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$2k_F$ Peierls Transition for a Half-Filled Band from a Hubbard Hamiltonian Extended with Intersite-Dependent Transfer

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We report a model calculation with the Hubbard Hamiltonian, extended with an exponentially dependent intersite transfer, on a half-filled band system. The calculation shows a phase transition which changes from an electronic (at low U/t) to a spin Peierls at high U/t.

In the presence of an external magnetic field a new phase ($2k_F + k_F$) was found. The specific heat, spin susceptibility, and intensity of the charge transfer absorption was calculated; the results compare reasonably well with experiment. In addition the pressure dependence of the phase transition temperature could be estimated.

INTRODUCTION

The properties of one-dimensional band systems have become a subject of considerable interest.[1] It has been found to be extremely difficult to solve the band structure of these relatively simple systems analytically in the presence of electron-electron correlation, such as the on-site interaction U. Therefore, recently we performed a numerical calculation on the quarter-filled band to obtain the $4k_F$ and $2k_F$ phase transitions, which occur in these systems.[2]

Half-filled bands show $2k_F$ phase transitions, and it therefore seemed useful to perform a model calculation for these systems as well. For undistorted half-filled bands numerical calculations were performed earlier by Bonner and Fisher[3] in the limit of large U, by Shiba and Pincus[4] for a set of values of t/U, where t is the transfer integral, and by Bray *et al.*[5] None

of these, however, included the effect of lattice distortions, leading to the $2k_F$ transition.

In addition to the phase transition, other properties, such as the spin susceptibility, the magnetic field and pressure dependence of the phase transition temperature, and the charge transfer band intensity could be calculated as well. It also turned out, that some properties could profitably be compared with experiment, and the rather surprisingly good agreement has lent considerable credence to the validity of the model.

THEORETICAL CONSIDERATIONS

A group theoretical justification of our model was given elsewhere.[2] The normal modes giving the $2k_F$ and k_F distortions are Q_3 and Q_5,Q_6 respectively (Q_5 and Q_6 are degenerate); they are displayed in Figure 1a. The Landau series expansion[6] up to fourth order of the free energy (F) in terms of these modes then is:

$$F(Q_3,Q_5,Q_6) = AQ_3^2 + B(Q_5^2 + Q_6^2) + CQ_3(Q_5^2 - Q_6^2) + DQ_3^4 + E(Q_5^4 + Q_6^4) + FQ_5^2Q_6^2 + GQ_3^2(Q_5^2 + Q_6^2)$$

By sampling the minima of $F(Q_3,Q_5,Q_6)$ we find for the half-filled band system the following relevant phases of the linear chain:

I: $Q_3 = Q_5 = Q_6 = 0$, the regular chain ($4k_F$)

II: $Q_3 \neq 0$ and $Q_5 = Q_6 = 0$, a $2k_F$ distorted chain (dimers)

III: $Q_3 \neq 0$ and $Q_5 = 0$ or $Q_6 = 0$, a mixed $2k_F + k_F$ distorted chain (dimerized dimers)

Other solutions can be found as described for the quarter-filled band.[2]

The regular $4k_F$ phase has a first or a second order transition to the $2k_F$ phase because there is no third order term in Q_3. The $2k_F$ and the $4k_F$ phase both have first or second order transitions to the $2k_F + k_F$ phase because there is no third order term in the order parameter Q_5.

The stability of a phase depends on the coefficients of the Landau expression, which in turn are determined by the electronic and lattice properties of the chain. To get a more quantitative insight we performed a calculation including electronic correlation as given by the on-site electron-electron interaction U. The inter-site electron-phonon interaction is obtained by making the transfer integral t exponentially dependent on the inter-site separation.

The electronic system is described by the Hubbard Hamiltonian:

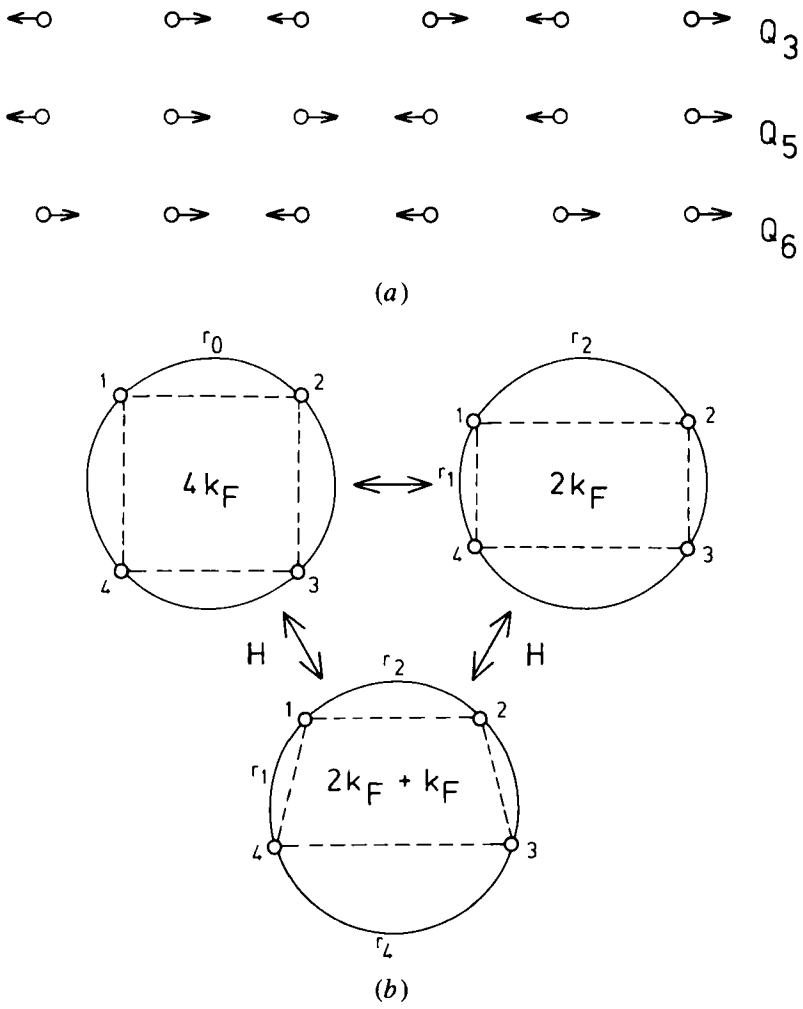

FIGURE 1a, b The $2k_F$ and k_F distortions for a half-filled one-dimensional chain (a). Q_3 denotes the $2k_F$ distortion, Q_5 and Q_6 the degenerate k_F distortions. Conformations of the four sites (b). The square ($4k_F$) has no distortion, the rectangle ($2k_F$) has distortion Q_3, and the trapezoid ($2k_F + k_F$) has Q_3 and Q_5 or Q_6. The possible phase transitions are indicated by arrows. H indicates that the transition can only be realized in the presence of an external magnetic field.

$$H = -\sum_{l \neq m} t_{lm} c^{+}_{l,\sigma} c_{m,\sigma} + U \sum_{l} n_{l,\sigma} n_{l,-\sigma}$$

where l and m label the sites, $c^{+}_{l,\sigma}$ and $c_{l,\sigma}$ are the creation and annihilation operators for an electron with spin σ at site l and $n_{l,\sigma}$ is the number operator

$c^+_{l,\sigma}c_{l,\sigma}$. As basis set we take the $m_s = 0$ four electron states:

$$A[c^+_{l,\sigma}c^+_{m,\sigma}c^+_{n,\sigma}c^+_{p,\sigma} \mid 0>],$$

where A is the antisymmetrization operator, which is permitted in the absence of a magnetic field and spin-orbit coupling. The basis set is transformed to form bases for the irreducible representation of the full rotation group R_3, yielding eigenfunctions of S^2. We obtain a set of twenty singlet functions, fifteen triplet functions, and one quintet function.

The numbering of the sites is depicted in Figure 1b. The electronic inter-site interaction is described by the transfer integral:[2]

$$t_i(R_i)\,(:)R_i^3 \exp - CR_i$$

with $C = Z'/2a_0$, where R_i is the intersite distance, Z' is the effective nuclear charge and a_0 the Bohr radius. This expression derives from the fact that in organic materials, showing $2k_F$ transitions, the transfer is between π-orbitals, which can be considered as LCAO's of $2p\sigma$-atomic orbitals. For the electron-nuclear attraction interaction operator $(1/r)$ between such orbitals situated on two fairly distant sites (i.e., in the order 3.5 Å) one finds analytically:

$$t_i(R_i) = \frac{Z'}{a_0}\left[\frac{(CR_i)^3}{12} - \frac{CR_i}{4} - \frac{1}{4}\right] \exp - CR_i$$

For the large separations considered we neglected the last two terms in the pre-exponential factor. This neglect, or even neglecting the R_i^3 term makes no qualitative differences in the calculation. The exponential term, however, is crucial. To simplify the description of the distortions we introduce the parameter ξ and η.[2] We find for the intersite distances:

$$R_{1,3} = [1 - \xi]R_0$$

$$R_{2,4} = [1 + \xi][1 \mp \eta]R_0$$

where R_0 is the intersite distance at zero distortion. By keeping R_0 constant we impose the condition that no expansion or contraction of the lattice occurs. (Pressure effects can be included by decreasing R_0.) For the transfer integrals we obtain

$$t_{1,3} = t_0[1 - \xi]^3 \exp \xi CR_0$$

$$t_{2,4} = t_0[1 + \xi]^3[1 \mp \eta]^3 \exp -[\mp\eta(1 + \xi) + \xi]CR_0$$

$$t_0\,(:)\,R_0^3 \exp - CR_0$$

CR_0 is treated as a parameter of the system, t_0 is used as the unit of energy in our calculations. The lattice is included by using the Born expression for

the lattice free energy, but the lattice dynamics and by consequence the lattice entropy is neglected. We then find for the lattice free energy:

$$F_{\text{lat}} = B \sum_i R_i^{-n}$$

where B is a constant and n is the repulsive exponent. In terms of ξ, η_1, and η_2 we find

$$F_{\text{lat}} = BR_0^{-n}[2(1 - \xi)^{-n} + (1 + \xi)^{-n}\{(1 - n)^{-n} + (1 + \eta)^{-n}\} + (1 + \xi)^{-n}\{(1 - \eta_2)^{-n} + (1 + \eta_2)^{-n}\}]$$

We introduce a parameter:

$$\alpha/4n(n + 1) = BR_0^{-n}$$

which can be related to the linear lattice compressibility.[2] For the parameters we use the values evaluated for the quarter-filled band systems of TCNQ salts.[2] The numbers are: $CR_0 = 10$, $n = 12$, and $\alpha = 160t_0$. [This corresponds to a linear lattice compressibility of 4.10^{-11} cm^2/dyne (graphite) and for the one-electron transfer integral $t_0 \approx 0.1$ eV.] A computer program was written for a Control Data 170/760 computer to perform the calculations. By computing eigenvalues and eigenvectors and by introducing a temperature the free energy is obtained for a large set of ξ and η values at different values of U. The free energies were evaluated from:

$$F = -kT \ln Z_{\text{el}} + F_{\text{lat}}$$

in which:

$$Z_{\text{el}} = \sum_i g_i \exp -(\varepsilon_i - \varepsilon_0)/kT$$

where the ε_i are the electronic energies of the ensemble of our model system and ε_0 is the energy of the lowest electronic state. By requiring all systems to show the same distortion at the same time, we build in the cooperativeness required to obtain a phase transition. A magnetic field was introduced by including the appropriate Zeeman energies of the triplet and quintet states in the free energy. The molar spin susceptibility was obtained by evaluating:

$$\chi_{\text{reduced}} = \chi \frac{6t_0}{Ng^2\beta^2} = \sum_i S_i(S_i + 1) \frac{g_i \exp -(\varepsilon_i - \varepsilon_0)/kT}{N.Z_{\text{el}}.T}$$

the summation runs over all quintet (Q) and triplet (T) states. The energies of the optical transitions are evaluated by taking the differences of the eigenvalues obtained by diagonalization of the Hubbard Hamiltonian inter-

action matrix. Because of the absence of spin-orbit coupling only singlet-singlet and triplet-triplet excitations are considered. For the calculation of the oscillator strengths of the transitions we assume a Boltzmann distribution over the available electronic states. For the oscillator strength of the transition $i \rightarrow j$ we then find:

$$f_{i\rightarrow j} = (\varepsilon_i - \varepsilon_j)g_i \frac{\exp -(\varepsilon_i - \varepsilon_0)/kT - \exp -(\varepsilon_j - \varepsilon_0)/kT}{Z} M^2_{i\rightarrow j}$$

where g is the degeneracy of the states i and j, $\varepsilon_i, \varepsilon_j$ their eigenvalues, ε_0 the value of the lowest eigenvalue and $M_{i\rightarrow j}$ the transition moment:

$$\mathbf{M}_{i\rightarrow j} = \sum_k c_{ik} c_{jk} \mathbf{R}_k$$

where $\mathbf{R}_k$ is the position vector of site k and c_{ik}, c_{jk} the coefficients of the eigenfunctions i, j on site k. Because our transfer integrals vary with the distortion and their sum is not constant, one does not expect the sum rule for oscillator strengths to hold, except for the undistorted case. Our model allows only the calculation of charge transfer states and will never give any information about intra-site excitations. By consequence no information will be obtained about the mechanism by which transitions "steal" their intensity, as is quite obvious in real one-dimensional systems.[7]

For the calculation of the pressure dependence of the phase transition temperature we assume Hooke's Law:

$$dR_0/dP = -\gamma R_0$$

Thus, a change of pressure will be reflected in a change of the equilibrium inter-site distance of the undistorted chain, R_0. For the effect of pressure on the transfer integral we use:

$$d[CR_0]/dP = -\gamma C R_0$$

assuming the effective atomic charge to be independent of pressure, i.e., assuming the internal structure of the molecules or ions not to change. Similarly for the lattice energy of the regular chain:

$$dE_l/dP = d/dR_0[BR_0^{-n}]dR_0/dP = n\gamma E_l$$

We also assume that the on-site electron repulsion U is not affected by external pressure.

Care was taken in the calculation to finally express all energy quantities in the original unit t_0 of the undistorted chain t_0^0, since in our calculation t_0^0 (i.e., the energy unit) will change with pressure. It should be noted that with our assumptions increasing the pressure (and the concomitant increase

of t) leads to a lower value of U/t, making the system more metal-like. Finally, in order to compare the phase transition temperatures at different pressures, all temperatures have to be multiplied by t_0^p/t_0^0 to reference them to the same scale.

The entropy and the electronic contribution to the specific heat at constant volume were evaluated from:

$$S = Nk[\ln Z + T\, d \ln Z/dT]/4$$

$$C_v = Nk[T^2 d^2 \ln Z/dT^2 + 2T\, d \ln Z/dT]/4$$

It should be noted that they are obtained in real energy units per reduced unit of temperature.

RESULTS

Figure 2 shows the phase diagram of the transition temperature vs U/t_0. Only two phases occur, the undistorted $4k_F$ and the dimerized $2k_F$ phase. The transition temperature between the two phases drops sharply with increasing U/t_0, similar to what was observed for the $2k_F$-transition of the

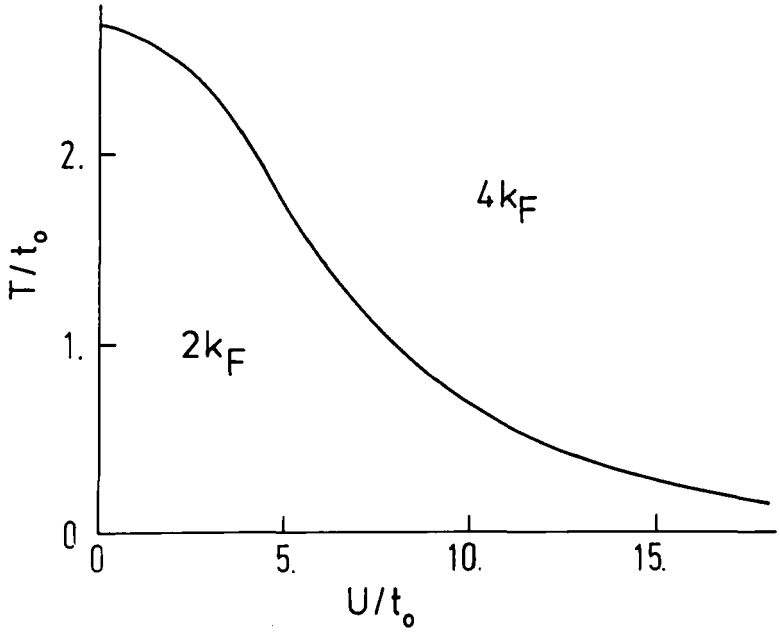

FIGURE 2 The phase-diagram of the various phases of a half-filled one-dimensional chain as a function of U/t_0. $4k_F$ denotes the regular chain and $2k_F$ the dimers.

quarter-filled band. As $U \rightarrow \infty$, the transition temperature goes to zero. Figure 3 gives the temperature dependence of the $2k_F$ distortion parameter ξ for $U = 6t_0$ and $U = 0$. In the high U case ξ drops sharply to zero near the transition temperature. Figure 4 shows the reduced magnetic susceptibility vs the temperature for a series of U/t_0 values. As U increases, the $2k_F$ phase transition is accompanied by a sharp drop in the susceptibility showing the loss of spin entropy in the lattice upon distortion.

In the electronic spectrum a strong charge-transfer excitation, polarized along the chain axis is only observed in the low temperature $2k_F$-phase. The drawn line in Figure 5 shows the temperature dependence of the oscillator strength of the charge transfer excitation. As the transition temperature is approached the oscillator strength drops to zero. This decrease is entirely due to the decrease of the transfer integral in the dimer.

The pressure dependence of the $2k_F$-transition for the present choice of parameters is given in Figure 6a. Because we did not calculate a pressure dependence for the quarter-filled band earlier, we give the results for it (2 electrons on 4 sites)[2] as well (Figure 6b). There appear to be two effects determining the sign of the pressure dependence. Increasing P

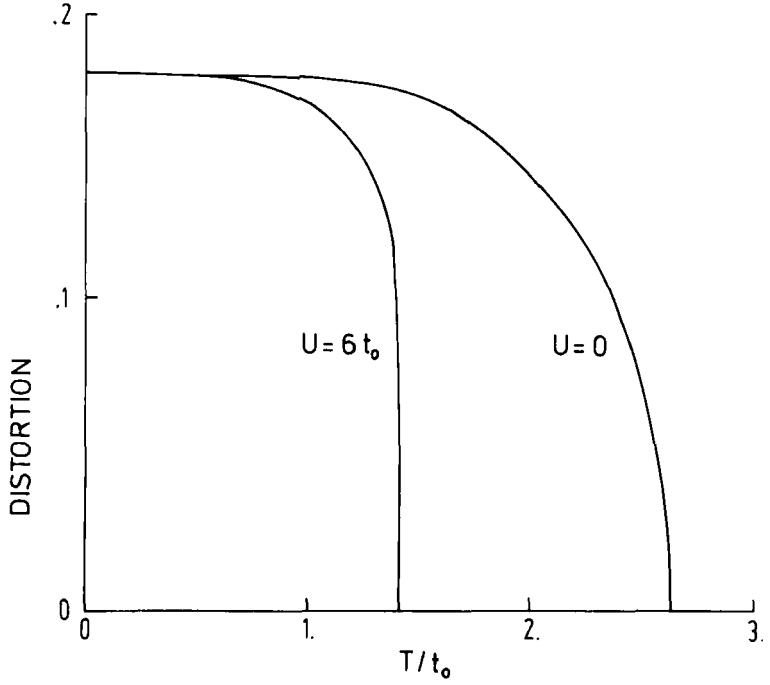

FIGURE 3 Temperature dependence of the $2k_F$ distortion parameter at $U/t_0 = 0$ and $U/t_0 = 6$.

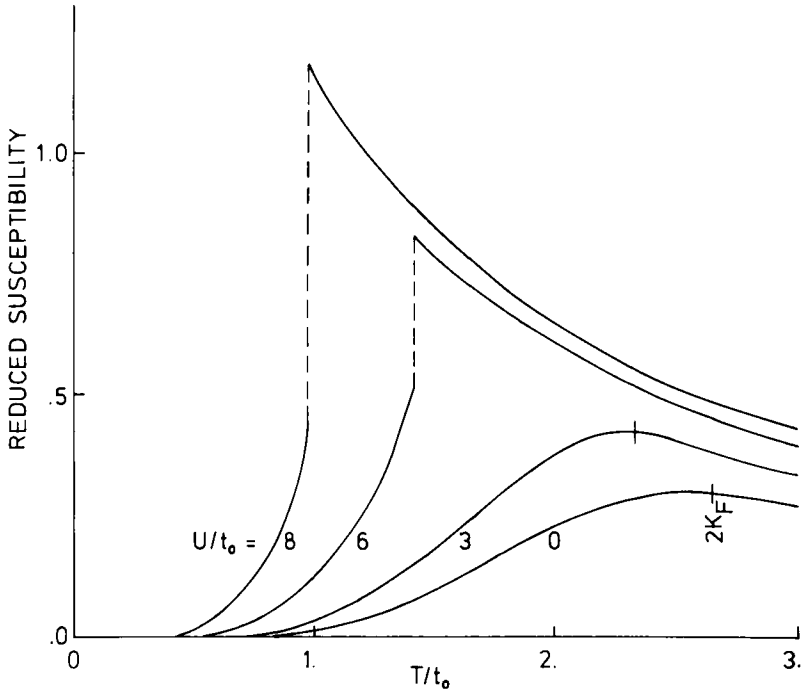

FIGURE 4 Temperature dependence of the reduced magnetic susceptibility for a set of U/t_0 values. The vertical bars denote the $2k_F$ phase transitions.

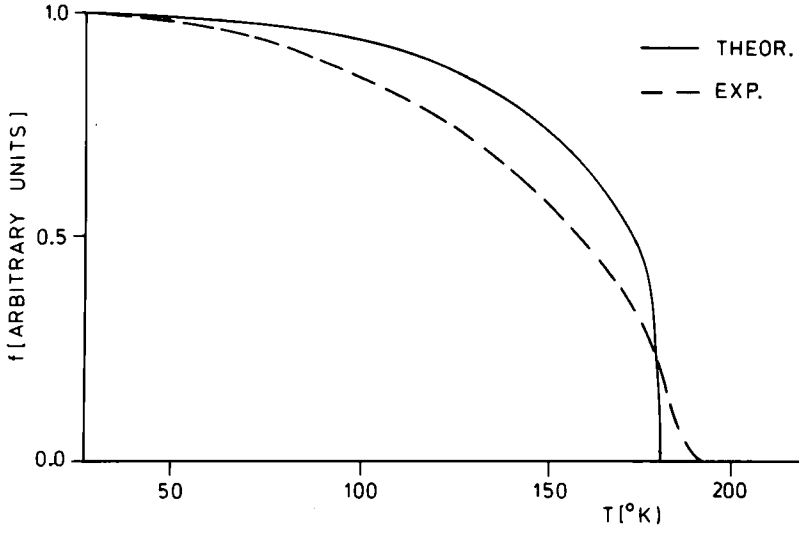

FIGURE 5 Comparison of the calculated and experimental[19] strength of the charge-transfer absorption in Wurster's Blue Perchlorate as a function of temperature. The parameters used are given in Table I.

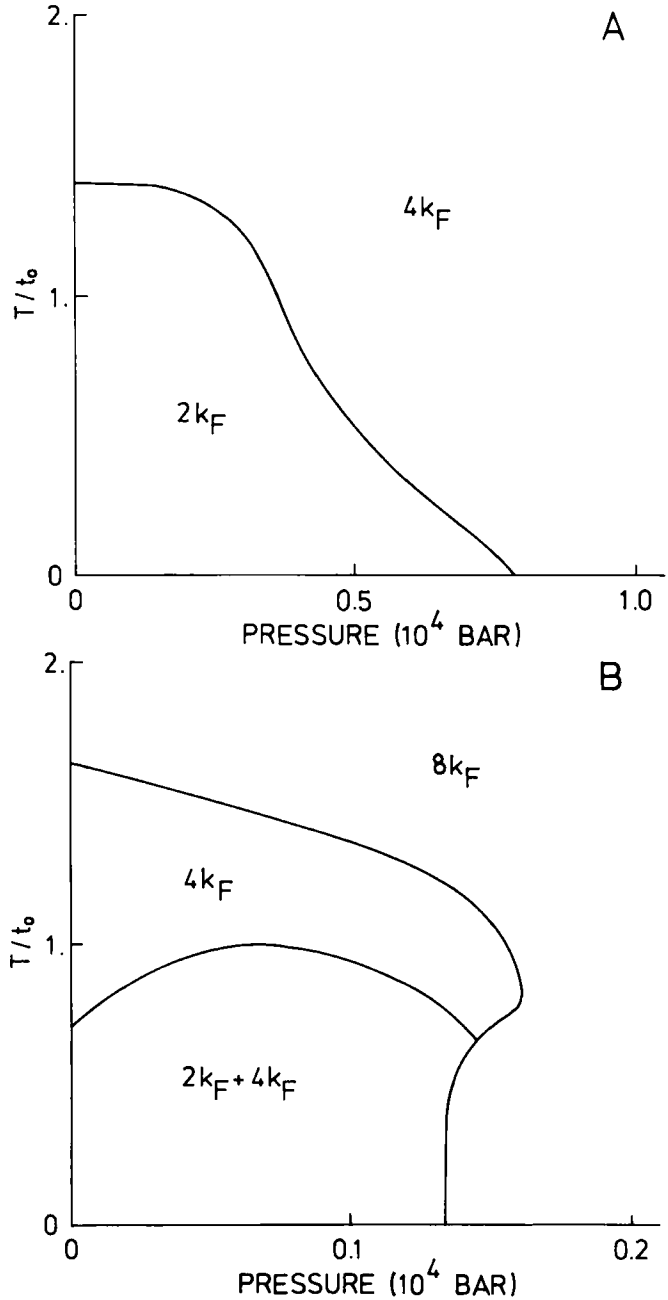

FIGURE 6a, b Pressure dependence of the phase transition temperature at $U = 6t_0$ for a half-filled band system (a) and a quarter-filled bank system (b). $\gamma = 1.10^{-11}$ em^2/dyne.

increases t and therefore decreases U/t. For the $2k_F$-transitions this should in both the half-filled and the quarter-filled band lead to an initial increase in T_c, as is clear from the phase diagram of T_c vs U/t. However, as the pressure goes up, the lattice stiffness increases and the energy gained by deforming the lattice gets smaller with a concomitant decrease in T_c. Therefore, in our calculations the sign of the pressure dependence of $T_c(2k_F)$ depends on the choice of parameters. Our preference at this point would be for the parameters given in this paper. Both signs of $dT_c(2k_F)/dP$ seem to have been observed.[8,9] The disappearance of $2k_F$, and the $(2k_F + 4k_F)$ phase in the half-filled and quarter-filled band systems, respectively, is an artifact of the finite ring size. In the 4 electrons on 4-sites case it does really persist albeit very small, in the 2 electron on 4-site case it disappears, because its occurrence depends on numbers.[2]

The $4k_F$-transition in the quarter-filled band is less sensitive to the value of U/t, and the initial increase of $T_c(4k_F)$ will be much less, if not absent. Its temperature dependence appears always to be negative. For $MEM(TCNQ)_2$ this is also what was observed.[9]

Figure 7 displays the magnetic field effect on the phase transition for $U = 6t_0$. As would be expected, the $2k_F$ transition is continuously shifted

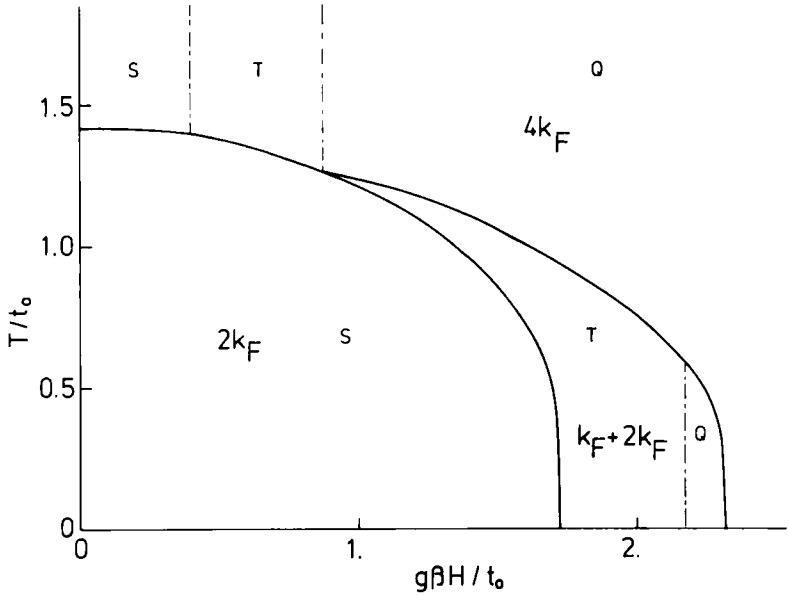

FIGURE 7 Dependence of the phase transition temperature on an external magnetic field. Note the appearance of a new phase $(2k_F + k_F)$ at a value of $g\beta H/t_0 \geqq \pm 0.8$. The character of the electronic groundstate of the system is indicated by the letters S (Singlet), T (Triplet) and Q (Quintet).

to lower temperatures, since the energy of the $4k_F$ magnetic phase is decreased more strongly by the field. At $g\beta H = 0.8t_0$ the $2k_F$ phase becomes unstable at some temperature and a new phase appears, which can be characterized as containing the distortions $2k_F$ and k_F. The $2k_F$ phase becomes unstable at all temperatures at $g\beta H = 1.7t_0$, while the $2k_F + k_F$ phase disappears at $g\beta H = 2.3t_0$. The spin multiplicity of the lowest electronic state of a particular configuration is indicated, always a singlet for the $2k_F$ phase. Note that at the point where the $2k_F + k_F$ phase appears in the phase diagram, the character of the ground state of the regular phase changes from triplet to quintet, while that of the new distorted phase remains triplet.

Figure 8 finally shows the change of the specific heat C_v with temperature for $U/t_0 = 6$.

COMPARISON WITH EXPERIMENT

As for the quarter-filled band, the model calculation displays the behavior of a half-filled band system very well. The present calculations should even

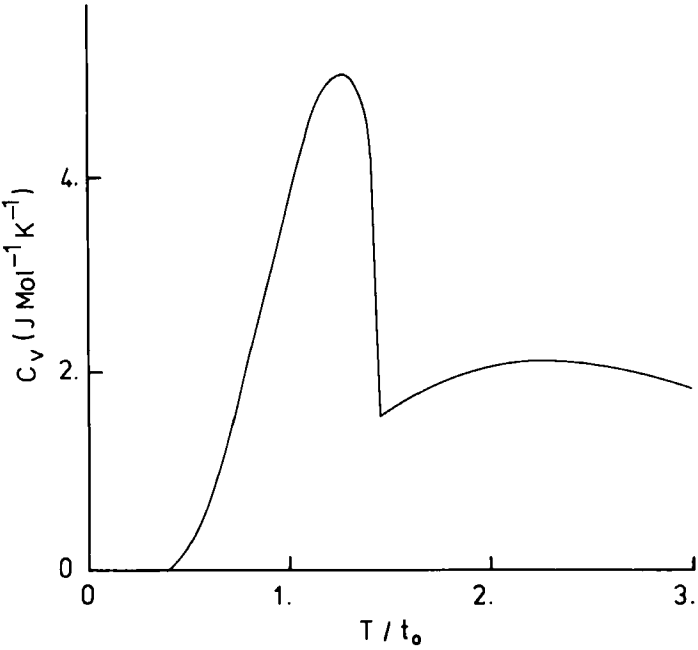

FIGURE 8 Temperature dependence of the specific heat at constant volume (C_V) at $U/t_0 = 6$.

correspond somewhat more to reality, since more states are considered (70 vs 28).

The Peierls transition is found for $U = 0$ and it changes gradually into a spin Peierls when U increases. The distinction between spin Peierls and electronic Peierls, which should be made for a less than half-filled band is not necessary here. The effect of increasing U on the transition temperature at sufficiently high U accords with the decrease in the effective exchange integral $J \approx 2t^2/U$. As this energy decreases the gain in energy upon dimerization decreases and the transition temperature is driven towards lower values.

It was surprising to see the new magnetic field induced $2k_F + k_F$ phase appear, but it was soon realized that such structures, consisting of partially paired and unpaired spin were also predicted by Cross, by Bray, and by Bulaevski[10] on more general theoretical grounds.

Experimental examples are TTF-BDT(Cu), where such a new phase was recently reported.[11,12] There should be many such phases, but in our present model, containing only four electrons, no more can be obtained. For the quarter-filled band having only two electrons, this is even more severely so, therefore the recently reported new phase of $MEM(TCNQ)_2$ in a magnetic field[13] lies outside the scope of our calculation. The electronic spectrum imitates reality very well. The charge transfer band in the $2k_F$ phase corresponds to the charge transfer band found in the low temperature phase of Wurster's Blue Perchlorate,[14] as well as to the band found at low temperatures in the alkali salts of TCNQ.[15] One has to note, that in those cases the charge transfer intensity is stolen from the *intra* molecular bands.[16] In our calculation the strong intensity originates from the exponential increase of the transfer integrals upon dimerization, the source of this increase not specified.

The position of the charge transfer band is often taken as an indication of the value of U. As this calculation shows, this is only very approximately true. Figure 9 gives the position of the charge transfer band at 0 K as a function of U/t_0. Considerable mixing occurs in the excited state, which shifts the frequency of the transition, particularly in the lower range of U.

In general, therefore, the properties of half-filled band systems are fairly well displayed by our calculations. One can, of course, try to go beyond this point and try to fit the results to real experiment. There is some risk involved, because we deal with a multi-parameter problem, the main parameters being the values of t_0, CR_0, U, n (the steepness of the lattice repulsion) and the lattice stiffness α. There are some guidelines, however:

(i) The stiffness of the lattice (α) has a decisive effect on the temperature

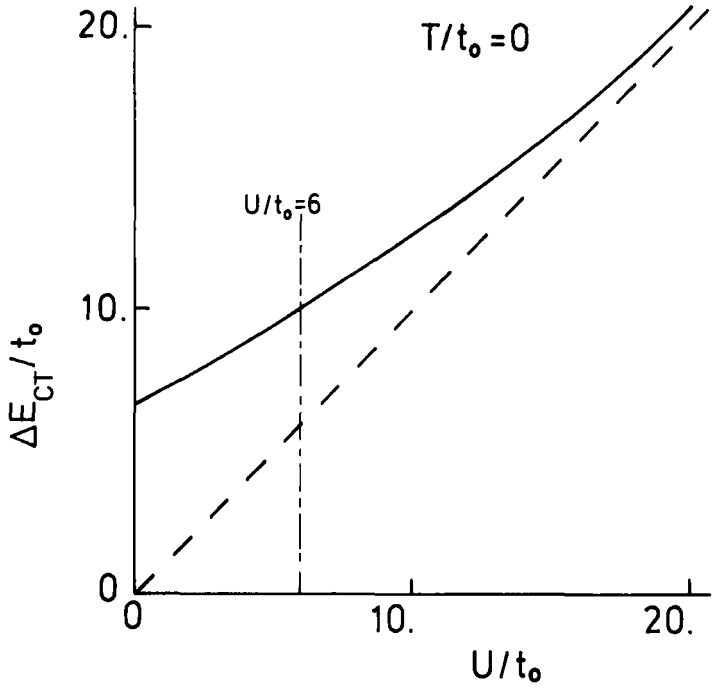

FIGURE 9 The position of the charge-transfer absorption ($\Delta E_{CT}/t_0$) as a function of U/t_0 at zero degree Kelvin.

of the phase transition. Its value can be estimated from data on the linear compressibility[2] or the Debye temperature of the lattice.[17]

(ii) The steepness of the lattice repulsion (n) is one of the decisive factors for the behavior of the order parameter below the phase transition temperature, its value should lie between 11 and 14.

(iii) The electron-electron repulsion (U) determines the value and variation with temperature of the spin susceptibility and its value can be estimated by fitting experimental and theoretical χT vs $1/T$ curves. (Note χT does not contain the parameter t_0.)

(iv) CR_0 determines the rate of change of the transfer integral with the distortion parameter and makes it possible to discriminate between longitudinal (steep) and transverse (less steep) distortions.

(v) The transfer integral at zero distortion t_0 does *not* appear in the actual calculation but is a scaling parameter for all properties derived from the partition function.

With these guidelines we proceed to fit some properties of a number of half-filled band systems.

An intriguing case is the temperature dependence of the spin susceptibility of Wurster's Blue Perchlorate.[18] Figure 10 compares the experimental result with the results of our calculation, keeping the above mentioned guidelines in mind. The agreement between experiment and our crude calculation is excellent. In order to obtain this fit we need $U/t_0 = 40$. The value of the transfer integral t_0, which is needed to simultaneously scale the value of the spin susceptibility and the phase transition temperature is low: $t_0 = 0.025$ eV, which yields a value of U of about 1 eV. In addition we compared in Figure 5 the increase of the experimental[19] and calculated oscillator strengths of the charge transfer transition below the phase transition temperature, which is a measure for the parameter n, the steepness of the lattice repulsion. The agreement was good for $n = 12$ or 13. The position of the charge transfer band we find at $h\nu_{CT} = U$, when $U = 40t_0$, and thus appears at 1 eV, which in view of the uncertainties involved compares reasonably well with the experimental value of 1.4 eV. Or inversely,

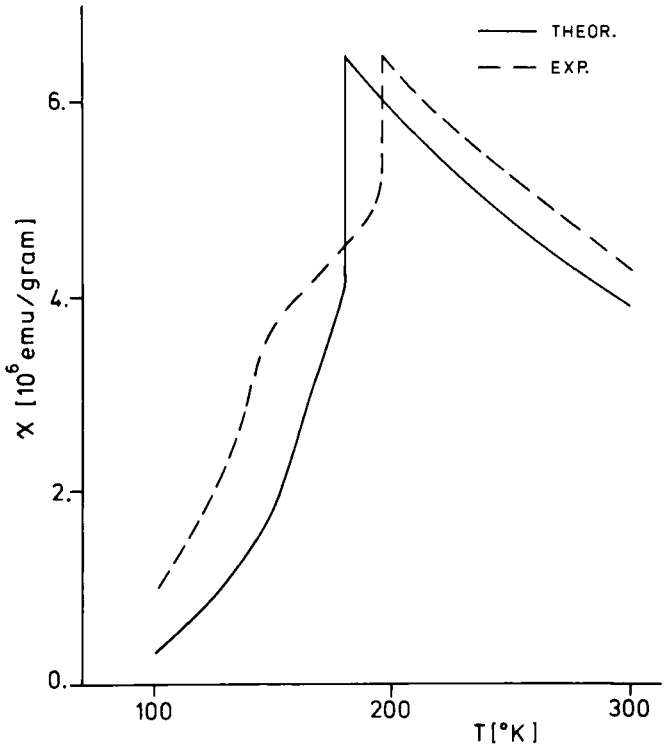

FIGURE 10 Calculated and experimental[18] spin susceptibility of Wurster's Blue Perchlorate as a function of temperature. The parameters used are given in Table I.

the values of t_0 evaluated from the spin susceptibility and the position of the charge transfer band are close (0.025 vs 0.035 eV).

Another class of materials with half-filled bands showing $2k_F$ transitions are the simple TCNQ salts.[20] We also fitted some of their spin susceptibilities. They all have exponentially increasing susceptibilities in the relevant temperature range, and they all have t_0 much larger than f.i. in $TMPD^+ClO_4^-$. Since the experiments then are all in a range, where $kT < t_0$ our fits are dependent on much fewer states than in Wurster's Blue Perchlorate. Of necessity, they are therefore less reliable, although of course much better than a simple singlet triplet model.

The results for all the relevant parameters are collected in Table I. As expected, the transfer integral for $TCNQ^-$ is much higher than for $TMPD^+$, while U is of about the same order of magnitude. Also the transfer integral t_0 is larger for the smaller counter ions in the alkali salts, which may derive from the closer equilibrium contacts possible. A major difference occurs in the value of CR_0 between $TMPD^+$ (9.0) and $TCNQ^-$ (5.8–6.6). Considering the displacements, longitudinal in $TMPD^+$[21] and transverse in TCNQ,[22] this seems not at all unreasonable. Finally another major difference occurs in the lattice stiffness (α/t_0), which for $TCNQ^-$ must be taken much higher than for $TMPD^+$. A number of reasons can be given for this difference:

(i) The $TMPD^+$-$TMPD^+$ distance is 3.49 A, while the undistorted TCNQ distances are in the order of 3.32, which accounts for a factor of two of the difference.

(ii) The repulsion of negative ions (TCNQ) will usually be stronger than that of positive ions, because of the bulkier nature of the former's orbitals.

(iii) The longitudinal motion of $TMPD^+$ upon dimerization[21] may be much softer than the transverse distortion observed in the TNCQ salts.[22]

Even though the difference is large there is no doubt that with the much smaller transfer integral in $TMPD^+$ (no conductivity to speak of) and U of

TABLE I

Fitting parameters for some half-filled band systems

	U/t_0	CR_0	U(eV)	t_0(eV)	T_c(K)	$T_{c,exp}(K)$	α/t_0
TMPD $C10_4$	40.0	9.0	1.00	0.025	190	196	17
NaTCNQ	6.0	6.5	2.27	0.38	305	345	160
KTCNQ	6.0	6.6	1.72	0.29	367	396	160
RbTCNQ (II)	4.0	6.0	1.08	0.27	238	220	160
CsTCNQ	4.0	6.0	0.88	0.21	195	217	160
RbTCNQ (I)	3.0	5.8	0.76	0.25	282	310	160

about 1 eV, one needs a much softer lattice to obtain a distortion at such a relatively high temperature.

CONCLUSIONS

As for the quarter-filled band, our model calculations appear to mimic the behavior of a one-dimensional half-filled band very well. We were even able to compare our calculated results with experiment, with at least reasonable success.

A limit is set by the discreetness of the calculation. When the phase transitions occur at temperatures low compared to the differences between the transfer integrals, the entropy of at least the low temperature phase is too approximative and the phase transition temperatures are bound to be unreliable. One way to overcome this problem is to increase the size of the ring. Although the numerical problems are formidable we are doing so at present for a quarter-filled band mimicked by four electrons on eight sites. The first results indicate that not too much changes, lending again more credence to the present work.

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