The role of phonon-modulated transfer integrals in the electrical and magnetic properties of an extended Hubbard model*

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The coupling of a narrow band of electrons to lattice vibrations is described in terms of the modulation of the one-electron transfer integrals due to phonons. The electrical conductivity due to phonon-assisted processes is calculated for the Mott insulator. These processes modify the temperature dependence of the conductivity and introduce lifetimes related to the phonon density of states. The magnetic susceptibility is calculated at high temperatures and it is seen that the effects of the phonons can be described in terms of a reduced Curie constant and an enhanced Curie-Weiss temperature. Possible applications to the tetracyanoquinodimethan salts are briefly mentioned.

I. INTRODUCTION

It has become increasingly recognized in recent years that the description of the electron-phonon interaction in narrow electron bands should not be based on the same assumptions as those for wide bands. In a wide band, one normally describes the electron-phonon interaction in terms of the change in the interaction between the electron and the (screened) ion as a result of the displacement of the ion from its regular lattice position. On the other hand, when the one-electron Wannier function is fairly localized on the scale of the interatomic spacing, it is more appropriate to start by assuming that the electron wave function is based on the instantaneous position of the ions. As has been noted by several workers,[1-6] this latter description leads to the modulation of the one-electron transfer integrals in Wannier-site space. In comparison, the more familiar electron-phonon interaction is only site diagonal with respect to one-electron transfer.

We have studied the role of the phonon-modulated transfer integrals in an extended Hubbard model. It has been suggested that the one-dimensional Hubbard model[7] has been experimentally realized in N-methylphenazium-tetracyanoquinodimethan (NMP-TCNQ).[8,9] However, this suggestion has been the subject of some criticism, because, although there appears to be some qualitative agreement between theory and experiment, there is strong evidence that the experiments cannot be accounted for in terms of the Hubbard model alone and that modifications of the model would be required.

Therefore, in view of the narrowness of the bandwidth in many of the TCNQ salts, the extremely short mean free paths and the relatively low Debye temperatures, an investigation of a modified Hubbard model that includes the coupling of the electrons to lattice phonons is warranted.

We consider a single nondegenerate half-filled band of electrons, described by a modified Hubbard Hamiltonian

$$H_M = U\sum_i n_{i\uparrow}n_{i\downarrow} + \sum_{\substack{i,\sigma\\ \delta=\pm1}} \tilde{b}(X_{i+\delta}-X_i)C^\dagger_{i\sigma}C_{i+\delta,\sigma} + \sum_q \omega(q)a_q^\dagger a_q \ . \tag{1}$$

$C^\dagger_{i\sigma}$ and $C_{i\sigma}$ respectively create and destroy an electron with spin σ in a Wannier site centered at the *instantaneous* position X_i of lattice site i. $n_{i\sigma}$ is the electron-number operator, while $a_q^\dagger$ and a_q are phonon operators. We assume that we have a harmonic lattice with nearest-neighbor interactions, so that the frequency $\omega(q)$ of the phonon mode of wave vector q is[10]

$$\omega(q) = \omega_M|\sin\tfrac{1}{2}qa| \ , \tag{2}$$

ω_M and a being the maximum-allowed frequency and the lattice spacing, respectively.

U is the on-site Coulomb repulsion and $\tilde{b}(X_{i+\delta}-X_i)$ is the amplitude for an electron in a Wannier state centered around $X_{i+\delta}$ to tunnel into one centered around X_i. We expand $\tilde{b}(X_{i+\delta}-X_i)$ to first order in the phonon operators and obtain

$$\tilde{b}(X_{i+\delta}-X_i) \approx \tilde{b}(R_{i+\delta}-R_i) + \left.\frac{\partial\tilde{b}(r)}{\partial r}\right|_{r=a} \times(\mathrm{sgn}\delta)\sum_q\left(\frac{1}{2MN\omega(q)}\right)^{1/2}(e^{iqR_{i+\delta}} - e^{iqR_i})(a_q + a_{-q}^\dagger) \ , \tag{3}$$

where R_i is the mean position of site i and r is a dummy variable. M is the mass of the lattice site, and N is the number of sites. Assuming that $\tilde{b}(r)$ describes tunneling in the region of exponentially decaying localized electronic wave functions, we may write[5]

$$\tilde{b}(r) = be^{-q_0(r-a)} .$$

Here $b = \tilde{b}(r=a)$ and q_0 is the inverse decay length of the exponentially dying-out wave function. Then

$$\left.\frac{\partial \tilde{b}(r)}{\partial r}\right|_{r=a} = -q_0 b \tag{4}$$

and putting Eqs. (1), (3), and (4) together, we obtain the Hamiltonian

$$H = U\sum_i n_{i\uparrow}n_{i\downarrow} + \sum_q \omega(q)a_q^\dagger a_q + b\sum_{\substack{i,\sigma \\ \delta=\pm1}} C_{i\sigma}^\dagger C_{i+\delta,\sigma} - q_0 b \sum_{\substack{q,i,\sigma \\ \delta=\pm1}} \left(\frac{1}{2MN\omega(q)}\right)^{1/2} (e^{iqR_{i+\delta}} - e^{iqR_i})\,\mathrm{sgn}\delta\,(a_q + a_{-q}^\dagger) C_{i\sigma}^\dagger C_{i+\delta,\sigma} . \tag{5}$$

Unlike Barišić *et al.*,[5] who regard the on-site Coulomb repulsion in a secondary fashion (only insofar as it enters the MacMillan expression for T_c) in their studies of superconductivity, we take U to be the largest parameter in the problem and consequently describe a Mott insulator or semiconductor.

II. CONDUCTIVITY

The electrical conductivity of the Mott semiconductor has been calculated by Bari and Kaplan[11] for the Hubbard model in the absence of electron-phonon coupling. They found that the temperature dependence of the dc conductivity is similar to that of an ordinary two-band semiconductor with the band gap replaced by the Mott-Hubbard correlation gap. We find important modifications to their result, due to phonon-assisted processes, as noted below.

In the system described here, an electron can move by either of two distinct mechanisms: (a) It can hop from site to site, a process that may be assisted (hindered) by a temporarily increased (decreased) value of $\tilde{b}(X_{i+\delta} - X_i)$, caused by neighboring sites being closer together (farther apart) than usual, due to phonons. (b) It can participate, with the site on which it is in residence, in the thermal motion of the site.

Measurements of the electronic dc conductivity probe only contributions from process (a), as that is the process by which electrons are transferred from site to site. The operator which corresponds to a direct electronic current is

$$J = e\sum_{i,\sigma} X_i \dot{n}_{i\sigma} = J_1 + J_2 , \tag{6}$$

where e is the electric charge and

$$J_1 = ieba \sum_{\substack{i,\sigma \\ \delta=\pm1}} (-\mathrm{sgn}\delta) C_{i\sigma}^\dagger C_{i+\delta,\sigma} \tag{7}$$

and

$$J_2 = ieb(q_0 a - 1)\sum_{\substack{i,\sigma,q \\ \delta=\pm1}} \left(\frac{1}{2MN\omega(q)}\right)^{1/2} \times (e^{iqR_i} - e^{iqR_{i+\delta}})(a_q + a_{-q}^\dagger) \times C_{i\sigma}^\dagger C_{i+\delta,\sigma} . \tag{8}$$

J_1 is the current operator one would obtain in the absence of phonons, whereas J_2 is the phonon-assisted current and arises from modulation of the electron hopping matrix element by phonons.

The response, at frequency ω, of the current to a uniform electric field is described by the conductivity[12]

$$\sigma[\omega] = (1/L)\int_0^\infty dt\, e^{i\omega t} \times \int_0^\beta d\lambda \langle \tilde{J} J(t + i\lambda)\rangle ,$$

where L is the crystal volume, β is the inverse temperature, $J(t + i\lambda)$ is related to J by the usual Heisenberg time evolution, and

$$\tilde{J} = \frac{d}{dt}\left(e\sum_{i\sigma} X_i n_{i\sigma}\right) \tag{9a}$$

$$= J_1 + J_2 + J_3 . \tag{9b}$$

J_1 and J_2 have been defined above.

$$J_3 = e\sum_{i\sigma} \mathring{X}_i n_{i\sigma} = -ie\sum_{i,q,\sigma} \frac{\omega(q)}{2MN} e^{iqR_i}(a_q - a_{-q}^\dagger) . \tag{10}$$

J_3 represents the operator corresponding to process (b) above and consequently it does not appear in the current operator J in the calculation of the dc electronic response. On the other hand, in the calculation of the ac energy dissipation it should, of course, be included in J.

The expression for the conductivity given above differs from the more familiar expression in terms of the current autocorrelation function since the current response J is distinct from the quantity, Eq. (9a), that couples to the external field.

The real part of $\sigma[\omega]$ can be written in the form

$$\sigma(\omega)=\sum_{a=1}^{3}\sum_{b=1}^{2}\sigma_{ab}(\omega)\,, \tag{11}$$

where

$$\sigma_{ab}(\omega)=(\tanh\tfrac{1}{2}\beta\omega/2\omega L)\int_{-\infty}^{\infty}dt\,e^{-i\omega t}[\langle J_a(t)J_b(0)\rangle+\langle J_b(0)J_a(t)\rangle] \tag{12}$$

and

$$\langle J_b(0)J_a(t)\rangle=\frac{\mathrm{Tr}e^{-\beta(\tilde{H}-\mu N+V)}e^{i(\tilde{H}+V)t}J_a e^{-i(\tilde{H}+V)t}J_b}{\mathrm{Tr}e^{-\beta(\tilde{H}-\mu\hat{N}+V)}}\,. \tag{13}$$

Here μ is the chemical potential, $\hat{N}=\sum n_{i\uparrow}+n_{i\downarrow}$, and

$$\tilde{H}=U\sum_i n_{i\uparrow}n_{i\downarrow}+\sum_q\omega(q)a_q^\dagger a_q \tag{14}$$

and

$$V=b\sum_{\substack{i,\sigma\\ \delta=\pm1}}C_{i\sigma}^\dagger C_{i+\delta\,\sigma}-q_0 b\sum_{\substack{q,i,\sigma\\ \delta=\pm1}}\left(\frac{1}{2MN\omega(q)}\right)^{1/2}(e^{iqR_{i+\delta}}-e^{iqR_i})(\mathrm{sgn}\delta)(a_q+a_{-q}^\dagger)C_{i\sigma}^\dagger C_{i+\delta,\sigma}\,. \tag{15}$$

We carry out the calculations of σ to order b^2. Since J_1 and J_2 are both explicitly proportional to b [Eqs. (7) and (8)], whereas J_3 [Eq. (10)] is not, we see that in calculating σ_{11}, σ_{12}, σ_{21}, and σ_{22}, we may drop V in the density operator and the time-evolution operators in Eq. (13), whereas in our calculations of σ_{31} and σ_{32} we need first-order (in V) contributions from both thermal and time operators.

$\sigma_{11}(\omega)$ is the conductivity of the phononless Hubbard model, and we obtain the results of Bari and Kaplan.[10] The dc contribution, which we denote by σ_{elec} is

$$\sigma_{\mathrm{elec}}=[2\pi e^2b^2a^2n/(1+e^{\beta U/2})^2]\times\beta e^{\beta U/2}\delta(\omega)\,. \tag{16}$$

Here n is the concentration and $\delta(\omega)$ is the δ function.

$\sigma_{12}(\omega)$ and $\sigma_{21}(\omega)$ are seen to vanish to the order we are interested. $\sigma_{22}(\omega)$, $\sigma_{31}(\omega)$, and $\sigma_{32}(\omega)$ are contributions to the conductivity due to phonon-assisted processes. The response, which was limited to δ-function peaks at $\omega=0$ and $\omega=\pm U$ in the calculations of Bari and Kaplan is, in these contributions to the conductivity, seen to be spread over a frequency range $\pm\omega_M$ within each of the peaks. The contribution to the dc conductivity from phonon-assisted processes, which we shall denote σ_{phon} is

$$\sigma_{\mathrm{phon}}=\frac{4e^2b^2n}{M\omega_M^2(1+e^{\beta U/2})^2}\left[2q_0a\beta e^{\beta U/2}\times\left(\int_0^{\omega_M}d\epsilon\,\frac{\epsilon\coth\frac{1}{2}\beta\epsilon}{(\omega_M^2-\epsilon^2)^{1/2}}\right)\delta(\omega)+\frac{2e^{\beta U/2}}{\omega_M}(q_0^2a^2-3q_0a+1)\right]. \tag{17}$$

We see that the contribution to the conductivity from phonon-assisted processes is a sensitive function of q_0, the inverse decay length of the localized molecular wave functions. We also see that for $T\gg\omega_M$, σ_{phon} tends to a constant value. From Eq. (16) we see that σ_{elec} falls off as $1/T$ at large temperatures. Thus the relative importance of phonon-assisted processes grows with temperature.

For the purpose of comparison, and in order to obtain a measure of the two terms in Eq. (17), we replace $\pi\delta(\omega)$ by a relaxation time τ which we assume to be caused by a temperature-independent scattering mechanism[13] (e.g., scattering from impurities). Making a similar replacement in Eq. (16), we find from Eqs. (16) and (17),

$$\frac{\sigma_{\mathrm{phon}}}{\sigma_{\mathrm{elec}}}=\frac{2q_0a}{\frac{1}{2}M\omega_M^2a^2\beta}\left[\frac{1}{\pi}\left(\int_0^{\omega_M}d\epsilon\,\frac{\beta\epsilon\coth\frac{1}{2}\beta\epsilon}{(\omega_M^2-\epsilon^2)^{1/2}}\right)+\frac{q_0a-3+1/q_0a}{\omega_M\tau}\right]. \tag{18}$$

In Fig. 1 we have plotted $\sigma_{phon}/\sigma_{elec}$ versus temperature using values of M, a, U, b, and ω_M which are believed to be appropriate to NMP-TCNQ.[8] For q_0 we have used a value of 3Å^{-1} which is appropriate to the $2p$ orbitals in an isolated carbon atom.[14,15] The curve is plotted with τ set equal to ∞ (corresponding to no scattering). Using the impurity concentration quoted in Ref. 9, we find a scattering time[13] of 10^{-10} sec. With τ set equal to this value in Eq. (18) the curve in Fig. 1 is not perceptibly altered.

Figure 2 exhibits the temperature dependence of the conductivity, $\sigma = \sigma_{elec} + \sigma_{phon}$, assuming no scattering is present ($\tau = \infty$). The parameter Λ which is plotted is related to the conductivity σ by a temperature-independent multiplicative factor:

$$\sigma = \Lambda(e^2 b^2 a^2 n/2U)\delta(\omega) .$$

For comparison we have also plotted Λ_{elec} which is related to σ_{elec} by the same factor as that relating Λ to σ.

Both Figs. 1 and 2 show that at high temperatures the phonon-assisted contribution to σ is appreciable. This suggests that the interpretation of the high-temperature behavior of some TCNQ salts in terms of a simple power-law dependence[16,17] ($\sigma \sim T^{-n}$) may be misleading.

We see that the phonon-assisted contribution to the dc conductivity is significant for $q_0 a \gtrsim 1$. In the opposite limit or $q_0 a \ll 1$, we see that Eq. (17) remains finite even as $q_0 \to 0$. This result can be understood in terms of the phonon-assisted current operator J_2 given by Eq. (8). The current operator is basically a velocity operator and in the terminology of the cell space of our model, the velocity is constructed in terms of a hopping time and a hopping distance. The hopping time is associated with the hopping parameter given in Eq. (3) and the hopping distance is just $X_{i-\delta} - X_i$. The modulation of the hopping time is reflected in the term proportional to q_0 in Eq. (8) and the term that is independent of q_0 reflects the modulation of the hopping distance due to the phonons.

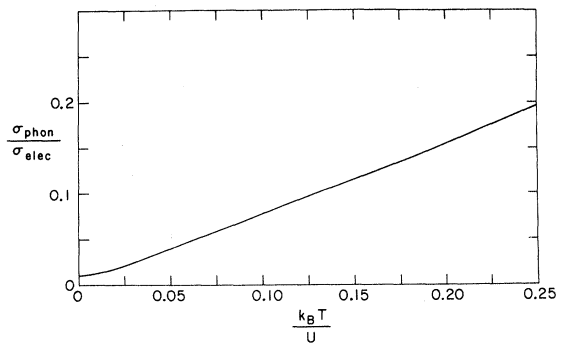

FIG. 1. Ratio of the phononic to the electronic contribution to the conductivity is plotted vs the temperature in units of U.

III. SUSCEPTIBILITY

We now turn to the effect of the electron-phonon interaction on the magnetic susceptibility at high temperatures.

The Hamiltonian of the system in a uniform magnetic field B is

$$H' = H - B\sum_i (n_{i\uparrow} - n_{i\downarrow}) , \tag{19}$$

where H was defined in (5). The partition function is

$$Z = \mathrm{Tr}\, e^{-\beta(H' - \mu\hat{N})}$$

$$= \mathrm{Tr}\exp\{-\beta[\tilde{H} - B\sum_i (n_{i\uparrow} - n_{i\downarrow})$$

$$- \mu\hat{N} + V]\} . \tag{20}$$

Z may be evaluated straightforwardly provided we retain only second-order terms in βV. We then find

$$Z = Z_0(1 + \Delta) , \tag{21}$$

where

$$Z_0 = [2(1 + e^{\beta U/2}\cosh\beta B)]^N \tag{22}$$

and

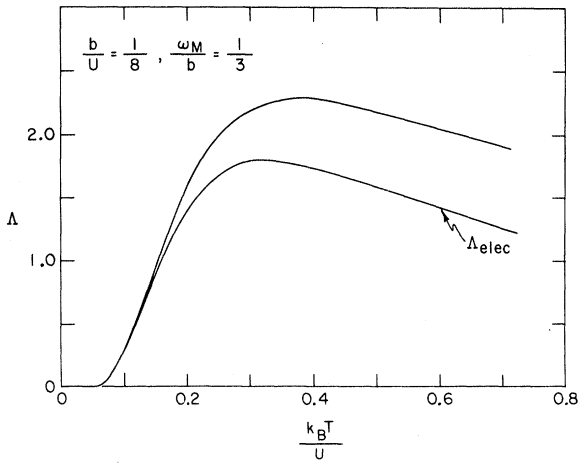

FIG. 2. Temperature dependence of the conductivity is exhibited. Λ is related to the conductivity σ by a temperature-independent multiplicative factor. Λ_{elec}, which is similarly related to σ_{elec}, is also plotted for comparison.

$$\Delta = \frac{\beta b^2}{(1+e^{\beta U/2}\cosh\beta B)^2}\left[\left(\frac{e^{\beta U}-1}{U}+\beta e^{\beta U/2}\cosh\beta B\right)\right.$$

$$\left.+\frac{1}{T_R}\left(e^{\beta U/2}\cosh\beta B+\frac{e^{\beta U}-1}{\pi}\int_0^{\omega_M}\frac{d\epsilon}{(\omega_M^2-\epsilon^2)^{1/2}}\,\frac{\epsilon U\cosh\frac{1}{2}\beta\epsilon-\epsilon^2}{U^2-\epsilon^2}\right)\right]. \tag{23}$$

The magnetic susceptibility χ is obtained by differentiating:

$$\chi = \frac{1}{\beta}\frac{\partial^2}{\partial B^2}\ln Z\Big|_{B=0}$$

$$\approx \frac{1}{\beta}\frac{\partial^2}{\partial B^2}\ln Z_0\Big|_{B=0}$$

$$+\frac{1}{\beta}\frac{\partial^2}{\partial B^2}\Delta\Big|_{B=0}. \tag{24}$$

We find

$$\chi = \frac{\beta}{1+e^{-\beta U/2}}\left[1-\frac{\beta b^2}{U}\tanh\tfrac{1}{4}\beta U\left(2[1+S(\beta)]\right.\right.$$

$$\left.\left.+\frac{\beta U}{1+e^{\beta U/2}}[1+R(\beta)]\right)\right], \tag{25}$$

where

$$R(\beta) = 1/\beta T_R, \tag{26}$$

$$S(\beta) = \frac{U}{2T_R}\int_0^{\omega_M}\frac{d\epsilon}{(\omega_M^2-\epsilon^2)^{1/2}}$$

$$\times\frac{U\epsilon\coth\frac{1}{2}\beta\epsilon-\epsilon^2}{U^2-\epsilon^2}, \tag{27}$$

and

$$T_R = M\omega_M^2/4q_0^2. \tag{28}$$

Setting $q_0 = 0$ in Eq. (25) we recover the result of Hone and Pincus.[18] In the temperature range $b^2/U \ll T \ll U$ Hone and Pincus showed that the susceptibility reduced to the form expected for an antiferromagnet at temperatures much larger than the Néel temperature:

$$1/\chi = T+\Theta, \tag{29}$$

where $\Theta = 2b^2/U$ is the effective exchange constant.

The effect of the electron-phonon interaction is to renormalize both the effective magnetic moment and the Néel temperature. In Fig. 3 we have plotted the inverse susceptibility versus temperature for various values of b/U and q_0.

We may simplify Eq. (25) for the susceptibility provided the temperature is in the range $U \gg T \gg R\Theta, \omega_M$.

In this regime

$$\frac{1}{\chi} = R(T+R\Theta), \tag{30}$$

where

$$R = \frac{1}{1-\Theta/T_R} \tag{31}$$

is the factor by which the Néel temperature is raised and the square of the effective magnetic moment is lowered.

In the derivation of Eq. (25) for the susceptibility we have assumed that

$$\beta^2\tilde{b}^2(X_{i+\delta}-X_i) \ll 1. \tag{32}$$

Evaluating

$$\langle\tilde{b}^2(X_{i+\delta}-X_i)\rangle_{\text{phon}},$$

where the thermal average is taken over the phonon states, we find that the condition (32) is satisfied provided

$$T \gg b, b^2/T_R. \tag{33}$$

The experimentally measured value of μ_{eff}^2 in NMP-TCNQ is $\frac{1}{3}$ (where μ_{eff} is the effective magnetic moment expressed in units for which the Bohr magneton is unity). Epstein *et al.*[8] noted that the discrepancy with the Hubbard-model prediction of $\mu_{\text{eff}}^2 = 1$ (in the limit $b/U \ll 1$) might result if the ground state (for $b/U = \frac{1}{8}$) contained large admixtures of polar states. However, calculations by Cabib and Kaplan[19] for a four-site Hubbard model showed that with $b/U = \frac{1}{8}$, the effective magnetic moment of the Hubbard model is not sufficiently different from the $b \ll U$ result.

Although agreement with the apparent reduced moment in NMP-TCNQ can be formally achieved as a result of an appropriate choice of the parameter q_0 in Eq. (25), there are at least two reasons for not taking this agreement too seriously. First, this choice of q_0 would violate the condition [Eq. (33)] required for the validity of Eqs. (25) and (30). Second, and more generally, if the value $b = 0.021$ eV in Ref. 8 is to be believed, then in the temperature regime $T < 200\,^\circ$K, the analysis of the susceptibility in terms of the high-temperature expansion is inappropriate. This point has also been noted by Kaplan.[20]

We also comment that the phonon mechanism studied here does not lend support to the suggestions in Ref. 8 that NMP-TCNQ can be understood in terms of a Hubbard model with different values of the parameters in the high- and low-temperature regimes.

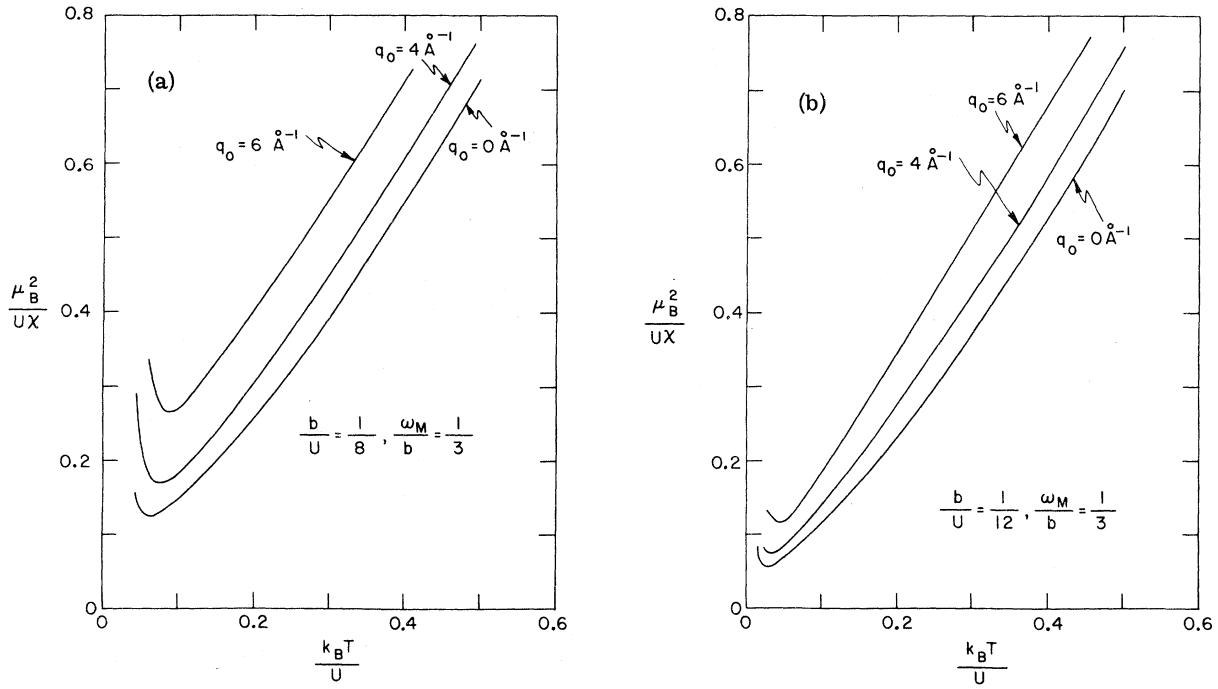

FIG. 3. Reciprocal of the susceptibility, in units of U/μ_B^2, is plotted versus the temperature in units of U. (μ_B is the Böhr magneton.) We have used values of M, a, and U quoted in Ref. 8. The effect of changing q_0 is exhibited with $b/U = \frac{1}{8}$ and $\frac{1}{12}$.

IV. SUMMARY

We have studied the consequences of the phonon modulation of the transfer integrals in a Hubbard model.

The current operator for the system contains a part which depends explicitly on the phonons. Consequently the conductivity has a phononic contribution, and is enhanced over its value in the absence of phonons. The enhancement increases with temperature, reflecting the fact that more phonons are available at higher temperatures to assist electron hopping.

From a high-temperature expansion of the susceptibility we showed that the phonons have a twofold effect: (a) They cause the Néel temperature to rise; (b) they result in a lowering of the effective magnetic moment. In a restricted temperature range the susceptibility took on a particularly simple form [Eq. (30)].

Both the conductivity and the susceptibility depended strongly on q_0, the inverse decay range of the localized electronic wave function. In this connection we remark that the value 3Å^{-1} for q_0 is its value for a $2p$ orbital in a carbon atom. In NMP-TCNQ the electrons are trapped by the highly withdrawing cyanide groups, and this may result in a larger value of q_0.

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[10]The calculations have been performed for a one-dimensional Hubbard model coupled to the vibrational modes of a one-dimensional lattice. It is known that such a lattice is unstable, i.e., $\langle u_i^2 \rangle_{\text{phonons}}$ is infinite. However, the quantities which appear in our calculations are invariably of the form $\langle u_{i+1} - u_i)^2 \rangle_{\text{phonons}}$, and are finite. A generalization of our calculations to higher dimensions is straightforward and in qualitative agreement with those presented here.

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