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MOTT’S $T^{1/4}$ LAW AS AN EVIDENCE OF A WIGNER INSTABILITY

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Résumé. — En analysant la perméabilité diélectrique statique nous constatons que, si les états électroniques sont localisés autour du niveau de Fermi, les électrons subissent une instabilité de Wigner à cause du champ d'Hartree, avec une période de base du réseau proportionnelle à $T^{-1/4}$. Nous utilisons ce résultat pour la discussion de la loi de Mott.

Abstract. — From an analysis of the static dielectric constant it is suggested that, if the electron states are localized around the Fermi energy, electrons there undergo a Wigner instability as a result of the Hartree field, with a lattice spacing proportional to $T^{-1/4}$. This result is used to discuss Mott’s law.

When electron states are localized around the Fermi energy, static conduction can occur by phonon-assisted hopping, the energy required in hops being available from the phonon field. Mott [1] first suggested that at sufficiently low temperatures such a mechanism should lead to the formula for the conductivity $\sigma$ as a function of temperature $T$:

$$\sigma = \sigma_0 \exp(-T_0/T)^{1/4}$$  \hspace{1cm} (1)

where $\sigma_0$ and $T_0$ are constants.

Some methods proposed so far [2, 3, 4] to derive this law have contained the common assumption that both the positions and energies of the traps are uncorrelated and have ignored the effect of long-range spatial correlations on the hopping process due to the electron-electron interaction.

Whether eq. (1) is modified on taking correlation into account is still controversial.

Efros et al. [5, 6] find that the density of states around the Fermi surface is modified from a constant value, which leads to (1), as a result of the Coulomb term $e^2/R$, $R$ being the hopping distance, and that this leads to an exponent 1/2 in (1). A recent analysis of Mott [7, 8] on the other hand indicates a persistence of the exponent 1/4 a result, presumably, of the screening of the Coulomb field.

Having in mind a correlated state of the type described by Wigner [9] we investigate this problem in two successive stages: first we calculate the wave-vector dependent static dielectric constant and detect an eventually long-ranged correlated state as a zero of it and second the results are used to discuss Mott’s law (1).

Actual calculations are carried on by using a self-consistent decoupling procedure proposed by us recently [10] and successfully applied to both the electron density of states and localization problems and by considering low temperatures where the electron-electron interaction can be introduced as a Hartree field [11].

Let us then consider a model system where a random potential is applied to the electrons: when a weak external potential $V(r)$ is applied to it the electron charge changes according to:

$$\langle \Delta \rho(r) \rangle = e \int \text{d}f(e) \text{Im} \langle \text{d}r' G(r, r') V(r') G(r', r) \rangle$$  \hspace{1cm} (2)

where $\langle \cdots \rangle$ is an ensemble average taking the randomness of the potential into account, $f(e)$ is the Fermi-Dirac distribution and $G(r, r')$ is the single particle electronic Green’s function of the system. From (2) a self-consistent field is generated, by means of Poisson’s equation, due to the Hartree field, and this is included in $V(r)$ in a self-consistent way, following closely a standard procedure [12].

In the limit of small $q$ the static dielectric constant $\varepsilon(q)$ is found to be:

$$\varepsilon(q) = 1 - (4\pi e^2/q^2) \Sigma_k \frac{F(k - q) - F(k)}{E(k - q) - E(k)}$$  \hspace{1cm} (3)
where $E(k)$ is the solution of the eigenvalue equation:

$$E(k) - \epsilon(k) - \Sigma_R(k, E(k)) = 0 \quad (4)$$

and $F(k)$ is given by:

$$F(k) = \text{Im} \int \frac{1}{\epsilon - \epsilon(k)} \Sigma(k, \epsilon) \times \left(1 - \frac{\partial}{\partial \epsilon} \Sigma(k, \epsilon) \right) \quad (5)$$

$\Sigma(k, \epsilon)$ being the self-energy in the absence of the Coulomb interaction and $\Sigma_R = \text{Re} \Sigma$, $\epsilon(k) = \frac{\hbar^2}{2m} k^2$.

We omit the derivation as it is straightforward and makes use of the decoupling of the product of the Green’s functions in (2) as described in reference [10].

As a limiting case, which serves as a test of the approximation used, we note that when the degree of disorder is negligible, eq. (3) becomes the usual Lindhard expression [12] for the free Fermi gas.

If now the Fermi energy lies well inside a region of energy where states are localized, the integration in (5) receives the largest contribution from a negative integrand, as follows by splitting $\Sigma(k, \epsilon)$ into its real and imaginary parts $\Sigma_R(k, \epsilon)$ and $\Sigma_I(k, \epsilon)$ and using the results $\Sigma_I = \eta$, $\eta$ being an infinitesimal [10] and

$$1 - \frac{\partial}{\partial \epsilon} \Sigma_R < 0 \quad [13, 14].$$

This implies on the other hand that $\epsilon(q) = 0$ at a certain $q_0$. The calculation of $q_0$ is easy enough at long wave-lengths giving:

$$q_0^2 = 4 \pi e^2 \Sigma_k - \frac{\partial \epsilon(E(k))}{\partial E(k)} \quad (6).$$

We have interpreted the $q_0$ instability as a Wigner state instability [9] corresponding to the electrons being accommodated on a lattice whose spacing is $R \cong q_0^{-1}$ essentially due to the fact that it corresponds to the vanishing of the static wavevector dependent dielectric constant. It is to be emphasized that this does not apply to the whole electron gas, but just to electrons excited from the Fermi sea, which constitute a low-density, weakly interacting, quasi-particle gas at low temperatures; these are the electrons which participate in the hopping when the electron-phonon coupling is introduced so that the Wigner-like arrangement is expected to provide a hopping distance of the order of $R$.

For the calculation the solutions to eq. (4) and then (6) are needed. For the electrons considered here we look for a solution of eq. (4) such that $E(k) \approx E_F$ where $E_F$ is the Fermi energy, thus

$$E(k) \approx \epsilon(k) + \Sigma_R(k_F, E_F) \quad (7)$$

which is the definition of the Fermi momentum $k_F$.

Consistently with the previous assumption that $E_F$ lies well inside the region of localized states, which is equivalent to have taken $\partial \Sigma_R/\partial \epsilon \gg 1$ we can now suppose that $\Sigma_R(k_F, E_F) \gg \epsilon(k_F)$ which, on interpreting eq. (7) as an energy conservation, amounts to saying that the potential energy dominates the kinetic energy. The solution of eq. (4) can then be written, under these circumstances, as:

$$E(k) \approx \epsilon(k) + E_F \quad (8)$$

On substituting this result in eq. (6), after some algebra, we get:

$$q_0 = \pi T^{1/4} \quad (9)$$

which carries that $1/4$ characteristic exponent of the hopping law (1), where:

$$r = (4 \pi e^2 / \sqrt{\pi} \cdot \hbar^3 / 2m^2)^{1/2} k^{1/4} \times \left( \int_0^{1/2} \ln \left( \frac{1-x}{x} \right)^{1/2} dx \right)^{1/2} \quad (10).$$

The discussion on hopping can be made quantitative by considering now transition probabilities of the form [2,7]:

$$P(R) = K \exp(-2 \alpha R - \Delta E/kT) \quad (11)$$

between any two localized states distant $R$ apart, $\alpha$ being a constant describing the exponential decay in space of each state, $\Delta E$ the activation energy and $K$ a constant characteristic of the electron-phonon coupling. For the electrons considered here we can calculate $\Delta E$ from the unperturbed density of localized states $N(0)$ at the Fermi surface:

$$\Delta E = \left( \frac{4}{3} \pi N(0) \right)^{-1} R^{-3}$$

as the main effect of the Hartree field is to produce the crystalline arrangement without appreciable change of the energy spectrum. By then using $q_0^{-1}$ as the hopping distance as discussed previously one finds eq. (1) with

$$T_0 = [2 \alpha \gamma + (4/3) k \pi \gamma^3 N(0)^{-1}]^4, \quad \gamma = RT^{1/4}. \quad$$

As a conclusion we can say that the hopping $T^{1/4}$ law continues to hold when electron-electron interactions are introduced as a result of the formation of the Wigner state.

Our results agree with Mott’s conclusion [8] as far as the conductivity is concerned and show that the Coulomb term $\sim e^2 / R$ turns out to be small, in contrast
with Efros et al. [5, 6], the hopping distance being large.

We note that we have implicitly used, during the calculations, an average description of the system in terms of an ensemble averaged Green’s function in the region of localized states and have used localization conditions consistent with such a description following Mattis and Yonezawa [13] and ourselves [10].

An alternative description based on averaged probabilities and hence on averages of products of Green’s functions seems to be hopeless here and it is a controversial matter to decide whether it would give a different answer. The fact that one localization criterion, namely the vanishing of the imaginary part of the self energy follows from the vanishing of the conductivity [10] is a strong suggestion for the equivalence of the two approaches.

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References