Abstract

The two-chain, inverted band model for TTF-TCNQ is solved by the exact methods developed by Luther and Emery and by Chui and Lee. On each chain, there are intrachain interactions $g_1$ and $g_2$, and there are interchain interactions $w_1$ and $w_2$. We investigate all of the possible two-particle correlation functions, of which the new divergent ones not present in the single chain problem are of the excitonic insulator type. In addition, we investigate essentially all of the many possible four-particle correlation functions. For the single chain, there are two divergent ones: the $4k_F$ response found by Emery, and a four-particle condensation of two Cooper pairs. For the two-chain problem, there are many others, the most unusual of which are of the excitonic molecule type. In addition, the $4k_F$ response is enhanced by the interchain coupling, and is divergent for weak intrachain coupling as well as for strong coupling. Using renormalization group techniques, we find that the essential features of the temperature dependence of the relative size of the $4k_F$ and $2k_F$ excitations recently observed can be explained in terms of a crossover from a region in which the $4k_F$ excitation is dominant to one in which the $2k_F$ charge density wave response is dominant.
I. Introduction

Recent observation of the $4k_F$ as well as the $2k_F$ scattering in TTF-TCNQ has generated a great deal of excitement. As regards the theorist, this is particularly important, as it enables him at last to be able to say something about the size and sign of the effective electron-electron interaction strengths, which until now had only been the subject of conjecture. In order to help clarify this situation, and to investigate the possibility of new additional types of excitations, we have studied a two-chain model for TTF-TCNQ in which the electrons on the TTF chains have a band inverted relative to the normal TCNQ band.

II. The Model

We consider the free Hamiltonian to be of the form

$$\mathcal{H}_{oa} = \sum_{k,s} v_F k (a_1^\dagger, ks a_1, ks - a_2^\dagger, ks a_2, ks)$$  \hspace{1cm} (1)

$$\mathcal{H}_{ob} = \sum_{k,s} (v_F k)(b_1^\dagger, ks b_1, ks - b_2^\dagger, ks b_2, ks)$$  \hspace{1cm} (2)

where $a_i, ks (b_i, ks)$ annihilates an electron of the a, or TCNQ, (b, or TTF) chain with spin $s = \pm 1$, and momentum $k$ relative to the Fermi momentum $k_F$ on the $i = 1, 2$ branch. For simplicity, we assume the Fermi velocities to be the same in magnitude, although opposite in sign. Although this is not exactly the case in TTF-TCNQ, we expect that this model will contain most of the essential features of that and similar charge-transfer systems. Using the transformation $b_1, ks \rightarrow c_2^\dagger, -ks$, etc., Eq. (2) may be written as

$$\mathcal{H}_{ob} = \sum_{k,s} v_F k (c_1^\dagger, ks c_1, ks - c_2^\dagger, ks c_2, ks)$$  \hspace{1cm} (3)

Thus, an electron on the inverted band TTF chain corresponds to a hole with a normal band structure, and vice-versa. The interactions are shown in Fig. (1). The intrachain interactions $g_1$ and $g_2$ are backward and forward scattering interactions, as in the single chain problem, and are assumed to be the same on both chains. The interchain interactions are $w_1$ and $w_2$. These interactions are between electrons, and we remark that the transformation to the $c$-notation changes the sign of $w_1$ and $w_2$ (although the sign of $w_1$ is unimportant).