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Self-Consistent Electron-Phonon Coupling in the Tight-Binding Approximation. II[*]

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The validity of the rigid-atom model for electron-phonon coupling in the tight-binding approximation is examined within the linearized self-consistent theory. It is shown that the deformation-induced charge-density wave will generally reduce the strength of the coupling, thus reducing the Kohn anomaly in the phonon spectrum and the superconducting transition temperature computed from the rigid-atom model. The charge-density wave does not appear for certain modes; the optimal situation is that of the (nearly) half-filled band, when the rigid-atom model gives approximately correct results.

I. INTRODUCTION

In Paper I of this work, referred to as I, an electron-phonon coupling model was examined. In I the long-range repulsive force acting between tightly bound electrons displaced by deformation was neglected. The elimination of the long-range part of the interaction can be attributed, by usual but more or less hand-waving arguments, to light conduction electrons, which, owing to their high mobility, are the only electrons effectively contributing to the screening. In particular, the model Hamiltonian describing the deformed lattice was shown, in this approximation, to be just a simple extension[1] of the Hubbard Hamiltonian of a narrow band. Such a picture probably gives a fairly correct physical description of transitional metals, but is not entirely satisfactory as far as a basic understanding is concerned.

There exists, on the contrary, a simple situation, which can be, at least mentally, formulated from first principles, with successive approximations which are much more clearly distinguishable. This is the case of an isolated narrow band, i.e., of the band which is assumed to be also the only conducting band present. Then, if any long-range forces appear in the crystal, they can only be screened by the narrow-band electrons. It is probable that the real physical situation in transition metals is intermediate[2,3] between these two models—one of complete screening and one of no screening by s-p electrons. It is thus of interest to examine this latter model too. In this model, there is added to the coupling which arises from the rigid-atom potential a term coming from the potential due to the redistribution of electrons over sites in the deformed state. This correction to the electron-phonon coupling will be shown to arise from the same kind of approach as that now currently used[4,5] in the study of the stability of one-dimensional systems.

The resulting self-consistency problem can be solved for some simple situations in the adiabatic approximation. However, the complete adiabatic solution is available only for one-dimensional systems. New effects are found for a partially filled band (nonintegral number of electrons per atom). Of course, such a supposition is, strictly speaking, inconsistent with the initial assumptions of a nondegenerate band and a perfect crystal; it can, however, occur when several narrow bands overlap, as in actual transition metals. The author believes that the present results extend to this latter case, although he has not examined it in detail.

General expressions are given for an arbitrary frequency ω; however, in actual computations the adiabatic ($\omega = 0$) limit is always used, except in the computation of the lifetime of a one-dimensional phonon. The notations used here are the same as in I.

II. SELF-CONSISTENT POTENTIAL AND CORRESPONDING PHONON SELF-ENERGY

In Sec. II of Paper I we argued that, owing to the breakdown of the translational symmetry, the probability density of an electron on site i,

$$\rho_i = 2\sum_{l\,\mathrm{occ}} |a_i^l|^2 ,$$

is generally altered in the deformed state. Therefore an excess charge $e\delta\rho_i d^2(\vec{r}-\vec{R}_i-\vec{u}_i)$ appears on the site i. $\delta\rho_i$ is the charge-density wave (CDW) on the site i and $\delta\rho_i = \rho_i - Q$ where Q is the number of electrons per atom in the band. $d(\vec{r}-\vec{R}_i-\vec{u}_i)$ is the local tight-binding wave function, centered on the position $\vec{R}_i+\vec{u}_i$, where $\vec{R}_i$ is the equilibrium position of the ion and $\vec{u}_i$ its displacement. This excess charge gives rise to a potential seen at the point $\vec{r}$:

$$\delta V(\vec{r}) = \sum_i \delta\rho_i \int \frac{e^2 d^2(\vec{r}\,'-\vec{R}_i-\vec{u}_i)}{|\vec{r}-\vec{r}\,'|}\, d^3r' . \qquad (2.1)$$

This potential is a superposition of long-range contributions from all sites i of the crystal, since we assume the long-range forces to act between d electrons. It represents a correction to the rigid-atom potential, this latter being self-consistent, when d functions are moved as in Eq. (2.1), only with a uniform electron distribution over sites.

This potential should thus be added to the rigid-atom potential acting on the left-hand side of Eq. (2.6) of I, which in this way becomes

$$\left[\left\langle d(\vec{r}-\vec{R}_j-\vec{u}_j)\right|\left(\frac{p^2}{2m}+V(\vec{r}-\vec{R}_j-\vec{u}_j)+\delta V(\vec{r})\right)\left|d(\vec{r}-\vec{R}_j-\vec{u}_j)\right\rangle - E_l\right] a_j^l$$

$$= -\sum_{\delta\neq 0}\langle d(\vec{r}-\vec{R}_j-\vec{u}_j)|\,V(\vec{r}-\vec{R}_{j+\delta}-\vec{u}_{j+\delta})\,|d(\vec{r}-\vec{R}_{j+\delta}-\vec{u}_{j+\delta})\rangle a_{j+\delta}^l . \qquad (2.2)$$

Here we retain only the forces of the longest range and thus neglect the matrix elements of the type $\langle d_{j+\delta}|\,\delta V(\vec{r})\,|d_j\rangle$ for $\delta \neq 0$.

The potential which acts on the electron is the superposition of the rigid-atom potential and a corrective term arising from small departures at each site from electrical neutrality. Here we treat the Hartree term (2.1) in the linearized approximation, i.e., we calculate the linear self-consistent response in $\delta\rho_i$ to the deformation $\vec{u}_j$. This completes the linearization procedure undertaken in Eq. (3.2) of I.

In order to shorten the actual calculations, we establish the mathematical analogy of such an approach with the more usual jellium calculation. First, we take the matrix element of the potential (2.1) on the left-hand side of the Eq. (2.2) so that the Eq. (3.3) of I is extended to

$$(E_l - \delta U_j - E_0)a_j^l = (K + V_{\mathrm{BS}})a_j^l , \qquad (2.3)$$

where

TABLE I. The formal correspondence between the jellium and tight-bonding quantities entering the computation of the electron-phonon interaction.

	Direct space	Unperturbed state	Unperturbed energy	Charge variation	Potential independent of charge variations $\delta\rho$	Induced potential	Zeroth-order phonon frequency
Jellium	$\vec{r}$	$e^{i\vec{p}\vec{r}}$	$\frac{p^2}{2m}$	$\delta\rho(\vec{r})$	potential of the external field	$\int \frac{e^2\delta\rho(\vec{r}\,')}{\lvert\vec{r}-\vec{r}\,'\rvert} d^3\vec{r}\,'$	Ω_p (ion plasma fr.)
Tight binding	j	$\exp(i\sum_\alpha l_\alpha j_\alpha)$	$2\sum_\alpha J(\vec{a}_\alpha)\cos l_\alpha$	$\delta\rho_j$	V_{BS}	$\delta U_j \approx \sum_i \frac{e^2\delta\rho_i}{\lvert\vec{R}_j-\vec{R}_i\rvert}$	$\omega^0_{s\lambda}$ (see Sec. III of I)

$$\delta U_j = \textstyle\sum_i \delta\rho_i V(\vec{R}_j, \vec{R}_i) \,, \tag{2.4}$$

with

$$V(\vec{R}_j, \vec{R}_i) = \int \frac{e^2 d^2(\vec{r}-\vec{R}_j) d^2(\vec{r}\,'-\vec{R}_i)}{\lvert\vec{r}-\vec{r}\,'\rvert} d^3r\, d^3r' \,. \tag{2.5}$$

For large distance $\lvert\vec{R}_j-\vec{R}_i\rvert$, the matrix element (2.5) reduces to $e^2/\lvert\vec{R}_j-\vec{R}_i\rvert$. This long-range behavior requires, by usual arguments, a self-consistent treatment of $\delta\rho_i$. We can thus establish the correspondence between the quantities appearing in the jellium and the tight-binding approach shown in Table I. Thus the rigid-atom coupling constant (3.7) of I arising from V_{BS} plays the role of the unscreened coupling constant in the jellium case. The charge variations are described by the correlation function $\langle \rho_{j+\delta}(t), \rho_j\rangle$ instead of $\langle \rho(\vec{r}\,', t)\rho(\vec{r}, 0)\rangle$. In the calculation of this correlation function we can obviously use the same diagram rules as in the free-electron case,[6] but keeping in mind that the space dual to j is l. Physically at least the nontrivial modification arises from the fact that the rigid-atom coupling constant depends not only on the momentum transfer s, but also on the initial electron state l, unlike the free-electron bare-coupling term.

In respect to Table I the zeroth-order Green's functions are to be taken as

$$G^0(l, \omega') = [\omega' - E_l + i\delta \operatorname{sgn}(E_l - E_F)]^{-1} \tag{2.6}$$

for electrons with energy $E_l = 2\sum_\alpha J(\vec{a}_\alpha)\cos l_\alpha$ and wave vector l, and

$$D^0_\lambda(s, \omega) = 2\omega^0_{s\lambda}/(\omega^2 - \omega^{0\,2}_{s\lambda} + i\delta) \tag{2.7}$$

for phonons of wave vector s, polarization λ, and frequency $\omega^0_{s\lambda}$. As pointed out in I, $\omega^0_{s\lambda}$ should vanish in the long-wavelength limit.

The "screened" electron-phonon interaction $\bar{g}^\lambda_{ls}$ is given by the usual diagrammatic expression[6] shown in Fig. 1. g^λ_{ls} is the coupling constant arising from the rigid-atom potential V_{BS}, Eq. (3.7) of I, and V^s_{SC} is the Fourier component of the matrix element $V(R_j)$, Eq. (2.5), screened within random phase approximation (RPA), as shown in Fig. 2. V^s is the Fourier transform of $V(\vec{R}_j)$ itself:

$$V^s = (1/N)\textstyle\sum_j V(\vec{R}_j)\exp(i\sum_\alpha s_\alpha j_\alpha) \,. \tag{2.8}$$

Defining

$$P_s(\omega) = \frac{2i}{N}\sum_l \int \frac{d\omega'}{2\pi} G^0(l, \omega') G^0(l+s, \omega+\omega') \,, \tag{2.9}$$

$$Q_s(\omega) = \frac{2i}{N}\sum_l g^\lambda_{ls} \int \frac{d\omega'}{2\pi} G^0(l, \omega') G^0(l+s, \omega+\omega') \,, \tag{2.10}$$

and using the usual diagram rules, we read Figs. 1 and 2 and obtain

$$\bar{g}^\lambda_{ls} = \left(\frac{\hbar^2}{2NM\omega^0_{s\lambda}}\right)^{1/2} \bar{I}^\lambda_{ls} = g^\lambda_{ls} - V^s_{SC} Q^\lambda_s \,, \tag{2.11}$$

$$V^s_{SC} = V^s - V^s P_s V^s_{SC} \,, \tag{2.12}$$

from which

$$\bar{g}^\lambda_{ls} = g^\lambda_{ls} - V^s Q^\lambda_s/(1 + V^s P_s) \,. \tag{2.13}$$

The final expression (2.13) for the coupling constant is built up of two parts—the rigid-atom part g^λ_{ls} and the appropriately normalized matrix element of $\delta U^{s\lambda}_j$, calculated within RPA, $\langle l+s \lvert \delta U^{s\lambda}_j \rvert l\rangle$. Unlike the almost-free-electron case, the dielectric constant does not appear in the rigid-atom part simply because in order to calculate the charge distribution around an ion we use the tight-binding approximation instead of the linearized Hartree approximation. On the contrary, the "dielectric constant" $\epsilon_s = 1 + V^s P_s$, corresponding to the correlation function $\langle \rho_j(t)\rho_i(0)\rangle$, appears in the second part since the small variations of the probability density on a site can presumably be treated by the linearized self-consistent theory.

If the band is almost empty (or almost full), one would be tempted to put $g^\lambda_{ls} \approx g^\lambda_s$, as in Eq. (3.8) of I, for the occupied (or unoccupied) states. For these states one would then have $Q^\lambda_s \approx g^\lambda_{ls} P_s$ and Eq. (2.13) would formally reduce to the free-electron expression[6]

$$\bar{g}^\lambda_s \approx g^\lambda_s/\epsilon_s \quad \text{for arbitrary } s \,. \tag{2.14}$$

But even[7] in the tight-binding limit this approximation is inconsistent because in order to have

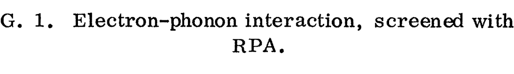

FIG. 1. Electron-phonon interaction, screened within RPA.

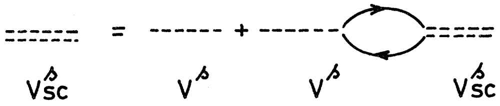

FIG. 2. Screened Coulomb interaction.

$\epsilon_s \neq 1$ over the finite portion of the phase space s (and with RPA valid) we must have a finite number of electron states filled, and hence take into account the l dependence of g^{λ}_{ls}.

However, before leaving Eq. (2.14), it is interesting to exhibit its physical meaning. In the Bardeen-Shockley limit[8] (l small or large, s small) I^{λ}_{s}, defined by Eq. (3.7) of I is linear in s, as, for example, in Eq. (3.8) of I. This limit corresponds to the Thomas-Fermi (s-small) approximation for ϵ_s, which thus diverges as $|s|^{-2}$. Hence $\bar{I}^{\lambda}_{s}$, Eq. (2.11), vanishes as a third power of s. More physically, the Thomas-Fermi electron redistribution $\delta\rho_j$ in an almost empty or almost filled narrow band is such that δU_j compensates primarily for the Bardeen-Shockley deformation potential V_{BS} created by the deformation. This in order to have $\delta\rho_j$ as small as possible: The remaining coupling term is weak since it is two orders higher in s.

Although inconsistent, this approximation exhibits the role of CDW in electron-phonon coupling. The l dependence of g^{λ}_{ls} will diminish both the rigid-atom coupling and the CDW, relative to the values corresponding to Eq. (2.14). The CDW is decreased more than the rigid-atom coupling, so that the linear s dependence of $\bar{I}^{\lambda}_{ls}$ for small s is recovered. The l dependence of I^{λ}_{ls} leads even to rather spectacular effects. Thus in Sec. III, we shall show that, when the band in the linear lattice of equidistant identical atoms is half-filled, Q_s vanishes in the adiabatic limit for any s, i.e., $\bar{I}_{ls} \equiv I_{ls}$ for arbitrary l and s. There is no charge transfer among the atoms in this case. The same property is derived in Sec. IV for a half-filled s band in the simple square lattice and a family of deformations containing the longitudinal long-wavelength deformation. The physical origin of the effect and its generalization to three dimensions are also discussed in this section. These results are to be contrasted to the free-electron theory, where just the longitudinal long-wavelength deformations produce the RPA variations of the charge density.

On the other hand, it is easy to see from Eq. (2.10) that the (110) shear deformation of the simple cubic lattice does not produce the linear charge variation, whatever its wavelength and whatever the s-band occupation.

In order to calculate the energy of electron redistribution we can proceed by the simple second-order time-independent self-consistent perturbation theory applied to the Hamiltonian (2.3). When one-half of the Coulomb energy of the electron redistribution is subtracted from this result we obtain the required energy $E^{(2)}_{s\lambda}$. However, $E^{(2)}_{s\lambda}$ still counts some of the electron-electron interactions twice, since the matrix elements are related to the one-electron potential including a part of the electron-electron interaction. With a suitable choice[9] of d functions and potentials this correction is thought to be small, and is usually neglected.[10]

The energy $E^{(2)}_{s\lambda}$, arising from the variation of the band energy in a static periodic deformation, gives in the Born-Oppenheimer adiabatic approximation the phonon self-energy, i.e., the renormalization of phonon frequencies:

$$\omega^2_{s\lambda} = \omega^{0\,2}_{s\lambda} + (E^{(2)}_{s\lambda} + E^{(2)\prime}_{s\lambda})/NM|u^{\lambda}_{s}|^2\hbar^{\,2} . \tag{2.15}$$

u^{λ}_{s} is the amplitude of the deformation. $E^{(2)\prime}_{s\lambda}$ is an energy term, at present uninteresting, arising from the second-order terms in the effective Hamiltonian, such as those mentioned at the beginning of Sec. III of I.

The phonon self-energy corresponding to $E^{(2)}_{s\lambda}$ can also be calculated by the use of diagrammatic methods. In fact, it can be readily shown (Appendix A), that if we calculate the phonon self-energy $\Pi^{\lambda}_{s}(\omega)$ from the graph shown in Fig. 3, then

$$\hbar^2 E^{(2)}_{s\lambda}/NM|u^{\lambda}_{s}|^2 = 2\omega^{0}_{s\lambda}\pi^{\lambda}_{s}(0) ,$$

as expected on physical grounds.

Inserting the coupling constant (2.13) and using the definition (2.10) of Q_s, Fig. 3 reads

$$\pi^{\lambda}_{s} = \pi^{0\lambda}_{s} - NV^{s}(Q^{\lambda}_{s})^2/(1 + V^{s}P_{s}) . \tag{2.16}$$

Here, $\pi^{0\lambda}_{s}$ is the self-energy corresponding only to the rigid-atom interaction $V^{s\lambda}_{\mathrm{BS}}$:

$$\pi^{0\lambda}_{s} = -2i\textstyle\sum_l |g^{\lambda}_{ls}|^2 \int_{-\infty}^{\infty} (d\omega'/2\pi) \times G^{0}(l, \omega')G^{0}(l+s, \omega+\omega') . \tag{2.17}$$

Such an energy was first studied by Migdal,[10] with g^{λ}_{ls} replaced by g^{λ}_{s} and a spherical Fermi surface. In Sec. III of I, we pointed out that Labbé's[11] variational approach to the electronic deformation energy is equivalent to the perturbation approach to the rigid-atom deformation potential, [Eq. (3.5) of I], which is in turn (see Appendix A) equivalent to the Born-Oppenheimer treatment of (2.17). Thus the effect of the anisotropy of the Fermi surface on the energy

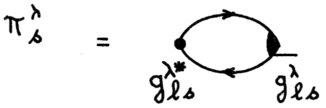

FIG. 3. Phonon self-energy due to the electron-phonon interaction.

(2.17) was already studied in Ref. 11.

The second term in the Eq. (2.16) arises from the self-consistent potential. By Eq. (2.16) its calculation is reduced to the calculation of Q_s^λ; thus it vanishes for the special cases mentioned above. Physically, we expect that, being related to the term which reduces the charge variation, it will reduce the Kohn anomaly. This will be shown in the one-dimensional case where the Kohn anomaly in (2.17) is so strong that it leads to the instability of the linear chain of equidistant atoms.

III. ONE-DIMENSIONAL CASE

In one dimension[12] our approach is in many respects similar to the Pariser-Parr-Pople approach to π electrons in polyens, used by Harris and Falicov[4] and more recently by Tric[5] in Hartree-Fock self-consistent calculations of the band energy of π electrons. These allow for band alternation combined with CDW's and spin-density waves (SDW) over the sites. In the present work only the terms linear in displacement are retained and we look for Hartree-self-consistent CDW (we ignore the SDW) with the same spatial phase as the phase of the deformation, which, as far as a linear response is concerned, amounts to RPA. Within these approximations we are able to extend the study of the band alternation to any periodic deformation of the chain. However we are restricted to energetic terms of second order in the deformation.

For bond-alternating deformation, our solution agrees with that of the above-mentioned Refs. 4 and 5: No bond alternation is required to minimize long-range Coulomb interaction, or, the other way around, for such a deformation a CDW does not exist in RPA. But CDW appears for deformations other than doubling of the lattice period, for arbitrary occupation of the band, and compensates partially for the gain of energy due to the rigid-atom potential. If the band is not half-filled, this can even lead to the disappearance of the instability of the lattice against the critical (longitudinal) deformation $q_s = 2k_F$.

Since we are primarily interested in the stability of the lattice we can use the adiabatic approximation for Π_s. If, for some s, the gain of energy $E_s^{(2)}$ due to the electron redistribution is larger than the increase in the remaining terms, the lattice is unstable. In another way, the instability occurs if the "Dyson equation" has a solution with $\omega = 0$,

$$-\omega_s^{0^2} = 2\omega_s^0 \pi_s(0) = \hbar^2 E^{(2)}/NM|u_s|^2 \; . \tag{3.1}$$

Strictly speaking, we should add on the right-hand side of the Eq. (3.1) the term arising from the second-order terms in the effective Hamiltonian, as explained in Sec. II, but this term is not of interest here and can be considered as included in a renormalization of the phonon pulsation ω_s^0.

If the solution of Eq. (3.1) exists (and it always exists for a rigid-atom interaction; Appendix B) it is of no great interest to consider the complete Dyson equation with $\pi_s(\omega \neq 0)$, since the lattice will be deformed by a static deformation and the vibrations must then be considered about a new equilibrium position of the ions. It can be expected on physical grounds that the hardening of the phonon spectra by this effect is much more important than nonadiabatic corrections to ω_s calculated[13] with respect to the lattice of equidistant equilibrium sites.

The coupling constant g_{ls} for the one-dimensional case is obtained from Eq. (3.7) of I on retaining only one component of the electron and phonon wave vectors and on assuming $\vec{\epsilon}_{s\lambda}$ parallel to the chain. When such a g_{ls} is inserted in the expression (A5) of the Appendix A the integration can be carried out in the closed form in the adiabatic ($\omega = 0$) limit, and one obtains

$$(2NM\hbar^{-2}\omega_s^0)^{1/2} Q_s = 4iq_0 T_s \sin\tfrac{1}{2}s \; , \tag{3.2}$$

where

$$2\pi T_s \sin\tfrac{1}{2}s = \ln\left|\frac{\tan l_F^0 + \tan\frac{1}{2}s}{\tan l_F^0 - \tan\frac{1}{2}s}\right| \; . \tag{3.3}$$

P_s is obtained on replacing g_{ls} by unity in Q_s:

$$P_s = -(1/J)L_s \; , \tag{3.4}$$

where

$$2\pi L_s \sin\tfrac{1}{2}s = \ln\left|\frac{\sin l_F^0 + \sin\frac{1}{2}s}{\sin l_F^0 - \sin\frac{1}{2}s}\right| \; , \tag{3.5}$$

l_F^0 is the Fermi vector of the narrow band

$$l_F^0 = ak_F = \tfrac{1}{2}\pi Q, \qquad 0 < Q < 2 \tag{3.6}$$

and Q is the number of electrons per atom present in the narrow band.

Both Q_s and P_s diverge logarithmically for the deformation with the wave vector

$$\begin{aligned} |s| &= 2l_F^0 \; , \qquad Q < 1 \\ &= 2\pi - 2l_F^0 \; , \quad Q > 1 \; . \end{aligned}$$

A useful relation in this limit is

$$2\pi(T_s - L_s)\sin\tfrac{1}{2}s = 2\ln|\cos l_F^0| \; . \tag{3.7}$$

A glance at Eq. (2.13) shows that in the one-dimensional case RPA is required not only by the divergence in V^s but also in Q_s. Actually, by Eq. (3.7), the divergences in Q_s and P_s compensate one another, except in the vicinity of the half-filled band $l_F^0 = \frac{1}{2}\pi$. However, a word of caution should be inserted at this point: The RPA bubble graph is not the only divergent diagram[14] in, say, the series for the irreducible polarizability in the one-dimensional case. From this point of view mean-field calcula-

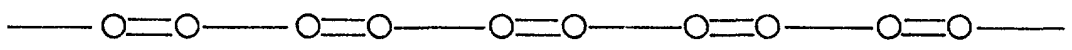

FIG. 4. —— and ═══ denote the long and short interatomic distances, respectively, and thus (in absolute value) the small and large overlap integrals. Each site is surrounded by one large and one small overlap: Thus all sites are electronically equivalent.

tions such as ours[4,5] may be oversimplified. Note in this respect that T_s (or Q_s) vanishes for $|s| = \pi$, whatever the occupation of the band. Within RPA the bond alternation, Fig. 4, does not introduce CDW for any band occupation. As seen in Fig. 4, the existence of CDW would break the symmetry of the electron Hamiltonian contained in $K + V_{\mathrm{BS}}$ and would thus be related to a supplementary phase transition.[14] The RPA solution is a symmetry-conserving solution. Moreover CDW does not exist for a half-filled band whatever the wavelength of the deformation. The physical origin of this effect is explained in Sec. IV.

The only mathematical difficulty appears in the point $l_F^0 = |\frac{1}{2}s| = \frac{1}{2}\pi$ where Eq. (3.3) has an essential singularity in the l_F^0, s plane. The limiting value depends on the path chosen to approach a singular point. Two "physical" paths are $l_F^0 = \frac{1}{2}\pi$, $|s| \to \pi$ and $|s| = \pi$, $l_F^0 \to \frac{1}{2}\pi$, both yielding $T_s = 0$ in this limit. This value should also be chosen by inspection of the integral before integration (see Sec. IV), or with regard to the fact that the exact diagonalization (Paper I) of $K + V_{\mathrm{BS}}^{s=\pi}$ does not give rise[5] to charge fluctuations, i.e., $\delta U_j^{s=\pi} \equiv 0$. The vanishing of CDW in the above situations can, on comparing with Eq. (2.14), be traced back to the l dependence of g_{ls}, i.e., to the nonlocality of the potential V_{BS}, Eq. (3.5) of I.

With Q_s known we can calculate the energy contribution produced by CDW in Eq. (2.16), and compare it to the rigid-atom term (2.17). First, from Eq. (A2), we find the self-energy arising from the rigid-atom potential

$$2MN\omega_s^0\hbar^{-2}\pi_s^0(0) = 16q_0^2 J \sin^2(\tfrac{1}{2}s)(L_s - S) ,$$

where (3.8)

$$S = (1/\pi)\sin l_F^0 .$$

Equation (3.8) is only a slight generalization to arbitrary band occupation of the expression obtained[13] by Ovchinnikov for the half-filled band. Also, it is the first of the series of divergent terms summed approximately[15] by Labbé.

In agreement with this latter result this term, by itself, leads to the instability of the lattice at $|s| = 2l_F^0$ or $|s| = 2\pi - 2l_F^0$, for $Q \lessgtr 1$, respectively, whatever the parameters determining ω_s^0.

The estimated[15] energy gap for this instability is small[16] when l_F^0 is small or close to π. But when the CDW RPA contribution to the phonon self-energy is added even this weak instability can completely disappear, i.e., the lattice is stable at 0 °K. In fact the total self-energy, obtained on combining Eqs. (2.16), (3.2), and (3.8), is

$$2MN\omega_s^0\hbar^{-2}\pi_s(0) = 16q_0^2 J \sin^2(\tfrac{1}{2}s)$$

$$\times\left(\frac{L_s^2 - T_s^2}{L_s} - S + \frac{JT_s^2}{(J - V^s L_s)L_s}\right) . \quad (3.9)$$

As readily seen from Eq. (3.7) the divergence, if it exists, is contained in the term $(L_s^2 - T_s^2)/L_s$. This term is plotted on Fig. 5 for three different Fermi vectors. We see that for small (or large) band occupations the divergence is eliminated. It develops when the number of electrons in the band increases towards the half-filled band, due to the fact that the CDW becomes smaller for the critical deformation $|s| = 2l_F^0$ as this deformation gets closer to the highly symmetric bond alternation (Fig. 4).

It is perhaps worthwhile to note that an analogous result is obtained in the RPA linearized Hartree-Fock approximation, with short-range electron-electron interaction. In this case V_s in Eq. (2.13) has to be replaced by $\frac{1}{2}V_0$, where V_0 is the intra-atomic matrix element of the short-range interaction.

In conclusion, the CDW reduces (within RPA) the Kohn anomaly in the phonon spectrum of the linear chain of equidistant atoms for small and large oc-

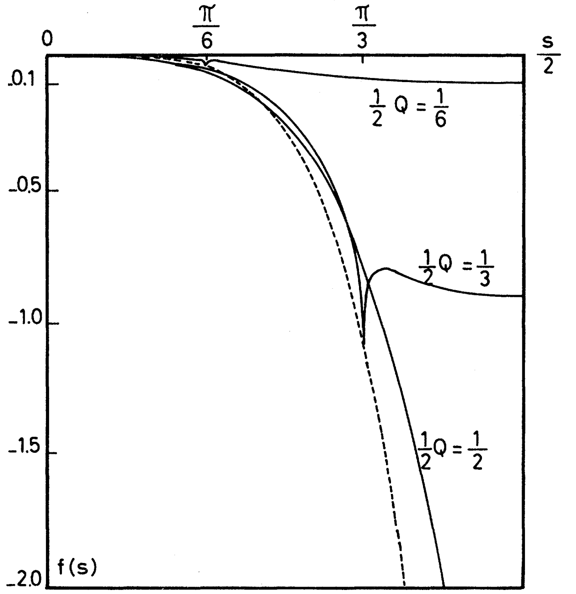

FIG. 5. Plot of the function $f(s) = 2\pi\sin^2(\frac{1}{2}s)\,[(T_s^2 - L_s^2)/L_s + S]$ leading to the instability in the vicinity of the half-filled band for occupation numbers $\frac{1}{2}Q$ (or $1 - \frac{1}{2}Q$) equal to $\frac{1}{6}$, $\frac{1}{3}$, $\frac{1}{2}$. The dotted line gives the position of turning points occurring for $|s/2\pi| = \frac{1}{2}Q$ (or $1 - \frac{1}{2}Q$).

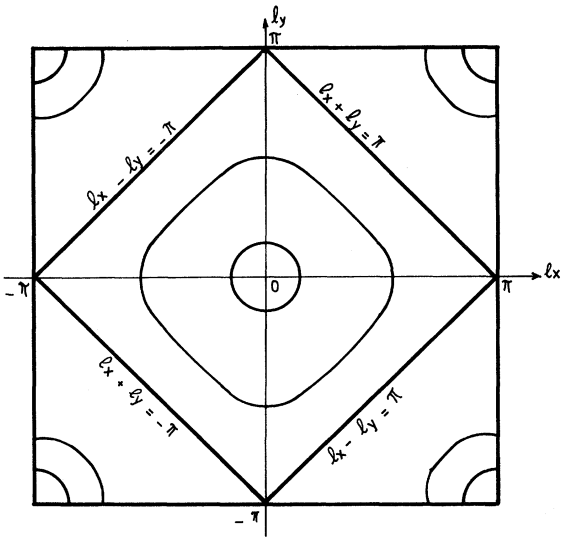

FIG. 6. Band structure of the tightly bound s band in the simple square lattice.

cupations of the band. In the vicinity of the half-filled band the equidistant lattice is always unstable. The width of the instability interval depends on various parameters contained in ω_s^0, and on the relative strength of the bare electron-phonon coupling $-q_0 J$ and the Coulomb interaction.

Before closing this section we note that $\text{Im}\,\pi_s(\omega)$ shows some interesting peculiarities arising from the one dimensionality of the problem, discussed in some detail in Appendix B.

IV. PLURIDIMENSIONAL CASE

In this section we shall indicate which of the particular properties of an almost half-filled band subsist in more than one dimension. Let us first consider a half-filled s band in the simple square lattice, deformed by a longitudinal static deformation along the direction (11), i.e., $s_x = s_y = s_0$. The variation of the band energy due to the rigid-atom part of the coupling constant is obtained from Eq. (A2) by the equivalence (A4):

$$\frac{E^{\text{rigid}}_{s_0 L}}{|u^L_{s_0}|^2} = 16 q_0^2 J \sin(\tfrac{1}{2}s_0)$$

$$\times \sum_{l_x l_y} \frac{\cos^2[\frac{1}{2}(l_x + l_y + s_0)] \cos[\frac{1}{2}(l_x - l_y)]}{\sin[\frac{1}{2}(l_x + l_y + s_0)]} \quad . \quad (4.1)$$

The trigonometric transformation to variables $\frac{1}{2}(l_x + l_y)$ and $\frac{1}{2}(l_x - l_y)$ in Eq. (4.1) is introduced because the limits of summation are simple in terms of these variables. From Fig. 6, we see that a half-filled band is characterized by

$$-\tfrac{1}{2}\pi < \tfrac{1}{2}(l_x \pm l_y) < \tfrac{1}{2}\pi \quad . \qquad (4.2)$$

Thus we have

$$\frac{E^{\text{rigid}}_{s_0 L}}{N |u^L_{s_0}|^2} = \frac{8}{\pi^2} q_0^2 |J| \sin(\tfrac{1}{2}s_0)$$

$$\times \left(\ln \frac{1 - \sin(\frac{1}{2}s_0)}{1 + \sin(\frac{1}{2}s_0)} + 2 \sin(\tfrac{1}{2}s_0) \right) \quad . \qquad (4.3)$$

When s_0 tends towards π the same type of instability occurs as in the one-dimensional case, Eq. (3.8). This instability obviously arises from the existence of straight lines in the Fermi "surface" of the half-filled band, so that the contact[11] of these Fermi "surfaces" corresponding to E_l and E_{l+s_0} for the critical s_0 is pathologically[17] strong. On the contrary, the Fermi surfaces of arbitrarily filled band *are curved* so that,[11] unlike the one-dimensional case, the instability disappears from the rigid-atom part of the phonon self-energy. For the same reason, it would be considerably reduced or even would not exist for a half-filled s band but with a more elaborate band structure. This would also occur if the overlap integrals differed along different axes (non-s band; nonsimple square lattice).

Note that the l dependence of the coupling constant is not essential in this calculation: The same physical conclusions would be obtained with a coupling constant depending only on the momentum transfer. On the contrary, this dependence is essential in showing that the considered modes do not produce CDW when the band is half-filled, i.e., that Eq. (4.3) gives the total variation of the band energy in the linearized theory. From Eq. (A5) one easily finds

$$Q^L_{s_0}(0) \sim P \sum_{-\pi/2 < (l_x + l_y)/2 < \pi/2} \cot\tfrac{1}{2}(l_x + l_y + s_0) \equiv 0 \ . \qquad (4.4)$$

$Q^L_{s_0}(0)$ vanishes for an arbitrary s_0 because the integration with respect to $\frac{1}{2}(l_x + l_y)$ runs over the complete period of the cotangent. Note that neglecting the l dependence of the coupling amounts to replacing $\cot\frac{1}{2}(l_x + l_y + s_0)$ in Eq. (4.4) by $1/\sin\frac{1}{2}(l_x + l_y + s_0)$. This would make the CDW reappear.

Next, we show that the vanishing of the CDW for a half-filled band is related not to the existence of planar parts of the Fermi surface, as is the instability, but rather to the fact that the band "breathes" about its center (at least for long-wavelength deformations). Thus we consider the case of a half-filled band with overlap integrals differing along different axes. Generally this situation will not present the lattice instability, and still the CDW will vanish. In the long-wavelength limit for deformations of, say, the orthorhombic lattice, V_{BS} [Eq. (3.5) of I] becomes

$$V_{\text{BS}} \approx 2 q_0 \sum_\alpha J(\vec{\text{a}}_\alpha) \frac{\partial u_j^\alpha}{\partial j_\alpha} \cos\left(-i \frac{\partial}{\partial j_\alpha}\right) . \qquad (4.5)$$

Further we assume that $\partial u_j^\alpha / \partial j_\alpha$ is independent of

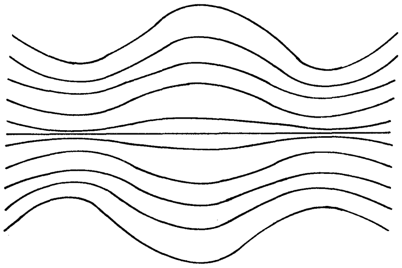

FIG. 7. Thomas-Fermi local band structure in presence of the long-wavelength "breathing" deformation.

α, i.e., we consider the "breathing modes." In this case the Hamiltonian $K+V_{\mathrm{BS}}$ still has the "free states" $\exp(i\sum_\alpha l_\alpha j_\alpha)$ as eigenstates if l_α are such that $\sum_\alpha J(\vec{a}_\alpha)\cos l_\alpha = 0$. But this equation defines the Fermi energy of the half-filled band. The energy of the states on the top of the distribution is not altered by the "breathing" deformation. For lower states we use the Thomas-Fermi approximation, solving for the local band structure. As seen on Fig. 7 the number of states on both sides of the Fermi level remains locally unchanged, the Fermi level itself being unaltered by the deformation. Therefore the deformation considered does not produce the CDW.

The reason for the vanishing of the CDW in the opposite, short-wavelength limit is related to the conservation of the symmetry of the system. The short-wavelength deformations, such as (π, π, π) or (π, 0, 0) longitudinal modes, for example (Fig. 8) may produce an array which is highly symmetric when seen by electrons. The nonvanishing CDW would break this symmetry on the electronic level and therefore does not appear within RPA. The arguments following Eq. (4.5) are of course independent of the dimensionality of the lattice.

Some of the above arguments are quite general. Let us briefly consider the static long-wavelength limit for deformations. The eventual screening of the electron-phonon coupling is most effective in this limit. A necessary and sufficient condition that the linear CDW does not appear is that the corresponding homogeneous deformation does not alter the Fermi level position to the first order in the deformation. Then there is no linear charge transfer between the unit cells deformed by the long-wavelength mode, since it can be considered as locally homogeneous.

The shift of the Fermi level positions, $E_F' - E_F$, in a cubic crystal deformed by the homogeneous deformation $\epsilon_{\alpha\beta}$ is

$$E_F' = E_F + A\sum_\alpha \epsilon_{\alpha\alpha} + \cdots \,.$$

Hence all long-wavelength volume-conserving (shear) modes are coupled to tightly bound electrons by an unscreened Mitra-like coupling. Unlike the free electrons, the tightly bound electrons are scattered by shear modes from one point of the Fermi surface to another. This has been established in the present model in Sec. III of I. However, the resulting charge redistribution is such that the unit cell remains neutral to the first order in deformation.

On the other hand, the vanishing of the coefficient A is related by Eq. (4.5) to the vanishing of the electron-phonon coupling over the Fermi surface. In more complicated band structures this need not be so. A will vanish if the Fermi level coincides with the energy which separates the *over-all* density of states in two regions which contain the same number of states before and after the hydrostatic deformation. In order to establish this "breathing" property of the over-all density of states it will usually be sufficient to consider its several first moments. In the bcc transition metals the mean displacement of the density of states is much smaller than the variation of the over-all bandwidth.[9] The density of states is rather symmetric and hence $A\approx 0$ close to the half-filled "band."

If the mean displacement of the over-all density of states is much larger than the variation of all other moments, the CDW appears. In the present

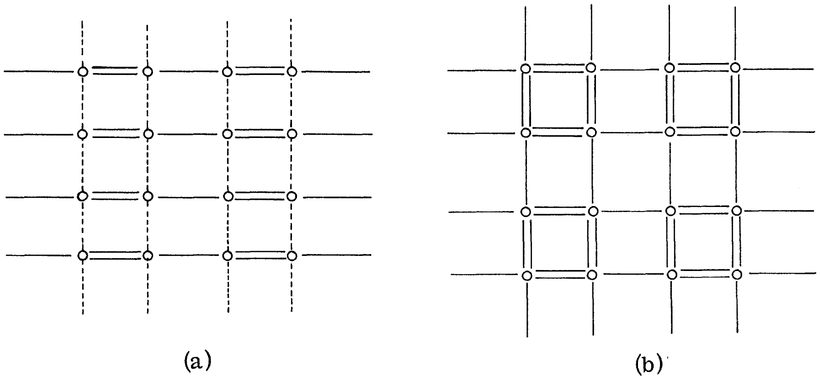

FIG. 8. Lattice of overlap integrals, like that of Fig. 1, for (a) (π, 0) and (b) (π, π) longitudinal modes of the simple square lattice. Dashed lines are the unperturbed overlaps. Again all sites are electronically equivalent.

simplified model this would occur if the only important bare electron-phonon coupling arises from the variation of the two center integrals $\langle d_j | V_{j+\delta} | d_j \rangle$, neglected in Eqs. (2.6) of I and (2.2). Such coupling depends only on the momentum transfer s, in a linear way. It is therefore strongly screened according to Eq. (2.14). However, in real metals the above mentioned integrals appear in both, the over-all "bandwidth" and the mean position of the band. They may contribute to some extent to the self-consistent electron-phonon coupling. But the variation of the overlap integrals remains essential[9] for transition metals.

Our results indicate that the superconducting transition temperature T_c is overestimated in computations (Paper I) using the rigid-atom electron-phonon coupling, but that this approach probably gives the correct order of magnitude in the middle of the transition series. At the extremities of the series T_c should fall somewhat more steeply than predicted by the rigid-atom model. This effect should go together with the reduction of the Kohn anomaly in the phonon spectrum.

V. CONCLUSION

In this paper an additive self-consistency term is derived which completes the rigid-atom electron-phonon coupling. This term arises from the long-range interaction between narrow-band electrons. The self-consistent treatment of this term shows some striking (and misleading) formal analogies with the free-electron case but also fundamental physical differences. These differences are emphasized for deformations in the long-wavelength limit, in which it is sometimes incorrectly believed that it is not necessary to distinguish between $\vec{r}$ and j spaces; a belief based on the statement (subject to criticism) that long-wavelength phonons do not see the details of the lattice.

It is shown that the self-consistent correction simply translates into the language of the electron-phonon interaction some concepts well established in the calculation of the stability of one-dimensional systems. This is achieved by the use of an effective self-consistent one-electron Hamiltonian. The stability of the partially filled band is examined and it is shown that the energy loss due to the induced CDW can compensate the corresponding gain of the band energy, i.e., to reduce the Kohn anomaly in the phonon spectrum.

This reduction of the electron-phonon coupling does not occur for certain modes. In the long-wavelength limit these are the shear modes, while for the "breathing" modes this occurs only for a given band occupation corresponding to nearly half-full bands. The elastic anomalies are thus more "probable" in shear modes. They actually occur[15,16] in V_3Si-like compounds.

The main shortcoming of the present theory arises from the incomplete treatment of electron correlations when several bands of different nature are present.

ACKNOWLEDGMENTS

Professor Friedel called my attention to the self-consistency problem. I have also benefited from discussions concerning the lattice instability with Dr. J. Labbé.

APPENDIX A

The integral appearing in Eqs. (2.9), (2.10), and (2.17) is given by the well-known expression

$$\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\, G^0(l,\, \omega')\, G^0(l+s,\, \omega+\omega')$$

$$= i\left(\frac{n_l(1-n_{l+s})}{E_l - E_{l+s} + \omega + i\delta} + \frac{n_{l+s}(1-n_l)}{E_{l+s} - E_l - \omega + i\delta} \right). \quad \text{(A1)}$$

Inserting it in Eq. (2.17), for example, we find

$$\mathrm{Re}\Pi_s^{0\lambda}(\omega) = 4P \sum_{l\,\mathrm{occ}} |g_{ls}^{\lambda}|^2 \frac{E_l - E_{l+s}}{(E_l - E_{l+s})^2 - \omega^2}\,, \quad \text{(A2)}$$

$$\mathrm{Im}\Pi_s^{0\lambda}(\omega) = -2\pi \sum_{l} |g_{ls}^{\lambda}|^2 n_l(1-n_{l+s})$$

$$\times[\delta(E_l - E_{l+s} + \omega) + \delta(E_l - E_{l+s} - \omega)]\,, \quad \text{(A3)}$$

We note that for $\omega = 0$ $\mathrm{Re}\Pi_s^{0\lambda}$ is proportional to the perturbative second-order energy arising from the rigid-atom potential $V_{\mathrm{BS}}^{s\lambda}$.

In Fig. 3 we replaced one g_{ls}^{λ} by $\bar{g}_{ls}^{\lambda}$. The same result for Π_s^{λ} would have been obtained if we took $\bar{g}_{ls}^{\lambda}$ on both sides of Fig. 3 but subtracted from such a contribution one-half of the electron-electron interaction between the charges $\delta\rho_j^{s\lambda}$ displaced in the presence of a phonon. The diagram with $\bar{g}_{ls}^{\lambda}$ on both sides corresponds, at $\omega = 0$, to the second-order perturbation energy arising from linearized $V_{\mathrm{BS}}^{s\lambda} + \delta U_j^{s\lambda}$, from which we also subtract one-half of the electron-electron interaction between the displaced charges $\delta\rho_j^{s\lambda}$ in order to obtain $E_{s\lambda}^{(2)}$ as defined in Sec. II.

The details of the calculation of $E_{s\lambda}^{(2)}$ are given in Ref. (12), but the relation

$$\frac{E_{s\lambda}^{(2)}}{N} = \frac{|u_s^{\lambda}|^2}{\hbar^2/2M\omega_{s\lambda}^0}\Pi_s^{\lambda} \quad \text{(A4)}$$

can be established already from the preceding discussion, since the factor

$$\frac{|u_s^{\lambda}|^2}{\hbar^2/2M\omega_{s\lambda}^0}\,,$$

deduced from the rigid-atom calculation, represents just the ratio of the amplitude of the ion displacement in the classical treatment to that created by the presence of one phonon. The steps in both methods are the same, only the amplitude of the ion

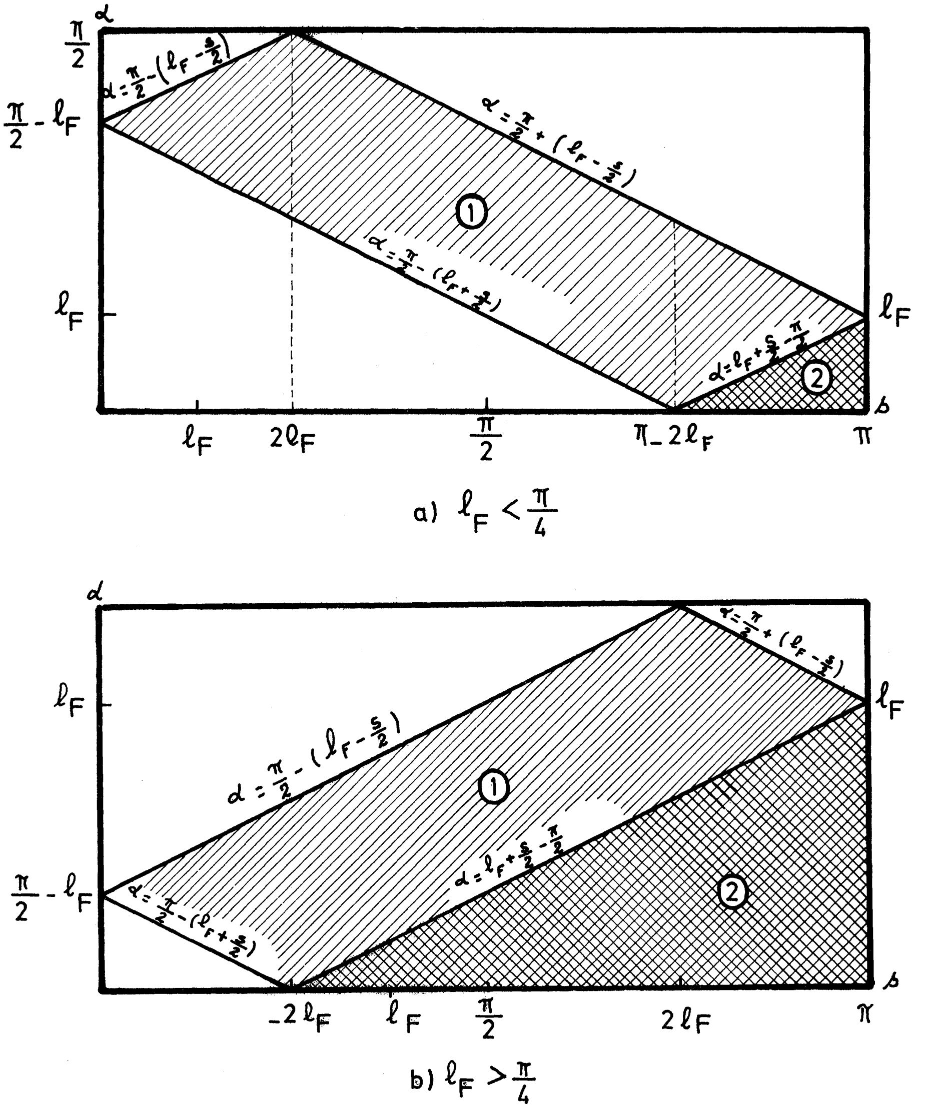

FIG. 9. The one-dimensional phonon lifetime arising from electron-phonon interaction for $l_F < \frac{1}{4}\pi$ and $l_F > \frac{1}{4}\pi$. $\alpha = \arccos(\omega/4|J|\sin\frac{1}{2}s)$ and the shaded regions denote the pairs (s, α) for which one pole (region①) or both poles (region②) contribute.

displacement may be different.

Finally, analogous to Eq. (A2), we have from Eqs. (2.10) and (A1)

$$Q_s^\lambda(0) = -\frac{4}{N} P \sum_{l\,\mathrm{occ}} \frac{g_{ls}^\lambda}{E_l - E_{l+s}} . \qquad \text{(A5)}$$

APPENDIX B

In this Appendix, we consider the particular properties of the phonon attenuation due to the one dimensionality of the system.

Using the Eq. (A1) and the relation $g_{ls}^\lambda = -g_{-l-s}^\lambda$ it can be easily seen that $\Pi_s(\omega) = \Pi_s(-\omega) = \Pi_{-s}(-\omega)$. Thus we can take without loss of generality

$$\omega > 0, \quad 0 < s < \pi, \quad 0 < l_F^0 < \tfrac{1}{2}\pi. \qquad \text{(B1)}$$

l_F^0 can be restricted to the above interval owing to the electron-hole symmetry of our model with respect to the half-filled band.

Then Eq. (A3) reduces to

$$\mathrm{Im}\,\Pi_s^0(\omega) = -2\pi \sum_l \frac{|g_{ls}|^2}{4|J| \sin(\frac{1}{2}s)\cos(\frac{1}{2}\pi - \alpha)}\, n_l(1 - n_{l+s}) \times [\delta(l - l_0^{(1)}) + \delta(l - l_0^{(2)})] . \qquad \text{(B2)}$$

The poles retained in Eq. (B2) arise from two physically distinguishable zeros of the function $E_l - E_{l+s} + \omega$:

$$E_l - E_{l+s} + \omega \approx 4J \sin(\tfrac{1}{2}s)\cos(l_0^{(i)} + \tfrac{1}{2}s)\,(l - l_0^{(i)}),$$

where

$$l_0^{(1,2)} = \tfrac{1}{2}\pi - \tfrac{1}{2}s \mp \alpha,$$
$$\alpha = \arccos \frac{\omega}{4|J| \sin\frac{1}{2}s}, \quad 0 < \alpha < \tfrac{1}{2}\pi. \qquad \text{(B3)}$$

$l^{(1)}$ appears in usual calculations of the electron-

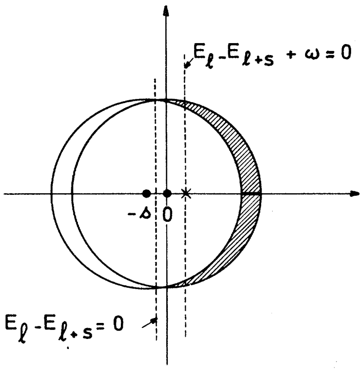

FIG. 10. Line in two dimensions, or the plane in three dimensions, defined by $E_l - E_{l+s} + \omega = 0$, always intersects the region of integration for small $|s|$ ($|s| < 2l_F^0$) and small ω, but the corresponding point * in one dimension may fall outside the region of integration (bold line).

phonon phonon self-energy, while $l^{(2)}$ arises from the introduction of the periodicity in the electron energy E_l.

Note that the expressions for $\mathrm{Im}P_s(\omega)$ and $\mathrm{Im}[Q_s(\omega)/i]$ are obtained on replacing $|g_{ls}|^2$ in Eq. (B2) by $-1/N$ and ig_{ls}/N, respectively. From (P_s, Q_s Π_s^0), the form of $\mathrm{Im}\Pi_s(\omega)$ is easily deduced.

In Fig. 9 we show the pairs (α, s) such that $l^{(1)}$ and/or $l^{(2)}$ fall in the region of integration $n_l(1 - n_{l+s}) = 1$ for a given l_F^0. In the (open) region ① only $l^{(1)}$ contributes while in the region ② both $l^{(1)}$ and $l^{(2)}$ contribute.

Since

$$g_{l_0 s}^{(i)} = -4\, iq_0 \left(\frac{\hbar^2}{2MN\omega_s^0}\right)^{1/2} J \sin(\tfrac{1}{2}s) \cos(\tfrac{1}{2}\pi \pm \alpha), \quad \text{(B4)}$$

the residuals of both poles in $\mathrm{Im}\pi_s^0(\omega)$ are the same and add in the region ②. This happens also in $\mathrm{Im}P_s(\omega)$. On the contrary, $\mathrm{Im}[Q_s(\omega)/i]$ vanishes in the region ② because, as seen from Eq. (B4), the residuals in $l^{(1)}$ and $l^{(2)}$ are in this case of the opposite sign.

The region ② will usually be of little interest since with $\omega \lesssim \omega_s^0$, $\alpha \gtrsim \frac{1}{2}\pi - \omega_D/4|J|$, i.e., with normal values of the parameters $\omega_D/4|J| \ll 1$. The physically interesting values of α fall very close to $\alpha = \frac{1}{2}\pi$.

Unlike the three-dimensional case the phonons with arbitrary $s < 2l_F^0$ are not attenuated. This is easily understood from Fig. 10. The attenuation exists only in the close vicinity of $s = 2l_F^0$.

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