Pramāṇa Vol. 7, No. 2, 1976, pp. 63–94. © Printed in India.

Electron-electron interaction and instabilities in one-dimensional metals

T V RAMAKRISHNAN
Department of Physics, Indian Institute of Technology, Kanpur 208016

MS received 26 July 1975; after revision 8 June 1976

Keywords. One-dimensional metals; electron interaction; instability

Abstract. The possible instabilities of a 1-dimensional itinerant electron gas are discussed, assuming electron-electron interaction to play the dominant role. As is well known, in the RPA, a 1-dimensional metal is prone to spin density wave (SDW), charge density wave (CDW) and Cooper pair (CP) instabilities. The spin channel decomposition of the irreducible scattering amplitude I is made and the spin channel projections are evaluated in terms of the matrix elements of bare electron-electron interaction $V(x)$ for momenta of interest. It is found that if the bare electron interaction $V(x)$ is repulsive and decreases monotonically with separation, only the SDW instability will occur. If the small separation $\left(x \lesssim (2k_F)^{-1}\right)$ part of the interaction is greatly reduced or is made attractive, $V(x)$ is non-monotonic, $V_q(q \cong 2k_F)$ is negative, and a CDW instability is preferred. A CP instability is possible if the electron interaction is attractive, *i.e.*, if $[V_q(0 < q < k_F) + V_q(q \simeq 2k_F)] < 0$.

The above RPA results serve only as rough indicators, since in general there are important two-electron configurations with two-electron momentum close to zero and with electron hole momentum close to $2k_F$, an example being the near Fermi energy configuration $k_1 \simeq k_F, k_2 \simeq -k_F, k_3 \simeq -k_F$ $k_4 \simeq k_F$. Therefore as pointed out first by Bychkov, Gorkov and Dzhyaloshinskii (BGD), cross channel coupling is especially significant. It is shown that the cross channel coupling is constructive in some cases, *eg.*, exchange of CD fluctuations leads to an effective electron-electron spin singlet attraction and vice-versa. A formalism for studying such effects is set up, and the particular example mentioned above is discussed. An RPA-like approximation is made for the form of the reducible singlet electron hole scattering amplitude γ_s^d and the resulting induced Cooper pair attraction is calculated to be

$$[I_s^c]_{\text{ind.}} \rho \epsilon_F = [\ln(\lambda\beta\omega_0)]^{-1} \ln \{[1 + 2\pi^{-1} \ln(\lambda\beta\omega_0)^2]/ 1 + [8\pi^{-1} \gamma_s^d (q = 2k_F)^{-1})^2]\}$$

where $\lambda = 1{\cdot}14$, $\beta = (k_B T)^{-1}$ and ω_0 is an electronic energy cut-off $\sim \epsilon_F$. The nduced electron hole attraction due to the exchange of virtual Cooper pairs has a similar expression, but with a factor of $(\frac{1}{4})$ and with $\gamma_s^c (q = 0)$ replacing $\gamma_s^d (q = 2k_F)$. The induced Cooper pair attraction is seen to be quite large over a broad range of temperatures close to but above T_{CDW} [*i.e.*, above T such that $\gamma_s^d (q = 2k_F)^{-1} = 0$]. There is no requirement that $\gamma_s^d (q = 2k_F)$ and $\gamma_s^c (q = 0)$ become singular at the same temperature, as found by BGD. The BGD prediction is seen to arise from the neglect of real particle hole and particle-particle excitations while calculating γ_s^d and γ_s^c. The effect of impurities, of electron-phonon coupling, of interchain coupling and of interaction between thermal order parameter fluctuations is discussed. The results are then applied to a discussion of the properties of TTF-TCNQ, where it is suggested that a CDW instability occurs because $V_q(q = 2k_F) < 0$,

i.e., because the small separation electron repulsion is strongly reduced by highly polarizable TTF. Because of substantial interchain coupling, the b CDW instability occurs close to the RPA instability temperature. The giant condu vity observed by Coleman *et al* is attributed to superconductive fluctuations i 1-dimensional system with large mean field superconductive transition tempera T_{CP}^{MF} of order 300 °K. Such a large T_{CP}^{MF} is shown to result from the indu Cooper pair attraction due to CD fluctuation exchange.

1. Introduction

A number of quasilinear metallic systems have been studied recently (Z 1973; Epstein *et al* 1972; Ferraris *et al* 1973). The solids studied consis parallel, linear and independent chains of molecules along which electrons relatively free to move. There is generally a transition from a metallic to an i lating phase as the temperature decreases. The insulating phase can be an ferromagnetic (Zeller 1973; Epstein *et al* 1972) (spin density wave) state charge density wave state (Zeller 1973; Coleman *et al* 1973). In the latter for the organic metal TTF-TCNQ (tetrathiofulvalinium-tetracyanonoquinod thane) the electrical condutivity shows a peak (Ferraris *et al* 1973; Coleman 1973) above but near the relatively sharply defined metal insulator trans temperature. In some samples, a giant conductivity peak, with $(\sigma/\sigma_{RT}) \sim$ has been reported (Coleman *et al* 1973).

Theoretical models for such systems have been basically of three types. the first, one considers a system of free electrons interacting with the vibra lattice (Peierls 1953; Frohlich 1954; Patton and Sham 1973). In the sec one considers a collection of tightly bound Coulomb correlated electrons hop to their nearest neighbours, *i.e.*, a 1-dimensional Hubbard model (Ovchinn *et al* 1973). The third type of model is that of a 1-dimensional interac itinerant electron system (Overhauser 1960; Bychkov *et al* 1966). The re obtained in this paper pertain to this third type of model. We now briefly line these three models and the conclusions obtained. We then summarize method and results of this paper, and their application to experimentally stu systems.

In the electron-phonon model, the electrons are regarded as moving independe along the chain. The electrons are coupled to the lattice. Thus the Hamilto is

$$H = H_e + H_{ep} + H_p$$
$$= \sum_k \epsilon_k a_k^+ a_k + \sum_{k,q} g(k, q)\, a_k^+ a_{k+q} (b_q^+ + b_{-q}) + \sum_q \omega_q b_q^+ b_q, \qquad (1$$

where the 1-electron energies are ϵ_k, the phonon energies are ω_q, and $g(k, q)$ the electron-phonon coupling matrix elements. As first shown by Peierls (1 in 1-dimension the metallic phase is necessarily unstable with respect to a la distortion of periodicity $\lambda = 2\pi (2k_F)^{-1}$ which opens up a gap in the electr energy spectrum at $k = \pm k_F$, and leads to the formation of an insulating ph The theory of a weakly coupled electron-phonon system has been developed Frohlich (1954), Kuper (1955), Rice and Strässler (1973) and Patton and Sl (1973). Rice and Strässler (1973) and Patton and Sham (1973) find that

temperature decreases, the $q = 2k_F$ LA phonon softens and "condenses" below the Peierls instability temperature T_P so that there is, below T_P, a static lattice distortion of periodicity $\lambda = 2\pi(2k_F)^{-1}$. A number of properties of the Peierls insulator have been calculated, *eg.*, the effect of thermal order parameter fluctuations (Lee *et al* 1973), the electrical conductivity (Lee *et al* 1974), the dielectric properties (Rice and Strässler 1973) and the phonon spectrum (Patton and Sham 1973). The metal insulator transition in $K_2Pt(CN)_4Br_{0\cdot3}.3H_2O$ (KCP) is believed to be basically a Peierls transition, as evidenced by the softening of the $q = 2k_F$ LA phonon mode (Renker *et al* 1973; Zeller 1973). Results obtained in this model have also been applied (Lee *et al* 1974) to the metal insulator transition in TTF-TCNQ.

The 1-dimensional metals investigated so for have rather narrow electronic energy bands. Optical absorption studies indicate (Zellet 1973) that the width of the conduction band in KCP is ~ 2 eV. The conduction bandwidth and the Fermi energy in TCNQ based compounds are estimated to be in the 0·1–0·4 eV range. For example a fairly successful Hubbard model analysis (Epstein *et al* 1972) of the properties of NMP-TCNQ leads to a bandwidth $\triangle_{\text{NMP-TCNQ}} = 0{\cdot}04$ eV. The high temperature thermoelectric power (Chaikin and Heeger 1973) and other properties (Garito and Heeger 1974) of TTF-TCNQ are consistent with a Fermi energy $\epsilon_F \sim 0{\cdot}25$ eV and thus $\triangle_{\text{TTF-TCNQ}} \sim 0{\cdot}50$ eV. Magnetic properties of a number of TCNQ compounds have been analysed in a free electron model (Vegter *et al* 1973) with bandwidths of order 0·06 eV and a bandgap $\sim 0{\cdot}14$ eV. Since the significance of electron-electron interaction depends on its size vis-a-vis the bandwidth $\triangle$ or Fermi energy ϵ_F, if the latter are small, we can expect electron-electron interaction effects to be of importance. We can therefore expect electron-electron interaction to play an important role in 1-dimensional systems, especially TCNQ based systems. This belief is supported by estimates (Epstein *et al* 1972) of the Hubbard correlation repulsion U, *i.e.*, of the difference between the Coulomb repulsion energy U_0 when the two electrons are on the same site and the repulsion U_1 when they are nearest neighbours (*i.e.*, $U = U_0 - U_1$). U_0 is reduced by the tendency of same site electrons to segregate on different parts of the molecule, or by the presence of a polarizable side chain (*eg.*, NMP or TTF side chains in TCNQ compounds). The estimated values are $U_0 \cong 3$ eV and $U_1 \simeq 2$ eV in TCNQ, so that $U = U_0 - U_1 \simeq 1$ eV. In NMP-TCNQ, U_0 is reduced because of NMP polarizability, and is estimated to be $U_0 \simeq 2{\cdot}25$ eV so that $U_{\text{NMP-TCNQ}} \simeq 0{\cdot}25$ eV. Replacement of NMP by the smaller, more polarizable, TTF may reduce U_0 and even change the sign of U, but there is no reason why, except by accident, it should not be comparable in magnitude to $\triangle$. In general, therefore, at least in TCNQ based systems, electron-electron interaction will not be negligible in comparison to one electron energies. Indeed, usually (*eg.*, in TCNQ, Na TCNQ, NMP-TCNQ) U is much greater than $\triangle$. This may be the reason why these compounds are insulators (Mott-Hubbard insulators) even though they have one conduction electron per molecule.

In view of the above, it is natural to consider a 1-dimensional Hubbard model for describing the strongly correlated narrow band system. The Hamiltonian is

$$H = t\sum_i a_i^+ a_{i+1} + U\sum_i n_{i\uparrow}\, n_{i\downarrow}. \qquad (1.2)$$

This Hamiltonian has been studied extensively (Ovchinnikov *et al* 1973), ma at $T = 0$, for a half-filled band, and for $U > 0$. The ground state is an ferromagnetic insulator, and the elementary excitations are spin waves. thermal ($T \neq 0$) properties have been studied (Hone and Pincus 1973) app mately and there has been a preliminary study (Pincus *et al* 1973) of the pro for $U < 0$. Since the electron-electron interaction can be reduced by the i duction of a polarizable side chain and thus can be made comparable with ty 1-electron energies, it is of interest to study a 1-dimensional model of itin interacting electrons, *i.e.*, a model with

$$H = \sum_{k,\sigma} \epsilon_k \, a^+_{k\sigma} \, a_{k\sigma} + \tfrac{1}{2} \sum_{\substack{k_i \, \sigma_i \\ i=1,4}} a^+_{k_1 \, \sigma_1} \, a^+_{k_2 \sigma_2} \, a_{k_3 \sigma_3} \, a_{k_4 \sigma_4} \, V_{k_1 - k_4}$$

$$\times \, \delta_{k_1 + k_2 - k_3 - k_4} \, \delta_{\sigma_1 \sigma_4} \, \delta_{\sigma_2 \sigma_3}.$$

This model has been discussed in detail by Bychkov, Gorkov and Dzhyalosh (1966) [see also Overhauser (1960), and the work of Tomonaga (1950), Lut (1963) and others on an exactly soluble 1-dimensional interacting electro model]. We summarize below the results of these authors and those ob in this paper for the model described by eq. (1.3).

It was pointed out by Overhauser that a 1-dimensional metal is prone t density wave (SDW), charge density wave (CDW) and Cooper pair (CP) i lities. The former two arise because the irreducible free electron hole po bility $\chi_0^{\,d}(q, z_m)$ in a 1-dimensional metal has (at $T = 0$) a logarithmic sing for electron hole momentum transfer $q = \pm 2k_F$ and energy transfer $z_m =$ a non-zero temperature, $\chi_0^{\,d}(\pm 2k_F, 0) = -(\tfrac{1}{2}) \rho \epsilon_F \ln(\lambda \beta \omega_c)$, where $\rho \epsilon_F$ density of electronic states (per spin) at the Fermi energy, $\lambda = 1{\cdot}14$, $\beta =$ (and ω_c is an electronic cut-off energy. In the usual random phase or H Fock approximation (Brout 1965), an instability occurs for an irreducible action I if $I\chi_0^{\,d} = 1$. Since $\chi_0^{\,d}(2k_F, 0)$ decreases monotonically with tempe a SDW or CDW instability will necessarily occur if the irreducible electro interaction I has the right sign in the appropriate spin state. Similarly, an e pair instability will necessarily occur if I is positive (attractive) in the ele electron channel for the appropriate spin state. Thus, in the RPA, the occ of one or the other kind of instability is determined by the relevant chann projection of I. We determine these projections in § 3 and, on that basis, the physical conditions on the electron-electron interaction which favou rent kinds of instability of the normal metallic phase. It is seen that no *i.e.*, for a repulsive electron-electron interaction which monotonically de with distance, a SDW instability is favoured over a CDW instability. No e pairing instability can occur. If the small separation part of the electron sion is strongly reduced or is made attractive, the CDW instability is fa over the SDW, and under some conditions a Cooper pair instability may

The above conclusions have been obtained in the RPA where the sca in different channels can be considered independently. It was first point by Bychkov, Gorkov and Dzhyaloshinskii (1966) that the coupling betwee tering in different channels is specially significant in a 1-dimensional r system. Physically, the cross channel coupling arises from the fact that

2-electron scattering, there are significant electron configurations with total 2-electron momentum close to zero and electron hole momentum transfer close to $2k_F$. For example, consider figure 1, which schematically represents the 2-electron scattering amplitude $\Gamma(p_1\sigma_1, p_2\sigma_2, p_3\sigma_3, p_4\sigma_4)$, p_i being the energy

$$\nu_{li} \left[= \frac{(2l_i+1)\, i\pi}{\beta}\right]$$ and momentum k_i of the electron i in the spin state σ_i.

The configuration $k_1 \simeq -k_2 \simeq -k_3 \simeq k_4 \simeq k_F$ and $\nu_{li} \simeq 0$ corresponds to two electrons of total momentum nearly zero, and to a momentum transfer $(k_1 - k_3) \simeq 2k_F$ in the electron hole channel 13. Thus, if the scattering amplitude is large in the electron hole channel 13 because of an incipient SDW or CDW instability, the electron pair scattering amplitude will be strongly affected. Bychkov, Gorkov and Dzhyaloshinskii considered the 2-particle scattering in the logarithmic approximation to the parquet diagram scheme (See for example Roulet *et al* 1969). The most important result is that the cross channel coupling is very coherent and leads to degenerate instability temperatures. For example, if the bare interaction is such that a CDW instability is expected at a temperature T^0_{CDW} the cross channel coupling will lead to both CDW and CP instabilities occurring at the *same* temperature, this temperature being different from T^0_{CDW} because of the cross channel coupling.

In this paper, we investigate the effect of interchannel coupling on instabilities in 1-dimensional metals. We first set up and describe the formalism for obtaining the 2-particle scattering amplitude Γ in different channels (§ 2). The RPA solution for Γ is then discussed in § 3. In § 4 the coupled channel equations are solved for a particular case (coupling between CDW and CP instabilities). The approximations made are discussed and justified. We find, for example, that the exchange of charge density fluctuations leads to considerable Cooper pair attraction, and vice versa. This induced attraction is calculated. There appears to be no reason why the instability temperatures in the two coupled channels should be the same. We find that the degeneracy in the instability temperatures obtained by BGD is spurious and arises from their neglect of the existence of real particle hole and particle-particle excitation continua.

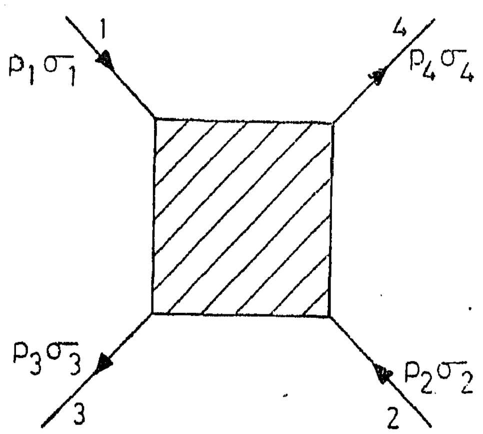

Figure 1. The 2-particle scattering amplitude $\Gamma\,(p_1\sigma_1, p_2\sigma_2, p_3\sigma_3, p_4\sigma_4)$ with momentum energy indices $p_i\,(i = 1, 4)$ and spin indices $\sigma_i(i = 1, 4)$ labelled.

In § 5 we discuss the effect of rigid random impurities, of electron phonon interaction, of interchain coupling and of thermal order parameter fluctuations on the results obtained in the previous section. The last effect is especially important, since it precludes the existence of true long-range order in a strictly 1-dimensional system. In this connection we point out that there can be sizeable electrostatic coupling between electron density fluctuations on parallel chains. The interchain coupling between pair fluctuations is much weaker. One can thus have a bulk CDW transition but perhaps no CP transition.

In § 6, the results obtained earlier are applied to TTF-TCNQ which undergoes a rather sharp metal insulator transition at $T_{\mathrm{CDW}}^{\mathrm{bulk}} \simeq 60°$ K. We find that there is substantial interchain coupling so that $T_{\mathrm{CDW}}^{\mathrm{bulk}}$ is close to the instability temperature computed in RPA or its modification in § 4. The induced Cooper pair attraction is estimated to be quite strong and to lead to a mean field transition temperature $T_{\mathrm{CP}}^{\mathrm{MF}}$ of nearly 400° K. As pointed out by Lee, Saitoh and Anderson (1973), the observed giant conductivity can be explained quantitatively by a thermally activated phase slippage process if a mean field gap or mean field superconducting (Cooper pairing) transition temperature $T_{\mathrm{CP}}^{\mathrm{MF}}$ of about 550° K is assumed. The work of this paper describes a mechanism (CD fluctuation exchange) for such a large $T_{\mathrm{CP}}^{\mathrm{MF}}$. We conclude by discussing the prospects for high temperature superconductivity with such a mechanism.

2. Many-body formalism

We review and describe in this section the many-body formalism used subsequently) Since our aim is to study the scattering amplitude for two electrons or for an electron and a hole in a definite total spin state, we obtain here the channel (electron-electron or electron hole) and spin state (triplet or singlet) decompositions of quantities like the bare interaction and the scattering amplitude. The Bethe-Salpeter equation is also analysed in terms of such decompositions of the irreducible and reducible scattering amplitude. This kind of channel spin decomposition has been done partially earlier by BGD (1966), by Weiner (1971) and by Amit, Kane and Wagner (1968). We present here a reasonably detailed account, since the formalism may be of some general interest.

The model for the 1-dimensional metal consists of a collection of itinerant electrons interacting with each other. The 1-electron Bloch states are denoted by a momentum k and a spin σ, with energy ϵ_k. Thus

$$H_0 = \sum_{k,\sigma} \epsilon_k \, a_{k\sigma}^{+} \, a_{k\sigma} \tag{2.1}$$

where $a_{k\sigma}^{+}$ creates an electron in the state $k\sigma$. There is Coulomb interaction between the electrons. This interaction is mediated in the systems of interest by many objects with degrees of freedom which do not consider, *eg.*, by side chain ions, molecules, and by electrons other than conduction electrons. Thus the " bare " electron-electron interaction (*i.e.*, the electron-electron interaction mediated by everything except the conduction electrons) can be expected to have a fairly complicated dependence on the electron separation. We do not, therefore, assume an explicit form for the bare interaction $V(12)$, taking it, however, to be a function only of the separation $(x_1 - x_2)$. The interaction Hamiltonian is

$$H_{\text{int}} = \tfrac{1}{2} \sum_{\substack{k_i,\sigma_i \\ i=1,4}} a^{+}_{k_1\sigma_1}\, a^{+}_{k_2\sigma_2}\, a_{k_3\sigma_3}\, a_{k_4\sigma_4}\, V_{k_1-k_4}\, \delta_{k_1+k_2-k_3-k_4}\, \delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}. \tag{2.2}$$

The bare irreducible interaction $\langle k_1\sigma_1, k_2\sigma_2 \mid I \mid k_3\sigma_3, k_4\sigma_4\rangle$ (See figure 1 for momentum and spin labels) is defined as the negative of the matrix element of H_{int} between initial electron states $k_3\sigma_3$, $k_4\sigma_4$ and final states $k_1\sigma_1$, $k_2\sigma_2$. Considering the antisymmetry of H_{int} with respect to the exchange of electron 1, 2 (or 3, 4), we see that

$$\langle k_1\sigma_1, k_2\sigma_2 \mid I \mid k_3\sigma_3, k_4\sigma_4\rangle$$
$$= -\tfrac{1}{2}\left[V_{k_1-k_4}\,\delta_{\sigma_1\sigma_4}\,\delta_{\sigma_2\sigma_3} - V_{k_1-k_3}\,\delta_{\sigma_1\sigma_3}\,\delta_{\sigma_2\sigma_4}\right]\,\delta_{k_1+k_2-k_3-k_4}. \tag{2.3}$$

We now divide this into spin triplet and spin singlet parts in various channels. We can view I as the irreducible interaction matrix element corresponding to the interaction between the electrons 1 and 2, electron 1 and hole 3, or electron 1 and hole 4. These three possibilities are called electron-electron (12), electron hole direct (13) and electron hole crossed (14) channels, respectively. Since the interacting entities have spin $\frac{1}{2}$ and since total spin is a good quantum number, it is natural to perform a decomposition of the interaction in various channels into spin triplet ($S = 1$) and spin singlet ($S = 0$) parts. This is best done by the use of spin projection operators P. For example, the spin triplet and spin singlet projection operators P_t^c and P_s^c in the electron-electron channel are

$$P_t^c = \tfrac{1}{2}\left[\delta_{\sigma_1\sigma_4}\,\delta_{\sigma_2\sigma_3} + \delta_{\sigma_1\sigma_3}\,\delta_{\sigma_2\sigma_4}\right] \tag{2.4 a}$$

$$P_s^c = \tfrac{1}{2}\left[\delta_{\sigma_1\sigma_4}\,\delta_{\sigma_2\sigma_3} - \delta_{\sigma_1\sigma_3}\,\delta_{\sigma_2\sigma_4}\right]. \tag{2.4 b}$$

The projection operators are easily obtained by inspection. The irreducible interaction I [eq. (2.3)] is then written as

$$I = \langle k_1\sigma_1, k_2\sigma_2 \mid I \mid k_3\sigma_3, k_4\sigma_4\rangle$$
$$= \delta_{k_1+k_2-k_3-k_4}\left[I_t^{\text{e}}\, P_t^{\text{e}} + I_s^{\text{e}}\, P_s^{\text{e}}\right] \tag{2.5}$$

where the irreducible interaction

$$I_t^{\text{e}} = \tfrac{1}{2}\left[V_{k_1-k_3} - V_{k_1-k_4}\right] \tag{2.6 a}$$

$$I_s^{\text{e}} = -\tfrac{1}{2}\left[V_{k_1-k_3} + V_{k_1-k_4}\right]. \tag{2.6 b}$$

One can perform a similar spin state decomposition in the direct electron hole channel (13) where the projection operators are

$$P_t^d = \delta_{\sigma_1\sigma_4}\,\delta_{\sigma_2\sigma_3} - \tfrac{1}{2}\,\delta_{\sigma_1\sigma_2}\,\delta_{\sigma_2\sigma},$$

$$P_s^d = \tfrac{1}{2}\,\delta_{\sigma_1\sigma_3}\,\delta_{\sigma_2\sigma_4}. \tag{2.7 a}$$

One finds that

$$I_t^d = -\tfrac{1}{2}\,V_{k_1-k_4}, \tag{2.8 a}$$

$$I_s^d = \left(V_{k_1-k_3} - \tfrac{1}{2}\,V_{k_1-k_4}\right). \tag{2.8 b}$$

The spin projection operator and the irreducible interaction for the crossed electron hole channel 14 are obtained from eqs (2.7) and (2.8), respectively, by interchanging the indices 3 and 4 and changing the sign. The results (2.6) and

(2.8) obtained above for the irreducible interaction are relevant for a discussion of the channel and the spin state in which instability can occur (See § 3).

We now discuss the 2-particle scattering amplitude $\Gamma(p_1\sigma_1, p_2\sigma_2, p_3\sigma_3, p_4\sigma_4)$ where p_1 is the momentum energy variable $p_1 = k_1, \nu_{l_1} = \frac{(2l_1+1)\,i\pi}{\beta}$. It is diagrammatically obvious that can be written as a sum

$$\Gamma = I + \gamma^e + \gamma^d + \gamma^c, \tag{2.9}$$

where the momentum energy and spin indices have been suppressed. In eq. (2.9), I is the totally irreducible bare scattering amplitude, γ^e is reducible in the electron-electron channel, γ^d is reducible in the direct electron hole channel and γ^c in the crossed electron hole channel. The result (2.9) is obvious since it is topologically impossible to construct a diagram for Γ which is simultaneously reducible in more than one channel. In order to obtain Γ, we need to know γ^e, γ^d and γ^c. These satisfy a Bethe-Salpeter like equation. For example,

$$\gamma^e(p_1\sigma_1, p_2\sigma_2, p_3\sigma_3, p_4\sigma_4) = \sum_{\substack{p'_3\sigma'_3 \\ p'_4\sigma'_4}} \Lambda^e(p_1\sigma_1, p_2\sigma_2, p'_3\sigma'_3, p'_4\sigma'_4)\, G_{p'_3\sigma'_3} \times G_{p'_4\sigma'_4}\, \Gamma(p'_3\sigma'_3, p'_4\sigma'_4, p_3\sigma_3, p_4\sigma_4), \tag{2.10}$$

where Λ^e is irreducible in the electron-electron channel. Clearly Λ^e consists of a totally irreducible part and of parts reducible in the electron hole channels 13 and 14. We can thus write schematically

$$\Lambda^e = I^e + \gamma^d + \gamma^c. \tag{2.11}$$

Pairs of equations similar to (2.10) and (2.11) can be written for γ^d and γ^c. We thus see that γ^e, γ^d and γ^c are dynamically coupled to each other. In principle, these quantities, and hence Γ are obtained by solving the coupled equations for a given I. It is again natural to work with equations for the singlet and triplet spin projections of the γ's. The equation for $\gamma^e_{t,s}$ (where t and s signify spin triplet and singlet projection in the electron-electron channel) is readily obtained from (2.10) to be

$$\gamma^e_{t,s} = \Lambda^e_{t,s}\, GG\, \Gamma^e_{t,s}. \tag{2.12}$$

In eq. (2.12), $\Lambda^e_{t,s}$ and $\Gamma^e_{t,s}$ are the spin triplet and singlet projections of Λ and Γ in the electron-electron channel. The momentum energy variables in eq. (2.12) are the same as in eq. (2.10). To write down an equation for $\Lambda^e_{t,s}$ similar to (2.11), we need to know $[\gamma^d]^e_{t,s}$ and $[\gamma^c]^e_{t,s}$ in terms of $\gamma^d_{t,s}$ and $\gamma^c_{s,t}$ *i.e.*, a spin state in the *ee* channel in terms of spin states in the *eh* channels. We need to relate, therefore, $P^e_{t,s}$ to $P^d_{t,s}$ and $P^c_{t,s}$. The relation is easily obtained from the definitions, *i.e.*, eqs (2.4) and (2.7). We then find that

$$\Lambda^e_t = I^e_t + \tfrac{1}{2}(\gamma^d_t + 3\gamma^d_s) - \tfrac{1}{2}(\gamma^c_t + 3\gamma^c_s), \tag{2.13 a}$$

$$\Lambda^e_s = I^e_s + \tfrac{1}{2}(\gamma^d_t - \gamma^d_s) + \tfrac{1}{2}(\gamma^c_t - \gamma^c_s). \tag{2.13 b}$$

Equations similar to (2.12) and (2.13) can be written for $\gamma^{d,c}_{t,s}$ and $\gamma^{d,c}_{t,s}$, respectively.

Since $\gamma^e_{t,s}$ and $\gamma^e_{s,t}$ are related by crossing symmetry (Amit, Kane and Wagner, 1968; Nozieres, 1965), in effect we have coupled equations for the four quantities $\gamma^e_{t,s}$ and $\gamma^d_{t,s}$. Each of these quantities depends on six variables (three momenta and three energies) since conservation of total momentum and total energy eliminates two out of the eight variables p_1, p_2, p_3, p_4. These six variables can be conveniently chosen to be the momentum and energy transfers in the three channels 12, 13 and 14. For this purpose we rename the variables as in figure 2 *a*, so that the momentum energy transfers are, respectively,

$$r\left[=q, z_m=\frac{2\pi i m}{\beta}\right], (p+p'-r) \quad \text{and} \quad (p-p').$$

Equation (2.10) now becomes (figure 2 *b*)

$$\gamma^e_{t,s}(r, p+p'-r, p-p') = \sum_{p''} \Lambda^e_{t,s}(r, p+p''-r, p-p'')\, G_{p''}\, G_{-p''+r} \times [\Lambda^e_{t,s}(r, p''+p'-r, p''-p') + \gamma^e_{t,s}(r, p'+p''-r, p''-p')] \tag{2.14}$$

where $\Lambda^e_{t,s}$ is defined by eq. (2.11). $\gamma^d_{t,s}$ satisfies a corresponding equation. The total scattering amplitude is given by eq. (2.8). In principle, to obtain Γ, we have to solve, for a given I, a coupled set of integral equations [eqs (2.14) and (2.11)], and a corresponding set for $\gamma^d_{t,s}$ in six variables. This manifestly impossible task is made feasible by several simplifications and approximations, which we briefly mention now. The description of these approximations and of the solutions obtained constitutes the remainder of this paper. In § 3 we assume that interchannel coupling can be neglected. This is the well-known random phase approximation (RPA). In § 4 we take interchannel coupling into account in an approximate way, by using an RPA-like form for the cross channel γ. We

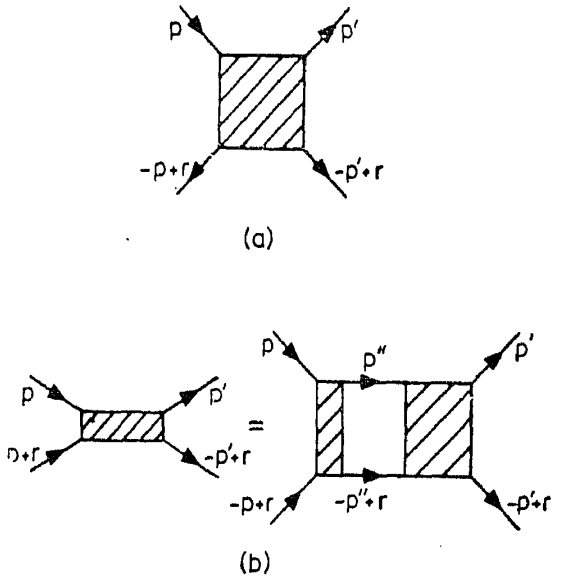

Figure 2. (*a*) The 2-particle scattering amplitude Γ with momentum energy transfers r, $(p-p')$ and $(p+p'-r)$ in the electron-electron (12), direct electron hole (13) and crossed electron hole (14) channels, respectively.

(*b*) The Bethe-Salpeter equation for γ^e, *i.e.* the equation $\gamma^e = \Lambda^e GG\Gamma$ (Eq. (2.10)) with the momentum energy variables $p\,(=k, \nu_l)$, etc. of the electrons shown.

also discuss there the method of BGD for taking interchannel coupling into account.

3. Random phase approximation

The most commonly used simplification of the coupled equations of the type (2.14) and (2.11) for γ is to assume them to be uncoupled. One assumes that the irreducible interaction in a particular channel is the bare interaction I in that channel, *eg.*, [see eq. (2.11)]

$$\Lambda^e_{t,s} = I^e_{t,s}. \tag{3.1}$$

In such a case, the equations for $\gamma^e_{t,s}$, etc., are all independent integral equations. For example eq. (2.13) becomes

$$\gamma^e_s(r, p+p'-r, p-p') = \sum_{p''} I^e_s(k+k''-q, k-k'')\, G_{p''}\, G_{-p''+r}$$

$$\times [I^e_s(k''+k'-q, k''-k') + \gamma^e_s(r, p''+p'-r, p''-p')]. \tag{3.2}$$

This is the RPA equation for γ^e_s. It can be further simplified by assuming $I^e_s(k+k''-q, k-k'') = -\frac{1}{2}(V_{k+k''-q} - V_{k-k''})$, see eq. (2.6 *a*) to be an insensitive function of its momentum variables in the range of values of interest. See below, *e.g.*, eq. (3.16). Then we have

$$\gamma^e_{t,s}(r) = I^e_{t,s}\left[\sum_{p''} G_{p''}\, G_{-p''+r}\right][I^e_{t,s} + \gamma^e_{t,s}(r)] \tag{3.3}$$

so that

$$\gamma^e_{t,s}(r) = \frac{I^{e\,2}_{ts}\,\chi_0{}^e(r)}{1 - I^e_{os}\,\chi_0{}^e(r)}, \tag{3.4}$$

where

$$\chi_0{}^e(r) = \sum_{p''} G_{p''}\, G_{-p''+r}. \tag{3.5}$$

The quantity $\chi_0{}^e(r)$ can easily be calculated for bare propagators, *i.e.*, with

$$G_{p''} = G^0_{p''} = (\nu_l'' - \tilde{\epsilon}_{k''})^{-1}. \tag{3.6}$$

For not too large deviations of k'' from the Fermi momentum k_F, we can write

$$\tilde{\epsilon}_{k''} = \frac{(k''-k_F)\,k_F}{m^*}. \tag{3.7}$$

In this approximation,

$$\chi_0{}^e(r) = \chi_0{}^e(q, z_m)$$

$$= \frac{\rho\epsilon_F}{2}\left[\phi^+(q, z_m) + \phi^-(q, z_m)\right], \tag{3.8}$$

where

$$\phi^{\pm}(q, z_m) = \sum_{l=0}^{l_c}\left[\, l + \tfrac{1}{2} + \frac{m}{2} \pm \frac{q\beta}{8i\pi k_F\,\rho\epsilon_F}\right]^{-1}. \tag{3.9}$$

In eq. (3.8), $\rho\epsilon_F$ is the density of electronic states at the Fermi energy, and in eq. (3.9) l_c is an electronic upper energy cut-off $\left(\frac{(2l_c+1)\pi}{\beta} = \text{the cut-off energy } \omega_c \simeq \text{bandwidth}\right)$. From eq. (3.9) it is clear that $\chi_0^e(r)$ is largest for $q = 0$, $z_m = 0$ and then has the value

$$\chi_c^e(0) = \chi_c^e(0, 0) = \rho\epsilon_F [\psi(l_c + \tfrac{1}{2}) - \psi(\tfrac{1}{2})]$$
$$= \rho\epsilon_F \ln(1.14\,\beta\omega_c) \qquad (3.10)$$

We thus see from eqs. (3.4) and (3.10) that there will necessarily be an electron pair instability if $I^e_{t,s} > 0$, *i.e.*, if the BCS condition is satisfied. The instability then occurs at the BCS transition temperature

$$(T_c)^e_{t,s} = 1.14\,\omega_c \exp -(I^c_{t,s}\,\rho\epsilon_F)^{-1}. \qquad (3.11)$$

We can similarly obtain $\gamma^d_{t,s}(r)$ where now r is the momentum energy transfer in the direct particle hole channel.

We find

$$\gamma^e_{t,s}(r) = \frac{I^{d\,2}_{t,s}\,\chi_0{}^d(r)}{1 - I^d_{t,s}\,\chi^d{}_0(r)} \qquad (3.12)$$

where $\chi_0{}^d(r)$ is

$$\chi_0{}^d(r) = \sum_p G_p\,G_{p+r}. \qquad (3.13)$$

Under the same approximations as used for $\chi_0{}^e(r)$, one finds that $\chi_0{}^d(r)$ has a logarithmic behaviour [similar to that of eq. (3.10)] for momentum $q = \pm 2k_F$ and $z_m = 0$. As a function of the variables $(|q| - 2k_F) = \delta$ and z_m, $\chi_0{}^d(r)$ is seen to be

$$\chi_0{}^d(r) = -\frac{\rho\epsilon_F}{4}\left[\phi^+(\delta, z_m) + \phi^-(\,,z_m)\right] \qquad (3.14)$$

where the $\phi^{\pm}(\delta, z_m)$ have been defined earlier (eq. (3.9)). Since $\chi_0{}^d(r)$ is largest for $\delta = 0$ ($|q| = 2k_F$) and $z_m = 0$, and there has the value $-\frac{\rho\epsilon_F}{2}\ln(1.14\,\beta\omega_c)$, we see from eq. (3.12) that there is necessarily an instability in the electron hole channel for $\delta = 0$ (*i.e.*, for $|q| = 2k_F$) and $z_m = 0$ provided $I^d_{t,s} < 0$, *i.e.*, provided the electron hole interaction in the appropriate spin state is attractive. The temperature at which the instability occurs is given by

$$[T_c]^d_{t,s} = (1.14\omega_c)\exp(\tfrac{1}{2}\,I_s{}^d\,\rho\epsilon_F)^{-1}. \qquad (3.15)$$

This electron hole instability with $q = 2k_F$ leads to the formation of a static spin or charge density wave below $T_c{}^d_{t,s}$, with wavelength $\lambda = 2\pi(2k_F)^{-1}$. The former occurs if the instability is in the spin triplet channel, the latter if the instability is in the spin singlet channel. This was first pointed out by Overhauser (1960).

We see from the above that in the RPA the occurrence of a particular kind of instability of the normal metallic phase depends entirely on the sign of the totally irreducible or bare inteaction in the spin channel state corresponding to that kind of instability. We, therefore, now look into the factors affecting the sign of $I^e_{t,s}$ and $I^d_{t,s}$ (given in terms of electron-electron interaction potential by eqs (2.6) and (2.8)). Consider first $I^e_{t,s}$ For scattering in the electron-electron channel the electrons 1 and 2 have nearly opposite momenta, $k_1 \cong -k_2 \cong k_F$. Further, the intermediate states for two electron scattering are the two electron states $p'', -p''$. Since $\frac{1}{\beta}\sum_{\nu l''} G^0_{p''} G^0_{-p''} \sim \left(\tanh \frac{\beta \tilde{\epsilon}_{k''}}{2} \Big/ \tilde{\epsilon}_{k''}\right)$ electron states with small $\tilde{\epsilon}_{k''}$, *i.e.*, states close to $k'' = k_F$, are weighted strongly. So a typically important set of momentum values is $k_1 \simeq -k_2 \simeq k_F$, $k_3 \simeq -k_4 \simeq -k_F$. This set of momentum values is also important for electron hole instability in the direct channel, since $|k_1 - k_3| \simeq 2k_F$ and the momenta are all close to the Fermi level. The irreducible interactions $I^e_{t,s}$ and $I^d_{t,s}$ should therefore be evaluated in this region of momentum values. We then find that

$$I_t^e = \tfrac{1}{2}(V_{k_1-k_3} - V_{k_1-k_1}) \simeq \tfrac{1}{2}(V_{2k_F} - V_0) \qquad (3.16\,a)$$

$$I_s^e = -\tfrac{1}{2}(V_{k_1-k_3} + V_{k_1-k_1}) \simeq -\tfrac{1}{2}(V_{2k_F} + V_0) \qquad (3.16\,b)$$

$$I_t^d = -\tfrac{1}{2} V_{k_1-k_4} \simeq -\tfrac{1}{2} V_0 \qquad (3.16\,c)$$

$$I_s^d = -\tfrac{1}{2} V_{k_1-k_4} + V_{k_1-k_3} \simeq -\tfrac{1}{2} V_0 + V_{2k_F}. \qquad (3.16\,d)$$

Here V_0 is the bare interaction for small values of the momentum transfer, *i.e.*, for $0 < |k_1 - k_4| < k_F$ while V_{2k_F} is the direct interaction for large values of the momentum transfer, *i.e.*, for $|k_1 - k_3| \sim 2k_F$.

Normally, the electron-electron interaction is repulsive and decreases monotonically with the distance between electrons. In that case, $V_0 > V_{2k_F} > 0$. We then see from eq. (3.16) that indeed the electron-electron interaction is repulsive in both spin states ($I^e_{t,s} < 0$) so there can be no instability in this channel. Further, both I_t^d and I_s^d are negative, and $I_t^d < I_s^d$, *i.e.*, the spin triplet electron interaction is more attractive than the singlet. Thus, in the RPA, an SDW instability must necessarily occur. This is perhaps the situation in NMP–TCNQ, which undergoes a transformation from a metal to an antiferromagnetic insulator with a doubling of the period, *i.e.*, to an SDW state with $q = 2k_F$.

Now suppose that V_{2k_F} is made negative; we then see from eqs (3.16 *c*) and (3.16 *d*) that a CDW instability is favoured over the SDW. V_{2k_F} can be negative if the small separation electron-electron repulsion (for separation $x \sim (2k_F)^{-1}$) is strongly reduced or is made attractive so that $V(x)$ has a non-monotonic dependence on x. In the site space language of the Hubbard model, we expect V_{2k_F} to be negative if the same site electron repulsion U_0 is less than the nearest neighbour repulsion U_1. This can be achieved in TCNQ based compounds by the introduction of a very highly polarizable side chain. This considerably reduces the same

site repulsion because there is now a large polarization induced attractive term in the same site electron interaction. This is perhaps what happens when the polarizable NMP in NMP-TCNQ is replaced by the even more polarizable and smaller TTF to form TTF-TCNQ. TTF-TCNQ also undergoes a metal insulator transition, and the insulating phase is a CDW, thus supporting our conjecture above. The condition for electron pair instability is more stringent. We first notice that if $V_{2k_F} < 0, I_s^e < I_t^e$. Next, $I_s^e > 0$ if $V_0 + V_{2k_F} < 0$, *i.e.*, if the small separation electron interaction ($V(x)$ for $x \sim (2k_F)^{-1}$) is attractive enough. This is not impossible, but has perhaps not yet been achieved experimentally.

The above discussion also brings out clearly a possible limitation of the RPA. It was found that a typical important electron scattering configuration is $k_1 \simeq -k_2 \simeq -k_3 \simeq k_F$. [With $k_1 + k_2 = k_3 + k_4$ exactly]. This has total electron momentum $\simeq 0$ and also electron hole momentum in direct channel $\simeq 2k_F$. Thus one is close to momentum conditions appropriate for a possible instability in both the channels. Since such electron configurations are important, we expect considerable coupling between singularities in *ee* and *eh* channels. This is discussed in the next section.

4. Interchannel coupling

We have seen above that there are important 2-electron momentum configurations which are simultaneously close to configurations for electron-electron and for electron hole instabilities. This clearly implies, through eqs (2.14) and (2.13) that the reducible electron-electron scattering amplitude $\gamma^e_{t,s}$ for small total 2-electron energy and momentum will be strongly affected by the reducible electron hole scattering amplitude $\gamma^d_{t,s}$, being large for electron hole momentum transfer $\simeq \pm 2k_F$ and small energy transfer. The converse is also true. In this section we analyse this interchannel coupling for a particular case in a certain approximation. We compare the results of BGD (1966) for this case with ours at the end of this section.

In general both γ_t^e and γ_s^e are coupled to γ_t^d and γ_s^d so that the interchannel coupling problem is in principle quite complicated. It is, however, evident physically as well as from eqs (2.14) and (2.13) that some of these interchannel couplings are especially significant in that they tend to drive the scattering amplitude in the other channel to instability. For example, suppose that the normal metal has a tendency to a CDW instability. This means that γ_s^d is negative and is large in size. We then see from eqs (2.14) and (2.13) that this will contribute a positive term to γ_s^e through the presence of $-\frac{1}{2}\gamma_s^d$ and $-\frac{1}{2}\gamma_s^c$ in the expression for A_s^e. Thus, there is an effective Cooper pair attraction due physically to the coupling of the electron pairs through the repeatedly scattering enhanced electron density fluctuations. It is difficult to be definite about the effect on γ_t^e, since from eq. (2.13 *a*) it appears that in A_t^e, γ_s^d and γ_s^c occur with opposite signs. Perhaps the effect will be small. On the other hand, suppose one is close to an SDW instability, *i.e.*, γ_t^d is negative and large. Then, again from eqs (2.14) and (2.13), it is clear that this gives rise to a repulsive contribution to γ_s^e (Berk and Schrieffer 1966). One can make similar statements about the converse effect.

Thus, we see that proximity to a CDW instability leads to enhanced Cooper pair scattering amplitude which in turn leads to an increased γ_s^d. The coupling between γ_s^e and γ_s^d is therefore specially significant. We study this case now. We therefore assume that the scattering amplitude in other channel spin states, (*i.e.*, γ_t^e and γ_t^d) have no incipient singularity, are not large and depend only weakly on temperature. To simplify matters, we shall omit γ_t^e and γ_t^d henceforth.

We see from eqs (2.14) and (2.13) that in order to calculate $\gamma_s^e(r, p+p'-r, p-p')$ we need $\gamma_{t,s}^{d,c}(r, p+p''-r, p-p'')$. We first make the simplifying assumption that a reducible scattering amplitude depends sensitively only on the momentum energy transfer in the channel in which it is reducible. For example, $\gamma_s^d(r, p+p''-r, p-p'')$ is assumed to be a sensitive function only of the momentum energy transfer $(p+p''-r)$ in the direct electron hole channel. This is reasonable, especially near an instability in the electron hole channel, since then for $(k+k''-q)$ away from $\pm 2k_F$, and $(\nu_l+\nu_{l''}-z_m)$ away from zero, the size of the scattering amplitude decreases rapidly. From the (ladder type) diagrams for γ_s^d we see that by definition the internal momentum energy transfer is always $(p+p''-r)$ in the direct *eh* channel, whereas it is a summed-over variable for the crossed *eh* and the *ee* channels. Thus the dependence of $\gamma_s^d(r, p+p''-r, p-p'')$ on r and on $(p-p'')$ is smoothened out, and can be neglected in the first approximation, especially if these variables are limited to a relatively narrow range by other considerations (*eg.*, r is small, p and p'' are close to Fermi level for cases of interest). Next, we assume that the dependence of γ_s^d on $(p+p''-r)$ has the same form as in the RPA, with at most an effective $\tilde{I}_s^d$ replacing the bare $\tilde{I}_s^d$. Thus we take over the RPA expression eq. (3.12) for ${}_s^d(r)$ where r is the momentum energy transfer in the electron hole channel, with $\tilde{I}_s^d$ instead of I_s^d. This assumption is discussed later below. One thus writes.

$$\begin{aligned}
\gamma_s^d(r) &= \gamma_s^d(q, z_m) = \gamma_s^d(\pm 2k_F + \delta, z_m) \\
&= -f_s^d(\delta, z_m)(\rho\epsilon_F)^{-1} \\
&= \tilde{I}_s^{d\,2}\,\chi_o^d(\delta, z_m)\{1-\tilde{I}_s^d\,\chi_o^d(\delta, z_m)\}^{-1} && (4.1)\\
&\simeq \tilde{I}_s^d\{1-\tilde{I}_s^d\,\chi_o^d(\delta, z_m)\}^{-1} && (4.2\,a)\\
&= -\{f_s^d(0)^{-1}+\chi_o^d(0,0)-\chi_o^d(\delta, z_m)\}^{-1}\rho\epsilon_F^{-1} && (4.2\,b)
\end{aligned}$$

where $f_s^d(0)$ is $\gamma_s^d(q, z_m)$ for $|q| = 2k_F$ and $z_m = 0$, multiplied by $(-\rho\epsilon_F)^{-1}$. The equality (4.2 *a*) is true near a singularity of $\gamma_s^d(r)$, *i.e.*, if $I_s^d\,\chi_o^d(\delta, z_m) \simeq 1$. Equations similar to (4.1) and (4.2) can be written for γ_t^d and for $\gamma_{t,s}^c$, $\gamma_{t,s}^c$.

We now use the above simplifications to calculate γ_s^e and γ_s^d. The eqs (2.14) and (2.13) for γ_s^e simplify to

$$\begin{aligned}
\gamma_s^e = (r)\sum_{p''}\{I_s^e - \tfrac{1}{2}[\gamma_s^d(p+p''-r)+\gamma_s^e(p-p'')]\}\,G_{p''}\,G_{-p''+r} \\
\times\{I_s^e - \tfrac{1}{2}[\gamma_s^d(p''+p'-r)+\gamma_s^e(p''-p')]+\gamma_s^e(r)\}. \qquad (4.3)
\end{aligned}$$

We first note from eq. (4.3) that, contrary to the assumption above, γ_s^c does depend on p and p'. However, this dependence can be shown (by explicit evaluation of eq. (4.3) using eq. (4.2)) to be weak. We therefore evaluate eq. (4.3) for (p, p') on the Fermi level, *i.e.*, for $|k|, |k'| = k_F$ and $\nu_l, \nu_{l'} = i\pi/\beta$. Since the singularity first occurs for $r = 0$, *i.e.*, for both the electrons at the Fermi level with equal and opposite momenta, we calculate $\gamma_s^c(0)$. Since $\gamma_s^d(q, z_m)$ is peaked near momentum transfer $q = \pm 2k_F$, it is convenient to change the momentum integration variable on the right-hand side of eq. (4.3) from k'' to $k'' \mp k_F = \delta$. The minus sign is appropriate for $\gamma_s^d(k''+k_F, \nu_l''+(i\pi/\beta)) = \gamma_s^d(2k_F+\delta, \nu_l''+(i\pi/\beta))$ and the plus sign for $\gamma_s^c(k_F-k'', (i\pi/\beta)-\nu_l'') = \gamma_s^c(2k_F-\delta, (i\pi/\beta)-\nu_l'')$. Changing over to this variable, eq. (4.3) becomes (for $r = 0$, and p, p' on the Fermi level)

$$\gamma_s^c(0) = A + B\gamma_s^c(0), \tag{4.4}$$

where

$$A = A_1 + A_2 + A_3 + A_4 \tag{4.5 a}$$

$$A_1 = (I_s^c)^2 \chi_0^c(0)$$

$$A_2 = 2I_s^c \rho\epsilon_F^{-1}\left[\frac{1}{\beta}\sum_{\nu l} G_{k_F+\delta}(\nu_l)\, G_{-k_F-\delta}(-\nu_l) f_s^d\left(\delta, \nu_l + \frac{i\pi}{\beta}\right)\right]$$

$$A_3 = \frac{1}{2}\rho\epsilon_F^{-2}\left\{\frac{1}{\beta}\sum_{\nu l,\,\delta} f_s^d\left(\delta, \nu_l + \frac{i\pi}{\beta}\right) f_s^d\left(-2k_F, \nu_l - \frac{i\pi}{\beta}\right)\right.$$

$$\left.\times\, G_{k_F+\delta}(\nu_l)\, G_{-k_F\delta}(-\nu_l)\right\}$$

$$A_4 = \frac{1}{2}\rho\epsilon_F^{-2}\frac{1}{\beta}\sum_{\nu l,\,\delta} f^d\left(\delta, \nu_l + \frac{i\pi}{\beta}\right)^2 G_{k_F+\delta}(\nu_l)\, G_{-k_F-\delta}(-\nu_l). \tag{4.5 b}$$

$$B = I_s^c \chi_s^c(0) + \rho\epsilon_F^{-1}\left[\frac{1}{\beta}\sum_{\nu l,\,\delta} f_s^d\left(\delta, \nu_l + \frac{i\pi}{\beta}\right)\right.$$

$$\left.\times\, G_{k_F+\delta}(\nu_l)\, G_{-k_F-\delta}(-\nu_l)\right]. \tag{4.6}$$

In eq. (4.4), A is the inhomogeneous part, and B is the coefficient of the homogeneous part. The effective Cooper pair interaction is determined by B, since the solution of eq. (4.4) is

$$\gamma_s^c(0) = A(1-B)^{-1}. \tag{4.7}$$

The instability is determined by the condition $B = 1$. In the absence of cross channel coupling, $\gamma_s^c(0)$ is given by eq (3.4) so that B is then related to the bare interaction I_s^c by

$$B_{\text{RPA}} = I_s^c \rho\epsilon_F \ln(1.14\beta\omega_c). \tag{4.8}$$

Thus one can generally define an effective interaction I_s^c such that

$$I_s^c \rho_{\epsilon_F} = B \ln(1.14\beta\omega_c)^{-1} \tag{4.9 a}$$

$$= [I_s^c + (I_s^c)_{\text{ind.}}]\, \rho_{\epsilon_F} \tag{4.9 b}$$

We now calculate B from eq. (4.6), using the expression (4.2) and (3.14) for f_s^a. The integration over the momentum variable δ is easily performed by deforming the contour in the complex plane. In doing this integration, the quantities in the integrand are expanded in powers of δ and only the linear term is retained. This is obviously valid for $\delta \ll k_F$, the momentum region of greatest importance. So the error introduced by this approximation is not expected to be serious. The energy summation over the Matsubara frequencies ν_l is done in the usual way by deforming the contour so that

$$\frac{1}{\beta}\sum_{\nu_l}\phi(\nu_l) = \int_{-\infty}^{+\infty}\frac{d\omega}{\pi}\left\{\mathrm{Im}\left[\phi(\omega^-)\right]\right\}\left\{e^{\beta\omega}+1\right\}^{-1} \tag{4.10}$$

where $\phi(\nu_l)$ is the summand in eq. (4.6) after the momentum integration (over δ) has been carried out. In doing the sum according to (4.10), we consider on the right-hand side only the discontinuity of the pair propagator part across the real axis, *i e*, the discontinuity of $\gamma_s^a(\delta, \tilde{\nu})$ ($\tilde{\nu}$ complex) across the real axis is neglected. That is, we consider only the effective electron-electron interaction arising from exchange of virtual electron density fluctuations of wave number $q \simeq \pm 2k_F$. The contribution of real electron density fluctuations (given by the term involving the discontinuity of $\gamma_s^a(\delta, \tilde{\nu})$ across the real axis) is limited by the Bose factor $[e^{\beta\nu} - 1]^{-1}$ to those of energy less than k_BT and is therefore likely to be small. We do not consider it here. It contributes a further atractive term to $\gamma_s^a(0)$. The integration over energies in (4·10) is restricted to an energy range $\pm\,\omega'_c$ (from the Fermi energy). This range is determined by the bandwidth and by the fall-off of electron propagators and of the scattering amplitude γ_s^a with energy. For simplicity, we take this electronic energy ω_c' to be the cut-off energy ω_c used in eqs (3.9) and (3.10) for example. Performing the energy summation under the above conditions, we obtain for B the expression

$$B = I_s^a\,\rho_{e_F} + \tfrac{1}{2}\int_0^{\omega_c} d\nu\,\frac{\tanh\left(\frac{\beta\nu}{2}\right)}{\nu}$$

$$\times\,\mathrm{Re}\left\{f_s^a(0)^{-1} + \tfrac{1}{4}\left[\psi\left(-\frac{i\beta\nu}{2\pi}\right) - \psi\left(\tfrac{1}{2}\right)\right]\right\}^{-1} \tag{4.11 a}$$

$$= I_s^a\,\rho_{eF} + \ln\left\{\frac{[+\,12\pi^{-1}\ln(\lambda\beta\omega_c)]^2}{1+[8\pi^{-1}f_s^a(0)^{-1}]^2}\right\} \tag{4.11 b}$$

where, in going from (4.11 *a*) to (4.11 *b*), we have simulated the effect of the factor $[\tanh(\beta\nu/2)/\nu]$ by $1/\nu$ and by cutting off the ν integration at $\nu_{\min} \sim k_BT$ or for convenience at $\nu_{\min} = k_BT\,\lambda^{-1} = k_BT\,(1.14)^{-1}$. We see from the second term of eq. (4.11 *b*) that the exchange of virtual electron density fluctuations leads to a Cooper pair attraction (see eq. (4.9)) equal to

$$(I_s^a)_{\text{ind.}}\,\rho_{e_F} = \ln(\lambda\beta\omega_c)^{-1}\,\ln\left\{\frac{1+[2\pi^{-1}\ln(\lambda\beta\omega_c)]^2}{1+[8\pi^{-1}f_s^a(0)^{-1}]^2}\right\}. \tag{4·12}$$

We see that the induced attraction is large (of order unity) and increases slowly as $f_s^a(0)^{-1} \to 0$, *i.e.*, as the CDW instability is approached.

We now evaluate the quantity A defined by eq. (4.5). We have

$$A_1 = (I_s^e)^2 \rho_{e_F} \ln (\lambda\beta\omega_c) \tag{4.13 a}$$

$$A_2 = 2I_s^e \ln \left\{ \frac{1 + [(2/\pi) \ln (\lambda\beta\omega_c)]^2}{1 + [(8/\pi) f_s^d (0)^{-1}]^2} \right\} \tag{4.13 b}$$

$$A_4 = -\rho\epsilon_F^{-1} \frac{16}{\pi} \frac{[f_s^d (0)^{-1} + \frac{1}{4} \ln (\lambda\beta\omega_c)]}{[1 + (8/\pi)(f_s^d (0)^{-1} + \frac{1}{4} \ln (\lambda\beta\omega_c))^2]}$$

$$+ \rho\epsilon_F^{-1} \frac{16}{\pi} \frac{f_s^d (0)^{-1}}{1 + [(8/\pi) f_s^d (0)^{-1}]^2} \tag{4.13 c}$$

A_3 cannot be calculated exactly, since it depends on $f_s^d (\delta, \nu_l + (i\pi/\beta) \times f_s^d [\delta - 2k_F, \nu_l - (i\pi/\beta)]$, *i.e.*, on a product of f_s^d's one of which necessarily has a large momentum transfer $(\delta - 2k_F)$. A rough estimate can be obtained by assuming $f_s^d (\delta - 2k_F, \nu_l - (i\pi/\beta)) \simeq f_s^d (-2k_F, 0)$. In that case we find

$$A_3 = \tfrac{1}{2} f_s^d (-2k_F, 0) \rho\epsilon_F^{-1} \ln \frac{[1 + (2\pi^{-1} \ln (\lambda\omega_0))^2]}{1 + [8\pi^{-1} f_s^d (0)^{-1})^2]} \tag{4.13 d}$$

The inhomogeneous term A in the reducible scattering amplitude γ_s^e is thus a fairly complicated function of the parameters I_s^e, f_s^d and $k_B T$. It is, however, a smooth function of these and in particular of $k_B T$.

A similar calculation can be carried out of the effect of interchannel coupling on γ_s^d. Assuming that $\gamma_s^e (q, z_m)$ can be described by an RPA-like form, we find that there is an induced electron hole attraction in the spin singlet (CDW) channel due to the exchange of virtual Cooper pairs between the electron and the hole. The induced attraction is computed to be

$$I_s^d{}_{\text{ind.}} \rho_{\epsilon_F} = -\tfrac{1}{4} \ln \frac{[1 + (2\pi^{-1} \ln (\lambda\beta\omega_c))^2]}{[1 + (4\pi^{-1} \gamma_s^e (0)^{-1})^2]} . \tag{4.14}$$

We note that this term is of the same form as $I_s^e{}_{\text{ind.}} \rho_{\epsilon_F}$ (eq. (4.12)). However, there is an extra factor of $(\frac{1}{4})$ in the expression (4.14). This is partly due to the difference in the RPA expressions for γ_s^e and for γ_s^d, and partly to the fact that the induced attraction in the electron-electron channel is contributed to by interchannel coupling with *both* direct and crossed electron hole scattering, while for, the induced electron hole interaction only one channel, the electron-electron channel, contributes. As a result, even at its maximum, the induced electron hole attraction is expected to be considerably smaller than the induced electron-electron attraction.

We now discuss our assumption of the RPA form for γ_s^d and γ_s^e. We first note that while the cross-channel induced attraction may be considerable, there is no requirement that $f_s^d (0)$ and $\gamma_s^e (0)$ tend to ∞ at the same temperature. Thus, in a certain temperature regime, one of them, *e.g.*, f_s^d or γ_s^d, may be large while the other (γ_s^e in that case) is not. Then, in V_s^d, γ_s^e is not large and is not sharply peaked as a function of the momentum energy transfer in the cross (electron-electron) channel. It can be taken to be a constant and thus the RPA form is quite accurate for γ_s^d. Further, we have seen that the effect of cross channel

coupling is much smaller in some cases than in others. For example, as mentioned above, $(I_s^d)_{\text{ind.}}$ due to coupling to γ_s^e is expected to be small. Thus, even if γ_s^e were large, there would be some justification in ignoring the effect of cross-channel coupling with γ_s^e on γ_s^d and in calculating γ_s^d in the RPA. Lastly, in the RPA, one assumes that the irreducible or effective interaction is independent of momentum energy transfer in all channels up to a certain cut-off energy transfer, whereafter it vanishes. The cross channel coupling term has a definite energy dependence; it is larger for small energy transfers in the crossed channels. However it decreases smoothly over a typical electronic cut-off energy, and can be approximately replaced by a properly averaged constant, *i.e.*, by $I_{\text{ind.}}$

We now compare our results with those of BGD (1966) and of Dzhyaloshinskii and Larkin (1972). These authors calculate the scattering amplitude in the logarithmic approximation to the parquet diagrams scheme. The method is easily applied to the case considered above, namely when there is strong inter-channel coupling between γ_s^d and γ_s^e. One finds (see Dzhyaloshinskii and Larkin (1972) or Roulet *et al* (1969) for details of the method)

$$\gamma_s^d(x) = -\tfrac{1}{2}\int_0^x [I_s^d - \gamma_s^d(y) + \gamma_s^e(y)]^2\, dy \qquad (4.15\,a)$$

$$\gamma_s^e(x) = \int_0^x [I_s^e - \tfrac{1}{2}\gamma_s^d(y) + \gamma_s^e(y)]^2\, dy. \qquad (4.15\,b)$$

Here x is the logarithmic momentum energy variable $x = \ln\{\lceil\omega_c/\min(\omega, q v_F, k_B T)\rceil\}$ where q is the momentum transfer (or momentum transfer $\pm 2k_F$ for the *eh* channel case) and ω is the energy transfer. We have not been able to solve eqs (4.15) analytically. However, it is clear from the symmetric structure of these equations (convertible into differential equations by simple differentiation) that if $\gamma_s^e(0)$ becomes singular at some temperature, $\gamma_s^d(0)$ will also necessarily do so at the same temperature. This is made evident, for example, by using the form $A/(B+x)$ for $\gamma_s^e(x)$ or $\gamma_s^d(x)$, the form being seen to be valid near the poles of these functions. A numerical solution of the coupled integral eqs (4.15) confirms this degeneracy of singularities in $\gamma_s^e(x)$ and $\gamma_s^d(x)$. BGD and Dzhyaloshinskii and Larkin (1969) also found such degenerate instability temperatures in the mathematically and physically similar cases treated by them. In terms of our earlier analysis, the source of this spurious degeneracy is the term A_4 in eqs (4.4) and (4.5) for $\gamma_s^e(0)$. This term is of the form $\frac{1}{2}\sum_{p''}\gamma_s^d(p-p'')\,G_{p''}\,G_{-p''}\,\gamma_s^d(p''-p')$. On evaluation in the logarithmic approximation (for p, p' close to the Fermi level) this leads to an expression of the form $\int_0^x [\gamma_s^d(y)]^2\, dy$, where $x \sim \ln(\beta\omega_c)$. This expression, present in the parquet eq. (4.15), is responsible for the degeneracy in the singularities of γ_s^e and γ_s^d. On evaluating it in our approximation, we obtain eq. (4.13 *c*), whose second term can be written as $[\pi/(4\rho\epsilon_F)]f_s^d(0)^{-1}[(\pi/8)^2 + f_s^d(0)^{-2}]^{-1}$. In this, the expression $(\pi/8)^2$ in the denominator arises from $\text{Im}\, f_s^d(\delta, \omega^-)$ being non-zero, *i.e.*, from the real particle hole excitation continuum. Suppose this is ignored, *i.e.*, we take $\text{Im}\, f_s^d(\delta, \omega^-) = 0$, as is effectively done in Bychkov *et al*

(1966) and Dzhyaloshinskii and Larkin (1969). Then the term mentioned above becomes $\pi/(4\rho\epsilon_F) f_s^a(0)$, *i.e.*, we have the result that $\gamma_s^e(0)$ has a part proportional to $f_s^a(0)$. Thus they have common singularities as a function of temperature. However, if the imaginary part of $f_s^a(\delta, \omega^-)$ is retained, we see that this term contributes insignificantly to $\gamma_s^e(0)$ for $|f_s^a(0)^{-1}| \ll \pi/8$. Thus the degenerate singularity obtained by BGD and DL is spurious, being based on an incorrect approximation, *i.e.*, on the neglect of real electron hole and electron-electron excitation continua.

Comment should be made about recent theoretical papers which go beyond the simple parquet scheme of BGD (1966) by using a renormalization group method (Menyhard and Sólyom, 1973) or by solving the problem exactly in special cases (Luther and Peschel, 1974 *a*, 1974 *b*, Luther and Emery, 1974). We first discuss the former. These rely heavily on the logarithmic approximation, *i.e.*, the approximation that quantities like scattering amplitudes depend logarithmically on energy variables. This leads to the renormalization behaviour, *i.e.*, various quantities like G, Γ, etc. only change scale when energy momentum variables and bare coupling constants are scaled. After some general remarks a number of specific criticism of this approximation are made below.

Quite generally, as pointed out above, the neglect of imaginary parts and retention of only the logarithmic term does violence to analytic properties of the scattering amplitudes. As pointed out by Zawadowski (1974), there exists an analogy between the one-dimensional metal problem and the Kondo problem (*see, eg.*, Suhl, 1973). The various approaches used in the latter problem illuminate the differences between various approximations used in the former. The parquet approximation of Abrikosov (1965) leads in the Kondo problem, to an unphysical singularity in the conduction electron scattering amplitude. This is similar to the BGD result. This unphysical singularity was remedied by Suhl (1965 *a*, 1965 *b*), who used properly analytic functions (dispersion theory), confined himself to one particle intermediate states and found that the scattering amplitude approaches the unitarity limit as $T \to 0$. Our calculation above is similar to Suhl's in spirit, *i.e.*, we use analytically correct Γ's and restrict ourselves to one-particle one-hole intermediate states. Again in the Kondo problem, Fowler and Zawadowski (1971), and Abrikosov and Migdal (1970) went beyond the first order parquet scheme as did Menyhard and Sólyom (1973) in the one-dimensional metal case. The former showed that at low temperatures the invariant coupling is not small. The latter found singular behaviour for χ and Γ at $T = 0$. As noted in Zawadowski (1974), neither of these can, because of the neglect of imaginary parts, yield the expected unitarity limit for Γ at $T = 0$. Further, it is pointed out in that to get this limit, one has definitely to include nonlogarithmic terms. Quite crudely, one can omit the imaginary part for temperature such that $g\rho_{\epsilon_F} \ln(\beta\omega_c) \gg 1$, *i.e.*, at very low temperatures the logarithmic parts completely swamp the imaginary part. At such low temperatures, the approximation developed in this paper is not reliable, and the logarithmic approximation schemes are more useful.

There are two specific criticism of the renormalization group method, both pertaining again to the neglect of imaginary part. We note that whereas the

invariant couplings g'_i are indeed real (eqs 28 and 29 of Menyhard and Solyom (1973)), the $\tilde{\Gamma}_i$ are not, and in calculating $\Gamma_i(x)$ using the renormalization group procedure, the imaginary parts are omitted. If this is not done, $\Gamma_1(x)$ and $\Gamma_2(x)$ are seen not to have common poles, even with the bare interaction used by BGD. Thus inclusion of imaginary parts, even within the first order RG scheme, modifies greatly the first order parquet results. Secondly, an assumption regarding the scale invariance of the Dyson equation, *i.e.*, the equation $G = G^{(0)}\,\Gamma^{(0)}\,GGG\Gamma G$, is made. Now very generally, the quantities $G^{(0)}$, Γ, G have discontinuities across the real axis and thus the above equation involves different combinations of the analytic parts, say for $G(\omega^{\pm})$. Unless these combinations transform in the same way (which they will only if imaginary parts are omitted), the scaling relations will be different, and one will not obtain relations connecting various renormalization constants (eq. 15 of Menyhard and Solyom (1973)).

There is a well-known class of exactly soluble one-dimensional interacting fermion models due to Tomonaga (1950) and to Luttinger (1963). The model is exactly soluble because effectively V_{2k_F} is set to zero (Luther and Peschel 1974 *a*, 1974 *b*). When electron scattering from one end of the Fermi level $(+k_F)$ to the other $(-k_F)$ is allowed, the problem is no longer exactly soluble. Here, Luther and Emery (1974) claim that an exact solution can be obtained for a particular value of V_{2k_F}; and using scaling arguments something can be said about solutions in general. Lee (1975) has pointed out a mistake in this paper which invalidates some of their results. However, there is a more serious objection, namely, the use of the boson approximation for one fermion operators (Luther and Peschel 1974 *a*, 1974 *b*). This approximation is known to give the correct equation of motion in some cases but gives incorrect equal time commutation relations for fermion operators. The reduction of the Hamiltonian considered in Luther and Emery (1974) to an exactly soluble one results from an equal time operation using the above boson approximation for one fermion operators. It is therefore not reliable.

In the next section, we consider a number of effects omitted above, *e. g.*, the effects of impurities, of electron-phonon coupling, of interchain coupling and of thermal order parameter fluctuations.

5. Effects of impurities, of electron-phonon, interchain and thermal fluctuation coupling

5.1 *Impurities*

We briefly discuss below the effect of a small concentration of rigid random impurities so that the resulting electron lifetime $\tau \gg (4k_BT)^{-1}$. Qualitatively, the induced electron-electron attraction, discussed in § 4, arises from the exchange of virtual electron density fluctuations with excitation energy $\omega_c \sim \epsilon_F > \omega \gg k_BT$, and wave number $(q/k_F) \gg (k_BT/\omega_c)$. Rigid random impurities introduce disorder (modifying electronic properties considerably) on an energy scale $\omega \sim \tau^{-1}$ and on a wave number scale $q \sim \tau^{-1} k_F^{-1} \epsilon_F^{-1}$. Thus, if $\tau \gg (4\,k_BT)^{-1}$, we expect the effect of impurities on the induced interaction to be negligible. In general, the effect will be small provided $\tau\omega_c$ or $\tau\epsilon_F \gg 1$. These considerations are borne out by an explicit calculation described below.

We calculate the impurity averaged RPA function $f_s^d(\delta, z_m)$, the impurity effects being included in the manner conventional in superconductivity theory (Werthamer, 1969), for example. That is, the impurity centres are treated as completely random and as giving rise to s-wave scattering, the sattering rate for electrons near the Fermi surface being τ^{-1}. We find that

$$\langle f_s^d(\delta, z_m)\rangle_{\text{imp.}} = -\frac{I_s^{d\,2}\langle \chi_0^d(\delta, z_m)\rangle_{\text{imp.}}}{1 - I_s^d\langle \chi_0^d(\delta, z_m)\rangle_{\text{imp.}}}\rho\epsilon_F^{-1} \tag{5.1}$$

where

$$\langle \chi_0^d(\delta, z_m)\rangle_{\text{imp.}} = -\frac{\rho\epsilon_F}{2}\operatorname{Re}\langle \phi^+(\delta, z_m)\rangle_{\text{imp.}} \tag{5.2 a}$$

$$= -\frac{\rho\epsilon_F}{2}\operatorname{Re}\left[\sum_{l=0}^{l_c}\left(l + \frac{|m|+1}{2} + \frac{3\beta}{8\pi\tau} + \frac{|i\delta\beta}{4\pi}\right)^{-1}\right].$$

The temperature at which the CDW instability occurs is given by $\langle I_s^d\,\chi_0^d(0,0)\rangle_{\text{imp}} = 1$. We see that the addition of impurities lowers the transition temperature, $T_{\text{CDW}}^{\text{imp}}$ being given for $(\beta/4\pi\tau) \ll 1$ by

$$T_{\text{CDW}}^{\text{imp.}} = T_{\text{CDW}}^{\text{RPA}}\exp\left[-\psi'\left(\tfrac{1}{2}\right)\frac{3\beta_c}{8\pi\tau}\right]. \tag{5.3}$$

The quantity B (*e.g.*, eq. (4.4)) is obtained by using, in eq. (4.6), the impurity averaged $f_s^d(\delta, z_m)$ eqs (5.1) and (5.2) and the impurity averaged pair propagator $\langle GG\rangle_{\text{imp}}$. We thus neglect any impurity-induced coupling between f_s^d and GG. Since the impurity averaged Cooper pair propagator is the same as before (Werthamer, 1969), we obtain

$$B_{\text{imp.}} = I_s^e\rho\epsilon_F + \tfrac{1}{2}\int_0^{w_c} dv\,\frac{\tanh\left(\frac{\beta v}{2}\right)}{v}\operatorname{Re}\left\{\langle f_s^d(0)\rangle_{\text{imp}}^{-1} + \tfrac{1}{4}\left[\psi\left(-\frac{i\beta v}{2\pi} + \frac{3\beta}{8\pi\tau}\right) - \psi\left(\tfrac{1}{2} + \frac{3\beta}{8\pi\tau}\right)\right]\right\}^{-1} \tag{5.4}$$

Comparison of this with the corresponding expression for (4.11 *a*) for the pure case shows that for $(\beta/4\pi\tau) \ll 1$, the second or induced attraction term of B has the same maximum value. This value occurs, however, at a temperature between $f_s^d(0)^{-1} \to 0$ and $\langle f_s^d(0)\rangle_{\text{imp}}^{-1} \to 0$, *i.e.*, between the original T_{CDW} and the impurity lowered T_{CDW}. Since the induced attraction is a rather mild function of $f_s^d(0)^{-1}$ and of temperature, if T_{CDW} and $\langle T_{\text{CDW}}\rangle_{\text{imp.}}$ are close together, *i.e.*, if $(\beta/4\pi\tau) \ll 1$ the above-mentioned change is not significant.

5.2. *Electron-phonon interaction*

We have so far completely neglected electron-phonon interaction. Its inclusion leads to an additional phonon mediated interaction between electrons. In particular for electrons close to the Fermi level (*i.e.*, with energies ω away from the Fermi energy by $\omega \ll \Omega_{\text{ph.}} \simeq \omega_D$), I_s^d is replaced by

$$I_s^d \to I_s^d - \frac{2g^2{}_{2k_F}}{\Omega^0{}_{2k_F}}, \tag{5.5}$$

where g_{2k_F} is the electron-phonon matrix element coupling, a phonon of momentum $2k_F$ and (unperturbed) energy $\Omega^0{}_{2k_F}$ with initial and final electrons of momentum $\pm k_F$, $\mp k_F$. From eq. (5.5) we see that the RPA transition temperature T_{CDW}^{RPA} calculated in (3.15) increases because of electron-phonon coupling, the new temperature T^*_{CDW} being given by

$$T^*_{CDW} = (1.14\omega_c) \exp\left[\rho \epsilon_F \left(\tfrac{1}{2} I_s{}^d - \frac{g^2{}_{2k_F}}{\Omega^0{}_{2k_F}}\right)\right]. \tag{5.6}$$

Similarly, as is well-known (Abrikosov *et al* 1963; Werthamer, 1969), there is phonon mediated BCS attraction between electrons close to the Fermi level (*i.e.* total energy $\omega < \Omega_{ph.}$), so that to the electronic $I_s{}^e$ one should add the BCS term. As shown by Patton and Sham (1973) and by Rice and Strässler (1973), if the $a = 2k_F$ phonon frequency is very low, *i.e.*, if $\Omega_{2k_F} < 2k_BT$, these phonons contribute repulsively rather than attractively to the electron-electron interaction.

The above outlines the effect of electron-phonon interaction on $I_s{}^d$ and $I_s{}^e$, and thus on the instabilities in the RPA. We now discuss briefly interchannel coupling when electron-phonon interaction is included. For the case discussed in § 4, *i.e.*, the effect of $\gamma_s{}^d$ on $\gamma_s{}^e$, and vice versa, we need to calculate $\gamma_s{}^d$, for example, in an RPA-like approximation, including the electron-phonon interaction. It is easy to see that the sensitive denominator of $\gamma_s{}^d\ (q, z_m)$ is no longer $[1 - \tilde{I}_s{}^d\ \chi_0{}^d\ (q, z_m)]$ (eq. (3.12)) but is $[1 - (\tilde{I}_s{}^d + g_q{}^2\ D^0\ (q, z_m))\ \chi_0{}^d\ (q, z_m)]$, where $D^0\ (q, z_m)$ is the bare phonon propagator. The phonon propagator has the usual form $D^0\ (q, z_m) = 2\Omega_q{}^0\ (z_m{}^2 - \Omega_q{}^{02})^{-1}$.

It is clear from the above form for the denominator of $\gamma_s{}^d\ (q, z_m)$ that the calculation of B (eq (4.6)) using it, is not easy. One can say, in general, that for small cross channel energy transfer $z_m\ (\to \nu)$, *i.e.*, for $\nu \ll \Omega^0{}_{2k_F}$, one has the usual attractive contribution, but with $f_s{}^d\ (0)^{-1}$ (of eq. (4.1)) replaced by $f_s{}^{d*}\ (0)^{-1}$ (*i.e.*, $f_s{}^d\ (0)^{-1}$ calculated with $\tilde{I}_s{}^d - 2g^2{}_{2k_F}\ (\Omega^0{}_{2k_F})^{-1}$ replacing $\tilde{I}_s{}^d$). For energy transfer $\nu \gg \Omega^0_{2k_F}$, the phonon term drops out and one has the old $\gamma_s{}^d$ form (eq. (4.1)) and thus the contribution of this part to B is obtained merely by changing the lower cut-off in eq. (4.11) to $\Omega^0_{2k_F}$ from $\frac{k_BT}{\lambda}$. Since (see eq. (4.12)) the induced term in B depends very weakly on the lower cut-off ω_l, *i.e.*,

$$B_{ind.}\ (\omega_l) = \ln \left\{\frac{1 + [2\pi^{-1} \ln\ (\lambda\beta\omega_c) + 8\pi^{-1} f_s{}^d\ (0)^{-1}]^2}{1 + [2\pi^{-1} \ln\ (\lambda\beta\omega_c) + 8\pi^{-1} f_s{}^d\ (0)^{-1}]^2}\right\} \tag{5.7}$$

the induced attraction has very nearly the same value. In the most unfavourable case, *i.e.* $\Omega_{2k_F} \sim k_BT$, there is no BCS attraction resulting from the low frequency ($\nu < \Omega_{2k_F}$) part of $\gamma_s{}^d$, but perhaps only a repulsion (Patton and Sham 1973; Rice and Strässler 1973). It is difficult to estimate this contribution. The "high frequency" contribution is $B_{ind.}\ (\omega_l)$ eq. (5.7) with $\omega_l \sim k_BT$. This is just the old expression, *i.e*, the expression obtained when electron-phonon coupling is neglected. We note however that $B_{ind.}\ (\omega_l)$ is maximum at $f_s{}^d\ (0)^{-1} \to 0$ [*i.e.*

$-\frac{1}{2} I_s^d \rho \epsilon_F \ln(\lambda\beta\omega_c) = 1]$ while the CDW instability occurs in the RPA for $f_s^d(0)^{-1} \to 0$ *i.e.*, for

$$\left(-\tfrac{1}{2} I_s^d \rho \epsilon_F - \frac{g^2_{2k_F} \rho \epsilon_F}{\Omega^0_{2\epsilon_F}}\right) \ln(\lambda\beta\omega_c) = 1.$$

The latter is a higher temperature. Therefore, the CD fluctuation-induced attraction has less than its maximum value at the RPA-CDW transition temperature.

5.3. *Interchain coupling*

We have discussed above a purely 1-dimensional metallic system. The solids studied experimentally consist of parallel, nearly independent chains. The electron wave functions are confined closely to the chains, and so there is not much interchain wave function overlap. However, the small residual interchain coupling plays an important qualitative role, as we shall see below in § 5.4, § 6. Briefly a strictly 1-dimensional infinite sytem with short-range forces cannot exhibit long-range order because of divergent fluctuations. The residual interchain coupling renders the system qualitatively 3-dimensional, suppresses the fluctuations and makes long-range order possible. The electron hole fluctuations on different chains are coupled simply through the Coulomb interaction, since they are charge density fluctuations. Calculating this electrostatic coupling we find

$$H_{ii} = \frac{e^2}{\epsilon_\perp a} \sum_{l,l',q,} \rho_q(l)\, \rho_{-q}(l')\, K_0(q\,|\,l - l'\,|) \tag{5.8}$$

where $\epsilon_\perp$ is the dielectric constant perpendicular tc the chains, a is the number of electrons per unit length and $\rho_q(l)$ is the electron density fluctuation of wave number q on chain l. $K_0(x)$ is the modified Bessel function of order zero. In our case, q values of interest are $|\,q\,| \simeq 2k$ and so $q\,|\,l - l'\,| \simeq 2k_F\,|\,l - l'\,|$ is quite likely to be greater than unity. In that case $K_0(x) \sim \sqrt{\frac{\pi}{2x}}\, e^{-x}$, and so the interchain electrostatic coupling is of a short range ($\sim (2k_F)^{-1}$). We shall see in § 6 that its size can still be significant. The coupling between Cooper pair fluctuations on different chains is expected to be much weaker, since it depends on the overlap between electron wave functions on different chains, *i.e.*, on the electron interchain tunnelling probability. This is quite small, as is evident, for example, from the very high anisotropy of the electrical conductivity (*i.e.*, of electron flow in the solid). Thus the solid may be 1-dimensional as regards the behaviour of Cooper pair fluctuations, but may exhibit significant interchain coupling between electron hole fluctuations.

A simple approximate expression for H_{ic} is obtained as follows. Since the interchain coupling falls off exponentially with chain separation, one need consider only the coupling between nearest neighbours. In terms of the wave vector k of density fluctuations perpendicular to the chain, we find that

$$H_{ic} \simeq \sqrt{\frac{\pi}{4k_F b}}\, e^{-2k_F b}\, \frac{e^2}{\epsilon_\perp a} \sum_{q,\,k,\,i} \rho_{qk}\, \rho_{-q,\,-k} \cos(k.b_i) \tag{5.9}$$

where the constants have been evaluated for $q = 2k_F$, and a square lattice of lattice constant b has been assumed perpendicular to the chain direction (say z).

Therefore, $b_i = b\{0, 1\}$ or $b\{1, 0\}$. The interchain electrostatic coupling can be expected to be attractive when the charge density fluctuations on the nearest neighbours are exactly out of phase (Comés *et al* 1973). In terms of eq. (5.9), the dominant density fluctuation k_0 is such that $\boldsymbol{k}_0.\boldsymbol{b}_i = \pi$ so that the $\cos(\boldsymbol{k}_0.\boldsymbol{b}_i) = -1$. Expanding k around k_0 (*i.e.*, around the lines k_x or $k_y = \pm(\pi/b)$), we see for small deviations δk (labelled as η_i henceforth for brevity) that

$$H_{io} \simeq -\sqrt{\frac{\pi}{4k_F b}}\, e^{-2k_F b}\, \frac{e^2}{\epsilon_\perp a} \sum_{q,\,\eta_i} \rho_{q,\eta_i}\, \rho_{-q,-\eta_i}(1 - \tfrac{1}{2}\eta_i^2 b^2). \tag{5.10}$$

5.4. *Thermal fluctuations*

We now discuss the most serious qualitative omission in the discussion of § 3 and § 4. According to § 3, *i.e.*, in the RPA, the normal 1-dimensional metallic phase is unstable with respect to the formation of an ordered phase of the CDW, SDW or CP type, provided the bare interaction in the appropriate channel has the right sign. The instability temperature is determined by the interaction, *e.g.*, eq. (3.16). In § 4 we found that interchannel coupling leads to an effective interaction different from the bare interaction, *e.g.*, near a CDW instability, exchange of virtual CD fluctuations leads to an additional Cooper pair interaction $[I_s^e]_{\text{ind.}}$ given by eq. (4.12). However, there is still an instability, the condition for which [$B = 1$, see eq. (4.7) or $\tilde{I}_s^e \rho_{\epsilon_F} \ln(\lambda\beta\omega_c) = 1$] is different from the RPA condition $I_s^e \rho\epsilon_F \ln(\lambda\beta\omega_c) = 1$. However, it is well-known that due to interaction between thermal order parameter flufuations, an infinite strictly 1-dimensional system does not exhibit long-range order (Rice, 1965; Hohenberg 1967). In the RPA or mean field theory, this interaction is omitted, and hence, a phase transition occurs even in 1-dimension. In this sense, the inclusion of interchannel coupling (§ 4) still keeps us within the mean field theory; only the effect of superthermal ($\omega > k_B T$) fluctuations in one channel on the effective interaction in another channel is included. Thus, the mean field parameters are changed, but the crucial thermal fluctuation interaction $|\psi|^4$ term of the Ginzburg-Landau theory is not considered. To get a qualitatively correct result, therefore, one should include this interaction. This can be done following a functional integral formulation of the interacting electron gas problem due to Rice (1967). (See also the work of Hassing and Wilkins (1973), where this formulation is applied to discuss superconductivity). We briefly describe below the results obtained.

In the interacting electron gas under consideration, there is a significant coupling between electron pairs, as well as between electron hole pairs of momentum $\pm 2k_F$ We introduce the corresponding random fields x and y and expand the free energy functional as a power series in the random fields. On retaining only the static part of this coupling and expanding up to quartic terms, we find that the free energy functional $F\{(x_q), (y_{qk})\}$ is given by

$$\begin{aligned} F\{(x_q), (y_{qk})\} &= \sum_q |x_q|^2 (1 - I_s^o \rho\epsilon_F \ln(\lambda\beta\omega_c) + q^2\xi_e^2) \\ &+ \sum_{q,\,\eta_i} |y_{q,\,\eta_i}|^2 \left(1 + \frac{I_s'^d \rho\epsilon_F}{2} \ln(\lambda\beta\omega_c) + q^2\xi_d^2 + k^2\xi_k^2\right) \end{aligned}$$

$$+ g_e^{(4)} \sum_{\substack{q_i \\ i=1,3}} x^*_{q_1} x^*_{q_2} x_{q_3} x_{q_1+q_2-q_3}$$

$$+ g_d^{(4)} \sum_{\substack{q_i,k_i \\ i=1,3}} y^*_{q_1k_1} y^*_{q_1k_2} y_{q_3k_3} y_{q_1+q_2-q_3,\ k_1+k_2-k_3}$$

$$+ g_{ed}^{(4)} \sum_{\substack{q_i,k \\ i=1,3}} x^*_{q_1} x_{q_2} y^*_{q_3,\ k} y_{q_1-q_2+q_3,\ k} \tag{5.11}$$

The free energy is obtanied by averaging $F\{(x_q), (y_{qk})\}$ overall possible values of the complex random variables x_q and y_{qk}. In eq. (5.11), the first term is the free energy functional for Cooper pair fluctuations in the RPA. The interchannel coupling effect discussed in § 4 is not included above, but can be included on replacing I_s^e by $\tilde{I}_s^e$. The quantity ξ_e s the electron pair coherence length and, for a pure system, has a value

$$\xi_e^{\,2} = -\frac{\psi''(\frac{1}{2})}{128\pi^2(k_B T \rho\epsilon_F)^2} \frac{I_s^e \rho \epsilon_F}{k_F^{\,2}} . \tag{5.12}$$

The second term represents the free energy functional for *eh* fluctuations in the RPA. I'^d_s is the bare interaction to which the interchain electrostatic coupling energy has been added, *i.e.*,

$$I'^d_s = I^d_s - \sqrt{\frac{\pi}{4k_F b}}\, e^{-2k_F b} \frac{e^2}{\epsilon_\perp a} . \tag{5.13}$$

The antiphase interchain coupling energy is attractive, as discussed in § 5.3, and thus somewhat increases the RPA T_{CDW}. The interchannel effect of Cooper pair fluctuations exchange can be included by changing I^d_s to $\tilde{I}^d_s$. The density fluctuation coherence length along the chain is ξ_d, and perpendicular to the chain is ξ_k. For a pure system these are given by

$$\xi_d^{\,2} = (I^d_s \rho\epsilon_F)\, \psi''(\tfrac{1}{2})\, [256\pi^2 (k_F k_B T \rho_{\epsilon_F})^2]^{-1} \tag{5.14}$$

$$\xi_k^{\,2} = \frac{1}{8}\sqrt{\frac{\pi}{k_F b}}\, e^{-2k_F b} \ln(\lambda\beta\omega_c) \left(\frac{e^2 \rho_{\epsilon_F}}{a}\right) b^2 \tag{5.15}$$

The quartic coupling terms $g_e^{(4)}$, $g_d^{(4)}$ and $g_{ed}^{(4)}$ are given by

$$g_e^{(4)} = -(I^e_s \rho_{\epsilon_F})^2\, \psi''(\tfrac{1}{2})\, (16\pi^2)^{-1} \tag{5.16}$$

$$g_d^{(4)} = -(I^d_s \rho_{\epsilon_F})^2\, \psi''(\tfrac{1}{2})\, (16\pi^2)^{-1} \tag{5.17}$$

and

$$g_{ed}^{(4)} = (I^d_s\, I^e_s \rho^2 \epsilon_F)\, \psi''(\tfrac{1}{2})\, (32\pi^2)^{-1}. \tag{5.18}$$

These results are all for a pure system, and are obtained by the method followed in Rice (1967) or in Hassing and Wilkins (1973). We notice that the thermal CP-CDW fluctuaton coupling ($g_{ed}^{(4)}$) is repulsive.

As mentioned above, the considerations of § 4 imply that I^e_s and I^d_s in eq. (5.11) [see also eq. (5.13)] should be replaced by I^e_s and I^d_s to take into account coupling to super-thermal ($\omega > k_B T$) fluctuations in the other channel. We

make this modification in eq. (5.11). This interchannel coupling is exclusive of the repulsive CP-CDW fluctuation coupling g_{ed} appearing in (5.11), since an analysis similar to that carried out by Hassing and Wilkins (1973) shows that $g_{ed}^{(4)}$ for non-zero frequency CP and CDW fluctuations decreases rapidly with fluctuation frequency.

The thermodynamic properties of the above system, *i.e.*, a system comprised of a 1-dimensional superconductive fluctuation field x_q and a (weakly) 3-dimensional charge density fluctuation field y_{qk} with a free energy functional $F\{(x_q), (y_{qk})\}$ cannot be obtained exactly. A simple, qualitatively correct approximation is the Hartree or self-consistent field approximation for the fluctuation field (Tucker and Halperin 1971). This is quantitatively not bad if the mean fluctuation amplitude is small compared with unity. We shall use it now to obtain some estimates. First, there is no Cooper pair instability or superconductive long-range order, since the system is 1-dimensional for CP or superconductive fluctuations. Further if there is a CDW instability in the RPA or the coupled channel RPA, the instability is still present, but occurs at a lower temperature given by the condition

$$1 = -\frac{I_s^d \rho\epsilon_F}{2} \ln(\lambda\beta\omega_c) + \frac{e^2 \rho\epsilon_F}{2\epsilon_\perp a} \sqrt{\frac{\pi}{2k_F b}}\, e^{-2k_F b} - g_d^{(4)} \frac{ab^2 k_c}{\xi_d \xi_k} \tag{5.19}$$

where k_c is a cut-off wave vector for density fluctuations with wave vector η pr-e pendicular to the chain (see eq. (5.10)). In the absence of thermal fluctuation coupling, the last two terms on the right-hand side of eq. (5.19) are not presents. In the next section, we discuss the application to TTF-TCNQ of the result, obtained so far.

6. Application to TTF-TCNQ

As mentioned in the introduction, TTF-TCNQ, consisting of weakly coupled parallel metallic chains, undergoes a metal insulator transition at about 60° K. The room temperature electrical conductivity is reasonably high, and has been measured by various workers (Ferraris *et al* 1973; Coleman 1973; Chaikin and Heeger 1973) to be in the range 400–2000 (ohm cm)$^{-1}$. On cooling, the conductivity increases up to the metal insulator transition temperature, the ratio $(\sigma(T_{MI})/\sigma(T_R))$ ranging from 6–30 except in a few specimens where giant increases of order 10^3 are observed (Coleman *et al* 1973). The conductivity drops sharply below T_{MI}, and has an activation temperature dependence $\sigma(T) = \exp(-\beta E)$ for $T \ll T_{MI}$. The special interest in TTF-TCNQ stems from the large conductivity increase generally reported, the sharp phase transition at 60° K and most particularly from the giant conductivity anomalies which have been interpreted as arising from superconductive fluctuations (Coleman *et al* 1973; Anderson *et al* 1973). These three features are all absent in NMP-TCNQ, expected to be broadly similar to it. NMP-TCNQ (Epstein *et al* 1972) shows a relatively moderate conductivity rise as the temperature is lowered; the rise does not, for pure specimens, vary very much from sample to sample. The metal insulator transition sets in gradually over a temperature range 50° K; and there are no cases of a giant conductivity anomaly.

Theoretical explanations proposed (Bardeen 1973; Anderson *et al* 1973) for TTF-TCNQ behaviour have been based mainly on the electron-phonon model. Patton and Sham (1973) showed that in the exactly half-filled band case there is a decrease in the conductivity due to the fluctuation effects associated with the incipient formation of a semiconducting phase. Bardeen (1973) revived the suggestion of Fröhlich that a superconductive strongly coupled electron-lattice density wave state can occur in a 1-dimensional system. In more conventional language, this corresponds to calculating the conductivity of such a coupled 1-dimensional electron-phonon system, including phonon drag and seeing whether it can be infinite. Such calculations have been done above the Peierls metal insulator transition temperature by Patton and Sham (1973), by Allender *et al* (1973) and by Strässler and Toombs (1973). The latter two groups of authors find, for the not half-filled band case and a pure system, a rather moderate conductivity increase $\sigma(T) \sim \sigma_0 (T - T_P/T_P)^{-\frac{1}{2}}$. Lee *et al* (1974) have shown that at $T = 0$, *i.e.*, in the Peierls CDW ground state, $\sigma(0)$ is infinite for the not half-filled band (or $(2k_F)^{-1}$ incommensurate with the lattice constant) case. Commensurability and impurities make the $T = 0$ conductivity finite. The above considerations are within the mean field approximation for the $|q| \sim 2k_F$ ion density fluctuations and neglect electron-electron interaction and interchain coupling. They are, moreover, quite at variance with the experimental facts.

We propose in this section an alternative explanation based on the view that electron-electron interaction plays a dominant role in TTF-TCNQ. As mentioned earlier (§ 1) the TCNQ based compounds have a narrow 1-electron band (bandwidth $\triangle \sim 0{\cdot}05$ to $0{\cdot}4$ eV), and the electron-electron repulsion typified by the same site repulsion U_0 and nearest neighbour repulsion U_1 has values of order 3 and 2 eV. By introducing polarizable side chains, U_0 is reduced in comparison to U_1 so that the Hubbard correlation energy $U = U_0 - U_1$ is greatly reduced. It is possible that if the side chain ion is sufficiently polarizable, U_0 may become smaller than U_1. Then the interelectron potential, instead of being relatively flat but monotonic, has a dip for small distances (figure 3). The former corresponds to the general dependence of V on x in NMP-TCNQ, and the latter, we suggest, to $V(x)$ for TTF-TCNQ. In consequence, V_{2k_F} is negative in TTF-TCNQ, $I_s^d < I_t^d$ (see eq. (3.16)), and, in the RPA, the CDW instability is favoured over the SDW.

The CDW transition may occur at a temperature very different from T_{CDW}^{RPA} if there is a substantial contribution to the electron hole coupling from virtual Cooper pair excitations (§ 4, eq. (4.14)) and may not occur at all if the system is strictly 1-dimensional. We argue later that a consistent view is to regard the mean field Cooper pair instability temperature as being very different from T_{CDW}^{RPA} so that for $T \simeq T_{CDW}^{RPA}$, the scattering amplitude $\gamma_s^e(q, z_m)$ is not near a singularity and thus very large, nor is it sharply peaked. Thus the interchannel term eq. (4.14) is small and can be neglected. The presence of interchain coupling suppresses fluctuations which make ordering impossible in a strictly 1-dimensional system. We perform a simple calculation of its effect using the Hartree approximation result eq. (5.19). As we shall see, interchain coupling is strong enough so that $T_{CDW}^{bulk} \simeq T_{CDW}^{RPA}$. Therefore, in estimating $g_d^{(4)}$, we use this approximation equality. The experimentally knowphysical paramn eters are $a = 3{\cdot}8$ Å, $b = 7{\cdot}6$ Å,

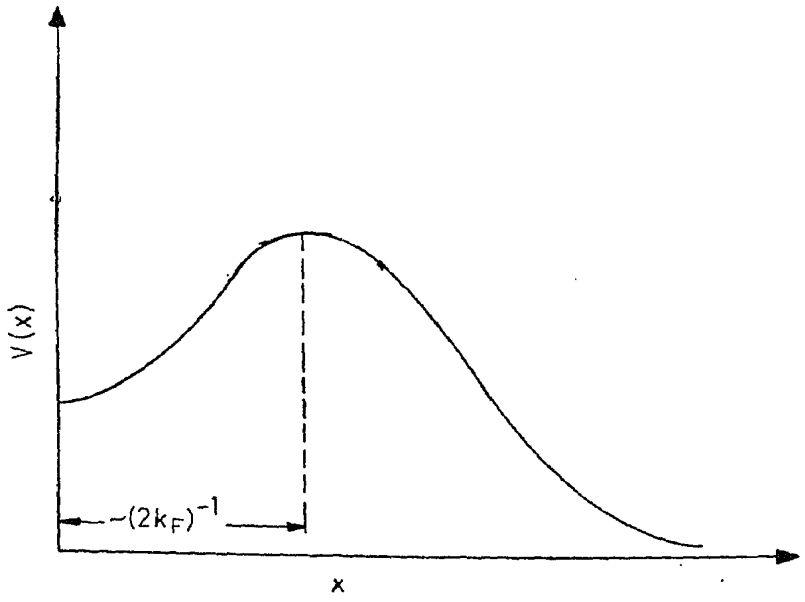

Figure 3. A schematic sketch of the bare electron-electron interaction $V(x)$ as a function of the inter-electron separation x. A CDW instability is favoured over an SDW instability if $V(x)$ has the dip shown for $x \lesssim (2k_F)^{-1}$.

$T_{CDW} \simeq 60°K$, $\epsilon_\perp = 3$, $\rho_{\epsilon_F} \simeq 0{\cdot}27$ eV. We assume $\omega_c = \epsilon_F = 0{\cdot}25$ eV. From these we calculate $k_F = 4 \times 10^7$ cm^{-1} (half-filled band), ρ_{ϵ_F} 0·92/eV/spin, and $I_s^d \rho_{\epsilon_F} \simeq -0{\cdot}5$ the last using $1 \simeq -(I_s^d \rho_{\epsilon_F}/2)\ln(1{\cdot}14\beta\omega_c)$. On using these numbers to estimate the last term on the right-hand side of eq. (5.19), *i.e.*, the interchain coupling limited fluctuation term, we find that it has the value 0·03. The mean fluctuation amplitude is indeed small, thus justifying *a posteriori* the use of the Hartree approximation. The downward shift in T_{CDW} is given through the equation

$$T_{CDW}^{bulk} = 1{\cdot}14\,\omega_c \exp\left[-(1{\cdot}03)\left(\tfrac{1}{2} I_s^d \rho_{\epsilon_F}\right)^{-1}\right]$$

$$= T_{CDW}^{RAP} \exp(-0{\cdot}12)$$

which is directly obtainable from eq. (5·19). We thus see that fluctuation effects lead to $\sim 10\%$ lowering in T_{CDW}^{RPA}, a rather moderate effect. This result implies that there should be a rather sharp transition to the CDW phase, with a relatively narrow transition regime. This is indeed observed in TTF-TCNQ. In contrast KCP exhibits a very broad CDW transition region. This is perhaps due to the much smaller interchain coupling in KCP, the interchain separation there being ~ 10 Å rather than 7·6 Å as in TTF-TCNQ. The coupling energy H_{ic} depends exponentially on the separation. Further, the interchain energies (*e.g.*, Fermi energy) are higher in KCP. Thus we picture TTF-TCNQ as undergoing a CDW metal insulator phase transition due to attractive electron hole coupling, at a temperature close to the RPA value. The inclusion of electron-phonon coupling will increase this transition temperature, according to eq. (5.6).

We now consider the effect of this incipient CDW instability on electron-electron or Cooper pairing interaction. This has been done in § 4, where we obtained the induced Cooper pair attraction, eq. (4.12). This has its maximum value for $f_s^d(0)^{-1} \to 0$, *i.e.*, at $T = T_{\mathrm{CDW}}^{\mathrm{MF}} \simeq T_{\mathrm{CDW}}^{\mathrm{bulk}}$. The value here is $I_{\mathrm{ind.}\ s}^{\ d}\ \rho\epsilon_F = 0.50$. This is clearly a large attractive interaction. Assuming that the direct interaction $I_s^e\,\rho\epsilon_F$ is small so that all the *ee* attraction is induced, we find that this $I_s^e\,\rho\epsilon_F$ corresponds a mean field transition temperature $T_{\mathrm{CP}}^{\mathrm{MF}} \sim 450°$ K. The induced attraction decreases as T increases, since $f_s^d(0)^{-1}$ increases from zero. At $T = 2T_{\mathrm{CDW}}^{\mathrm{bulk}} = 120°$ K, $I_{\mathrm{ind}}^{\ e}{}_s\ \rho\epsilon_F = 0{\cdot}35$, corresponding to a $T_{\mathrm{CP}}^{\mathrm{MF}}$ of $\sim 290°$ K. Thus the induced Cooper pair attraction is quite large and can lead to mean field transition temperatures of several times T_{CDW} over a wide temperature range. One does not, however, expect superconductive long-range order since the system is 1-dimensional as far as pair fluctuations are concerned eq. (5.11).

In order to calculate the conductivity of this system, one needs to determine the current transported by the thermal CP fluctuations by solving the Ginzburg-Landau equation with the modified $|x_q|^2$ coefficient

$$[1 - \tilde{I}_s^e(T)\,\rho\tilde{\epsilon}_F \ln(\lambda\beta\omega_c) + \xi_s^2 q^2]$$

(see eq. (5.11)) and determining the equilibrium phase slippage rate (Langer and Ambegaokar 1967). For a simple model, this was done by Anderson, Lee and Saitoh (1973) who found a paraconductivity $\sigma(T) \sim \sigma_0 \exp \alpha\,(T_{\mathrm{CP}}^{\mathrm{MF}}/T)$, where α is a constant of order unity. They found that the giant conductivity data of Coleman *et al* (1973) could be explained if $T_{\mathrm{CP}}^{\mathrm{MF}} \sim 550°$ K. The work in this paper provides a microscopic theory for such large mean field transition temperatures. The paraconductivity is quite sensitive to impurities (Tucker and Halperin 1967; Langer and Ambegaokar 1967) since the coherence length ξ_s, which determines the effect of fluctuation interaction, decreases considerably as the system become impure. The paraconductivity can therefore be expected to decrease with the presence of impurities. It is generally believed that there are many strand interruptions in such systems (Zeller 1973). The effect of these on the current transported by Cooper fluctuations has not been calculated, but a considerable reduction is likely. Therefore, it is plausible that depending on the presence of impurities, strand interruptions and other kinds of disorder, the paraconductivity will vary a great deal, and only ideally will exhibit the giant values sometimes observed.

We have not discussed so far what happens below the CDW instability temperature. Clearly, one has a new phase, an insulator with a gap which increases as the temperature decreases below $T_{\mathrm{CDW}}^{\mathrm{bulk}}$. We are mainly interested in the behaviour of pair fluctuations in this CDW phase, and the effect of this behaviour on the (para) conductivity. Consider for concreteness the free energy functional for superconductive fluctuations, *i.e.*, first and third terms of eq. (5.12). The first term has the RPA part $I_s^e(\sum_p G_p\, G_{-p+Q})$ in it. This must now be evaluated with bare 1-electron propagators in the CDW phase. The CDW energy gap

will clearly reduce the pair propagator, and so the RPA term will decrease. Similarly, the induced attraction is to be calculated with f_s^a and G_p evaluated in the CDW phase. Again, we expect f_s^a to be non-singular and smaller because of the gap in the spectrum of electronic excitations. Therefore, the coefficient of the $|x_q|^2$ term, which was negative (and fairly large in size) above T_{CDW}^{bulk}, will decrease in magnitude, and may even change sign to become positive. This will tend to reduce the amplitude of pair fluctuations. Further, the contribution of pair fluctuations to conductivity will decrease as the temperature decreases, because of the gap. For example, consider the usual Aslamazov-Larkin diagram (Aslamazov and Larkin 1968) for paraconductivity. In this, the electron hole pair which normally carries the current is coupled to the CP propagators which transport the electric current. Below T_{CDW}^{bulk}, since there is a gap in the electron hole excitation spectrum, this paraconductivity term will decrease as $\exp\{-\Delta(T)/T\}$ where $\Delta(T)$ is the CDW gap. Thus we expect that because of the reasons mentioned above, the paraconductivity due to pair fluctuations will decrease rapidly (exponentially) with temperature below T_{CDW}^{bulk}. This is observed.

We conclude with some remarks regarding the prospects for (high temperature) superconductivity in 1-dimensional systems. Proposals (Little 1964; Ginzburg and Kirzhnits 1972) for this have concentrated on attempting to reduce the small separation electron repulsion by introducing polarizable side chains and even making the interchain attractive. We have seen above that the more likely result of this is a CDW metal insulator instability, especially since there appears to be considerable interchain electrostatic coupling. In the RPA, it is possible, by making the short-range part of $V(x)$ sufficiently attractive or more precisely by making $V_0 < 0$, to make $T_{CP}^{RPA} > T_{CDW}^{RPA}$. However, this will not lead to a superconductive state unless there is sufficient coupling between pair fluctuation on different chains. The induced Cooper pair attraction term (§ 4) seems to help in achieving temperature superconductivity as discussed above, where T_{CP}^{MF} of several hundred degrees has been estimated. Again, one cannot expect a superconductive phase in the absence of interchain coupling. Further, if superconductive ordering does occur, the electron momentum distribution will be smoothened, f_s^a will become smaller and the CD fluctuation induced attraction will decrease. The decrease will be greater as T decreases and the superconductive gap increases. Thus, in a sense, the induced attraction is self-destructive, and the metal may become normal as temperature is decreased. The main qualitative conclusion is that attempts to reduce and change the sign of the small separation electron repulsion will, if successful, lead most likely to a CDW insulating ground state. The CD fluctuation induced Cooper pair attraction discussed in § 4 can lead to the paraconductivity behaviour above $T_{CDW}^{bulk} \simeq T_{CDW}^{RPA}$, as observed for example in TTF-TCNQ. It can lead to high temperature superconductivity in perhaps a restricted temperature range above T_{CDW}^{RPA} if there is sufficient coupling between pair fluctuations on different chains.

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