PHYSICAL REVIEW B VOLUME 11, NUMBER 11 1 JUNE 1975

Peierls instability in pseudo-one-dimensional conductors

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(Received 27 March 1974; revised manuscript received 7 October 1974)

We investigate the properties of pseudo-one-dimensional systems which exhibit Peierls instability at $T_c(\mu)$, where μ is the Fermi energy as measured from the middle of a conduction band. We show that, except at $\mu = 0$ or $|\mu| \gg T$, the giant Kohn anomalies of the phonon spectrum do not occur at $2k_F$. For $|\mu| \ll W$, where $2W$ is the bandwidth, $T_c(\mu)$ decreases as $|\mu|$ increases, and, for $W \gg |\mu| \gg T$, $T_c(\mu)/T_c(0) = T_c(0)/2.26|\mu|$. As $|\mu|$ further increases towards W, the decrease of $T_c(\mu)$ towards zero need not in general be monotonic. The neutron scattering differential cross section shows a peak with magnitude proportional to $(T-T_c)^{-1}$.

I. INTRODUCTION

For some time, investigations have been made on those organic solids which, because of their peculiar crystal structures, show electrical conductivities so anisotropic that they may be considered as one-dimensional conductors. The charge-transfer salts of tetracyanoquinodimethane (TCNQ) and the mixed-vacancy planar (MVP) transition-metal compounds are two fairly large classes of compounds[1,2] that possess such anisotropy. In both cases, planar molecules are stacked in columns. The interactions between adjacent atoms in a column are sufficiently strong to form bands. The columns are, however, relatively far apart so that conductivities along the column are much larger than those perpendicular to it. Some of these solids are metallic at high temperature, and they undergo a metal-insulator phase transition[1-4] as the temperature decreases. One of the possible explanations for the phase transition is the occurrence of a Peierls instability[5] which produces linear superlattice distortion.[6,7]

So far in the literature on Peierls instability and the Kohn anomalies in one-dimensional systems, discussions have been limited to solids with exactly half-filled conduction bands.[8,9] In the present work, we investigate[10,11] the effects of μ on various properties of pure one-dimensional conductors, where μ denotes the Fermi energy as measured from the middle of the conduction band. We also investigate under what conditions is the tight-binding model equivalent to the free-electron model. One may apply methods similar to those presented here to calculate the effects of μ on fluctuation conductivity.[10-12]

In Sec. II we observe that the Fermi energy μ plays the role of paramagnetic[14-17] effect of a magnetic field on superconductors. We investigate the Kohn anomalies, Peierls instability, and neutron scattering for various values of μ. μ is a measure of the deviation from half-filledness since μ vanishes for exactly half-filled conduction bands. We show that, within the range $|\mu| \ll W$ (assuming $T \ll W$), as $|\mu|$ increases, the transition temperature $T_c(\mu)$, at which a Peierls distortion or a soft mode occurs, decreases, since the nonvanishing of μ produces a mismatching between the electron state k and the states $k \pm Q$. For $|\mu| < 1.056 T_c(0)$, the soft-phonon mode has wave number $Q = \pi/d$, where d is the interatomic distance and $T_c(0)$ is the transition temperature for an identical system, but with $\mu = 0$. For $|\mu| > 1.056 T_c(0)$, however, it is the phonon mode with wave number equal to $Q + q_0$ ($q_0 \neq 0$) that becomes soft first as T approaches $T_c(\mu)$. As $|\mu|$ further increases, q_0 increases, but $Q + q_0$ is not equal to $2k_F$ until $|\mu|/T$ becomes very large. Accordingly, the giant Kohn anomalies of the phonon spectrum do not occur at $2k_F$ in one-dimensional conductors except when $\mu = 0$ and $|\mu| \gg T$. In general, the Kohn anomalies occur at $k = Q + q_0$. For $W \gg W - |\mu| \gg T$, the tight-binding model becomes equivalent to the free-electron model, as far as Peierls instability is concerned. At $|\mu| = W$, $T_c = 0$; that is, there is no Peierls distortion for a completely filled or empty band, as one would expect intuitively.

In Sec. III we show that the critical fluctuation would produce in neutron scattering a central peak which diverges as $(T - T_c)^{-1}$.

According to some general theorems,[13] there can exist at finite temperature no phase transition in one-dimensional systems for short-range interactions. This is probably true in general for strictly one-dimensional systems. We assume, however, that we are dealing here with a model system in which, while the electron can move in only one direction, the lattice is three-dimensional, so that mean-field theory may be employed to deal with Peierls instability.

II. PEIERLS INSTABILITY

In a one-dimensional electron-phonon system, the model Hamiltonian may be taken as

$$\mathcal{H}=\sum_{k\sigma} E_k a^\dagger_{k\sigma}a_{k\sigma}+\Omega_0\sum_q b^\dagger_q b_q$$
$$+g\sum_{k\sigma}\sum_q a^\dagger_{k+q\sigma}a_{k\sigma}(b_q+b^\dagger_{-q}),$$

where g is the electron-phonon coupling constant and a_k and b_q are operators for electrons and phonons, respectively. In a tight-binding model, $E_k = -W\cos kd$, with d denoting the interatomic distance and $2W$ the width of the band; $\mu=-W\cos k_F d$ is the Fermi energy, and k_F is the Fermi momentum. We shall use frequently the relation

$$E_{k+Q}=-E_k\,, \tag{1}$$

where $Q=\pi/d$. When $\mu=0$, $Q=2k_F$. Ω_0 is here equal to Ω_{p_0} because, for our purposes, only phonon modes with $q\simeq p_0$ are important, where p_0 is the wave number of the phonon mode which goes soft at the temperature T_c, at which the Peierls instability occurs. It is convenient to write

$$p_0=Q+q_0\,.$$

In this section we shall derive the equations defining q_0 and T_c.

Using the familiar random-phase approximation, the renormalized phonon propagator is

$$D^{-1}(i\Omega_m,p)=D_0^{-1}(i\Omega_m,p)-g^2\Pi(i\Omega_m,p)\,,$$

with the polarization propagator

$$\Pi(i\Omega_m,p)=T\sum_\nu\sum_{k\sigma}G(i\omega_\nu,k)$$
$$\times G(i\omega_\nu+i\Omega_m,k+p)\,,$$

and the bare phonon propagator

$$D_0^{-1}(i\Omega_m,p)=[(i\Omega_m)^2-\Omega_0^2]/2\Omega_0\,,$$

where

$$p=p_0+q\,.$$

To bring out the physics of our calculation, it is preferable to write

$$\Pi(i\Omega_m,p)=T\sum_\nu\sum_{\substack{k>0\\ \sigma}}G(i\omega_\nu,k)$$
$$\times[G(i\omega_\nu+i\Omega_m,k+p)+G(i\omega_\nu+i\Omega_m,k-p)]\,.$$

The first term represents the coupling between the momentum states k and $k+p$, while the second term represents the coupling between the states k and $k-p$. The coupling between states k and $k\pm p\pm 2n\pi/d$ should not be included since one must keep the values of k within the range $|k|<\pi/d$. Using $G_R(i\omega_\nu,k)=(i\omega_\nu-E_k+\mu+1/2\tau)^{-1}$ and Eq. (1), one obtains, after some straightforward calculations,

$$\Pi(\Omega+i\delta,p)=-N(\mu)[\ln(4e^\gamma W/\pi T)-F(\mu,q_0,T;\rho)$$
$$+(-\alpha^2q^2+i\Omega b)/\lambda\Omega_0^2]\,,$$

where

$$\lambda=2N(\mu)g^2/\Omega_0\,, \tag{2}$$

$$F(\mu,q_0,T;\rho)=\tfrac{1}{2}\,\mathrm{Re}\sum_{j=\pm}\psi(\tfrac{1}{2}+\rho+i\mu_j)-\psi(\tfrac{1}{2})\,, \tag{3}$$

$$\mu_\pm=(2\mu\pm v_Fq_0)/4\pi T\,, \tag{4}$$

$$\rho=1/4\pi T\tau\,, \tag{5}$$

$$\alpha^2=\lambda\Omega_0^2\alpha_0^2\,, \tag{6}$$

$$\alpha_0^2=-(v_F/8\pi T)^2\,\mathrm{Re}\sum_{j=\pm}\psi^{(2)}(\tfrac{1}{2}+\rho+i\mu_j)\,, \tag{7}$$

$$b=\lambda\Omega_0^2B/8\pi T\,, \tag{8}$$

$$B=\mathrm{Re}\sum_{j=\pm}\psi^{(1)}(\tfrac{1}{2}+\rho+i\mu_j)\,. \tag{9}$$

τ is the lifetime of the electron states due to impurity scattering and the scatterings of those phonons with wave number not near to p_0; v_F is the Fermi velocity; γ is Euler's constant; $N(\mu)$ is the density of states at the Fermi surface. Since $\Pi(i\Omega_m,p)$ is an even function of μ, one readily observes that μ plays the role of paramagnetic effects[14-17] of a magnetic field on superconductivity. The above relations are valid only when $q_0d\ll 1$. In our calculations, we have, for simplicity, assumed the relation $|\mu|\ll W$. It is not difficult however to relax this limitation. Near T_c, at which the Peierls instability occurs the retarded dressed phonon propagator is

$$D_R(\Omega,p)=2\Omega_0/(\Omega^2-\lambda\Omega_0^2\epsilon-\alpha^2q^2+i\Omega b)\,, \tag{11}$$

where

$$\epsilon=(T-T_c)/T_c\,. \tag{12}$$

T_c and q_0 are functions of μ, obtained by solving the following equations in the pure limit $\tau T\gg 1$:

$$\ln(T_c/T_0)+F(\mu,q_0,T_c;0)=0 \tag{13}$$

and

$$-\frac{8\pi T_c}{v_F}\frac{\partial F(\mu,q_0,T_c;0)}{\partial q_0}$$
$$=\mathrm{Im}[\psi^{(1)}(\tfrac{1}{2}+i\mu_+)-\psi^{(1)}(\tfrac{1}{2}+i\mu_-)]=0\,, \tag{14}$$

where ψ is a digamma function,

$$\psi^{(n)}(z) = \frac{\partial^n \psi(z)}{\partial z^n}$$

and

$$T_0 = T_c(0) = (4We^{\gamma}/\pi)e^{-1/\lambda} \tag{15}$$

is the transition temperature of an identical system, but with $\mu = 0$. Explicitly, $4e^{\gamma}/\pi = 2.26$. At $\mu = 0$, $q_0 = 0$, it follows immediately from Eq. (3) that $F(0, 0, T_c; 0) = 0$. Since $F(\mu, q_0, T_c; 0)$ is always positive, T_c is smaller than T_0 for $\mu \neq 0$. Equation (14) ensures that the minimum of $F(\mu, q, T_c; 0)$, as a function of q, occurs at $q = q_0$. When $F(\mu, q, T_c; 0)$ is at its minimum as a function of q, it follows from Eq. (13) that T_c is at its maximum.

From these equations, one observes that for $|\mu| \ll W$, μ has the same effect as a magnetic field on the phase transition of one-dimensional conductors.[18] We define μ_L as the solution of the equation

$$\left(\frac{\partial^2 F}{\partial q_0^2}\right)_{q_0=0} = 0\,;$$

i.e.,

$$\mathrm{Re}\,\psi^{(2)}(\tfrac{1}{2} + i\mu_L/2\pi T) = 0\,.$$

In connection with paramagnetic effects on superconductors, Sarma[16] has solved this equation with

$$\mu_L = 1.056\,T_0\,. \tag{16}$$

q_0 vanishes for $|\mu| < \mu_L$, but is nonzero for $|\mu| > \mu_L$. When $|\mu| \gg T$, we expect $|\mu_-| \ll 1$ and $|\mu_+| \gg 1$. In such a case,

$$\mathrm{Im}\,\psi^{(1)}(\tfrac{1}{2} + i\mu_-) \simeq -14\zeta(3)\mu_-$$

and

$$\mathrm{Im}\,\psi^{(1)}(\tfrac{1}{2} + i\mu_+) \simeq -1/\mu_+\,.$$

Equation (14) therefore leads to the relation

$$\mu_- \approx [14\zeta(3)\mu_+]^{-1} \simeq 0\,, \tag{17}$$

which is equivalent to

$$2\mu \simeq v_F q_0\,. \tag{18}$$

Using the relation $|\frac{1}{2}Q - k_F|d \ll 1$ and the definition of μ, one readily obtains the relation

$$2k_F = p_0\,.$$

Accordingly, when $|\mu| \gg T$, one may replace μ_- in Eqs. (13) and (14) by $\mu_- = 0$ and use the approximation

$$\mathrm{Re}\,\psi(\tfrac{1}{2} + i\mu_+) = \ln \mu_+\,.$$

One obtains, then, from Eq. (13),

$$\frac{T_c}{T_0} = \frac{\pi}{4e^{\gamma}}\frac{T_0}{|\mu|}\,. \tag{19}$$

Assuming $|\mu| = 0.2$ eV and $T_0 = 500$ K, one obtains $T_c \sim 50$ K. To make physical interpretations more transparent, it is interesting to substitute the explicit expression Eq. (15) for T_0 into Eq. (19) to obtain[19]

$$T_c = (W/|\mu|)T_f\,, \tag{20}$$

where

$$T_f = (4e^{\gamma}/\pi)We^{-1/\lambda_f}\,, \tag{21}$$

with

$$\lambda_f = \tfrac{1}{2}\lambda\,. \tag{22}$$

T_f may be taken as the transition temperature for the free-electron model. As we have used the relation $q_0 d \ll 1$ in our calculation, Eqs. (20)–(22) are, strictly speaking, only valid for $|\mu| \ll W$. As $|\mu|$ approaches W so that $W \gg W - |\mu| \gg T$, one obtains

$$T_c(\mu) = (1 - |\mu|/W)(2e^{\gamma}W/\pi)e^{-1/\lambda_f} \tag{23}$$

from the equation

$$\Omega_0/2q^2 + \Pi(0, p) = 0\,. \tag{24}$$

At $|\mu| = W$, $T_c = 0$. The physical meanings of the above derivations are as follows. The Peierls distortions are due to coupling between the electron states k and the states $k \pm p_0$. We shall consider only $k > 0$; the reasoning for $k < 0$ is similar. At $\mu = 0$, $p_0 = Q = 2k_F$. The states k and $k \pm Q$ are symmetric with respect to the Fermi surface; by "symmetric," we mean $E_k - \mu = -(E_{k\pm Q} - \mu)$. Such symmetry gives rise to optimal coupling effects. $T_c(\mu)$ is accordingly largest at $\mu = 0$ (assuming λ constant). At $\mu = 0$, the giant Kohn anomalies of the phonon spectrum occur at $2k_F$. As $|\mu|$ increases but is still smaller than μ_L, p_0 remains equal to Q. However Q no longer equals $2k_F$ and consequently the coupling between k and $k \pm p_0$ is not symmetric with respect to the Fermi surface. Such a mismatch is reflected in the reduction in T_c as $|\mu|$ increases, T_c being determined by Eq. (13) with $q_0 = 0$. The Kohn anomalies occur at $Q(\neq 2k_F)$. As $|\mu|$ further increases so that $|\mu| > \mu_L$, the wave number of the soft phonon becomes $p_0 = Q + q_0$ with $q_0 \neq 0$. In this way, the electron states k and $k - p_0$ become more symmetric with respect to the Fermi surface. On the other hand, k and $k + p_0$ become less symmetric, giving rise to a further reduction in T_c. T_c and q_0 are now determined by Eqs. (13) and (14). The Kohn anomalies occur at $Q + q_0$, which is again not equal to $2k_F$. In the limit $|\mu| \gg T$, $p_0 = Q + q_0 = 2k_F$. The states k and $k - p_0$ become again completely symmetric with respect to the Fermi surface. Greater mismatching, however, exists between k and $k + p_0$. The transition temperature now has a very simple form, namely Eq. (19). The Kohn anomalies occurs again at $2k_F$ in this limit. As far as phase transition is concerned, the $W \gg |\mu| \gg T$ limit is not equivalent to the free-electron limit. This can be most easily seen from Eqs. (20)–(22). T_f has a form identical to T_0, the transition temperature for the half-filled case, except that λ_f is now equal to only half of λ. If $|\mu|$ were of the same order as W, T_c would be equal to T_f, and this would mean that the coupling between k and $k-p_0$ remains perfect while the coupling between the states k and $k+p_0$ becomes completely negligible. However, for $W \gg |\mu| \gg T$, $T_c \gg T_f$; which means that the coupling between the states k and $k+p_0$ remains nonnegligible in this limit. When $W \gg W - |\mu| \gg T$ becomes true, the tight-binding model is equivalent to the free-electron model for the Peierls instability. As far as the phonon lifetime and the fluctuation conductivity[10–12] are concerned, it actually reaches the free-electron limit when $W \gg |\mu| \gg T$, because only the states very near to k_F are important in determining the phonon lifetime (and conductivity). Thus, in this limit, the lifetime $2/b$ of the soft phonon is twice as long as in the case $\mu = 0$, because only the scattering of k into $k-p_0$ remains available.

In the above discussions, we have purposely kept λ independent of μ in order to bring out the physics of our derivations. For $|\mu| \ll W$, this assumption is reasonable. When $|\mu|$ is of the order of W, however, one must take into consideration the μ dependence of λ, since g, Ω_0, and $N(\mu)$ are all functions of μ. From the relations

$$N(\mu) = L/2\pi W d(1-\mu^2/W^2)^{1/2}$$

and Eq. (2), $\lambda(\mu)/\lambda(0)$ becomes large as $1-\mu^2/W^2$ decreases. Accordingly the decrease of $T_c(\mu)$ toward zero is, in general, not necessarily monotonic.

In the presence of a magnetic field H, we replace $\mu_\pm$ by $\mu_\sigma^\pm = \mu_\pm + \sigma\gamma_B H/2\pi T_c$, where $\sigma = \pm 1$, $\gamma_B = eh/2m^*c$; e and m^* are electron charge and mass, respectively. In this case F, α_0, and B, respectively, in Eqs. (3), (7), and (9) are replaced by

$$F_H = \frac{1}{4}\sum_\sigma \mathrm{Re}[\psi(\tfrac{1}{2}+\rho+i\mu_\sigma^+) + \psi(\tfrac{1}{2}+\rho+i\mu_\sigma^-)] - \psi(\tfrac{1}{2}),$$

$$\alpha_0^2 = -\left(\frac{v_F}{8\pi T}\right)^2 \sum_\sigma \tfrac{1}{2}\mathrm{Re}[\psi^{(2)}(\tfrac{1}{2}+\rho+i\mu_\sigma^+) + \psi^{(2)}(\tfrac{1}{2}+\rho+i\mu_\sigma^-)],$$

and

$$B_H = \frac{1}{2}\sum_\sigma [\psi^{(1)}(\tfrac{1}{2}+\rho+i\mu_\sigma^+) + \psi^{(1)}(\tfrac{1}{2}+\rho+i\mu_\sigma^-)].$$

For fixed μ, H_L is defined by the equation

$$\mathrm{Re}\sum_\sigma \psi^{(2)}\left(\frac{1}{2} + i\,\frac{\mu+\sigma\gamma_B H_L}{2\pi T_c}\right) = 0.$$

When[18] $\mu = 0$, $\gamma_B H_L = 1.056 T_0$; when $H > H_L$, $q_0 \neq 0$; but, for $H < H_L$, q_0 vanishes. In the presence of a magnetic field, one may in general have $q_0 \neq 0$, even though $|\mu| < 1.056 T_0$.

Using the model Hamiltonian

$$\mathcal{H} = N(\mu)\frac{|\Delta|^2}{\lambda} + \sum_{k\sigma}(E_k-\mu)a_k^\dagger a_k + \Delta\sum_k a_{k+p_0}^\dagger a_k + \Delta^*\sum_k a_{k-p_0}^\dagger a_k, \tag{25}$$

where

$$\Delta = 2g\langle b_{p_0}\rangle,$$

to describe the quasi-unidimensional system below T_c, one can easily show that the free energy near T_c is

$$\Delta\mathfrak{F} = N(\mu)[\ln(T/T_c)|\Delta|^2 + \tfrac{1}{2}\overline{B}|\Delta|^4],$$

where $\overline{B}$ is defined by Eqs. (A1)–(A4) in the Appendix and is never negative. The Peierls distortion is therefore a second-order phase transition for the various values of μ under consideration. For completeness, we have given a more detailed derivation for the free energy in the Appendix.

III. NEUTRON SCATTERING

The differential cross section of neutron scattering by lattice is given by[20]

$$\frac{d^2\sigma}{d\omega d\Omega} = u^2 S(\vec{k},\omega),$$

where

$$u^2 = \frac{N}{4\pi^2}\frac{|\vec{k}+\vec{k}'|}{k'}\frac{2\pi}{M}\int d\vec{r}\,\tilde{V}(\vec{r})e^{i\vec{k}\cdot\vec{r}};$$

$\vec{k}'$ is the momentum of the incident neutron. N and M are, respectively, the total number of the ions and the mass of the ion. $\tilde{V}(r)$ is the scattering potential between the neutrons and the ions. The magnitude of u^2 is independent of temperature but depends on the individual system. Including only one-phonon processes in the inelastic scattering, one obtains the structure factor as

$$S(\vec{k},\omega) = e^{-2W_k}\left(N\sum_{\vec{G}}\delta_{\vec{k}+\vec{G}} + \mathrm{Im}\sum_{ij} D_{ij}(\vec{k},\omega)\frac{k_i k_j}{1-e^{-\beta\omega}}\right).$$

e^{-2W_k} is the Debye-Waller factor; $\vec{G}$ is the reciprocal vector (parallel to the chain, $G=2nQ$, with $n=1,2,3\ldots$); $\delta_{\vec{k}+\vec{G}}=1$ if $\vec{k}+\vec{G}=\vec{0}$, and $\delta_{\vec{k}+\vec{G}}=0$ if $\vec{k}+\vec{G}\neq\vec{0}$. i,j are the 3 directions of the phonon. Choosing $\vec{k}$ parallel to the chain and $k=Q+q_0$, one obtains

$$S(p_0,\omega)=e^{-2W_{p_0}}p_0^2\,\mathrm{Im}D_R(p_0,\omega)/(1-e^{-\beta\omega}),$$

where D_R is the retarded propagator defined by Eq. (11). One therefore obtains

$$S(p_0,\omega)=e^{-2W_{p_0}}\frac{2\Omega_0p_0^2bT}{(\omega^2-\lambda\Omega_0^2\epsilon)^2+\omega^2b^2}. \tag{26}$$

As $T\to T_c$, the positions of the peaks of the $Q+q_0$ phonon shift towards $\omega=0$. In particular, when one puts $\omega=0$ in Eq. (26), one obtains

$$S(p_0,0)=e^{-2W_{p_0}}\frac{2bT_cp_0^2}{\lambda^2\Omega_0^3}\frac{T_c}{T-T_c},$$

which gives rise, near T_c, to a central peak with a magnitude diverging as $(T-T_c)^{-1}$.

ACKNOWLEDGMENTS

We are grateful to G. Eilenberger for his stimulating comments and have benefited from conversations with W. Dietrich, P. Fulde, W. Pesch, and H. Keiter.

APPENDIX

Using the model Hamiltonian (25), one may write free energy near T_c

$$\Delta\mathfrak{F}=N(\mu)\left[\left(\frac{1}{\lambda}-\frac{1}{N(\mu)}\Pi(0,p_0)\right)|\Delta|^2+\frac{\overline{B}}{2}|\Delta|^4\right],$$

where

$$\overline{B}=-\tfrac{1}{3}(2S_1+S_2) \tag{A1}$$

and $\Pi(0,p_0)$ is the contribution from Fig. 1(a), S_1 from Fig. 1(b), and S_2 from Fig. 1(c). The contribution from Fig. 1(a) is simply

$$\Pi(0,p_0)=-N(0)\left[\ln(4e^{\gamma}W/\pi T)-F(\mu,q_0,T_c;0)\right].$$

The contribution from Fig. 1(b) is

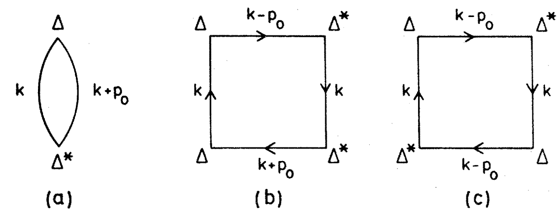

FIG. 1. Solid lines denote bare electron propagators.

$$S_1=-T\sum_{\nu,k}[G(i\omega_\nu,k)]^2\times G(i\omega_\nu,k+p_0)G(i\omega_\nu,k-p_0).$$

Integrating over k, one obtains

$$S_1=\frac{N(\mu)}{16\pi Tv_Fq_0}\mathrm{Im}\left[\psi^{(1)}(\tfrac{1}{2}+i\mu_+)-\psi^{(1)}(\tfrac{1}{2}+i\mu_-)\right]. \tag{A2}$$

We observe that, for $\mu>\mu_L$, $S_1=0$ because of Eq. (14). For $\mu<\mu_L$, however, $q_0=0$ and

$$S_1=\frac{1}{32\pi^2T^2}\mathrm{Re}\sum_{j=\pm}\psi^{(2)}(\tfrac{1}{2}+i\mu_j). \tag{A3}$$

The contribution from Fig. 1(c) is

$$S_2=-T\sum_{\nu,k}[G(i\omega_\nu,k)G(i\omega_\nu,k-p_0)]^2=\frac{1}{32\pi^2T^2}\mathrm{Re}\sum_{j=\pm}\psi^{(2)}(\tfrac{1}{2}+i\mu_j). \tag{A4}$$

Since S_1 and S_2 are never positive, the Peierls distortion is a second-order phase transition.

A similar calculation has been carried out by Nakanishi and Maki[21] for superconductivity in the presence of high magnetic fields. They show that the sinusoidal solution of the order parameter, $\Delta(r)=\Delta_0\cos qr$, gives rise to lower free energy than the solution, $\Delta(r)=\Delta_0e^{iqr}$, and the phase transition is of first order. Because the electrons can only move in one direction in our model, however, Peierls instability is a second-order phase transition, as we have shown. In passing, it is interesting to note that the sinusoidal solution implies resistance steps in superconducting thin films or whiskers in the presence of high magnetic fields.

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