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SUPERCONDUCTIVITY AND PEIERLS INSTABILITY IN COUPLED LINEAR CHAIN SYSTEMS*

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We study the superconducting transition temperature (T_c) and the Peierls instability temperature (T_p) using Eliashberg type equations for both T_c and T_p self consistently with finite interchain coupling. We show that $T_c > T_p$ below a critical electron–phonon coupling constant which depends on the bare phonon frequency. This determines an upper bound on T_c so that for higher transition temperatures $T_p > T_c$ and superconductivity is unlikely. Higher values of T_c are possible if the interchain coupling is increased above a critical value where the Peierls instability is suppressed.

THE POSSIBILITY of superconductivity in one-dimensional ($1d$) systems has been of interest for quite some time. Even before the BCS theory Frohlich[1] proposed a model of a $1d$ metal undergoing a Peierls transition[2] at a temperature T_p with a propagating lattice distortion. More recently this system was shown to possess some paraconductivity above T_p.[3] Below T_p the Frohlich mode is likely to be pinned down leading to an insulating phase.

In the present work we consider the true pairing (BCS) superconductivity (below T_c) and the Peierls phase (below T_p) which are both due to the same electron–phonon interaction.

Experimentally only few relevant systems are known up to date. $K_2Pt(CN)_4Br_{0.3}3H_2O$(KCP)[4] shows a Peierls instability at $T_p \simeq 100°K$ with no trace of superconductivity, while $(SN)_x$ is a superconductor[5] below $T_c = 0.25°K$. Tetrathiofulvalene tetracyanoquinodimethan (TTF–TCNQ) shows perhaps paraconductivity,[3] but below 53°K it is an insulator in the Peierls phase.[6] Also relevant are the intermetallic A-15 compounds, whose quasi $1d$ nature was proposed to contribute to their high T_c.[7] The martensitic transformation possible in these compounds was associated with a Peierls transition.[7,8]

Theoretically it was shown[9] that within logarithmic accuracy (Parquet approximation) the Peierls phase and superconductivity occur together in pure $1d$ systems. More advanced calculations show that the nature of the ground state[10,11] depends on the important couplings describing momentum transfer of $2p_F$ or zero along the chain direction Z, where p_F is the Fermi wavevector. For the electron–phonon coupling g_q we define

$$\begin{aligned} s_1 &= g^2_{q_z \sim 2p_F} \cdot 2N(0)/\omega_0 \\ s_2 &= g^2_{q_z \sim 0} \cdot 2N(0)/\omega_0 \end{aligned} \qquad (1)$$

where $N(0)$ is the electron density of states for both spins at the Fermi surface and ω_0 is the bare phonon frequency.

For the strictly $1d$ system the ordered phases exist only at $T = 0$ and may appear simultaneously in a region of the s_1, s_2 plane. However, once an interchain coupling is introduced, one of the phases would have a higher transition temperature and we expect just a line of coexistence in the s_1, s_2 plane on which $T_c = T_p$.

In an attempt to describe real systems we wish to improve upon these works[9–11] in two respects. (a) Introduce an interchain coupling so that a finite transition temperature is possible. (b) Attractive interactions ($s_1, s_2 > 0$) are due to phonons, therefore retardation effects as well as the soft phonon effect should be included.[12]

The interchain coupling can be introduced from the weak coupling limit,[13] or assume it is large enough so that the mean field (MF) theory is valid. Thus it was shown[14] for a non-retarded interaction that $s_1 = 2s_2$ is the coexistence line. Retardation and soft phonon effects have also been investigated[15–17] (with no interchain coupling) showing that the coexistence line has $s_1 > 0$ even for $s_2 = 0$.

We show here that these works[15–17] are qualitatively correct by accounting for both interchain coupling (assuming it is not too small) and retardation effects.

The interchain coupling η is introduced by the electronic dispersion

$$\epsilon_p = \epsilon(p_z) - \eta T_F(\cos ap_x + \cos ap_y) \qquad (2)$$

where a is the distance between the chains and T_F is the Fermi temperature. The Peierls instability for such a

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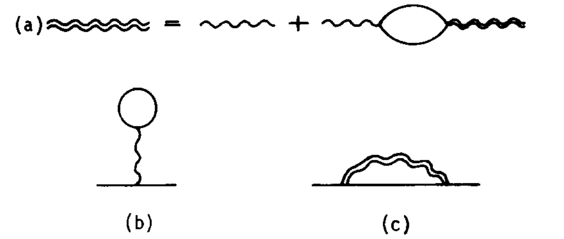

Fig. 1. The screened phonon propagator (a) and electron self mass corrections: The direct term (b) and the exchange term (c).

system was recently investigated[18] showing that the instability with the wavevector $q_0 = (\pi/a, \pi/a, 2p_F)$ exists even for large values of η. The Peierls instability is effectively described by a $1d$ theory for

$$\eta \gtrsim 4T/T_F. \qquad (3)$$

The lower bound on η is such that fluctuations reduce T_p by less than 20%. If $\epsilon(p_z)$ has electron–hole symmetry $\epsilon(p_F + \delta p_Z) = -\epsilon(p_F - \delta p_Z)$ then T_p is independent of η. (Electron energy is measured from the Fermi level.) In this case there is no upper bound on η due to the perfect nesting of the opposite Fermi surfaces, which leads to the "effective" one dimensionality. We first assume that electron–hole symmetry exists.

The interaction is represented by the screened phonon propagator $D(q, i\nu_n)$ and for the important momenta we obtain ($\nu_n = 2\pi Tn$)

$$Q_1(n) \equiv \tfrac{1}{8}s_1 D(q_0, i\nu_n) = \frac{1}{2}\left[\frac{2}{s_1}\left(\frac{\nu_n}{\omega_0}\right)^2 + \ln\frac{T}{T_p} + \alpha(n)\right]^{-1}$$

$$Q_2(n) \equiv \tfrac{1}{8}s_2 D(0, i\nu_n) = \frac{1}{4}s_2\left[\left(\frac{\nu_n}{\omega_0}\right)^2 + 1\right]^{-1}$$

$$\alpha(n) = \left(\frac{\pi n}{2}\right)^2 \int_0^\infty \frac{\tanh x}{x\left[\left(\frac{\pi n}{2}\right)^2 + x^2\right]}\,dx. \qquad (4)$$

$Q_1(n)$ is obtained[18] from Fig. 1(a) and the singularity at $n = 0$, $T = T_p$ is due to the soft phonon at the Peierls instability. The expression for $\alpha(n)$ is exact within MF [Fig. 1(a)] and reduces to the usual form[3] $\alpha(i\nu_n = \nu) = -i\pi\nu/8T$ for $\nu/T \to 0$. $Q_2(n)$ corresponds to the bare phonon propagator and screening effects which are concentrated near $q_z = 2p_F$ are neglected for $q_z \sim 0$. Equation (4) assumes that ω_0 is independent of q, which is reasonable for an optical phonon. However even a 3-dimensional acoustic phonon with $q_z \simeq 0$ contributes mainly with its large q_x, q_y momenta (higher density of states), hence a constant ω_0 is reasonable even in this case.[19]

We evaluate T_c (for a zero Peierls gap) using the linearized Eliashberg equations for the BCS gap function $\phi_n(p)$,[20] $[\omega_m = \pi T(2m + 1)]$

$$\phi_n(p) = -T\sum_{p',m}\frac{1}{[\omega_m Z_m(p')]^2 + [\epsilon_{p'} + \chi_m(p')]^2} \times g^2_{p-p'}D(p - p', i\nu_{n-m})\phi_m(p') \qquad (5)$$

$$Z_n(p) = 1 - \frac{T}{\omega_n}\sum_{p',m}\frac{\omega_m Z_m(p')}{[\omega_m Z_m(p')]^2 + [\epsilon_{p'} + \chi_m(p')]^2} \times g^2_{p-p'}D(p - p', i\nu_{n-m}) \qquad (6)$$

$$\chi_n(p) = T\sum_{p',m}\frac{\epsilon_{p'} + \chi_m(p')}{[\omega_m Z_m(p')]^2 + [\epsilon_{p'} + \chi_m(p')]^2} \times g^2_{p-p'}D(p - p', i\nu_{n-m}). \qquad (7)$$

These equations are derived within the Nambu notation[21] from the exchange term, Fig. 1(c). (The direct term, Fig. 1(b) does not contribute to superconductivity.)

The Nambu notation can also be used in the Peierls space[22] and an analogous equation for the Peierls gap $\Delta_n(p)$ is obtained

$$\Delta_n(p) = -T\sum_{p',m}\frac{\Delta_m(p')}{[\omega_m Z_m(p')]^2 + [\epsilon_{p'} + \chi_m(p')]^2} \times [g^2_{q_0}D_0(q_0, 0) - \tfrac{1}{2}g^2_q D(q, i\nu_{n-m})] \qquad (8)$$

with $q_z = |p_z| - |p_z'| \simeq 0$ and the same renormalizing functions of equations (6) and (7). Discussion of equation (8) and the effects of retardation on the Peierls gap are presented elsewhere.[23] The first term in equation (8) is due to the direct term, Fig. 1(b), and by iteration it is seen that screening is already included. Thus the bare phonon propagator $D_0(q_0, 0) = -2/\omega_0$ appears in this term. The second term in equation (8) is due to the exchange term, Fig. 1(c) and involves only small momentum transfer. By iterating the exchange term on the direct term it is seen that vertex corrections of the ladder type are included, and these indeed involve only $q_z \sim 0$ momenta.[24] An instability in the ladder summation is responsible for superconductivity[25] so that these vertex corrections represent the effect of T_c on T_p, analogous to the effect of T_p on T_c by screening the exchange term [equations (4) and (5)]. This demonstrates the self consistency of equations (5) and (8) which both correspond to Fig. 1 in their respective Nambu spaces. However the screened interaction is not fully consistent since $Q_1(n)$ [equation (4)] does not include vertex and mass corrections. We account for the main renormalizing effect by using for T_p in $Q_1(n)$ the actual solution of equation (8). As for other vertex corrections, we note the success of the Eliashberg equations in describing well known superconductors. Thus we expect the present formalism to be valid, at least for not too small η. [equation (3)].

We proceed to evaluate rhe renormalizing functions, equations (6) and (7). The terms with $n = m$ are singular at $p - p' = q_0$ for $T \to T_p$, thus we substitute $\epsilon_{p'} = \epsilon_{p-q_0} = -\epsilon_p$ and use[18]

$$\langle \Delta^2 \rangle = -g_{2p_F}^2 T \sum_q D(q, 0). \tag{9}$$

$\langle \Delta^2 \rangle$ is the fluctuation average of the Peierls gap. For the terms $n \neq m$ in (4), it can be shown that the momentum dependence of $D(q \simeq q_0, i\nu_n \neq 0)$ is strongly reduced and since these are not singular we neglect this dependence. These terms give a small correction q_n to Z_n and vanish in the equation for χ_n,

$$Z_n(p) = 1 + \frac{Z_n(p)\langle \Delta^2 \rangle}{[\omega_n Z_n(p)]^2 + [\epsilon_p + \chi_n(p)]^2} + q_n$$

$$\chi_n(p) = \frac{\epsilon_p + \chi_n(p)}{[\omega_n Z_n(p)]^2 + [\epsilon_p + \chi_n(p)]^2} \langle \Delta^2 \rangle. \tag{10}$$

The renormalized electron dispersion is $\tilde{\epsilon}_p = [\epsilon_p + \chi_n(p)]/Z_n(p) = \epsilon_p/(1 + q_n)$ so that the possibly divergent terms with $\langle \Delta^2 \rangle$ cancel and ϵ_p is only slightly modified. The Fermi velocity is reduced by this effect and we assume that the q_n are effectively absorbed in the definition of v_F [or $N(0)$]. Thus the renormalizing function $\chi_n(p)$, which is usually neglected,[21,22] is important in this case due to the singular behaviour of $D(q, 0)$.

Thus we obtain from (10)

$$\epsilon_p + \chi_n(p) = Z_n \epsilon_p$$

$$Z_n = \tfrac{1}{2}[1 + (1 + 4\langle \Delta^2 \rangle/\omega_n^2)^{1/2}] \tag{11}$$

and the momentum dependence of Z_n is negligible for $\epsilon_p \lesssim \pi T$. In the range (3) we have[18]

$$\langle \Delta^2 \rangle \simeq (2\pi T^2/\eta T_F)^2 \tag{12}$$

so that for $\eta \gtrsim 4T/T_F$, and $q_n = 0$, Z_n are indeed close to 1 and the MF approximation is valid.

In equation (5) for the BCS gap we treat the $n = m$ terms as above using equation (9), while in the $n \neq m$ terms the momentum integration involves mainly the electronic factor and the phonon part reduces to $Q(n) = Q_1(n) + Q_2(n)$. Since $\phi(-\omega_m) = \phi(\omega_m)$ we obtain for the coefficients of $\tilde{\phi}_n = \phi_n/Z_n^2\sqrt{2n+1}$ the symmetric matrix $(n, m \geqslant 0)$

$$A_{n,m} = \left[\frac{\langle \Delta^2 \rangle}{\omega_n^2} + \frac{Q(2n+1)}{2n+1} - Z_n^2\right]\delta_{n,m} + \frac{Q(n-m) + Q(n+m+1)}{[(2n+1)(2m+1)]^{1/2}}(1 - \delta_{n,m}). \tag{13}$$

T_c is the solution for det $(A) = 0$. From equation (8) the the Peierls gap satisfies

$$\Delta_n = \frac{2}{\pi}\sum_{m=0}^{\infty} \frac{\Delta_m}{Z_m^2(2m+1)} \tan^{-1}\frac{E_c}{\omega_m} \times [s_1 - Q_2(n-m) - Q_2(n+m+1)]. \tag{14}$$

Since the s_1 term is not retarded the electronic cutoff energy E_c has to be kept. In the limit $\omega_0/T \to \infty$, $Q_2(n) \to s_2/4$ and for $Z_n = 1$ the MF result[18,23] $T_p^0 = 1.13E_c \exp[-4/(2s_1 - s_2)]$ is obtained. We use $E_c = 4T_F$ which corresponds to the free electron dispersion for $\epsilon(p_z)$.[18] By iterating equation (14) a faster converging series is obtained,[23] and T_p is the temperature for which the determinant of the coefficients vanishes.

The renormalization Z_n is important as we move out of the MF range (3). Although the present formalism is not sufficient in this case, we can make some qualitative remarks. For $\eta \to 0$ for the fluctuations $\langle \Delta^2 \rangle$ diverge, but this is cancelled by a similar divergence of Z_n^2 in equation (13). Thus the solution for T_c/T_p depends weakly on η. However from (14) T_p is reduced if Z_n diverges so that both T_c and T_p are reduced due to renormalization at small η.

We solve equations (13) and (14) for T_c and T_p and plot the coexistence line ($T_c = T_p$) for $\eta = 0.1$ in Fig. 2. The dependence of the phase diagram on η is weak in the the range (3), and as mentioned above, is expected to remain weak even for small η. The main feature of the results is that for small coupling s_1, $T_c > T_p$ while for larger s_1, $T_p > T_c$. Thus for any ω_0 and s_2 there is an upper bound on T_c. For $3s_2 - s_1 > 4$ the system is unstable at $q = 0$[14,24] so that we limit the phase diagram to $0 \leqslant s_2 \lesssim 1$. In this range the maximal T_c is roughly given by max $(T_c/\omega_0) = 0.002 + 0.045s_2$, so that for $s_2 = 1$ the maximal T_c is roughly $\omega_0/20$. The dimension of the determinants in the calculation has to be larger than $\omega_0/2\pi T_c$, thus dimensions in the range 10–100 were used.

Comparison with the dashed line, $s_1 = 2s_2$, in Fig. 2 shows the effect of screening and retardation. For large couplings retardation effects are important – reducing T_c and enhancing T_p, so that the coexistence curve has $s_1 < 2s_2$. For small couplings (low T/ω_0), retardation is not important, while screening enhances T_c but not T_p, so that the coexistence curve has $s_1 > 2s_2$. If screening would not be included the coexistence curve would have joined the line $s_1 = 2s_2$ at low couplings.

In Fig. 3 we plot T_c and T_p along the line $s_1 = s_2$ for $\eta = 0.1$. Of course only the higher transition temperature is valid in our description. (The gap created at the higher transition temperature will possibly eliminate the other phase at lower temperatures.)[7,25] As ω_0 decreases T_p increases, and the soft phonons which become available at figher temperatures enhance T_c.

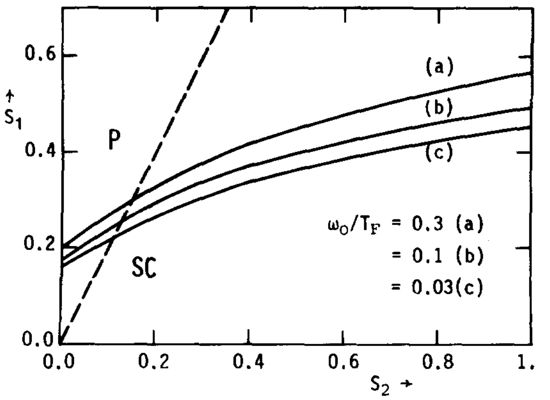

Fig. 2. Phase diagram for $\eta = 0.1$. The dashed line $s_1 = 2s_2$ is the coexistence line for an instantaneous interaction.

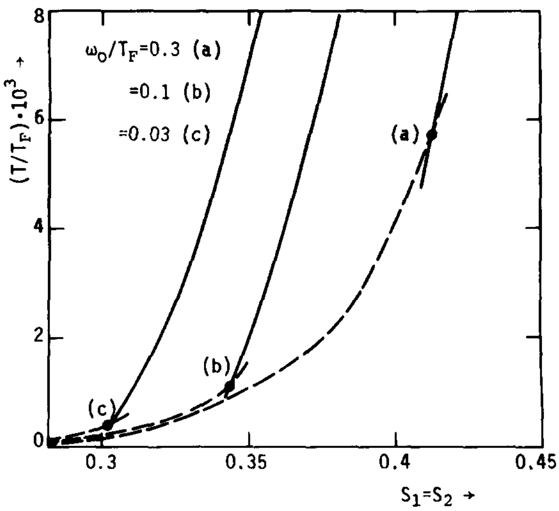

Fig. 3. T_p (full lines) and T_c (dashed lines) for $\eta = 0.1$. The crossing points are marked with a point.

Let us now extend the calculations to high values of η, above η_c, where the Peierls instability is suppressed. This happens if $\epsilon(p_Z)$ in (2) does not have electron–hole symmetry, as for the free electron dispersion. In this case the critical η_c is[18,23]

$$\eta_c = 8 \exp\left(\frac{-2}{2s_1 - s_2}\right). \tag{15}$$

For $\eta \gtrsim \eta_c$, $\sqrt{T/T_F}$, we can replace the factor $\ln T/T_p$ in equation (4) by $2 \ln \eta/\eta_c$[18] which represents the soft phonons with finite frequency at $\eta > \eta_c$. We plot in Fig. 4 T_c and T_p as functions of η for $s_1 = s_2 = 0.4$. The main feature is that T_c is enhanced as the phonons become softer ($\eta \to \eta_c$). For small η we observe the importance of renormalization in reducing T_c and T_p.

It has been claimed that phonons with frequency below $2\pi T_c$ are not very helpful. This is the case if one

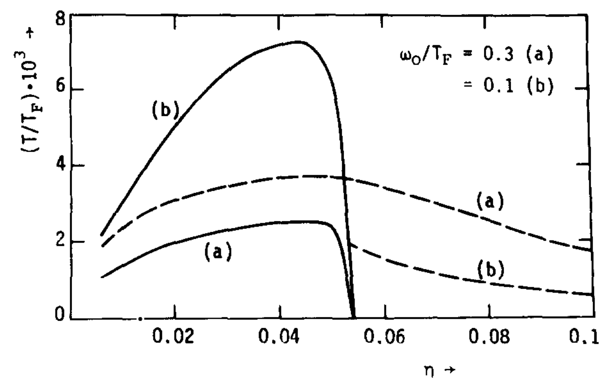

Fig. 4. T_p (full lines) and T_c (dashed lines) for $s_1 = s_2 = 0.4$, as functions of the interchain coupling.

compares different materials, so that the electron–phonon coupling g_q depends on the phonon frequency, and the total weight of the Eliashberg function $\alpha^2F(\omega)$ is constant.[26] However for a given material, phonon softening due to temperature variation does not change g_q and the relevant constraint is that $\int_0^\infty \omega\alpha^2F(\omega)\,d\omega$ is constant.[15,24] Thus in our case the functional derivative $\delta T_c/\delta\alpha^2F(\omega)$ has a maximum at $\omega = 0$ so that the phonon is more helpful for superconductivity as it is softer.[27]

In conclusion we have seen that superconductivity is limited by the lattice instability to roughly $T_c \lesssim \omega_0/20$. In order to achieve a higher T_c the Peierls phase must be suppressed by distorting the Fermi surface, and the soft phonons, which are still present, help to enhance T_c. The high T_c of the A15 compounds may be due in part to such a mechanism. Distortion of the Fermi surface can be achieved by increasing the interchain coupling (i.e. by pressure) or by other means, i.e., nonmagnetic impurities.[28]

Our results explain why for $(SN)_x$ at $T = 0.25°K$ T_c is favoured while for KCP at $T \simeq 100°K$ the Peierls instability is dominant. For TTF–TCNQ the answer depends upon which ω_0 we should use. For the acoustic phonon $T_p \gg T_c$ at 53°, but for high frequency bond vibrations[15,29] $T_c \simeq T_p$.

The possible degeneracy between T_p and T_c [8–11] is lifted by three factors. (a) Independent variation of both s_1, s_2. (b) Interchain coupling and (c) The retarded nature of the phonon induced interaction. In the present work we have demonstrated the practical importance of factor (c).

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