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Peierls transition in substitutionally disordered quasi-one-dimensional conductors

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In this paper, the mean-field transition temperature of the Peierls transition is obtained for a quasi-one-dimensional binary substitutional alloy A_xB_{1-x} as a function of the relative concentration x. The Peierls state is assumed to result from a soft-mode structural instability driven by the one-dimensional electronic system coupled to the intramolecular vibrational mode. We consider only diagonal disorder arising from fluctuations in the intrasite electron potential and electron-intramolecular vibrational-mode interaction. Its effect on the Peierls phase is evaluated using the coherent potential approximation for single dimers. The use of suitable approximations resulted in an analytic expression for the transition temperature. The transition temperature of a half-filled conduction-band system diluted with a substitutional impurity of a different valency is also studied.

I. INTRODUCTION

Considerable effort has been devoted to detailed examinations of the physical properties of pure quasi-one-dimensional systems[1-4] such as TTF-TCNQ (tetrathiofulvalene-tetracyanoquinodimethane) and KCP [$K_2Pt(CN)_4Br_{0.30}\cdot 3H_2O$]. The existence of a charge-density-wave ground state following a Peierls instability has been established experimentally in materials of low dimension[1-4] by a considerable number of experiments, e.g., experimental studies of the dc[5] and microwave conductivity,[6] optical,[7] electronic,[7] magnetic,[8] and elastic[9] properties of such systems. In this paper, we investigate the effect of substitutional disorder on the mean-field Peierls transition temperature.

Adopting the mean-field approximation, the Peierls instability is viewed as a soft-mode structural transition resulting from a condensation of $2k_F$ phonons driven by the one-dimensional electronic system, where k_F is the Fermi momentum. The lattice phase transition, regarded as a condensation of electron-hole pairs with momenta k_F and $-k_F$, is then shown[10] to occur at T_c^0 where the electron spectrum acquires a gap through a second-order phase transition analogous to the BCS phase transition. Going beyond the mean-field approximation, the one-dimensional (1D) fluctuations shift the phase transition to $T=0$ K in the absence of interchain interaction. Lee *et al.*,[11] allowing for fluctuations in the lattice dynamics, evaluated their influence, within the framework of the Ginzburg-Landau static approximation, on the Peierls transition. They showed, that strictly speaking, there should be no long-range order for the purely one-dimensional system, but that for $T < \frac{1}{4}T_c^0$, the correlation length becomes very large so that we can assume that a Peierls superlattice appears in the system with the resulting distortion giving rise to diffuse x-ray scattering.[12] The above discussion of the Peierls transition, ignored the interaction between displacements of atoms on neighboring chains. This interaction is due to the Coulomb forces between electrons and to the electrons transitions between the chains as a result of the overlap of the electrons wave functions. Allowance of these interactions permits the order parameter of the Peierls transition to become three dimensional. $t_\perp$ is defined to be the resonance integral between neighboring chains ($t_\perp << k_B T_c^0$ for typical quasi-one-dimensional crystals) and t is the equivalent quantity for intrachain nearest neighbors. Let $\xi(\xi \sim t/T_c^0)$ be the characteristic correlation length of the Peierls state along a chain expressed in intrachain lattice spacing. Treating the above interactions[13] in the static Ginzburg-Landau approximation, two different regimes for the quasi-one-dimensional system are discussed. First for $\xi t_\perp >> T_c^0$, the total interaction between the chains is much larger than the mean-field temperature and the fluctuations are important only in a very narrow temperature range near T_c^0. The mean-field theory results are applicable almost everywhere giving rise to a three-dimensionally ordered Peierls state. Second, for $\xi t_\perp \lesssim T_c^0$, the fluctuations are important even far below T_c^0 and the physical properties of the quasi-one-dimensional system follow from the fluctuating regime studied by Lee *et al.*[11] for the purely one-dimensional system. Our study of the mean-field Peierls transition temperature is justified for both of the above regimes where, however, in the second case ($\xi t_\perp \lesssim T_c^0$), T_c^0 is only a temperature scale below which the electrons and the $2k_F$ phonons are strongly coupled.

Attempts have been made to prepare chemical isomorphs of TTF-TCNQ[14] and KCP[14, 15] with a view to gain better understanding of the important physical mechanisms taking place in the pure materials from the effect of alloying and controlled disorder on the physical properties and phase transition parameters (T_c^0) of such materials. For example, Schultz and Craven[16] have made an experimental study of the series $(\mathrm{TSeF})_x\,(\mathrm{TTF})_{1-x}\mathrm{TCNQ}$. These alloys are isostructural to TTF-TCNQ with the TTF molecules which contain sulfur, replaced by TSeF molecules. They examined the behavior of the lattice parameters, the dc conductivity, the thermoelectric power, the spin susceptibility, the EPR linewidth, g shift and the diffuse x-ray scattering for these materials as a function of relative concentration. Chiang *et al.*[17] investigated the effect of controlled disorder on the electrical conductivity of TTF-TCNQ by irradiating the sample with a deuteron beam. They found that the temperature of the conductivity maximum increases with defect concentration, whereas the associated disorder shifts the transition temperatures T_1 and T_2 downward with initial slopes $dT_1/dc = 150$ K/(percent defects) and $dT_2/dc = 200$ K/(percent defects). $T_1 = 52.3$ K and $T_2 = 38$ K in pure samples. Moreover it is now widely accepted that, in KCP, only 50% of the sites available to K and 60% available to Br are occupied.[18] The position of both ions are random according to x-ray[19] structure data. Hence, the electrons moving along the Pt chains experience a random potential due to the random distribution of the Br and K ions. Further the random orientation of the water molecules,[20] which correspond to randomly oriented dipoles, has an important effect[21] on the charge-density-wave state along the Pt chains.

The effects of disorder and impurities on the Peierls transition have been examined by many authors having in mind the widely accepted hypothesis that the Peierls phase transition could be suppressed by impurities and hence the appearance of superconductivity being favored. The basis for the hypothesis was the result that nonmagnetic impurities have no appreciable effect on the superconducting transition in three-dimensional conductors.[22] However it was soon realized[23] that impurities in quasi-one-dimensional conductors suppress not only the metal-insulator transition but also the superconducting transition. Schuster[24] and Ono[25] showed that, within the Born approximation, dilute nonmagnetic impurities influence the transition temperature and the energy gap[10] of the Peierls phase in the same way that magnetic impurities[26] modify the corresponding quantities in a BCS superconductor. Sham and Patton,[27] using a functional integral formalism,[28] showed that a random distribution of impurities destroys the long-range order of the charge-density-wave state. Their calculation is based on a mapping of the chain onto a 1D spin system in which the action of the impurities is simulated by a random magnetic field. Bulaevskii and Sadovskii[29] considered the effect of disorder on the Peierls transition by using disorder models which allow an exact determination of the density of states. They considered the Lloyd and fragment models and obtained an expression for the transition temperature in the presence of disorder. The result obtained with the Lloyd model demonstrates quite clearly the analogy between the influence of the lattice disorder on the Peierls transition and the influence of magnetic impurities on the superconducting transition. Sen and Varma[30] calculated the reduction in the transition temperature due to the presence of impurities by working from the high-temperature phase. They obtained an expression for the ensemble averaged electronic polarizability at the nesting wave vector in the framework of the coherent potential approximation. This is equivalent to a coherent-potential-approximation (CPA) average of a product of two single-particle Green's functions.[31]

In this paper, we investigate the effect of disorder on the mean-field Peierls transition temperature from a different point of view.[32] The electrons are assumed to belong to a single half-filled tight-binding conduction band in a one-dimensional conductor. Furthermore they do not interact with each other but are coupled to the host lattice via the intramolecular vibrational mode of the molecules occupying the lattice sites. For tight-binding organic metals with a narrow bandwidth, this source of modulation of the electronic energies, where the various molecular bond lengths change with the addition of an extra electron, is more important than the interaction with intermolecular lattice phonons. For the pure system, it can then be shown[10] that an energy gap opens up at the Peierls transition temperature T_c^0 and that the lattice exhibits a corresponding distortion with a wave number $Q = 2k_F$. The magnitude of the distortion increases as T decreases below T_c^0 and for the half-filled band, the distortion is commensurate with the now dimerized lattice.[10] Even though Peierls transition existed in a non-half-filled conduction band[33] and, that it may be described by a bond scheme,[34] we will be concerned in this paper only with a half-filled band and the site description of the Peierls transition. Hence, we used a microscopic theory based on a representation which takes into account the symmetry of the low-temperature dimerized state of the chain. Next the scattering due to impurities is treated in this representation by using mean-field theory and the CPA. We will call the resultant approximation the single-dimer coherent-potential approximation (SDCPA). This approximation is different from the cluster[35] CPA and gives new results which compare well with previous theories. The Hamiltonian of the system and the formalism of the SDCPA are described in Sec. II. The expression for the mean-field transition temperature T_c of the Peierls transition for an impure 1D chain is obtained and analyzed in Sec. III. Numerical results are presented in Sec. IV, which contains a concluding discussion.

II. HAMILTONIAN AND FORMALISM

The Fröhlich Hamiltonian for the coupled electron intramolecular vibration-mode system in a one-dimensional conductor with a single conduction band may be written as follows:

$$\mathcal{H}=\sum_{i\sigma}\epsilon_{i\sigma}c_{i\sigma}^{\dagger}c_{i\sigma}+\sum_{ij\sigma}t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+\sum_{j\alpha}\omega_{j\alpha}(b_{j\alpha}^{\dagger}b_{j\alpha}+\tfrac{1}{2})+\sum_{j\alpha\sigma}g_{j}c_{j\sigma}^{\dagger}c_{j\sigma}(b_{j\alpha}^{\dagger}+b_{j\alpha}) \quad . \tag{1}$$

$c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are electron creation and annihilation operators and $b_{i\alpha}^{\dagger}$ and $b_{i\alpha}$ are intramolecular vibrational-mode creation and annihilation operators for the ith site. σ is the electron spin and α is a phonon branch. $\epsilon_{i\sigma}$ is the local electron pseudopotential of the ith site and $t_{ij}=t(\vec{R}_i-\vec{R}_j)$ is the resonance integral between sites i and j which is assumed to be translationally invariant for simplicity.

In this calculation, we treat the effect of the spatially fluctuating intramolecular electron potentials introduced by alloying with isostructural substitutional impurities. However, it is to be realized that substitutional alloying could also introduce important structural changes which will be the source of randomly fluctuating intrachain resonance integrals and interchain interaction potentials. Even though the latter may turn out to be important[16] in certain cases, they are not treated in the present study. $\omega_{j\alpha}$ represents the phonon frequency of the αth branch and g_i is the electron intramolecular vibrational-mode coupling constant at the ith site. For an impure one-dimensional conductor, $\epsilon_{i\sigma}$, $\omega_{j\alpha}$, and g_i are site dependent and therefore not translationally invariant. The Hamiltonian described in Eq. (1) was used by Rice *et al.*[36] in a study of the optical properties of K-TCNQ.

Next the chain is divided into a set of nearest-neighbor pairs of atoms in anticipation of the dimerization state. This requires a revised notation for all the operators and variables of the Hamiltonian of Eq. (1). i will now become a dimer index and therefore the subscripts $(i,1;\,i,2)$ will refer to the atoms 1 and 2 of the ith dimer. The new Hamiltonian in the mean-field approximation can now be written

$$\begin{aligned}\mathcal{H}_{\mathrm{mf}}=&\sum_{i}\epsilon_{i,1}c_{i,1}^{\dagger}c_{i,1}+\sum_{i}\epsilon_{i,2}c_{i,2}^{\dagger}c_{i,2}+\sum_{i}\omega_{i,1}(\Delta_{i,1}^{2}+\tfrac{1}{2})+\sum_{i}\omega_{i,2}(\Delta_{i,2}^{2}+\tfrac{1}{2})\\&-2\sum_{i}g_{i,1}\Delta_{i,1}c_{i,1}^{\dagger}c_{i,1}+2\sum_{i}g_{i,2}\Delta_{i,2}c_{i,2}^{\dagger}c_{i,2}+\sum_{i}t(c_{i,1}^{\dagger}c_{i,2}+c_{i,2}^{\dagger}c_{i+1,1}+c_{i,2}^{\dagger}c_{i,1}+c_{i+1,1}^{\dagger}c_{i,2}) \quad .\end{aligned} \tag{2}$$

$\Delta_{i,1}$ and $\Delta_{i,2}$ are the distortions of atoms 1 and 2 in the ith dimer and must be calculated self-consistently. They are given as follows:

$$\begin{aligned}\Delta_{i,1}&=(g_{i,1}/\omega_{i,1})\langle c_{i,1}^{\dagger}c_{i,1}\rangle_d \quad ,\\ \Delta_{i,2}&=-(g_{i,2}/\omega_{i,2})\langle c_{i,2}^{\dagger}c_{i,2}\rangle_d \quad ,\end{aligned} \tag{3}$$

where $\langle\ \rangle_d$ is a thermodynamic average over an ensemble in the deformed state described by $\mathcal{H}_{\mathrm{mf}}$ of Eq. (2).

The dynamics of the system for fixed values of $\epsilon_{i\alpha}$, $\omega_{i\alpha}$, and $\Delta_{i\alpha}$ $(\alpha=1,2)$ is now described in terms of a configuration dependent matrix propagator which can be written as follows in the dimer representation:

$$G_{ij}(z)=\begin{bmatrix}\mathcal{G}_{ij}^{11}(z) & \mathcal{G}_{ij}^{12}(z)\\ \mathcal{G}_{ij}^{21}(z) & \mathcal{G}_{ij}^{22}(z)\end{bmatrix} \quad , \tag{4}$$

where

$$\mathcal{G}_{ij}^{\alpha\beta}(z)=\langle\langle c_{i\alpha},c_{j\beta}^{\dagger}\rangle\rangle_z \quad .$$

Here $\langle\langle A,B\rangle\rangle_z$ is the Fourier transform in frequency space z of a double-time temperature Green's function (see Zubarev[37]).

The equation of motion for the propagator in Eq. (4) may be obtained in the standard manner from the Hamiltonian $\mathcal{H}_{\mathrm{mf}}$ of Eq. (2). We refer the reader to Ref. 37 for details of the method. The resultant equation of motion for the $\mathcal{G}_{ij}^{\alpha\beta}$ may then be written in matrix form as follows:

$$\begin{bmatrix}A(z) & E\\ D & C(z)\end{bmatrix}G(z)=1$$

with

$$
\begin{aligned}
G(z)&=[G_{ik}(z)]\ ,\\
A(z)&=[A_{ik}(z)]=[(z-\epsilon_{k,1}+2g_{k,1}\Delta_{k,1})\delta_{ik}]\ ,\\
C(z)&=[C_{ik}(z)]=[(z-\epsilon_{k,2}-2g_{k,2}\Delta_{k,2})\delta_{ik}]\ ,\\
E&=[E_{ik}]=[-t(\delta_{ki}+\delta_{k,i-1})]\ ,\\
D&=[D_{ik}]=[-t(\delta_{ki}+\delta_{k,i+1})]\ .
\end{aligned}
\tag{5}
$$

The next step is to apply the coherent-potential approximation (CPA) to the equations of motion of Eq. (5). The single-dimer coherent-potential approximation (SDCPA), derived in the framework of the multiple-scattering theory, corresponds to the determination of a translationally invariant effective medium such that the average scattering from a single dimer is equal to zero. CPA is a mean-field theory where the effective medium is determined self-consistently and we argue that treating the effect of impurities in the CPA approximation is consistent with the mean-field treatment of the Peierls phase transition. We follow the method of Weinkauf and Zittarz[38] as applied to the properties of superconducting alloys. The results of their theory have been confirmed experimentally[39] and have been extended by Dubovskii[40] in order to take into account off-diagonal disorder. In particular, Dubovskii was able to make an excellent fit to the data for the composition dependence of the superconducting transition temperature of the V-Ta system using his extended CPA theory. The use of the CPA requires the definition of a propagator $\langle G(z)\rangle_{\text{av}}$, which is the average of $G(z)$ over the ensemble of atomic configurations of the impure 1D chain. $\langle G(z)\rangle_{\text{av}}$ defines an effective translationally invariant medium and the matrix equation for $\langle G(z)\rangle_{\text{av}}$ is written as follows:

$$
\begin{bmatrix}\tilde{A}(z) & E\\ D & \tilde{C}(z)\end{bmatrix}\langle G(z)\rangle_{\text{av}}=1\ ,
$$

with

$$
\begin{aligned}
\tilde{A}(z)&=[\tilde{A}_{ik}(z)]=[[z-\epsilon_1(z)+2g_1\Delta_1(z)]\delta_{ik}]\ ,\\
\tilde{C}(z)&=[\tilde{C}_{ik}(z)]=[[z-\epsilon_2(z)-2g_2\Delta_2(z)]\delta_{ik}]\ .
\end{aligned}
\tag{6}
$$

Here $\epsilon_1(z)$ and $\epsilon_2(z)$ are self-energies corresponding to $\epsilon_{i,1}$ and $\epsilon_{i,2}$, $\Delta_1(z)$ and $\Delta_2(z)$ are self-consistent gap functions corresponding to the distortions $\Delta_{i,1}$ and $\Delta_{i,2}$, and g_1 and g_2 are the effective electron intramolecular vibration-mode coupling constants. The matrices E and D of Eq. (5) remain unchanged since only diagonal disorder is taken into account in Eqs. (5) and (6).

Use of Eqs. (5) and (6) enables us to write down the following expression for the t matrix due to excess scattering of the electrons over the average contained in $\langle G(z)\rangle_{\text{av}}$:

$$
T=W(1-\langle G\rangle_{\text{av}}W)^{-1};\quad T=[T_{ij}]\ ,
\tag{7}
$$

where

$$
W=\langle G\rangle_{\text{av}}^{-1}-G^{-1}=\begin{bmatrix}\tilde{A}(z)-A(z) & 0\\ 0 & \tilde{C}(z)-C(z)\end{bmatrix}\ .
\tag{8}
$$

We note that W in Eq. (8) is diagonal in the dimer representation but not in the site representation.[38] The CPA approximation is given by the requirement that the configurational average of the diagonal element T_{ii} which describes the excess multiple scattering of the electrons at a single-dimer site i is zero; i.e.,

$$
\langle T_{ii}\rangle_{\text{av}}=0\ .
\tag{9}
$$

Use of Eqs. (5) to (9) results in the following self-consistent equations:

$$
\langle\{\epsilon_{i,1}-\epsilon_1(z)+2[g_1\Delta_1(z)-g_{i,1}\Delta_{i,1}]\}/d_i(z)\rangle_{\text{av}}=0\ ,
\tag{10a}
$$

$$
\langle\{\epsilon_{i,2}-\epsilon_2(z)-2[g_2\Delta_2(z)-g_{i,2}\Delta_{i,2}]\}/d_i(z)\rangle_{\text{av}}=0\ ,
\tag{10b}
$$

$$
\langle[\epsilon_{i,1}-\epsilon_1(z)+2(g_1\Delta_1(z)-g_{i,1}\Delta_{i,1})][\epsilon_{i,2}-\epsilon_2(z)-2(g_2\Delta_2(z)-g_{i,2}\Delta_{i,2})]/d_i(z)\rangle_{\text{av}}=0\ .
\tag{10c}
$$

$d_i(z)$ is written as follows:

$$
d_i(z)=1-F_2(z)[\tilde{C}(z)-C]_{ii}-F_1(z)[\tilde{A}(z)-A]_{ii}+[F_1(z)F_2(z)-Z^2(z)][\tilde{A}(z)-A]_{ii}[\tilde{C}(z)-C]_{ii}\ .
\tag{11}
$$

F_1, F_2, and Z are given by

$$
\begin{aligned}
&F_1(z)=[z-\epsilon_2(z)-2g_2\Delta_2(z)]\Phi(z)\ ,\quad F_2(z)=[z-\epsilon_1(z)+2g_1\Delta_1(z)]\Phi(z)\ ,\\
&Z(z)=\frac{1}{N}\sum_k\frac{t(1+e^{-2iak})}{[z-\epsilon_1(z)+2g_1\Delta_1(z)][z-\epsilon_2(z)-2g_2\Delta_2(z)]-\epsilon^2(k)}\ ,\\
&\Phi(z)=\frac{1}{N}\sum_k\frac{1}{[z-\epsilon_1(z)+2g_1\Delta_1(z)][z-\epsilon_2(z)-2g_2\Delta_2(z)]-\epsilon^2(k)}\ ,
\end{aligned}
\tag{12}
$$

where N is the number of dimers. The sum over crystal momentum k is taken over the first Brillouin zone of the effective dimerized crystal whose lattice parameter is $2a$. $\epsilon(k)$ is the kinetic energy of an electron in a one-dimensional tight-binding band[10] for a crystal with lattice parameter a, i.e., $\epsilon(k) = 2t\cos ka$. Equations (10) to (12) are the basic equations of the SDCPA, from which the functions $\epsilon_\alpha(z)$ and $\Delta_\alpha(z)$ $(\alpha = 1, 2)$ are calculable, in terms of the local distortions $\Delta_{i,1}$ and $\Delta_{i,2}$. The equations for $\Delta_{i,1}$ and $\Delta_{i,2}$ in terms of $\mathcal{G}_{ij}^{\alpha\beta}(z)$ are given by

$$\Delta_{i,1} = \frac{g_{i,1}}{\omega_{i,1}\beta} \sum_{z_n} \mathcal{G}_{ii}^{11}(z_n) e^{z_n\delta} ,$$

$$\Delta_{i,2} = -\frac{g_{i,2}}{\omega_{i,2}\beta} \sum_{z_n} \mathcal{G}_{ii}^{22}(z_n) e^{z_n\delta} ; \tag{13}$$

$$z_n = (2n+1)i\pi/\beta, \quad n \in \mathfrak{Z}, \quad \delta = 0^+ ,$$

where $\beta = 1/k_B T$, T is the absolute temperature in K, and k_B is Boltzmann's constant. $\mathcal{G}_{ii}^{\alpha\alpha}(z_n)$ is the analytic continuation of $\mathcal{G}_{ii}^{\alpha\alpha}(z)$ onto the imaginary z axis at the point $z = z_n$ (the thermodynamic Green's function in the Matsubara representation). Equations (10) to (13) form a set of self-consistent equations. The addition of Eqs. (10a) and (10b) and the subsequent substitution of Eq. (13) for $\Delta_{i,\alpha}$ gives the following useful expression:

$$[g_1\Delta_1(z) + g_2\Delta_2(z)]\phi(z) = \left\langle \frac{g_{i,1}^2}{\omega_{i,1}\beta d_i(z)} \sum_{z_n} [\mathcal{G}_{ii}^{11}(z_n) - \mathcal{G}_{ii}^{22}(z_n)] e^{z_n\delta} \right\rangle_{\text{av}} , \tag{14}$$

where $\phi(z) = \langle 1/d_i(z) \rangle_{\text{av}}$.

The numerical analysis of the SDCPA equations is a formidable task. However the formalism may be simplified without loss of generality by assuming that there is no distinction between sublattices in the effective medium, i.e., we take

$$\Delta_{i,1} = \Delta_{i,2} , \quad g_1 = g_2 = g , \quad \Delta_1(z) = \Delta_2(z) = \Delta(z) . \tag{15}$$

Moreover we assume: $\epsilon_1(z) = \epsilon_2(z) = \epsilon(z)$ for simplicity. The SDCPA is used in the next section to obtain an expression for the Peierls transition temperature of an impure 1D conductor.

III. PEIERLS TRANSITION TEMPERATURE

The average distortions $\Delta_{i,1}$ and $\Delta_{i,2}$ and the related gap function $\Delta(z)$ are small for temperatures below, but close to the Peierls transition temperature. In consequence Eq. (14) will be linearized with respect to $\Delta_{i,\alpha}(\alpha = 1, 2)$ and $\Delta(z)$. The resultant equation for $\Delta(z)$ is given by

$$\Delta(z)\phi(z) = \left\langle \frac{2g_{i,1}^2}{(1+\delta_i)\omega_{i,1}\beta d_i^0(z)} \sum_n \frac{1}{d_i^0(z_n)} \{\chi^2(z_n)[z_n - \epsilon(z_n)]^2 - Z^2(z_n) - \chi(z_n)\}\Delta(z_n) \right\rangle_{\text{av}} , \tag{16a}$$

with

$$\chi(z) = \frac{1}{N} \sum_k \frac{1}{[z-\epsilon(z)]^2 - \epsilon^2(k)} \equiv \int \frac{\rho_0(\epsilon)d\epsilon}{[z-\epsilon(z)]^2 - \epsilon^2} \tag{16b}$$

and where δ_i is given by

$$\delta_i = -\frac{g_{i,1}^2}{\omega_{i,1}\beta} \sum_n \frac{2Z^2(z_n) - F_1^2(z_n) - F_2^2(z_n)}{d_i^0(z_n)} . \tag{16c}$$

$d_i^0(z)$ is the linearized function $d_i(z)$ with respect to the gaps and is given by

$$d_i^0(z) = 1 - 2[z-\epsilon(z)][\epsilon_i - \epsilon(z)]\chi(z) + \{\chi^2(z)[z-\epsilon(z)]^2 - Z^2(z)\}[\epsilon_i - \epsilon(z)]^2 . \tag{16d}$$

Further $\rho_0(\epsilon)$ is the density of states of the conduction band for the pure conductor.

Next we introduce the function $F^0(z)$ where

$$F^0(z) = [z - \epsilon(z)]\chi(z) . \tag{17}$$

From a symmetric density of states $\rho_0(\epsilon) = \rho_0(-\epsilon)$, $F^0(z)$ may be written as follows:

$$F^0(z) = \int \frac{\rho_0(\epsilon)d\epsilon}{z - \epsilon(z) - \epsilon} . \tag{18}$$

Equation (18) shows that $F^0(z)$ is the Hilbert transform[41] of the electronic density of states $\rho_0(\epsilon)$.

We now require an approximate functional form for $\rho_0(\epsilon)$ in order to proceed. It is convenient to choose a Lorentzian behavior for $\rho_0(\epsilon)$, i.e.,

$$\rho_0(\epsilon) = \frac{1}{\pi} \frac{D}{(1 + D^2\epsilon^2)} , \tag{19}$$

where $D = \pi N(0)$ is the density of states per spin at the Fermi level. The Lorentzian is useful in the sense that it enables us to proceed further analytically besides it does not alter drastically the nature of the Peierls transition. This is due to the fact that all the states contribute in providing us with the value of the transition temperature. Unfortunately, the Lorentzian density of states approximation breaks down in the case we are interested in calculating physical quantities to which we assign a fine mesh of states around the Fermi energy for instance or in the case where the density of states profile is crucial for the determination of a physical property. Use of Eqs. (18) and (19) gives the following expression for $F^0(z)$:

$$F^0(z) = 1/[z - \epsilon(z) + i\eta(z)/D] \ ,$$

where

$$\eta(z) = \mathrm{sgn}\{\mathrm{Im}[z - \epsilon(z)]\} \ . \tag{20}$$

Let $\epsilon_F^0 (=2t)$ and T_c be the half-width of the conduction band of the pure chain and the Peierls transition temperature, respectively. Then substitution of $F^0(z)$ as given in Eq. (20) into the gap equation (16) in conjunction with the approximation $\epsilon_F^0 >> k_B T_c$ gives the following equation for $\Delta(z)$:

$$\Delta(z) = \left\langle \frac{-2ig_{i,1}^2}{(1+\delta_i) D \omega_{i,1} \beta d_i^0(z)} \sum_n \frac{\eta(z_n)\Delta(z_n)}{[z_n + i\eta(z_n)/D - \epsilon_i]^2 [z_n - \epsilon(z_n)]} \right\rangle_{\mathrm{av}} . \tag{21}$$

We next make the standard approximation[42]

$$\Delta(z) = \left\langle \frac{-2ig_{i,1}^2}{(1+\delta_i) D \omega_{i,1} \beta d_i^0(z)} \right\rangle_{\mathrm{av}} \sum_n \left\langle \frac{\eta(z_n)\Delta(z_n)}{[z_n + i\eta(z_n)/D - \epsilon_i]^2 [z_n - \epsilon(z_n)]} \right\rangle_{\mathrm{av}} . \tag{22}$$

Use of the relationship $\phi(z) = 1$ then gives

$$\Delta(z) = \left\langle \frac{-2ig_{i,1}^2}{(1+\delta_i) D \omega_{i,1} \beta d_i^0(z)} \right\rangle_{\mathrm{av}} \sum_n \frac{\eta(z_n)[F^0(z_n)]^2 \Delta(z_n)}{z_n - \epsilon(z_n)} \ . \tag{23}$$

The symmetry relationships for the self-energy $\epsilon(z)$ and the gap function $\Delta(z)$ are

$$\epsilon(z) = \epsilon^*(z^*) \ , \quad \Delta(z) = \Delta^*(z^*) \ , \tag{24}$$

Then from Eqs. (23) and (24) the linearized equation for the gap function becomes

$$\Delta(z) = \left\langle \frac{4g_{i,1}^2}{(1+\delta_i) D \omega_{i,1} \beta d_i^0(z)} \right\rangle_{\mathrm{av}} \mathrm{Im} \left| \sum_{n \geq 0} \frac{\eta(z_n)[F^0(z_n)]^2}{z_n - \epsilon(z_n)} \Delta(z_n) \right| \ . \tag{25}$$

Since $\Delta(z)$ is a complex function of z, Eq. (25) is equivalent to two equations for $\mathrm{Re}\Delta(z)$ and $\mathrm{Im}\Delta(z)$, respectively. Since both equations are linear in these functions, the resulting equation for the Peierls transition temperature T_c is a 2×2 determinant. However Eq. (25) may be approximated directly without the necessity of analyzing the determinant. In the limit $\epsilon_F^0 >> k_B T_c$, $d_i^0(z)$, $F^0(z)$, and $\epsilon(z)$ may be replaced by their values at $z = i0$ in Eq. (25) and δ_i may be neglected as shown in Appendix A. Then the gap equation becomes

$$1 = \mathrm{Re} \langle [4g_{i,1}^2 F^2 / D \omega_{i,1} \beta_c d_i^0(i0)] \rangle_{\mathrm{av}} \sum_{n \geq 0} \frac{1}{\tau_n + v} \ , \tag{26}$$

where $F = \mathrm{Im} F^0(i0)$, $v = \mathrm{Im}\epsilon(i0)$, and $\tau_n = (2n+1)\pi\beta_c$; $\beta_c = 1/k_B T_c$. This is equivalent to expanding the right-hand side of the gap equation to first order in Db/a where

$$a = \left\langle \frac{1}{\epsilon_i^2 + 1/D^2} \right\rangle_{\mathrm{av}} ; \quad b = \left\langle \frac{\epsilon_i}{\epsilon_i^2 + 1/D^2} \right\rangle_{\mathrm{av}} \ . \tag{27}$$

The ratio Db/a is in general small since the sign of ϵ_i alternates due to the conditions imposed on the Fermi level (see below).

The first step is to show that Eq. (26) reduces to the results of Rice and Strässler[10] in the limit of a pure quasi-one-dimensional conductor with a single half-filled conduction band. In this limit $d_i^0(i0) = 1$, $v = 0$, $F^2 = D^2$, and $b = 0$. Then Eq. (26) reduces to the following equation:

$$1 = \frac{4g_0^2 D}{\omega_0} \sum_{n \geq 0} \frac{1}{(2n+1)\pi} \ , \tag{28}$$

where g_0 and ω_0 are the coupling constant of the electron-intramolecular vibration-mode interaction and the intramolecular vibration-mode frequency, respectively, of the pure conductor. Since the sum on the right-hand side of Eq. (28) diverges, a cutoff of the BCS type must be introduced. We take this to be $2\epsilon_F^0$ so that the sum over n in Eq. (28) is restricted to values of τ_n such that $\tau_n \leq 2\epsilon_F^0$. Use of this cutoff in conjunction with Eq. (28) yields the result of Rice and Strässler[10] for the Peierls transition temperature T_c^0 of the pure conductor with exactly the same numerical coefficient, i.e.,

$$k_B T_c^0 = (4e^c \epsilon_F^0/\pi)\exp[-\omega_0/2g_0^2 N(0)] \ , \tag{29}$$

where $c\,(=0.577)$ is Euler's constant.

The equation for the Peierls transition temperature of an impure quasi-one-dimensional conductor $A_x B_{1-x}$ is obtained using the cutoff $2\epsilon_F$ in Eq. (26), ϵ_F being the half-bandwidth of the conduction band of the alloy. The resultant equation for T_c is

$$\ln\left(\frac{\beta_c^0 \epsilon_F^0}{\pi}\right) - \psi\left(\tfrac{1}{2}\right) = \nu\left[\ln\left(\frac{\beta_c \epsilon_F}{\pi}\right) - \psi\left(\frac{1}{2} + \frac{\upsilon\beta_c}{2\pi}\right)\right] \ , \tag{30}$$

where $\psi(x)$ is the logarithmic derivative[43] of the gamma function and ν and υ are quantities, respectively, given by

$$\begin{aligned} \nu &= \left\langle \frac{g_i^2/g_0^2\,(1-D^2\epsilon_i^2)}{\omega_i/\omega_0(1+D^2\epsilon_i^2)^2} \right\rangle_{\text{av}} \ ; \\ \upsilon &= \left\langle \frac{D\epsilon_i^2}{D^2\epsilon_i^2+1} \right\rangle_{\text{av}} \Big/ \left\langle \frac{1}{D^2\epsilon_i^2+1} \right\rangle_{\text{av}} \ . \end{aligned} \tag{31}$$

g_i, ω_i, and $\epsilon_i\,(i=A,B)$ are the electron intramolecular vibration-mode coupling constant, the phonon frequency, and the electron pseudopotential, respectively, for the pure A or B crystals, $\beta_c^0 = 1/k_B T_c^0$ is the inverse transition temperature of the pure B material $(x=0)$. Clearly, the quantity ν which contains the lattice alloy parameters reduces in the dilute limit $(x \ll 1)$ to

$$\nu = 1 + O(x) \ , \tag{32}$$

whereas υ which corresponds to the inverse lifetime of the electrons that are scattered by the site static fluctuations of the intramolecular potential goes in the dilute $(x \ll 1)$ and weak scattering limits $(D|\epsilon_A - \epsilon_B| \ll 1)$ to

$$\upsilon = x\pi N(0)(\epsilon_A - \epsilon_B)^2 \ . \tag{33}$$

Equation (33) for υ is identical to that obtained by Abrikosov and Gorkov[26] for the impurity scattering of the electrons treated in the Born approximation for a site δ-function potential strength $(\epsilon_A - \epsilon_B)$ and a density of states at the Fermi surface equal to $N(0)$. In the above limit [see Eqs. (32) and (33)], Eq. (30) reduces to the result obtained by Bulaevskii and Sadovskii[29] and Schuster[24] where it was shown that nonmagnetic impurities influence the transition temperature of the Peierls phase transition in the same way as magnetic impurities change the critical temperature of a superconductor (see Appendix B for an analytical comparison). Note that the above two references did not treat the changes in the lattice upon alloying such that the quantity ν was then taken to be unity. Moreover, they considered a site independent order parameter Δ in the limit of weak disorder. This kind of treatment leads to an underestimation[38] of the mean-field alloy transition temperature with respect to ours where we take into account the site dependence of the order parameter Δ_i.

The final step is to show how the dependence of the critical temperature T_c may be obtained as a function of concentration x of A atoms in an $A_x B_{1-x}$ alloy. Let the number of valence electrons per A and B atoms be $(1+n_A)$ and 1, respectively, and let the Fermi level of the alloy be fixed at zero energy. The equation which fixes the chemical potential at zero energy is

$$(1+xn_A)/2 = \int_{-\infty}^{0} d\omega\,\rho(\omega) \ . \tag{34}$$

$\rho(\omega) = -(1/\pi)\,\mathrm{Im}F^0(\omega + i0)$ is the density of electron states in the alloy and is given in terms of the Lorentzian distribution by

$$\rho(\omega) = \frac{1}{\pi D}\left(\frac{x}{(\omega-\epsilon_A)^2 + 1/D^2} + \frac{1-x}{(\omega-\epsilon_B)^2 + 1/D^2}\right) \ . \tag{35}$$

Equations (34) and (35) then lead to the following relationship between x, $\epsilon_{A,B}$, and n_A:

$$x = \tan^{-1}\epsilon_B/(\tan^{-1}\epsilon_B - \tan^{-1}\epsilon_A - \pi n_A/2) \ . \tag{36}$$

Equations (30) and (36) enable us to calculate T_c as a function of x provided that the normalized coupling constants λ_i given by

$$\lambda_i = 2N(0)g_i^2/\omega_i \quad (i=A,B) \tag{37}$$

and the related half-bandwidths $\epsilon_{F,i}$ are known. The parameters and the half-bandwidths $\epsilon_{F,i}$ of the alloy are related as follows in the simplest approximation:

$$\epsilon_F = x\epsilon_{F,A} + (1-x)\epsilon_{F,B} \ . \tag{38}$$

In the next section $T_c(x)$ will be calculated for fixed values of $\delta = D|\epsilon_B - \epsilon_A|$. We note that the quantity $D(\epsilon_A + \epsilon_B)$ must be determined using Eq. (34) which fixes the chemical potential at zero energy.

IV. RESULTS AND DISCUSSIONS

The behavior of the alloy critical temperature T_c as a function of x at fixed δ is shown in Fig. 1. In the isoelectronic case, i.e., $n_A = 0$, one sees quite clearly that for small δ, i.e., small site energies difference, $T_c(x)$ changes linearly with x. As we increase δ the curves $T_c(x)$ start to bend downwards and for large δ, $T_c(x)$ even reaches zero at critical concentrations. Moreover one notes that a symmetry in the behavior of $T_c(x)$ as x is close to 0 or 1 since for these limits we have nearly the pure B or A materials. However,

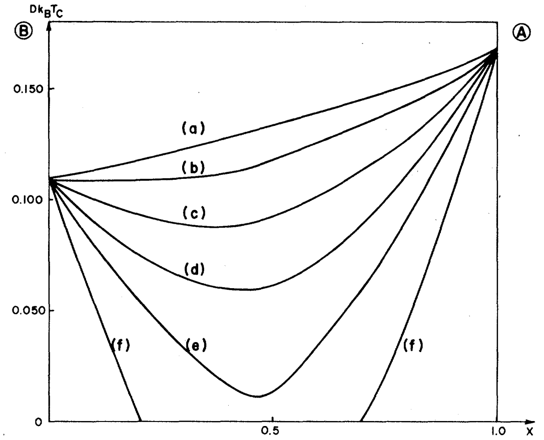

FIG. 1. Normalized transition temperature Dk_BT_c as a function of the concentration x of A species for fixed values of $\delta = D|\epsilon_B - \epsilon_A|$ in the isoelectronic case; i.e., $n_A = 0$. The normalized coupling constants are $\lambda_A = 0.4$ and $\lambda_B = 0.33$ for the pure A and B materials. The normalized half-bandwidths are $D\epsilon_{F,A} = 0.9$, and $D\epsilon_{F,B} = 1.0$. The curves (a), (b), (c), (d), (e), and (f) correspond to values of δ equal, respectively, to 0.1, 0.2, 0.3, 0.4, 0.5, and 0.7.

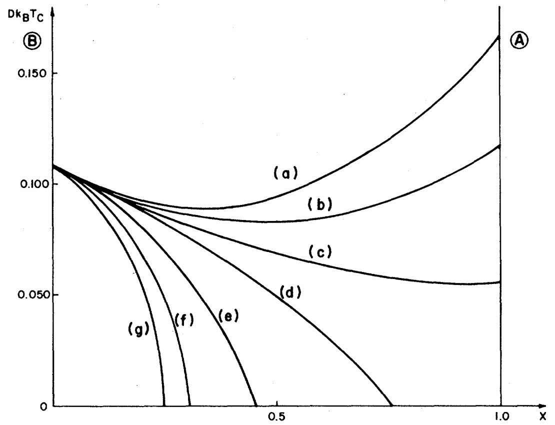

FIG. 3. These are curves of the transition temperature vs x at fixed $\delta(=0.3)$ for different values of n_A. The parameters of the pure material are the same as in Figs. 1 and 2 . Curves (a), (b), (d), (e), (f), and (g) are for n_A equal, respectively, to 0.0, 0.1, 0.2, 0.3, 0.4, and 0.5. The curve (c) corresponding to $n_A = 0.15$ is the borderline separating the curves belonging to a definite sign of concavity.

in the case where the valences are not equal, i.e., $n_A \neq 0$ the situation is quite different. We considered three cases of interest (see Figs. 2, 3, and 4). Firstly, for small δ, Fig. 2 shows that as we increase n_A, the quasilinear behavior of $T_c(x)$ obtained for $n_A = 0$, is strongly altered. The resulting $T_c(x)$ curves are bending progressively downwards as we increase n_A. Nevertheless one should keep in mind that our results for $T_c(x)$ are considered to be valid for regions where x is near zero since at large values of x $(x \simeq 1)$, one approaches the pure A material having a valence of $(1+n_A)$ where a commensurate-incommensurate phase transition occurs for increasing values of n_A. This possibility, which is left out of our formalism, limits the validity of our calculation of the reduced critical temperature $T_c(x)$ to small values of x, the maximum value of x decreasing with increasing value of n_A.

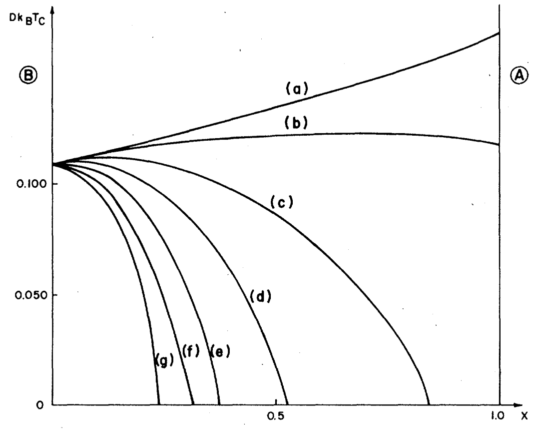

FIG. 2. Behavior of the normalized transition temperature Dk_BT_c vs x for different values of n_A. The pure B material has valence 1 whereas A has valence $(1+n_A)$. The curves are plotted for the same value of δ which is 0.1. Besides $\lambda_A = 0.4$, $\lambda_B = 0.33$, $D\epsilon_{F,A} = 0.9$, and $D\epsilon_{F,B} = 1.0$ as in Fig. 1. The curves (a), (b), (c), (d), (e), (f), and (g) are calculated for n_A equal, respectively, to 0.0, 0.1, 0.2, 0.3, 0.4, 0.5, and 0.6.

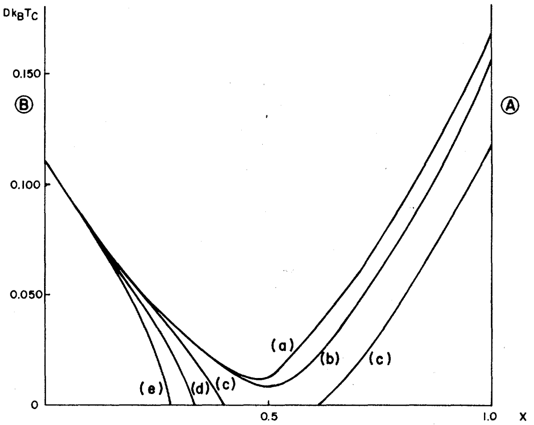

FIG. 4. Curves $Dk_BT_c(x)$ at fixed $\delta(=0.5)$ for different values of n_A. The parameters used are the same as in Figs. 1–3. Curves (a), (b), (c), (d), and (e) are for n_A equal to 0.0, 0.05, 0.1, 0.2, and 0.3, respectively.

Leung and Ono[33] studied separately the Peierls transition in a non-half-filled tight-binding band and have obtained expressions for the transition temperature reduction with the filling. In Fig. 5 we plotted the transition temperature obtained for the pure A material as a function of n_A. This was done by taking the limit $x \rightarrow 1$ of the transition temperature of the alloy A_xB_{1-x}. For comparison we show in the same figure the trend of the transition temperature as calculated for the same material in the framework of Leung[33] formalism. From this one concludes the SDCPA overestimates the transition temperature from the normal to the commensurate phase. Furthermore, Leung and Ono[33] predict the transition to the incommensurate phase to occur at $n_A = 0.04$ (for the parameters of Fig. 5). This means that the SDCPA should be restricted to values of $n_A << 1$. Now let us get back to discuss further the results of the SDCPA. In Fig. 3, we considered an intermediary value for δ. The characteristic feature happening in this case is the change of the sign of the concavity of the curve $T_c(x)$ as we increase n_A. This is not observed in the isoelectronic case ($n_A = 0$) where all the curves have positive concavity. A supplementary feature happens for large values of δ (Fig. 4) where $T_c(x)$ resumes increasing its value with x after falling down to zero at a lower critical concentration. This has been observed already in the isoelectronic case (Fig. 1). The observed depression of the transition temperature in the isoelectronic case (Fig. 1) stems from the additional scattering of electron-hole pairs by the potentials arising from disorder in the electronic states and electron intramolecular vibrational-mode coupled states. The presence of these two independent types of disorder calls for the determination of two effective potentials $\epsilon(z)$ and $\Delta(z)$. The electron-hole pairs hopping through the lattice are forced into different binding situations on sites occupied by different atoms with the accompanied pair breaking situation.

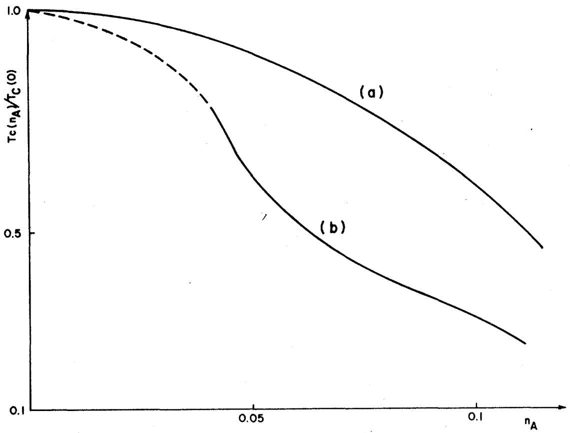

FIG. 5. Variation of the transition temperature for the A material vs n_A. (a) is given with SDCPA by taking the limit $x \rightarrow 1$ of the normal to commensurate transition temperature of the alloy A_xB_{1-x}. The parameters used are $\lambda_A = \frac{1}{3}$, $D\epsilon_{F,A} = 1.0$. (b) is given by Leung (Ref. 33) theory for the same parameters.

In this paper, we have evaluated the effect of alloying on the mean-field Peierls transition temperature T_c. An overall depression of $T_c(x)$ for intermediate concentration is predicted for alloying half-filled conduction-band system with impurities having a single electron. The depression is enlarged for larger deviations δ of the single-site intramolecular potentials. The additional effect of alloying with molecules having a valency larger than one ($n_A > 0$), is to produce additional reduction of T_c for x close to unity ($x \lesssim 1$) and an overall suppression of the mean-field Peierls state for large enough deviation of the valency from unity. Sen and Varma[30] have already obtained this kind of depression for the transition temperature, however it is difficult to make a direct comparison of our results with theirs: they treated the $\frac{5}{6}$-filled one-dimensional band, moreover they worked from the high-temperature uniform phase, i.e., for zero-order parameters Δ_i. Even though we worked from the low temperature phase considering site dependent Δ_i our results must be equivalent, at the same filling, to those of Sen and Varma[30] since our definition of the alloying transition is where all the effective order parameters are zero. A definite comparison fo $T_c(x)$ with the experimental results (like those of Schultz and Craven[16]) which are related to the establishment of three-dimensional long-range order may only proceed at a qualitative level since $T_c(x)$ is a scale temperature as indicated in the Introduction. Nevertheless, the results obtained above are in good agreement with the few experimental results[16] coming out on this subject.

APPENDIX A: EVALUATION OF δ_i

$$\delta_i = -\frac{g_{i,1}^2}{\omega_{i,1}\beta} \sum_n \frac{2Z^2(z_n) - F_1^2(z_n) - F_2^2(z_n)}{d_i^0(z_n)} . \tag{A1}$$

At T_c and in the limit $\beta_c \epsilon_F^0 >> 1$ one may write

$$F_1(z) = F_2(z) = F^0(z)$$

so that

$$\delta_i = \frac{2g_{i,1}^2}{\omega_{i,1}\beta_c} \sum_n \frac{[F^0(z_n)]^2}{\{1 - [\epsilon_i - \epsilon(z_n)]F^0(z_n)\}^2} . \tag{A2}$$

For a Lorentzian density of states one has

$$[F^0(z)]^{-1} = z + i\eta(z)/D - \epsilon(z) , \tag{A3}$$

where $\eta(z)=\operatorname{sgn}\{\operatorname{Im}[z-\epsilon(z)]\}$. Hence,

$$\delta_i=\frac{2g_{i,1}^2}{\omega_{i,1}\beta_c}\sum_n\frac{1}{[z_n+(i/D)\eta(z_n)-\epsilon_i]^2} \ .$$

One may now decompose this sum in two, for $n>0$ and $n<0$, further in conjunction with the symmetry properties of $\epsilon(z)$ and $\eta(z)$ one obtains

$$\delta_i=\frac{4g_{i,1}^2}{\omega_{i,1}\beta_c}\sum_{n=0}^{N}\operatorname{Re}\frac{1}{[\epsilon_i+z_n+(i/D)\eta(z_n)]^2} \ , \tag{A4}$$

where N is the usual cutoff $N=\beta_c\epsilon_F/\pi$. Hence,

$$\begin{aligned}\delta_i&\leqslant\frac{4g_{i,1}^2}{\omega_{i,1}\beta_c}\sum_{n=0}^{N}\frac{1}{|\epsilon_i+z_n+(i/D)\eta(z_n)|^2}\\&=\frac{4g_{i,1}^2}{\omega_{i,1}\beta_c}\sum_{n=0}^{N}\frac{1}{\epsilon_i^2+[\tau_n+\eta(z_n)/D]^2} \ .\end{aligned} \tag{A5}$$

Consequently

$$\delta_i\leqslant\frac{4g_{i,1}^2}{\omega_{i,1}\beta_c}\sum_{n=0}^{N}\frac{1}{[\tau_n+\eta(z_n)/D]^2} \ . \tag{A6}$$

The sum in Eq. (A6) is approximated by

$$\delta_i\leqslant\frac{4g_{i,1}^2}{\omega_{i,1}\beta_c}\sum_{n=0}^{N}D^2 \tag{A7}$$

for $\eta(z_n)=\pm1$ and $\tau_n \ll 1/D$. $D=\pi N(0)\sim1/\epsilon_F$ in one dimension. Equation (A7) yields

$$\delta_i\leqslant\frac{4g_{i,1}^2\beta_c}{\omega_{i,1}\pi}\left[\frac{1}{\beta_c\epsilon_F}\right] \ , \tag{A8}$$

which means that δ_i may be safely neglected in the limit $\beta_c\epsilon_F \gg 1$.

APPENDIX B: RELATION TO THE THEORY OF SUPERCONDUCTORS CONTAINING MAGNETIC IMPURITIES

Equation (5) for the electron propagator G_{ij} in the dimer representation can be written in the site notation as follows:

$$\begin{bmatrix}z-\epsilon_{i,1}+2g_{i,1}\Delta_{i,1} & 0\\ 0 & z-\epsilon_{i,2}-2g_{i,2}\Delta_{i,2}\end{bmatrix}G_{ij}=\delta_{ij}+\tau_1\sum_k t_{ik}G_{kj} \ . \tag{B1}$$

The Pauli matrices τ_1 and τ_3 are given by

$$\tau_1=\begin{bmatrix}0&1\\1&0\end{bmatrix} ; \quad \tau_3=\begin{bmatrix}1&0\\0&-1\end{bmatrix} \ .$$

The simplest approximation for nonmagnetic impurities in a quasi-1D conductor is given by the following equalities:

$$\begin{gathered}\Delta_{i,1}=\Delta_{i,2}=\tilde{\Delta} \ , \quad g_{i,1}=g_{i,2}=g \ , \quad \omega_{i,1}=\omega_{i,2}=\omega \ ,\\ \epsilon_{i,1}=\epsilon_{i,2}=\epsilon_i \ , \quad \Delta=2g\tilde{\Delta} \ .\end{gathered} \tag{B2}$$

Then Eq. (B1) can be written as follows using Eq. (B2):

$$(z+\Delta\tau_3)G_{ij}=\delta_{ij}+\tau_1\sum_k t_{ik}G_{kj}+\epsilon_iG_{ij} \ . \tag{B3}$$

For an A,B alloy, ϵ_i may be written as follows:

$$\epsilon_i=0, \quad i\in A \ , \quad \epsilon_i=\epsilon_B, \quad i\in B \ . \tag{B4}$$

The Fourier components of t_{ij} and G_{ij} may be written:

$$t_{ij}=\frac{1}{N}\sum_q\epsilon_q e^{iq(R_i-R_j)} \ , \quad G_{ij}=\frac{1}{N}\sum_{qq'}G_{qq'}e^{i(qR_i-q'R_j)} \ . \tag{B5}$$

Then use of Eqs. (B3) to (B5) in conjunction with the following rotation in pseudospin space

$$1,\tau_1,\tau_2,\tau_3\rightarrow1,\tau_3,\tau_2,\tau_1 \tag{B6}$$

gives the following equation for $G_{qq'}$

$$(z-\epsilon_q\tau_3+\Delta\tau_1)G_{qq'}=\delta_{qq'}+\sum_{q''}\epsilon_{qq''}G_{q''q'} \ , \tag{B7}$$

where

$$\epsilon_{qq'}=\frac{1}{N}\sum_{\gamma\in B}\epsilon_B e^{iR_\gamma(q-q')} \ . \tag{B8}$$

Δ now is given by the self-consistent equation

$$\Delta=\frac{g}{\beta\omega}\tau_1\sum_n\langle G_{ii}(z_n)\rangle_{\text{av}} \ . \tag{B9}$$

Equation (B7) is the equation of motion for an electron propagator corresponding to Schuster's Hamiltonian [Ref. 24, Eq. (6)]. Hence, Eq. (B7) is identical to the propagator equation for a BCS superconductor containing magnetic impurities following Schuster's argument, provided that we take $S(S+1)=1$ when S is the effective impurity spin. It is therefore not surprising that the equations for the Peierls transition temperature for impure quasi-1D conductors of Sec. III are so closely analogous to those for the superconducting critical temperature of a superconductor containing magnetic impurities.

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