SUPERCONDUCTIVITY IN QUASI ONE-DIMENSIONAL METALS AND THE OPTIMAL PHONON FREQUENCY

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Abstract

The transition temperature, T_s, to singlet superconductivity in quasi one-dimensional metals is studied as a function of the phonon frequency ω_0. When both electron–phonon and electron–electron couplings are present, T_s has a maximum at a finite ω_0. When the electron–phonon interaction dominates and ω_0 is too *small*, superconductivity is eliminated by charge density waves, while if the electron–electron interaction dominates and ω_0 is too *large*, superconductivity is eliminated by spin density waves.

The question of the maximum superconducting transition temperature in one-dimensional metals has been of interest for quite some time. The competition between the CDW Peierls–Frohlich transition at T_p and the BCS superconducting transition at T_s was pointed out by Bychkov *et al.* [1] who suggested that $T_p = T_s$. Taking into account the retarded nature of the interaction it was shown [2] that $T_s > T_p$ for a small electron–phonon coupling constant λ, and $T_s < T_p$ for large λ, and at the crossover, T_s attains its maximum value T_s^{max}. T_s^{max} is related to the phonon frequency and ranges from $T_s^{max} \cong \omega_{ph}/50$ to $T_s^{max} \cong \omega_{ph}/20$, depending on the relative strength of forward and backward scattering [2]. The recent discovery of superconductivity in organic metals [3] at temperatures around 1 - 2 K confirms this result, since the phonon frequency is of the order of 50 K. Thus, the phonon frequency plays a dominant role in determining the maximum transition temperature T_s. Organic metals consist of molecular crystals which in addition to the external mode phonons (translations and vibrations), also contain internal mode phonons — bond stretching vibrations, molecular twists, bends, rocking motions, etc. These phonons possess much higher frequencies; the C=C stretching vibrations are at about 1400 cm^{-1}, for example. Thus, if these modes are responsible for electron–phonon coupling, much higher values of

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T_s are in principle possible. This was pointed out quite some time ago [2], and the coupling of the electrons with these modes is indeed found to be rather strong [4].

In addition to CDW instabilities, SDW instabilities must also be considered. Indeed, most of the quasi one-dimensional systems are CDW or SDW. The parameter space of the problem includes coupling constants for backward scattering ($\bar{g}_{1e}$), forward scattering ($\bar{g}_{2e}$), umklapp scattering when the band is half full ($\bar{g}_{3e}$) and the corresponding retarded interactions via phonons: λ_1, λ_2, λ_3. In addition one needs the phonon frequency ω_0 and the electronic cut-off energy E_c [5]. More generally one needs to specify both the longitudinal transfer integral ($t_\parallel$) and the transverse one ($t_\perp$) [6]. Below, however, we consider the case of weak coupling and not too large anisotropy, *i.e.*, $\bar{g}_i \ln t_\parallel/t_\perp$, $\lambda_i \ln t_\parallel/t_\perp \ll 1$. If this condition is not satisfied, one may use in some cases a renormalization-group procedure [7, 8] to redefine the coupling constants and then $E_c \cong t_\perp$.

The umklapp process is of special importance in the superconductors known so far as the $(TMTSF)_2X$ family [3]. Superconductivity is possible only if the umklapp process is suppressed by either pressure or by disorder of the counter ions for $X = ClO_4$. This conclusion was first reached [5] by examining the pressure dependence of both T_s and T_{SDW} and by correlating the disorder feature of $X = ClO_4$ with the appearance of superconductivity at ambient pressure. This conclusion was further supported [8] by data on $(TMTTF)_2X$ compounds. Note that these arguments are independent of the type of umklapp, and the controversial issue [5, 8] of whether $\bar{g}_3$ or λ_3 is more pressure dependent should be settled by further experiments.

In the present study we consider the case $\bar{g}_3 = \lambda_3 = 0$, which is favorable to superconductivity. The transition temperature is given by [5]

$$T_s = \omega_0 \exp\left\{-\left(\lambda - \frac{\mu}{1 + \mu \ln E_c/\omega_0}\right)^{-1}\right\} \tag{1}$$

where $\lambda = (\lambda_1 + \lambda_2)/2$ and $\mu = (\bar{g}_{1e} + \bar{g}_{2e})/2$. This is the usual weak coupling form for T_s [9] and is valid here because of the decoupling of the superconducting channel from the $2k_F$ divergencies for $T_s \lesssim t_\perp$ [2].

The competing instabilities are those of the CDW, SDW and triplet superconductivity (TS) with the transition temperatures for $T_c \ll \omega_0 \ll E_c$ given by [5]

$$T_c = \omega_0 \exp\left\{-\left[\tfrac{1}{2}\bar{g}^R + \tfrac{1}{2}\left(\frac{\bar{g}^N}{1 - \frac{1}{2}\bar{g}^N \ln E_c/\omega_0}\right)\right]^{-1}\right\} \tag{2}$$

where $\bar{g}^N$, $\bar{g}^R$ are given in Table 1 for each phase. The phase diagram is shown in Fig. 1, where $\bar{g}_1 = \bar{g}_{1e} - \lambda_1$ and $\bar{g}_2 = \bar{g}_{2e} - \lambda_2$.

Consider first the region where attractive interactions dominate and assume then that $\mu_1 = \mu_2 = 0$. In this case, superconductivity competes with the CDW phase. This competition has been studied in detail [2]; in weak coupling the coexistence line is given by

TABLE 1

Values of $\bar{g}^N$ and $\bar{g}^R$ for each phase

	$\bar{g}^N$	$\bar{g}^R$
S	$-\bar{g}_{1e}-\bar{g}_{2e}$	$\lambda_1+\lambda_2$
TS	$\bar{g}_{1e}-\bar{g}_{2e}$	$-\lambda_1+\lambda_2$
CDW	$-2\bar{g}_{1e}+\bar{g}_{2e}+2\lambda_1$	$-\lambda_2$
SDW	$\bar{g}_{2e}$	$-\lambda_2$

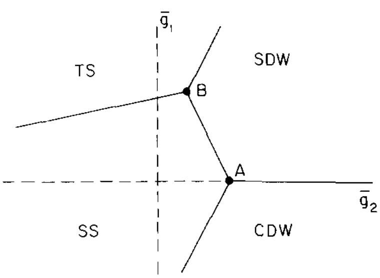


Fig. 1. Phase diagram in the $(\bar{g}_1, \bar{g}_2)$ plane $(\bar{g}_1 = \bar{g}_{1e} - \lambda_1, \bar{g}_2 = \bar{g}_{2e} - \lambda_2)$.

$$\lambda_2 = \tfrac{1}{2}\lambda_1 \frac{1+\lambda_1 \ln E_c/\omega_0}{1-\lambda_1 \ln E_c/\omega_0} \tag{3}$$

The transition temperature T_s increases with both λ_i and ω_0, but when the λ_i are beyond the line of eqn. (3), CDW takes over. The crossing line allows higher T_s as ω_0 increases, *e.g.*, for $\lambda_1 = \lambda_2 = \lambda$ the maximal T_s is $T_s^{max} = \omega_0^4/E_c^3$. This temperature increases with ω_0, and leads one to hope that high values of T_s are possible in organic metals where high frequency intra-molecular phonons are strongly coupled with electrons.

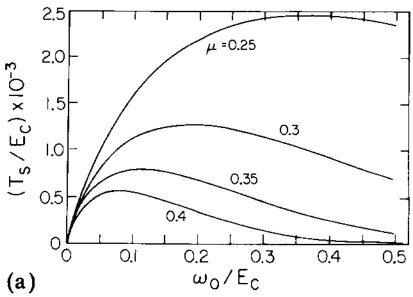
Consider next the region where repulsive interactions dominate, $\mu_i > \lambda_i$. In this case retardation renormalizes μ to $\mu^* = \mu/(1-\mu \ln \omega_0/E_c) < \mu$ and superconductvitity is allowed, as shown in Fig. 1. The competing phase here is the SDW phase. Apart from this competition, there is an interesting behavior of T_s, namely it has a maximum at an optimal values ω_0^{max} of the phonon frequency, given by

$$\omega_0^{max} = E_c \exp\left\{\frac{1}{\mu} - \frac{1}{\lambda}\right\} \tag{4}$$

The transition temperature at this frequency is

$$T_s^{max} = E_c \exp\left\{\frac{1}{\mu} - \frac{4}{\lambda}\right\} \tag{5}$$

T_s as a function of ω_0 is shown in Fig. 2(a) for $\mu < \lambda$ and in Fig. 2(b) for $\mu > \lambda$ with $\lambda = 0.4$. As μ becomes larger than λ the peak in $T_s(\omega_0)$ moves to lower frequencies and to lower transition temperatures.



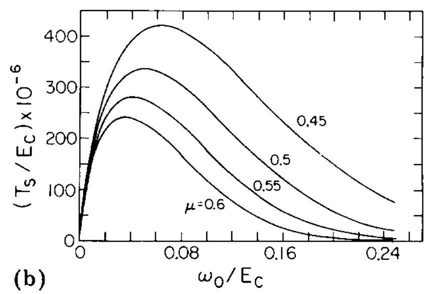


Fig. 2. T_s as a function of ω_0 (eqn. (1)) for $\lambda = 0.4$ and various values of μ.

For a fixed λ and μ the optimal ω_0 is given by eqn. (4). For this frequency the system becomes superconducting only if it is within its phase boundary of Fig. 1. Superconductivity is allowed for $\mu > \lambda$ because of retardation effects (the μ^* effect) and if ω_0 is too high this effect is weakened and SDW will take over. Thus superconductivity is allowed if ω_0 is sufficiently *small*, in contrast with the case $\lambda \gg \mu$, where superconductivity is allowed when ω_0 is sufficiently *large*. For $\lambda < \mu$ the optimal case is $\mu_1 = \lambda_1$ and then the value of ω_0 at the crossover is

$$\omega_0^* = E_c \exp\left\{-\frac{8(\mu-\lambda)}{\lambda_1(4\lambda-\lambda_1)}\right\} \tag{6}$$

This will limit the attainability of $T_s^{\max}$ (eqn. (5)) if $\omega_0^* < \omega_0^{\max}$. Figure 3 shows ω_0^* as a fucntion of λ_1 ($\lambda_1 = \mu_1$) for the λ, μ parameters of Fig. 2(b). The values of $\omega_0^{\max}$ are marked by a star; for values of λ_1 smaller than the abscissa of the star, then $\omega_0^* < \omega_0^{\max}$ and the SDW instability does not allow the maximal T_s (eqn. (5)) to be reached. This shows the importance of increasing λ_1, even if μ_1 is also increasing.

Finally we consider the region $\lambda_1 > \mu_1$ but $\lambda_2 < \mu_2$. In this case superconductivity is restricted to values of ω_0 which are neither too large or too small. To see how this happens, consider the S–CDW coexistence line in Fig. 1, whose equation is

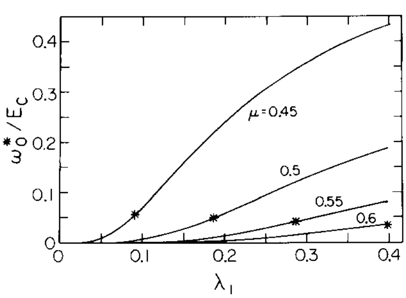


Fig. 3. The crossover frequency ω_0^* from superconductivity to SDW for $\lambda_1 = \bar{g}_{1e}$ ($\bar{g}_1 = 0$) as a function of λ_1 for $\lambda = 0.4$ and the values of μ corresponding to Fig. 2(b). The star marks the position of $\omega_0^{\max}$, the maximum of T_s in Fig. 2(b).

$$\bar{g}_1\left[1+\tfrac{3}{2}(\lambda_1+2\lambda_2)\ln E_c/\omega_0\right]-2\bar{g}_2=-\tfrac{1}{2}(\lambda_1+2\lambda_2)\ln E_c/\omega_0 \qquad (7)$$

As ω_0 increases, the intersection of this line with $\bar{g}_1 = 0$ moves to the left while its slope increases towards +2. Thus if for a given ω_0 a point is very close to the coexistence line on its superconducting side and $\lambda_1 > \bar{g}_{1e}$, $\lambda_2 < \bar{g}_{2e}$, then both an increase or a decrease in ω_0 will eliminate superconductivity by forming a CDW phase.

The conclusion that we reach from these calculations is that for the internal modes, which possess a high phonon frequency, the transition temperature is determined essentially by $\lambda - \mu$, where μ is the *unrenormalized* Coulomb coupling, which is large. As a result, $\lambda - \mu$ is small, (or even negative) and it is difficult to obtain a high value of T_s. For the external modes, which possess a low phonon frequency, the transition temperature is determined by $\lambda - \mu^*$, where μ^* is the renormalized Coulomb coupling, which is small. However, the small prefactor ω_{ph} limits T_c. Thus, a maximum value of T_c may be obtained for an intermediate value of ω_{ph}.

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