\rm ph} = \frac{N\hbar\omega_q\epsilon_q^2 V^2}{2|g_q|^2} = \frac{N_e E_F}{2\alpha\gamma}\left(\frac{q}{k_F}\right)^3\left(\frac{V}{\xi}\right)^2\epsilon_q^2\,, \tag{35}$$

where we have defined the important parameter

$$\gamma(q) = 2|g_q|^2(\phi_q\hbar\omega_q N/\Omega)^{-1}\,, \tag{36}$$

which will turn out to be decisive for the occur-

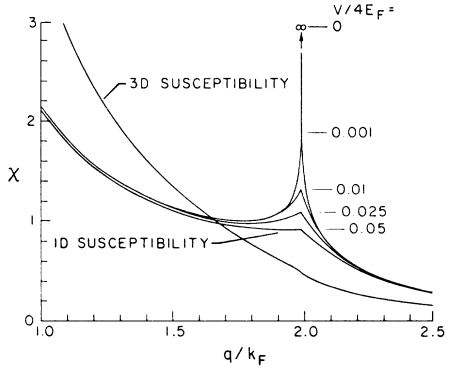

FIG. 1. Susceptibility in 1D and 3D. One-dimensional static susceptibility, $\chi(q,V) \equiv \epsilon_q - 1$ is plotted in units of $4m^*e^2/A\hbar^2k_F^3$. V is constant (not V/ξ) for each curve at the values shown alongside the respective peaks at $q = 2k_F$. The curve for $V = 0$ is the result obtained by nondegenerate perturbation theory. For comparison, the three-dimensional Lindhard susceptibility, $\chi(q)$, is also plotted, in units of $m^*e^2/\pi\hbar^2k_F$. The logarithmic singularity in the slope at $q = 2k_F$ is essentially invisible on this scale of q.

rence of the PI. Note that due to the dependence of ϵ_q near $2k_F$ on V (which is half the Peierls gap), ΔE_{ph} is *not* simply proportional to V^2 as for the unscreened (or even linearly screened) PI. Altogether Eqs. (27), (29), (31), and (35) give for ΔE

$$\frac{\Delta E}{N_e E_F}=\frac{1}{2}\left(\frac{q}{k_F}\right)^3\left(\frac{V}{\xi}\right)^2\left[-\frac{\delta^2}{2V^2}+\frac{1}{\alpha(q)\gamma(q)}+\left(\frac{2}{\gamma(q)}-1\right)\ln\left|\frac{2\xi\delta}{V^2}+1\right|+\alpha(q)\left(\frac{1}{\gamma(q)}-1\right)\ln^2\left|\frac{2\xi\delta}{V^2}+1\right|\right]. \tag{37}$$

The terms involving γ come from the phonon contribution. The remaining terms come from the electrons, with the $\ln^2$ term being the overcounting contribution. $\Delta E<0$ corresponds to an instability. Equation (37) is the central result of this paper. It can be shown, for an almost filled band (i.e., the "hole" case), that if interband coupling is ignored, Eq. (37) results again provided the effective mass and Fermi wave number of the holes are used for m^* and k_F.

IV. ONE-DIMENSIONAL PEIERLS INSTABILITY

A. Instability criteria

We now show that within the range of validity of perturbation theory ($V/\xi \ll 1$), a necessary condition for an instability (i.e., $\Delta E<0$) at any $q \leq 2k_F$ is

$$\gamma(q)>1\,, \tag{38}$$

and that a sufficient condition for an instability at $q=2k_F$ is

$$\gamma(2k_F)>1\,. \tag{39}$$

Later we will see that the greatest instability (i.e., minimum of ΔE) will not necessarily occur at $q=2k_F$, but that it may occur at some smaller value of q, corresponding to a gap *below* the Fermi level. We will comment about the situation for $q>2k_F$ later.

We assume that there is no static antiscreening; i.e., that $\alpha(q)>0$ so that $\epsilon_q>1$. We consider first the energetics at $q=2k_F$. In this case $\delta=V$, and Eq. (37) reduces to

$$\frac{\Delta E}{N_e E_F}=4\left(\frac{V}{4E_F}\right)^2\left[-\frac{1}{2}+\frac{1}{\alpha\gamma}+\left(\frac{2}{\gamma}-1\right)\ln\left(\frac{2\xi}{V}+1\right)+\alpha\left(\frac{1}{\gamma}-1\right)\ln^2\left(\frac{2\xi}{V}+1\right)\right]. \tag{40}$$

For small enough V the $\ln^2$ term dominates and if Eq. (39) is satisfied, $\Delta E(2k_F)<0$. Hence Eq. (39) is a sufficient condition for a PI to occur, at least at $q=2k_F$, with possibly an even lower energy for a different q.

In order to show that Eq. (38) is a necessary condition, consider $\gamma(q)=1$, for any $q \leq 2k_F$. Then by Eq. (37),

$$\frac{\Delta E(q,\gamma=1)}{N_e E_F}\geq\frac{1}{2}\left(\frac{q}{k_F}\right)^3\left(\frac{V}{\xi}\right)^2\left(-\frac{\delta^2}{2V^2}+\ln\left|\frac{2\xi\delta}{V^2}+1\right|\right). \tag{41}$$

In order to obtain $\Delta E(q,\gamma=1)<0$, Eq. (41) demands

$$\ln\left|2\xi\delta/V^2+1\right|<\delta^2/2V^2\,,$$

or

$$1+2\xi\delta/V^2<e^{\delta^2/2V^2}\,. \tag{42}$$

But for $q \leq 2k_F$, $0<\delta/V\leq 1$ and in this range of δ/V

$$e^{\delta^2/2V^2}\leq 1+(\sqrt{e}-1)\delta/V\,. \tag{43}$$

Thus Eq. (42) would demand

$$V/\xi>2/(\sqrt{e}-1)\approx 3.08>1\,.$$

But this lies outside the range of validity of our perturbation theory, and it probably reflects the breakdown of the approximations used rather than a true decrease in energy for such a large value of V. Moreover, we shall see that when $V\gtrsim\xi$, the lattice distortions are comparable to or larger than the lattice periodicity, and hence the details of the neglected anharmonic lattice interactions will be important. Thus Eq. (42) is not fulfilled in the region of validity of our perturbation theory, and hence, at least for this region, we must have $\Delta E(q\leq 2k_F,\gamma=1)>0$. Furthermore, by inspection of Eq. (37) for ΔE, one sees that

$$\Delta E(q,V,\gamma(q)<1)>\Delta E(q,V,\gamma(q)=1)\,.$$

Thus $\gamma(q)>1$ is a necessary condition to have $\Delta E(q\leq 2k_F)<0$, at least for $V\ll\xi$.

Our proof does not apply for $q>2k_F$ where $\delta<0$. However, using Eqs. (42) and (43), with appropriate sign changes, and also Eq. (23) for δ, one can show that if $V/\xi<1$, an instability for $q>2k_F$, not satisfying Eq. (38), would require at least $V/\xi>k_F/q$. This rules out such an instability for arbitrarily small V for any given $q>2k_F$. In the specific examples we have considered, no instabilities with $q>2k_F$ were found that did not satisfy Eq. (38), and we consider such instabilities unlikely. Furthermore, a $q>2k_F$ instability would lead to a gap above the Fermi level and would therefore not be particularly interesting.

Note that it is the coefficient of the $\ln^2$ term in ΔE that determines whether an instability will occur. The α/γ part of this coefficient is from part of the phonon contribution to ΔE due to

screening. The $-\alpha$ part of this coefficient is from the overcounting contribution to ΔE. This entire $\ln^2$ term is absent from the free-energy expression in the case of the unscreened PI. Thus, the temperature dependence of the gap cannot be assumed to be the BCS type as obtained in treatments of the unscreened PI.

It is also interesting to note that even if the *linear* response dielectric function were used, which diverges at $2k_F$, we would still obtain the instability requirement $\gamma > 1$ in the (appropriate!) limit of large ϵ.

B. Instability gap

The instability at $q \leq 2k_F$ that will occur for $\gamma(2k_F) > 1$, will put an energy gap of magnitude $2V$ at or below the Fermi level. For $q = 2k_F$, the value of V that minimizes Eq. (40) for ΔE is given by

$$\ln\left(\frac{V}{8E_F}\right) = \frac{a-b}{c} - \frac{1}{2} - \left[\left(\frac{a-b}{c} - \frac{1}{2}\right)^2 + \frac{b^2}{c} - \frac{b}{c}\right]^{1/2}, \tag{44}$$

where $a = \gamma/2\alpha$, $b = 1/\alpha$, and $c = \gamma - 1$. Equation (44) can be compared to the unscreened PI results of Refs. 1–4, obtainable by putting $\phi_q = 0$ for the implicit dependences on ϕ_q in Eqs. (37) or (44). At $q = 2k_F$, this results in an energy minimum at

$$\ln(V/8E_F) = -1/\gamma\alpha . \tag{45}$$

This differs from the literature[2-4] by a factor of 2 in the argument of the logarithm. The difference is due to our having included the state $|k+q\rangle$ in the perturbation analysis of $|k\rangle$, rather than just the more important states $|k\rangle$ and $|k-q\rangle$. If we had omitted $|k+q\rangle$, the only change in Eq. (37) would be in the argument of the logarithms, with

$$\ln|2\xi\delta/V^2 + 1| \to \ln|\xi\delta/V^2| .$$

Thus at $q = 2k_F$, $8E_F$ would have been replaced by $4E_F$ on the left-hand side of Eqs. (44) and (45), in agreement with the literature.

It is most important to realize that Eq. (44) is generally *not* useful for determining the actual magnitude of V. Equation (44) will generally give $V \gtrsim \xi$ for the value of V at the energy minimum, and is thus unreliable as our treatment is only valid for $V \ll \xi$. Only when γ is greater than but about equal to 1 is $V \ll \xi$ found by Eq. (44) for the energy minimum at $q = 2k_F$. There apparently is no simple expression, derived from Eq. (44), for how close γ has to be to 1 to have $V \ll \xi$. In practice, plots of Eq. (44) show that the upper limit γ_0 of this range is a quantity of the order of $1 + 1/\alpha(2k_F)$; $1/\alpha$ is typically less than or about equal to 1; although in the limit of no electron-electron interaction it is infinite.

When Eq. (44) predicts $V \gtrsim \xi$ the actual gap is probably determined by anharmonic couplings involving the entire lattice. In the special cases considered below we find that even when $V/\xi = \frac{1}{8}$, the lattice distortions have an amplitude of about 20% of the ion-ion distance.

When $1 < \gamma < \gamma_0$ so that Eq. (44) gives $V \ll \xi$, we find, in the special cases considered below, that the energy has a second minimum at $q < 2k_F$ and that this minimum is the absolute minimum in energy. In this case the gap would be below the Fermi surface. Thus Eq. (44), if used at all, must be used with reservations.

C. Two special cases of the Peierls instability

In order to proceed further, we have to become more specific about the nature of the solid. We shall assume the unscreened longitudinal phonon Hamiltonian to be

$$H_{\rm ph} = \frac{M}{2}\sum_j (\delta\dot{R}_j)^2 + \sum_j [c_1(\delta R_{j+1} - \delta R_j)^2 + c_2(\delta R_j)^2] , \tag{46}$$

where c_1 and c_2 are force constants and δR_j is the displacement of the jth ion of mass M ($\delta\vec{R}_j \| \vec{z}$). With certain assumptions, such a Hamiltonian may be used for an acoustic (Debye) phonon by putting $c_2 = 0$. It can also be used for an Einstein-like vibration by putting $c_1 = 0$. For this Hamiltonian, it can be shown, by the usual elementary techniques, that

$$\delta R_j = \sum_{\vec{k}} \left(\frac{\hbar}{2NM\omega_{\vec{k}}}\right)^{1/2} (b_{\vec{k}} + b^{\dagger}_{-\vec{k}}) e^{i\vec{k}\cdot\vec{R}_j} , \tag{47}$$

$$\omega_q^2 = (2/M)[2c_1(1 - \cos qd) + c_2] , \tag{48}$$

where the R_j are the undistorted equilibrium positions of the ions, which are separated by d, and where ω_q is the bare phonon frequency.

For ions of charge Ze that satisfy Eq. (47), the electron-phonon coupling constant is given by

$$g_q = i\left(\frac{\hbar}{2M\omega_q}\right)^{1/2} \frac{N}{\Omega} \frac{4\pi Ze^2}{q} \tag{49}$$

(see, for example, Pines,[24] pp. 230–240). Using Eqs. (47), (49), (12), (33), and (34), we find for the Peierls state

$$\langle \delta R_j \rangle = \Delta R \cos(\vec{q}\cdot\vec{R}_j) ,$$

where

$$\Delta R = \frac{2d}{\pi Z}\left(\frac{V}{\xi}\right)\left(\ln\left|\frac{2\xi\delta}{V^2} + 1\right| + \frac{1}{\alpha}\right) . \tag{50}$$

At $q = 2k_F$,

$$\Delta R \gtrsim \frac{2d}{\pi Z}\left(\frac{V}{4E_F}\right)\left(\ln\frac{8E_F}{V}\right). \tag{51}$$

The amplitude, ΔR, in Eq. (51) does not depend explicitly on q or ω_q. This allows some quantitative estimates. With $Z=1$, $V=0.1E_F$, $\Delta R \gtrsim 0.07d$, while at $V=0.5E_F=\frac{1}{8}\xi$, $\Delta R \gtrsim 0.22d$. For a distortion with a 20 Å period (as in KCP) and for $m^*=m_e$, $\xi=0.38$ eV. The gap is equal to $2V$, and so V's that are not too small a fraction of ξ are of interest. As we see, such V's lead to distortions that are sizable fractions of the interatomic distances. Moreover, in Sec. IV B, we saw that typically the gap would have $V \gtrsim \xi$ which implies still larger fractions. Thus we see the likely importance of anharmonic couplings. We can get an idea of the size of displacement at which anharmonicities are of critical importance by noting that the Lindemann melting criterion has sodium and a number of other metals melting when the rms vibration of an atom (associated with acoustic phonons) is about $\frac{1}{8}$ the interatomic spacing (Pines,[24] pp. 34–37).

The importance of anharmonicities in limiting the size of the Peierls gap suggests that the Peierls gap (or charge-density wave) may be tied to the entire lattice like the ordinary *immobile* gaps found in insulators and semiconductors, which do not exhibit a Fröhlich collective mode.

For our model, γ of Eq. (36) simplifies to

$$\gamma(q)=\omega_{pl}^2/\omega_q^2. \tag{52}$$

Equation (52) leads to the simple criterion $\omega_q<\omega_{pl}$ for the occurrence of a PI, at some $q \leq 2k_F$. Recall that this is a necessary criterion for $q \leq 2k_F$ and that it is also sufficient at $q=2k_F$. It is generally rather easy to satisfy though usually γ will be of order 1 rather than being much bigger (unless $\omega_q \propto q$ and q is small).

To carry our investigation of this particular example of a PI further, we first specialize Eq. (48) to $\omega_q=$ const, as for a phonon with an Einstein spectrum. Such would be the case for an ion "rattling loosely in a crystal cage."[25] (It corresponds to a longitudinal optical phonon.) Anharmonicities and the dipole associated with the vibration may favor such a phonon over an acoustic one.

We now describe an extensive graphical study of ΔE of Eq. (37). $\Delta E/N_eE_F$ depends on the independent variables $\gamma(2k_F)$, q/k_F, V/ξ, and $\alpha(2k_F)$. γ was varied between 0 and 20; q/k_F between 0.1 and 5, and V/ξ between 0 and about 0.5; $V/\xi \ll 1$ is required for our treatment to be valid. With ϕ_q of Eq. (18b), $m^*=m_e$, $A=(10\text{ Å})^2$ (as in KCP), and the wavelength of the Peierls distortion, $2\pi/q=20$ Å (as in KCP), one finds $\alpha(2k_F)\approx 5$. Since $\alpha(2k_F)$ goes as $m^*(2k_F)^{-3}$, a considerable range of α may be of interest. Thus, α was varied between 0.1 and 1000.

The behavior of ΔE as a function of q/k_F is shown in Figs. 2 and 3. In both the figures $\alpha(2k_F)=5$. Figure 2 shows $\Delta E(q/k_F)$ for fixed $V/\xi=0.05$ and different values of $\gamma(2k_F)$. Figure 3 shows $\Delta E(q/k_F)$ for fixed $\gamma(2k_F)=1.06$ and different values of V/ξ. It is found that an instability only occurs for $\gamma>1$, as was expected. [In this example, $\omega_q=$ const so that γ is independent of q and the instability conditions, Eqs. (38) and (39), coalesce.] When $\gamma>\gamma_0(\approx 1.05$ in Fig. 2) nothing unusual happens: There is a single energy minimum, which is at $q=2k_F$ for all $V \ll \xi$, and which gets deeper with increasing γ. However, when $1<\gamma<\gamma_0$ a second minimum for which $\Delta E<0$ appears at $q<2k_F$, typically for q between 1.0 and $1.5k_F$. Toward the smaller values of γ in this range, for fixed V/ξ, this secondary minimum is the absolute minimum, at least within the region of validity of our perturbation theory ($V \ll \xi$). Increasing V/ξ keeping γ fixed favors the secondary minimum and moves it slightly towards smaller q (Fig. 3).

The secondary minimum does not approach arbitrarily closely to $q=2k_F$. When the secondary minimum exists, it is unbounded for increasing V/ξ, at least within the region of validity of perturbation theory. Meanwhile, when there is a secondary minimum, the primary minimum at $q=2k_F$ *is* bounded by some value of V/ξ. This can be seen in Fig. 3.

The possibility of the gap preferentially forming *below* the Fermi level is connected with the fact that there are two peaks in the dielectric function (Fig. 1), the second being at $q=0$. To bring this out we rewrite Eq. (37) as

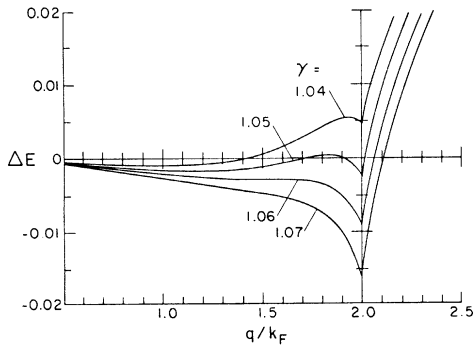

FIG. 2. $\Delta E(q/k_F)$ for different γ ($\omega_q=$ const). ΔE in units of N_eE_F is shown for different values of $\gamma(2k_F)$ and for fixed $\alpha(2k_F)=5$, and $V/\xi=0.05$. (V/ξ is constant, not $V/4E_F$.) When $\gamma>1$ is small enough, the absolute minimum is at $q<2k_F$.

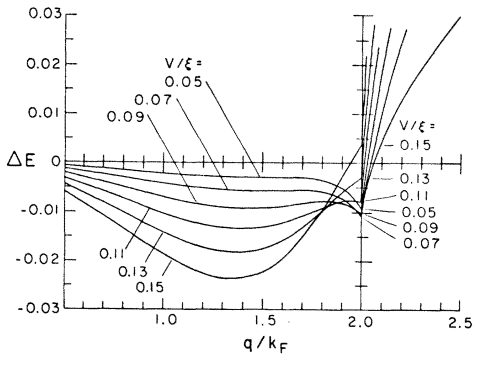

FIG. 3. $\Delta E(q/k_F)$ for different V/ξ ($\omega_q = \text{const}$). ΔE in units of $N_e E_F$ is shown for different values of V/ξ and for fixed $\gamma(2k_F) = 1.06$, and $\alpha(2k_F) = 5$. V/ξ, not $V/4E_F$, is constant along each curve. Absolute minimum is at $q < 2k_F$.

$$\frac{\Delta E}{N_e E_F} = \frac{1}{2}\left(\frac{q}{k_F}\right)^3\left(\frac{V}{\xi}\right)^2 \frac{1}{\alpha(q)} \times \left[\frac{-\alpha(q)\delta^2}{2V^2} + \epsilon_q + \epsilon_q^2\left(\frac{1}{\gamma} - 1\right)\right]. \quad (53)$$

The sum of the first two terms in the large square brackets is greater than one, at least for $q \lesssim 2k_F$. If we suppose γ is independent of q and just slightly greater than one, then ϵ_q must be large enough in order to make $\Delta E < 0$. At $q = 2k_F$, ϵ_q can be made large enough by decreasing V. Alternatively, ϵ_q can be made larger by going to smaller q. At $2k_F$, ϵ_q goes approximately as $\ln(8E_F/V)$ while for $q \lesssim k_F$, ϵ_q goes as $1/q^2$. Therefore, ϵ_q can be increased much faster by decreasing q than by decreasing V at $q = 2k_F$. In fact, V must be decreased exponentially to make a comparable change in ϵ_q. However, since ΔE has an overall factor of V^2, an exponential decrease in V will make $|\Delta E|$ very small so that energetically it is more favorable to increase ϵ_q by decreasing q—i.e., by forming the gap *below* the Fermi surface.

We cannot predict what will happen for $V \gtrsim \xi$, as this is too large a perturbation for our perturbation theory to be valid. Moreover, the distortions will then be larger than or comparable to the lattice period, as we saw below Eq. (51), and the neglected anharmonic interactions will then be quite important.

While our example has used $\omega_q = \text{const}$ so that $\gamma(q)$ of Eq. (52) is independent of q, similar behavior is obtained for an acoustic (Debye) type of dispersion, $\omega_q \propto q$. This is because the necessary condition for a PI, $\gamma(q) > 1$, is satisfied at $q < 2k_F$ before it is satisfied at $q = 2k_F$, as $\gamma \propto 1/q^2$ in this case. Thus if ϵ_q in Eq. (53) is large enough, ΔE will become negative first for $q < 2k_F$. Hence for an acoustic phonon the gap will also form first *below* the Fermi level and then move up to the Fermi level when γ becomes somewhat larger. This is seen in Fig. 4.

There are several differences from the first case for this Debye case. $|\Delta E|$ is considerably larger for the $q < 2k_F$ energy minimum and this minimum can approach continuously to $2k_F$. If we now define γ_0 more generally so that when $\gamma(2k_F) > \gamma_0 > 1$ the gap is at the Fermi level, then in the Debye case γ_0 is no longer roughly of order $1 + 1/\alpha(2k_F)$ as in the Einstein case. Furthermore, since $\gamma(q) \propto q^{-2}$ even if $\gamma(2k_F) \ll 1$, $\gamma(q)$ will be greater than one for small enough q so that a gap is always likely to form at small q. That this is indeed the case can be shown by examining the sign of $\Delta E(q)$ in the small q limit. However, the energy lowering due to such a gap forming may be almost negligible. In addition, the gap itself may be quite small since anharmonicities probably limit V to being less than ξ ($= \hbar^2 q^2/2m^*$) and ξ is small for small q. With these two examples we see a richness of possible effects that will depend on the size of γ and the actual q dependence for the crystal of interest.

It is interesting to consider how the instability requirement, $\gamma(q) > 1$, is related to the softening of the Kohn-screened[26] phonon frequencies. When both electron-electron and electron-phonon interactions are included, the screened phonon frequency, $\omega_s(q)$, is given, in our notation, by

$$\omega_s^2(q) = \omega_q^2 - \omega_q^2\gamma(q)(1 - 1/\epsilon_q) = \omega_q^2[1 - \gamma(q)] + \omega_q^2\gamma(q)/\epsilon_q$$

[Pines,[24] Eq. (5–29)]. Clearly $\gamma(q) > 1$ is a necessary condition to have $\omega_s^2(q) < 0$ and at $q = 2k_F$ it

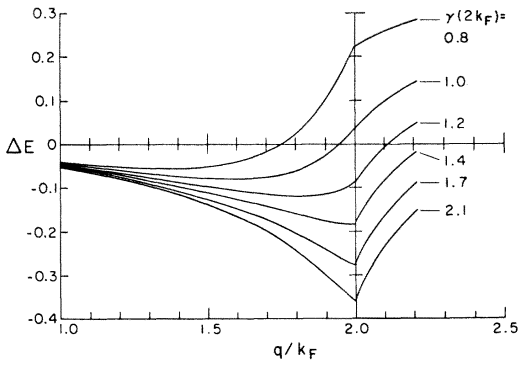

FIG. 4. $\Delta E(q/k_F)$ for different $\gamma(2k_F)$ ($\omega_q \propto q$). ΔE in units of $N_e E_F$ is shown for different values of $\gamma(2k_F)$ and for fixed $\alpha(2k_F) = 5$, and $V/\xi = 0.05$; $\omega_q \propto q$ is assumed here. For $\gamma(2k_F) \lesssim 1.4$ the minimum is at $q \lesssim 2k_F$. This could result in a gap very close to, but below, the Fermi level.

is also sufficient in the limit of small V, since ϵ_q at $q=2k_F$ then diverges. Thus we have the same necessary condition needed to make both $\Delta E(q)<0$ and $\omega_s^2(q)<0$, and the same sufficient condition for $q=2k_F$ at $V\to 0$. However, at finite V one may (and sometimes does!) have $\omega_s^2(q)>0$ for some $\gamma(q)>1$, while at the same time having $\Delta E(q)<0$. One may easily show that $\omega_s^2(q)>0$ whenever

$$0<\gamma(q)-1<(\epsilon_q-1)^{-1}.$$

However, it is possible to have $\gamma(q)-1$ in this range and at the same time have $\Delta E(q)<0$. An example is the curve for $\gamma(2k_F)=1.05(000)$ in Fig. 2. For the parameters in that figure $(\epsilon_q-1)^{-1}=0.054$, so $\gamma=1.050$ makes $\Delta E(2k_F)<0$ while having $\omega_s^2(2k_F)>0$ [here $\omega_s(q)=0.06\omega_q$ at $q=2k_F$]. Thus for finite V at $q=2k_F$, if $\omega_s^2(q)>0$, it is *possible* that an instability will occur, while if $\omega_s^2(q)<0$, it is *certain* that an instability will occur. Note that the distinction is only important in the region $1<\gamma(q)\approx 1$, the same region in which the gap may be at $k<k_F$.

V. EFFECT OF EXCHANGE AND CORRELATION

A Hartree treatment gives a better account of simple 3D metals than a Hartree-Fock treatment (Pines,[24] esp. pp. 81–85), with the worst problem of the Hartree-Fock treatment occurring in the important region near the Fermi surface, where it leads to a unrealistic vanishing of the density of states. To get an improvement over a Hartree treatment, exchange (that is Hartree-Fock) and correlation effects must be considered together. We will assume a local-field approximation for assessing the effects of exchange and correlation and base our expectations on an analogy with the much-studied 3D electron gas.

Ours is a perturbation problem. The perturbation of the local exchange-correlation field results in an additional induced potential which brings about a modification to ϵ_q. For the 3D electron gas, inclusion of the local-field correction results in[27]

$$\epsilon_q=1+\chi(q)\to\epsilon_q=1+\chi(q)[1-G(q)],$$

or since $\chi(q)\propto\phi_q$,

$$\phi_q\to\phi_q[1-G(q)].$$

A closer look will show that, in a local-field approximation, this modification of ϕ_q will appropriately correct each of the terms of ΔE in Eq. (37) for exchange and correlation.

In an approximate treatment, Hubbard[28] found

$$G(q)=\tfrac{1}{2}[q^2/(q^2+k_F^2)],$$

which varies between 0 and $\frac{1}{2}$. Recently, Niklasson[29] obtained the exact result $\frac{1}{3}<G(\infty)<\frac{2}{3}$, which suggests that $G(q)$ is between 0 and $\frac{2}{3}$. If this is so, then the effect of exchange and correlation is simply to modify ϕ_q by a factor between 1 and $\frac{1}{3}$. This is merely a quantitative, not qualitative, modification of ΔE of Eq. (37), since Eq. (37) is valid for general ϕ_q, not merely the ϕ_q given in Eq. (18). A reduced ϕ_q results in smaller $\alpha(q)$ and larger $\gamma(q)$. Since the instability criterion is $\gamma>1$, the instability occurs more readily; however, ΔE is not then necessarily more negative. In this sense exchange and correlation favor the PI.

APPENDIX: CALCULATION OF ρ_q

From Eqs. (17) and (24)

$$\rho(z)=\sum_{\substack{-k_F<k<k_F\\ \text{spins}}}|\psi_k|^2=\frac{2N_\perp}{\Omega}\sum_{\substack{0<k<k_F\\ \text{spins}}}(a_kb_k^*+a_k^*c_k)e^{iqz}+\text{c.c.}+\text{const.}+e^{\pm 2iqz}\times(\text{terms of higher order in } V/\xi).$$

From Eq. (17) we get

$$\rho_q=\frac{4N_\perp}{\Omega}\sum_{0<k<k_F}(a_kb_k^*+a_k^*c_k)=\frac{4LN_\perp}{2\pi\Omega}\int_0^{k_F}dk(a_kb_k^*+a_k^*c_k),\tag{A1}$$

where the additional factor of 2 comes from summing over two spin states. To perform this integral (and all others needed in this paper), we replace k in Eq. (A1) in favor of $\delta(k,q)$ of Eq. (23). This is fruitful because k^2 terms cancel leaving the simple result

$$k=\frac{[-\delta(k,q)+V^2/\delta(k,q)+\xi]m^*}{\hbar^2q}.$$

With the help of Eqs. (24), Eq. (A1) becomes, after a little algebra,

$$\rho_q=\frac{-q}{\pi A}\frac{V_q}{\xi}\int_{\delta(0,q)}^{\delta(k_F,q)}d\delta\frac{1}{\delta+V^2/2\xi},$$

where $A=\Omega/N_\perp L$ is the cross-sectional area of a unit cell. If $q\geq 2k_F$, the integration gives

$$\rho_q=\frac{-q}{\pi A}\frac{V_q}{\xi}\ln\left|\frac{\delta(k_F,q)+V^2/2\xi}{\delta(0,q)+V^2/2\xi}\right|.\tag{A2}$$

Using a Taylor expansion on $\delta(0,q)$ that requires $V<\frac{1}{2}\xi$:

$$\delta(0,q)=-V^2/\xi+O(V^4/\xi^3),\tag{A3}$$

we obtain

$$\rho_q = \frac{-q}{\pi A}\frac{V_q}{\xi}\ln\left|\frac{2\xi\delta(k_F,q)}{V^2}+1\right|. \tag{A4}$$

For $q<2k_F$, the integral must be broken up into two pieces at $k=\frac{1}{2}q$ because of the discontinuity in $\delta(k,q)$ at $k=\frac{1}{2}q$. When this is done and the approximation in Eq. (A3) is used, Eq. (A4) results again. Without such an approximation one would have to deal with two different expressions according to whether $q>2k_F$ or not.

Equations (A4) and (28) for ρ_q have a discontinuity at $q=2k_F$ that is an artifact of using the approximation (A3) and that is insignificant in this order of calculation. Without the approximation (A3), ρ_q is continuous. However, in addition, there is a real physical discontinuity in the *slope* of ρ_q at $q=2k_F$.

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