# ANHARMONISM AND THE METAL-INSULATOR TRANSITION

By M. Matlak*,**

Institut für Theoretische Physik II, Westfälische Wilhelms-Universität, Münster

The influence of anharmonism, in the pseudoharmonic approximation (pseudo-harmonic phonons), on the electron properties of the nondegenerate $s$-band has been investigated. The $s$-band is described by the Hubbard model. We have considered the case of weak coupling between electrons and lattice vibrations. Pseudoharmonic phonons renormalize the $s$-bandwidth making it temperature dependent. (A simple cubic lattice is considered for simplicity.) The numerical calculations, based on the Debye model for the lattice, show that the $s$-bandwidth slowly decreases with temperature. It seems that such a behaviour of the bandwidth should be qualitatively independent of any approximation. It has been shown that anharmonism alone cannot describe the insulator-metal transition in the frame of the Hubbard III approximation for a half-filled band but a metal-insulator transition. In this connection an explanation of the metal-insulator transition observed in $V_2O_3$ and $Ti_2O_3$ is suggested. Finally, the influence of the anharmonism (pseudoharmonic approximation, weak coupling between electrons and lattice vibrations) on the dc conductivity of the Mott insulator is discussed. The numerical calculations, based on the Debye model, show that the anharmonism enhances the conductivity at all temperatures.

## 1. Introduction

Many properties of solids depend on the influence of phonons on the electron system. This problem has been investigated by many authors. It was shown [1–4] that the coupling between electrons and phonons in materials with narrow bands is not so strong as in materials with wide bands. Therefore it seems that in the first case the influence of phonons on the properties of the electron system is small. Recently Barma and Bari [5] have investigated the influence of phonons on the properties of the electrons of the nondegenerate $s$-band, described by the Hubbard model [6]. They have shown that phonons modify the temperature dependence of the conductivity for a Mott insulator. These authors have taken the Hamiltonian of the lattice in the harmonic approximation. The hopping integral in their paper was expanded in the Taylor series including both the zero- and first-order terms in the displacements of the lattice atoms.

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* On leave from the Institute of Physics, Silesian University, Uniwersytecka 4, 40-007 Katowice, Poland.

** Mailing address until the end of July 1978: Institut für Theoretische Physik II, Westfälische Wilhelms-Universität, Steinfurther Str. 107, 4400 Münster, BRD.

However, we can take into account all terms in the expansion of both the potential energy of the lattice and hopping integral with respect to atomic displacements. In the present paper we investigate the influence of all these terms on the electron properties of the nondegenerate half-filled $s$-band, described by the Hubbard model [6]. For simplicity we consider a simple cubic lattice and we use the well known Green's function method [7]. It should be noted here that an analogous treatment of the anharmonism was worked out earlier in papers [8–10] and applied to ferromagnets and quantum crystals. In the present paper we shall follow the work of Konwent and Plakida [10]. These authors have considered the Heisenberg ferromagnet and treated the anharmonism of the lattice in the pseudoharmonic approximation. We also use the pseudoharmonic approximation and the simplest decoupling scheme of the higher order Green functions. This scheme is only valid for weak coupling between electrons and lattice vibrations (see (9), (10) and (11) of Section 2 for details).The pseudoharmonic approximation renormalizes the hopping integral $(T_{ij} \rightarrow \tilde{T}_{ij})$ making it temperature dependent. This means that the bandwidth is also temperature dependent $(\varDelta \rightarrow \tilde{\varDelta})$. In order to discuss the electron properties of a band (insulating phase, metallic phase, metal-insulator transition) with changing temperature we have to make an analogous approximation of the one-electron Green function to that of Hubbard III [11] (or the CPA formulation [12]). This approximation can easily be made. It suffices to replace $T_{ij} \rightarrow \tilde{T}_{ij}$ (pseudoharmonic approximation and the simplest decoupling scheme (9), (10) and (11) of Section 2) in the suitable expression for the one-particle Green function in Hubbards paper [11] and we obtain the desired result. In order to perform the numerical calculations of the bandwidth as a function of temperature we have to make further approximations. As the simplest approximation of the lattice Hamiltonian we use the Debye model. When taking into account three acoustic branches for the simple cubic lattice we find that the bandwidth slowly decreases with temperature. It seems that this result is physically reasonable. We feel that it should be qualitatively independent of any approximation. We then discuss, analogously to Ref. [11], the possibility of obtaining the different phases depending on the ratio $\varDelta/U$ where $U$ is the Coulomb integral. The only difference from Ref. [11] is that in our treatment the bandwidth is temperature dependent. Keeping $U = $ const we obtain two possibilities. The first of them is the appearance of the insulating phase at all temperatures. The second one is the metallic phase up to $T_{cr}$ and the insulating phase above it. The second case is a little analogous to that given by the small polaron theory [15–17, 19].

According to experimental data the oxides and sulfides of the transition metals show insulating behaviour at low temperatures and metallic behaviour above a critical temperature. Our result disagrees with these experimental data. The anharmonism cannot explain the insulating behaviour at low temperatures and the metallic behaviour at higher temperatures. But there exist some substances as $V_2O_3$ and $Ti_2O_3$ (cf. [18, 20–22]) which are insulating at low temperatures, exhibit an insulator-metal transition and thereafter come back to the insulating phase. We suggest that anharmonism can explain the properties of these substances after the metallic phase is reached.

Finally, we calculate in the pseudoharmonic approximation and in the case of weak coupling between electrons and phonons the dc conductivity of the Mott insulator. The

numerical calculations, again assuming the Debye model for the lattice, show the enhancement of the conductivity compared to that calculated when there are no lattice vibrations.

## 2. Pseudoharmonic approximation in the anharmonic crystal

We consider a crystal with a simple cubic structure containing $N$ atoms described by the Hamiltonian

$$H = H_1 + H_H, \tag{1}$$

where

$$H_1 = \sum_m \frac{P_m^2}{2M} + V(R_1, \dots R_N), \tag{2}$$

and

$$H_H = \sum_{\substack{ij \\ \sigma}} T_{ij} c_{i\sigma}^+ c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}. \tag{3}$$

The Hamiltonian (2) describes the lattice of the crystal (its kinetic and potential energy). The Hamiltonian (3) describes electrons of the $s$-band. If we write $R_m = R_m^0 + u_m$ where $R_m^0$ is the equilibrium position of the atom $m$ and $u_m$ a small deviation from it and expand (2) and (3) in a Taylor series (cf. e. g. [10]) we obtain

$$H_1 = \sum_m \frac{P_m^2}{2M} + \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\substack{m_1 \dots m_n \\ \alpha_1 \dots \alpha_n}} [\nabla_{m_1}^{\alpha_1} \dots \nabla_{m_n}^{\alpha_n} V(R_1^0 \dots R_N^0)] u_{m_1}^{\alpha_1} \dots u_{m_n}^{\alpha_n} \tag{4}$$

and

$$H_H = \sum_{\substack{ij \\ \sigma}} \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\alpha_1 \dots \alpha_n} [\nabla_i^{\alpha_1} \dots \nabla_i^{\alpha_n} T_{ij}^0] (u_i^{\alpha_1} - u_j^{\alpha_1}) \dots$$

$$\times (u_i^{\alpha_n} - u_j^{\alpha_n}) c_{i\sigma}^+ c_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \tag{5}$$

$$T_{ij}^0 \equiv T(|R_i^0 - R_j^0|). \tag{5'}$$

In order to obtain the thermodynamical properties of the crystal it is convenient to introduce the phonon Green function

$$F_{mm'}^{\alpha\beta}(t-t') = -i\theta(t-t') \langle [u_m^\alpha(t), u_{m'}^\beta(t')] \rangle \equiv \langle\langle u_m^\alpha(t) | u_{m'}^\beta(t') \rangle\rangle \tag{6}$$

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and the electron Green function

$$G_{ij}^{\sigma\sigma'}(t-t') = -i\theta(t-t')\langle\{c_{i\sigma}(t), c_{j\sigma'}^+(t')\}\rangle \equiv \langle\!\langle c_{i\sigma}(t)\,|\,c_{j\sigma'}^+(t')\rangle\!\rangle. \tag{7}$$

After performing the time Fourier transformation we obtain the following equation for the phonon Green function

$$E^2 F_{mm'}^{\alpha\beta}(E) = \frac{\delta_{mm'}\delta_{\alpha\beta}}{2\pi M} + \frac{1}{M}\sum_{n=1}^{\infty}\frac{1}{n!}\sum_{\substack{m_1\ldots m_n\\ \alpha_1\ldots\alpha_n}}[\nabla_m^\alpha\nabla_{m_1}^{\alpha_1}\ldots$$

$$\times\nabla_{m_n}^{\alpha_n}V(\boldsymbol{R}_1^0\ldots\boldsymbol{R}_N^0)]\,\langle\!\langle u_{m_1}^{\alpha_1}\ldots u_{m_n}^{\alpha_n}|u_{m'}^\beta\rangle\!\rangle_E$$

$$+\frac{1}{M}\sum_{j\sigma}\sum_{n=1}^{\infty}\frac{1}{n!}\sum_{\alpha_1\ldots\alpha_n}[\nabla_m^\alpha\nabla_{m_1}^{\alpha_1}\ldots\nabla_{m_n}^{\alpha_n}T_{mj}^0]$$

$$\times\langle\!\langle(u_m^{\alpha_1}-u_j^{\alpha_1})\ldots(u_m^{\alpha_n}-u_j^{\alpha_n})(c_{m\sigma}^+c_{j\sigma}-c_{m\sigma}c_{j\sigma}^+)\,|\,u_{m'}^\beta\rangle\!\rangle_E. \tag{8}$$

We use here the pseudoharmonic approximation [9]

$$\langle\!\langle u_1\ldots u_n|u_{m'}^\beta\rangle\!\rangle_E \approx \sum_{i=1}^{n}\langle\!\langle u_i|u_{m'}^\beta\rangle\!\rangle_E\langle\prod_{j\neq i}u_j\rangle, \tag{9}$$

$$\langle u_1\ldots u_n\rangle \approx n!!\langle u_1 u_2\rangle\ldots\langle u_{n-1}u_n\rangle. \tag{10}$$

Analogously to paper [10] we perform the following decoupling

$$\langle\!\langle(u_m^{\alpha_1}-u_j^{\alpha_1})\ldots(u_m^{\alpha_n}-u_j^{\alpha_n})(c_{m\sigma}^+c_{j\sigma}-c_{m\sigma}c_{j\sigma}^+)\,|\,u_{m'}^\beta\rangle\!\rangle_E$$

$$\approx \langle\!\langle(u_m^{\alpha_1}-u_j^{\alpha_1})\ldots(u_m^{\alpha_n}-u_j^{\alpha_n})\,|\,u_{m'}^\beta\rangle\!\rangle_E\langle c_{m\sigma}^+c_{j\sigma}-c_{m\sigma}c_{j\sigma}^+\rangle. \tag{11}$$

We define the space Fourier transformation

$$F_{mm'}^{\alpha\beta}(E) = \frac{1}{MN}\sum_{k,s,s'}e_{k,s}^\alpha e_{k,s'}^\beta F_{k,s,s'}(E)e^{ik\cdot(R_m^0-R_{m'}^0)}, \tag{12}$$

where the **k**-summation runs over the first Brillouin zone, $s$ and $s'$ labels the phonon branhes and $e_{k,s}$ denotes the polarization vector of the phonon. Making use of (9), (10), (11) and (12) we get

$$F_{k,s,s'}(E) = \frac{\delta_{ss'}}{2\pi(E^2-\omega_{k,s}^2)}, \tag{13}$$

where

$$\omega_{k,s}^2 = \frac{1}{M}\sum_{j\alpha\delta}e_{k,s}^\alpha e_{k,s}^\delta[e^{-ik\cdot(R_m^0-R_j^0)}\nabla_m^\alpha\nabla_j^\delta\tilde{V}(R_1^0\ldots R_N)$$

$$+(1-e^{-ik\cdot(R_m^0-R_j^0)})\nabla_m^\alpha\nabla_m^\delta\tilde{T}_{mj}\sum_\sigma\langle c_{m\sigma}^+c_{j\sigma}-c_{m\sigma}c_{j\sigma}^+\rangle], \tag{14}$$

and

$$\tilde{V}(R_1^0 \dots R_N^0) = \exp\left\{\frac{1}{2} \sum_{\substack{lm \\ \alpha\beta}} \langle u_l^\alpha u_m^\beta \rangle \nabla_l^\alpha \nabla_m^\beta \right\} V(R_1^0 \dots R_N^0), \qquad (15)$$

$$\tilde{T}_{mj} = \exp\left\{\frac{1}{2} \sum_{\beta_1 \beta_2} \langle (u_m^{\beta_1} - u_j^{\beta_1})(u_m^{\beta_2} - u_j^{\beta_2}) \rangle \nabla_m^{\beta_1} \nabla_m^{\beta_2} \right\} T_{mj}^0. \qquad (16)$$

According to the spectral theorem for the Green function (13) it is easy to obtain the phonon correlation function

$$\langle u_m^\alpha u_{m'}^\beta \rangle = \frac{1}{MN} \sum_{k,s} \frac{e_{k,s}^\alpha e_{k,s}^\beta}{2\omega_{k,s}} \operatorname{cth}\left(\frac{\omega_{k,s}}{2\theta}\right) e^{ik \cdot (R_m^0 - R_{m'}^0)}. \qquad (17)$$

We should now calculate the electron Green function (7). In order to do this we should make the same approximation as in (9), (10) and (11) for the higher order Green functions. We follow paper [11]. We obtain the same formula for the electron Green function as in [11] the only difference being that we have to replace the hopping integral $T_{ij}$ therein by $\tilde{T}_{ij}$ as given by formula (16).

### 3. Temperature depending bandwidth in the pseudoharmonic approximation

We define the space Fourier transformation of the hopping integral (5′) as usually (cf. [6])

$$T_{ij}^0 = \frac{1}{N} \sum_q (\varepsilon_q - T_0) e^{iq \cdot (R_i^0 - R_j^0)}, \qquad (18)$$

and

$$\varepsilon_q - T_0 = \sum_{(R_i^0 - R_j^0)} T_{ij}^0 e^{-iq \cdot (R_i^0 - R_j^0)}, \qquad (19)$$

where $\varepsilon_q$ is the $s$-band energy and $T_0 = T_{ii}^0$. Eq. (19) leads, for the simple cubic lattice restricted to the nearest neighbours, to the well known result

$$\varepsilon_q - T_0 = \frac{\Delta}{6}(\cos q_x a + \cos q_y a + \cos q_z a), \qquad (20)$$

where $\Delta$ is the bandwidth of the $s$-band and $a$ is the lattice constant. According to (18) and (19) the space Fourier transformation of the hopping integral (16) is

$$\tilde{\varepsilon}_q - T_0 = \sum_{(R_i^0 - R_j^0)} \tilde{T}_{ij} e^{-iq \cdot (R_i^0 - R_j^0)} \approx \frac{1}{N} \sum_{q'} \sum_{(R_i^0 - R_j^0)} (\varepsilon_{q'} - T_0)$$
$$\times \exp\left\{-\frac{1}{2} \sum_{\beta_1 \beta_2} \langle (u_i^{\beta_1} - u_j^{\beta_1})(u_i^{\beta_2} - u_j^{\beta_2}) \rangle q'^{\beta_1} q'^{\beta_2} \right\} e^{i(q'-q) \cdot (R_i^0 - R_j^0)}, \qquad (21)$$

where $\varepsilon_{q'} - T_0$ is given by formula (20). Taking into account (17) and performing the summation over $(R_i^0 - R_j^0)$ we get

$$\tilde{\varepsilon}_q - T_0 = \sum_{i=x,y,z} (A_i \cos q_i a + B_i \sin q_i a), \qquad (22)$$

where

$$A_x = \frac{2}{N} \sum_{q'} (\varepsilon_{q'} - T_0) \exp\left\{-\sum_{\beta_1 \beta_2} a^{\beta_1 \beta_2}(x) q'^{\beta_1} q'^{\beta_2}\right\} \cos q'_x a \qquad (23)$$

$$B_x = \frac{2}{N} \sum_{q'} (\varepsilon_{q'} - T_0) \exp\left\{-\sum_{\beta_1 \beta_2} a^{\beta_1 \beta_2}(x) q'^{\beta_1} q'^{\beta_2}\right\} \sin q'_x a \qquad (24)$$

and

$$a^{\beta_1 \beta_2}(x) = \sum_{k,s} \frac{e_{k,s}^{\beta_1} e_{k,s}^{\beta_2}}{NM\omega_{k,s}} \operatorname{cth}\left(\frac{\omega_{k,s}}{2\theta}\right) \sin^2\left(\frac{k_x a}{2}\right). \qquad (25)$$

Analogously to (23), (24) and (25) we may deduce the formulae for $A_y$, $A_z$, $B_y$, $B_z$, $a^{\beta_1 \beta_2}(y)$ and $a^{\beta_1 \beta_2}(z)$. It is easy to calculate the bandwidth of the $s$-band by finding the maximum and minimum of (22) as a function of $q$. This gives the bandwidth

$$\tilde{\Delta} = 2 \sum_{i=x,y,z} (A_i^2 + B_i^2)^{1/2}. \qquad (26)$$

As will be seen from (23), (24) and (25) this bandwidth is temperature dependent due to pseudoharmonic phonons.

## 4. Numerical calculation of the bandwidth as a function of temperature and the Metal-Insulator Transition

The calculation of the bandwidth (26) as a function of temperature is very difficult because we need to know $\omega_{k,s}$ and $e_{k,s}$ as a function of $k$, where $\omega_{k,s}$ is given by the very complicated formula (14) and $e_{k,s}$ is in general not known. For simplicity we assume that the lattice of the crystal can be described by the very well known Hamiltonian

$$H_1 = \sum_{k,s} \omega_{k,s}(a_{k,s}^+ a_{k,s} + \tfrac{1}{2}). \qquad (27)$$

But even in this case the calculation of the bandwidth is still not a simple task. To define $\omega_{k,s}$ as a function of $k$ we assume the Debye model for the heat capacity of the lattice. Since we considered a simple cubic lattice we have only three acoustic branches with $\omega_{k,s} = v_s k (s = 1, 2, 3)$, where $v_s$ is the sound velocity. We assume that the polarization vectors $e_{k,s}$ are directed in a way such that $e_{k,3}$ is parallel to $k$, $e_{k,1}$, $e_{k,2}$ are orthogonal to $k$, $e_{k,1} \perp e_{k,2}$, $|e_{k,s}| = 1$ and for $s = 1, 2$ we have $v_1 = v_2 = v_t$ (transverse branches) and for $s = 3$ we have a longitudinal branch with velocity $v_3 = v_l$. Under these assumptions the numerical calculations were performed. We can change the sums over $k$ and $q$ to

integrals, estimate the parameters $v_t$, $v_1$, $a$, $M$, $\Delta$ (see (20)) and the radius of the Debye sphere $k_{max}$ [1]. Fig. 1 shows the resulting temperature dependence of $\tilde{\Delta}$. We see that $\tilde{\Delta}$ behaves quite linearly and decreases with increasing temperature. For $T = 0$ K the bandwidth $\tilde{\Delta}$ is greater than $\Delta$ by about $\Delta/6$. For more complicated crystal structures with more than 1 atom per unit cell there exist optical phonons, too. In this case we expect a sharper dependence of $\tilde{\Delta}$ on $T$. For a half-filled band Hubbard has shown [11] that
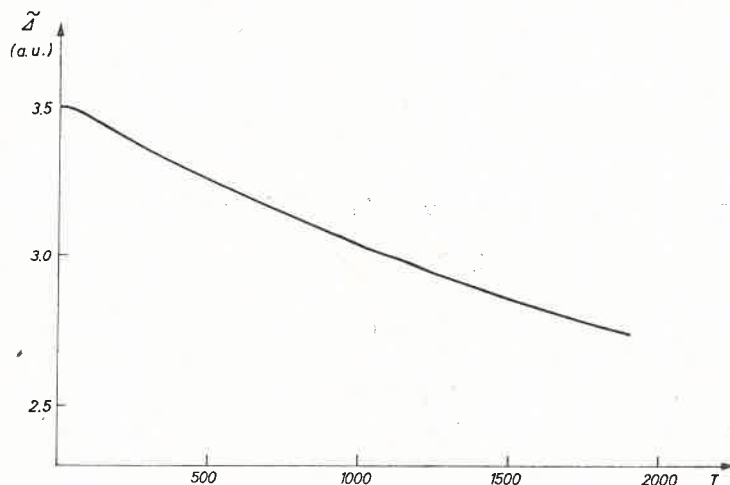


Fig. 1. Dependence of the bandwidth on temperature

the density of states depends on the ratio $\Delta/U^2$. $\Delta$ and $U$ in his considerations were temperature independent. In our treatment we have $\tilde{\Delta}$ temperature dependent due to pseudoharmonic phonons and $U$ temperature independent. Assuming $U = \mathrm{const}$ and $\tilde{\Delta}$ to be temperature dependent we can obtain two possibilities: an insulating phase at all temperatures, as well as a metallic phase at low temperatures and an insulating phase at higher temperatures[3]. We see that the second possibility is in disagreement with the experimental results [18] and reminds one a little of the prediction of the small polaron theory [15–17, 19]. Although we have considered only the simplest pseudoharmonic approximation, it seems, however, that the anharmonism alone cannot give the insulating

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[1] The following values of parameters were taken: $v_t = 950$ m/sec, $v_l = 2000$ m/sec, $a = 5.63$ Å (NaCl), $M = 3.84 \cdot 10^{-23}$ g(Na), $\Delta = 3$ (arbitrary unit), $k_{max} = 0.69$ Å$^{-1}$.

[2] Recently Sakoh and Shimizu [13], using the functional integral method with the static approximation, have shown that the density of states for the Hubbard model (without phonons) in the case of a half-filled band is temperature dependent. These authors say that the Hubbard treatment [11] is valid only for $T = 0$K, which is not true. The Hubbard treatment is true for $T \neq 0$K but the density of states is temperature independent. The functional integral method used by these authors in the static approximation gives for some values of the Coulomb integral $U$ a negative specific heat (see e.g. [14]). Calculations of the magnetic susceptibility may produce unphysical results.

[3] It depends on the choice of $U$. For $U = 1.7517$ and $\tilde{\Delta}(T = 0) = 3.5034$ we obtain the insulator phase at all temperatures. After choosing $U = 2.4773$ and $\tilde{\Delta}(T = 0) = 3.5034$ we obtain a metallic phase up to $T_{cr} = 1516$ K and insulating phase above.

phase at low temperatures and the metallic phase at higher temperatures in the frame of the Hubbard III approximation, but when the metallic phase is reached it leads with increasing temperature to a gradual transition back to the insulating phase. It is known from the experimental data (cf. [20, 21]) that $V_2O_3$ is an insulator at low temperatures and at about 160 K a transition to the metallic phase occurs. At 550 K, however, a gradual transition back to the insulating state takes place. Quite an analogous situation was found in $Ti_2O_3$. According to [22] the transition to the metallic state occurs at 660 K and a gradual transition back to an insulating state at about 1000 K. The existing theoretical models [23–28] are Hubbard-like. Because the back transition takes place at rather high temperatures, in our opinion the transition from a metallic to an insulating state can be caused by the anharmonism in the same way as described above for the Hubbard model.

### 5. Pseudoharmonic phonons and conductivity of the Mott insulator

There were many attempts to calculate the electrical conductivity for the Hubbard model. Most of them were based on the well known Kubo formula [29]. Because the conductivity $\sigma$ is represented by a two-particle Green function we can determine the conductivity only for some special cases. Bari, Adler and Lange [30] have calculated the conductivity in the atomic limit only. Kubo [31] has used the Kubo formula and the decoupling procedure introduced by Hubbard [6] and Sakurai [32]. Kikoin and Flerov [33] have presented in their paper another type of decoupling but it leads to the same result as [31]. Bari and Kaplan [34] with the aid of the Kubo formula have calculated

the conductivity in the limiting case $\lim\limits_{\Delta \to 0} \dfrac{\sigma}{\Delta^2}$. Barma and Bari [5] have considered the

coupling of narrow band electrons to lattice vibrations and the electrical conductivity for the Mott insulator. Eswaran and Kimball [35] have presented the calculations of the conductivity in the strong interaction limit in the presence of impurities. Nolting [36] has proposed an approximate expression for the conductivity by the method of spectral moments. His expression reproduces all limiting cases which can be calculated exactly. Recently, many authors try to calculate the electrical resistivity rather than the conductivity (cf. e. g. [37, 38]. Very recently De Marco, Economou and Licciardello [39] have calculated the dc conductivity for the Hubbard model by using a very restrictive approximation.

We now calculate the conductivity of the Mott insulator in the presence of pseudoharmonic phonons. We select the approach of Bari and Kaplan [34]. According to the Kubo formula the conductivity is given by

$$\sigma(\omega) = \frac{1}{2V} \int\limits_{-\infty}^{\infty} d\tau e^{i\omega\tau} \int\limits_{0}^{1/\theta} d\lambda \langle Je^{iH(\tau+i\lambda)} Je^{-iH(\tau+i\lambda)} \rangle, \tag{28}$$

where the current operator

$$J = -ie \sum (R_i - R_j) T_{ij} c_{i\sigma}^+ c_{j\sigma} \tag{29}$$

and $R_i$ are the components of the lattice-site position vectors parallel to the external electric field. Performing the same decoupling as in (11) and taking into account (29), formula (28) may be written in the form

$$\sigma(\omega) = -\frac{e^2}{2V} \int\limits_{-\infty}^{\infty} d\tau e^{i\omega\tau} \int\limits_{0}^{1/\theta} d\lambda \sum_{\substack{ij\sigma \\ lm\sigma'}} \langle (R_i - R_j) T_{ij} e^{iH(\tau+i\lambda)} (R_l - R_m)$$

$$\times T_{lm} e^{-iH(\tau+i\lambda)} \rangle \langle c_{i\sigma}^+ c_{j\sigma} e^{iH(\tau+i\lambda)} c_{l\sigma'}^+ c_{m\sigma'} e^{-iH(\tau+i\lambda)} \rangle. \tag{30}$$

According to [34] we have

$$\langle c_{i\sigma}^+ c_{j\sigma} e^{iH(\tau+i\lambda)} c_{l\sigma'}^+ c_{m\sigma'} e^{-iH(\tau+i\lambda)} \rangle$$

$$= \delta_{\sigma\sigma'} \delta_{jl} \delta_{im} \frac{e^{-\xi} + 2e^{U/\theta} + e^{\xi} e^{U/\theta}}{4(1+e^{U/\theta})^2}, \tag{31}$$

with $\xi = iU(\tau + i\lambda)$ and the chemical potential for the half-filled band $\mu = \dfrac{U}{2}$ (cf. [40, 41]).

To calculate the first average in (30) we make the simplest approximation

$$\langle (R_i - R_j) T_{ij} e^{iH(\tau+i\lambda)} (R_i - R_j) T_{ij} e^{-iH(\tau+i\lambda)} \rangle \approx a^2 \langle T_{ij} \rangle^2 = a^2 \tilde{T}_{ij}^2, \tag{32}$$

where $\tilde{T}_{ij}$ is given by formula (16). According to (21) and (25) we may write

$$\sum_{ij} \tilde{T}_{ij}^2 = \frac{1}{N^2} \sum_{\substack{q_1, q_2 \\ i,j}} (\varepsilon_{q_1} - T_0)(\varepsilon_{q_2} - T_0)$$

$$\times \exp\left\{-\frac{1}{2} \sum_{\alpha,\beta} \langle (u_i^\alpha - u_j^\alpha)(u_i^\beta - u_j^\beta) \rangle q_1^\alpha q_1^\beta \right\} \exp\left\{-\frac{1}{2} \sum_{\alpha,\beta} \langle (u_i^\alpha - u_j^\alpha)(u_i^\beta - u_j^\beta) \rangle q_2^\alpha q_2^\beta \right\} e^{iq_1 \cdot (R_i^0 - R_j^0)}$$

$$\times e^{iq_2 \cdot (R_i^0 - R_j^0)} = \frac{N}{2}(A_x^2 + A_y^2 + A_z^2 - B_x^2 - B_y^2 - B_z^2), \tag{33}$$

where $A_i$ and $B_i$ $(i = x, y, z)$ are given by (23) and (24). Thus the dc conductivity for the Mott insulator in the presence of pseudoharmonic phonons is

$$\sigma_A = \frac{\pi N e^2 a^2}{2V} \frac{e^{U/2\theta}}{\theta(1+e^{U/2\theta})^2}(A_x^2 + A_y^2 + A_z^2 - B_x^2 - B_y^2 - B_z^2). \tag{34}$$

Simultaneously the dc conductivity obtained in [34] is

$$\sigma = \frac{\pi N e^2 a^2 z \Delta^2}{144 V} \frac{e^{U/2\theta}}{\theta(1+e^{U/2\theta})^2}, \tag{35}$$

where $z$ is the number of nearest neighbours. When we define

$$\sigma_0 = \frac{e^{U/2\theta}}{\theta(1+e^{U/2\theta})^2}, \tag{36}$$

the normalized $\sigma_A$ can be written in the form

$$\sigma_A^{norm} = \frac{12}{\Delta^2}\,\sigma_0(A_x^2 + A_y^2 + A_z^2 - B_x^2 - B_y^2 - B_z^2), \tag{37}$$

where we have substituted $z = 6$ (simple cubic lattice). In the absence of lattice vibrations $A_x = A_y = A_z = \dfrac{\Delta}{6}$, $B_x = B_y = B_z = 0$ and $\sigma_A^{norm} = \sigma_0$ as it should be. The numerical calculations of $\sigma_A^{norm}$ as a function of temperature were made analogously to the calculations of the temperature dependent bandwidth described in Section 4. We again assume that the lattice can be described by the Debye model. In this way we calculate $A_i$ and $B_i$
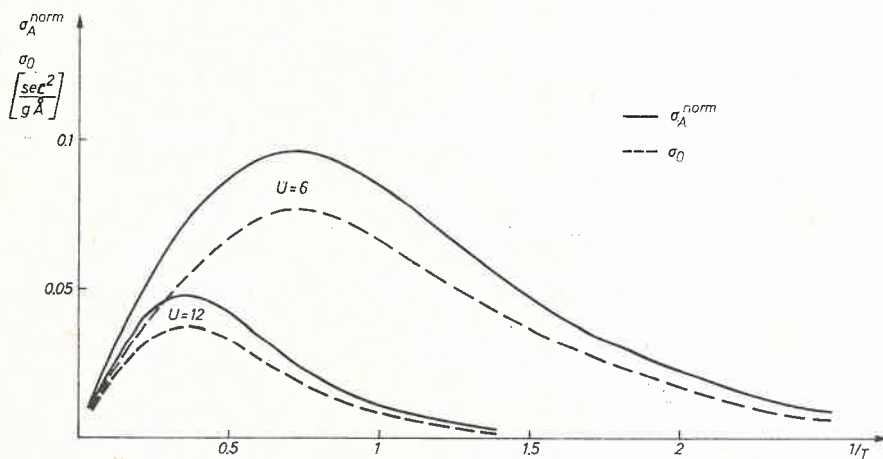


Fig. 2. Dependence of $\sigma_A^{norm}$ and $\sigma_0$ on reciprocal temperature

$(i = x, y, z)$ and subsequently $\sigma_A^{norm}$. The dependence of $\sigma_A^{norm}$ on the reciprocal temperature compared to $\sigma_0$ is given in Fig. 2. We see that the maxima of $\sigma_A^{norm}$ and $\sigma_0$ occur at the same temperature but $\sigma_A^{norm}$ exceeds $\sigma_0$ at all temperatures. The maxima of $\sigma_A^{norm}$ and $\sigma_0$ are shifted to higher temperatures with increasing $U$. The obtained result shown in Fig. 2 qualitatively agrees with the result of paper [5].

## 6. Conclusions

Assuming the Hubbard approximation [11] for the electron Green function we have investigated the influence of anharmonism in the pseudoharmonic approximation on the electron properties of the nondegenerated $s$-band. It leads to the conclusions that in order to obtain the insulating phase at low temperatures and the metallic phase at higher temperatures in the frame of the Hubbard model for a half-filled band with a bandwidth $\tilde{\Delta}$ depending on temperature and constant $U$ (there is no reason to keep $U$ temperature

dependent) $\tilde{\Delta}$ should be an increasing function of temperature between 0 K and $T_{cr}$. Above $T_{cr}$ the bandwidth $\tilde{\Delta}$ should be a constant and further, should decrease with temperature (as described by the anharmonism). We now see that besides the anharmonism there must exist some other mechanism responsible for such a behaviour of $\tilde{\Delta}$ with temperature. But up to now this mechanism is not known.

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