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LETTER TO THE EDITOR

Interaction effects and thermoelectric power in low-temperature hopping

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Abstract. The effect of electron–electron interactions on the thermoelectric power for hopping transport in two and three dimensions is calculated in the low-temperature limit. While the conductivity requires a very precise measurement to extract a temperature exponent with enough precision to determine the role of the interactions, it is shown that the thermopower behaviour will reflect the presence of interactions in an unambiguous manner. In contrast to a Mott variable-range hopping model where the thermopower decreases to zero as the temperature decreases ($S = 0$ at $T = 0$), the thermopower in an Efros interaction model should approach a non-zero constant as $T \rightarrow 0$.

While the problem of hopping between localised states has been around for several years (Miller and Abrahams 1960, Mott 1968, Efros and Shklovskii 1975), the role of any possible electron–electron interactions, and their physical manifestation in the transport properties such as conductivity and Hall effect, has never been very clear (Redfield 1973, Ambegaokar *et al* 1971, Pollak *et al* 1973, Mott 1975, 1976, 1980, Efros *et al* 1979, Benzaquen and Walsh 1984). Other transport properties have generally been neglected or have shed little light on the role interactions may play in the low-temperature properties of disordered systems (Clark 1967, Khosla and Fischer 1970, Clark *et al* 1974, Zvyagin 1973 and Overhof 1975). In this communication, we wish to point out that the role of an Efros-type pseudogap (Efros 1976) in the density of states will have a profound effect on the thermopower and allow an unambiguous determination of the presence of electron–electron interactions, if any, in the single-particle transport properties of a system. We also argue that the manifestation of any interaction effects should be more gradual and occur at higher temperatures than has been previously assumed.

Mott (1968) showed that if R_0 is the average spacing between localised states, and if the electronic wave-functions taper off as $\exp(-\alpha r)$, then if $\alpha R_0 < 1$ the DC conductivity of the system is determined by maximising the distance that a localised electron whose energy is within $k_B T$ of the Fermi level μ can hop under the opposing conditions of the exponential decrease of hopping probability with distance and between nearby states with large energy differences (as compared to $k_B T$). Such a process results in a DC conductivity of

$$\sigma(T) = \sigma_0 \exp[-(T_0/T)^{1/(d+1)}] \tag{1}$$

where d is the dimensionality,

$$T_0 = \left[(2\alpha)^d \frac{\Gamma(d/2+1)}{D(\mu)\pi^{d/2}k_b}\right](d^{1/(d+1)} + d^{-d/(d+1)})^{d+1} \tag{2}$$

the density of states $D(\mu)$ is assumed constant and σ_0 is only weakly dependent on temperature. The carriers in this model transport, on the average, an amount of energy

$$E_{\mathrm{h}} = \left[\frac{\Gamma(d/2+1)}{D(\mu)\pi^{d/2}}\right]^{1/(d+1)} \left[\frac{2\alpha K_b T}{d}\right]^{d/(d+1)} \tag{3}$$

where $\Gamma(x)$ is the gamma function, rather than $(E_{\mathrm{gap}} - \mu)$ for a semiconductor or $D_0(\mu)[k_{\mathrm{B}}T]^2$ for a metal.

Efros *et al* (1979: see also Efros 1976, Efros and Shklovskii 1975) consider the problem of electron–electron interactions in a system which would otherwise display Mott variable-range hopping. They describe the system with a Hamiltonian

$$H = \sum_i \varepsilon_i n_i + \sum_{i \neq j} \frac{e^2 n_i n_j}{K|\boldsymbol{r}_i - \boldsymbol{r}_j|} \tag{4}$$

where ε_i is the 'bare' energy of the ith electronic state, K is the dielectric constant of the medium and n_i is the occupation number of the ith state, which due to the Pauli exclusion principle is either 0 or 1. The ground state of such a system is given by the following condition. In the system ground state, all n_i for states with $\varepsilon < \mu$ are equal to 1 and all other n_i are equal to zero.

There is, however, one additional requirement. Suppose at $T = 0$ one considers two states i and j where in the system ground state i is occupied and j is empty. If the electron in the state i is removed and placed in state j, the system cannot be in its ground state (we have excited a particle), and so the energy of the system should have changed by

$$\Delta E_{i \to j} = \varepsilon_j - \varepsilon_i - \frac{e^2}{K|\boldsymbol{r}_i - \boldsymbol{r}_j|} > 0 \tag{5}$$

where the last term may be regarded as the energy of the resulting electron–hole pair. Since the system started in its ground state, any net rearrangement of the occupation of the states must increase the system energy.

Therefore, any two states, separated by the Fermi level (μ) in the ground state, must satisfy equation (5). This requires that the hopping energy (E_{h}) must obey (Efros *et al* 1979, Efros 1976, Efros and Shklovskii 1975)

$$E_{\mathrm{h}} > \left[\frac{\mathrm{e}^{2d}}{K^d} \frac{D_0(\mu)\pi^{d/2}}{\Gamma(d/2+1)}\right]^{1/(d-1)} \equiv \Delta. \tag{6}$$

This says that a hop from an occupied state below μ to an unoccupied state above μ is only possible if the resulting electron and hole have enough energy to resist recombination. Efros *et al* argue that a constant single-particle density of states would allow E_{h} to be arbitrarily small, which would contradict equation (6). The *minimum* criterion for equation (6) to hold is for the density of states to follow

$$D(\varepsilon) = \left[\frac{2|\varepsilon - \mu|}{\Delta}\right]^{d-1} D_0(\varepsilon) \tag{7}$$

for $|\varepsilon - \mu| < (\Delta/2)$ and $D(\varepsilon) = D_0(\varepsilon)$ for $|\varepsilon - \mu| > (\Delta/2)$, where $D_0(\varepsilon)$ is the 'non-interacting' density of states, resulting in

$$E_h(\text{Efros}) = (e^2/K)^{1/2}(2\alpha k_B T)^{1/2} \tag{8}$$

when $E_h(\text{Mott}) < \Delta$. In other words, a soft Coulomb gap must exist in the density of states about μ. In this model, Efros argues that Mott-type variable-range hopping should be valid above some critical temperature (T_c)

$$T_c = \frac{1}{k_B}\left(\frac{e^2}{K}\right)^{(d+1)/(d-1)}\left(\frac{d}{2\alpha}\right)\left[\frac{D_0\pi^{d/2}}{\Gamma(d/2+1)}\right]^{2/(d-1)}. \tag{9}$$

If however, $T \ll T_c$, the states within the Coulomb gap are extremely important, resulting in a conductivity (Efros 1976, Efros *et al* 1979)

$$\sigma(T) = \sigma_0 \exp[-(T'_0/T)^{1/2}] \tag{10}$$

independent of the system dimensionality, where

$$T'_0 = (8\alpha e^2)/k_B K \tag{11}$$

and again, σ_0 is only weakly temperature-dependent.

While the presence of a 'soft' gap in the single-particle density of states altering the conductivity from that given by equation (1) to that given by equation (10) is hardly dramatic, it is feasible, albeit not trivial, to perform measurements on 'hopping systems' covering enough dynamic range with sufficient accuracy to distinguish between a $\log(\sigma) \propto T^{1/4}$ and $\log(\sigma) \propto T^{1/2}$ dependence. Unfortunately, after over a decade of controversy the experimental situation is far from clear. In crystalline GaAs for example, Benzaquen and Walsh (1984) find $\log(\sigma) \propto T^{1/4}$, while in slightly more heavily doped samples Redfield (1973) found $\log(\sigma) \propto T^{1/2}$. In the following, we will show that the thermopower for a system described by an Efros-type model displays a radically different behaviour from the corresponding non-interacting Mott picture.

The thermopower can be calculated from the Peltier coefficient

$$\boldsymbol{Q} = \Pi \boldsymbol{J} \tag{12}$$

(where $\boldsymbol{Q}$ is the heat current of the carriers and $\boldsymbol{J}$ their electrical current) using the Onsager relation

$$\Pi = TS. \tag{13}$$

For a metal, the average heat per carrier is proportional to the specific heat C times the temperature, and the heat current is $v\int_0^T C(T)\,dT$, with v the average electronic drift velocity. The electrical current is $J = -nev$ with n the electron density, and the specific heat is $\sim nk_B[D(\mu)k_B T]$. The Peltier heat and the thermopower are then given by

$$\Pi \propto (1/ek_B)D(\mu)(k_B T)^2 \tag{14}$$

$$S(T) \propto (D(\mu)/e)k_B T \tag{15}$$

resulting in the familiar result for a metal of $S \to 0$ as $T \to 0$.

For both the Mott and the Efros variable-range hopping models, the distribution of electrons responsible for the conductivity has a characteristic width E_h rather than $k_B T$. One might then expect the expressions for the Peltier heat (equation (12)) to be modified to

$$\Pi \propto (1/ek_B)D(\mu)(E_h)^2 \tag{16}$$

where E_h is given by equation (3) for the Mott picture and equation (8) for the Efros picture, giving thermopowers of the form

$$S(T) \propto T^{(d-1)/(d+1)} \qquad \text{(Mott picture)} \tag{17}$$

$$S(T) \propto \text{constant} \qquad \text{(Efros picture)}. \tag{18}$$

The thermopower for the Mott picture has been predicted for three dimensions (Zvyagin 1973, Overhof 1975, Mott and Davis 1979) and an extension to d dimensions gives

$$S(T) = \frac{k_B}{2e}\left[\frac{\Gamma(d/2+1)}{D_0(\mu)\pi^{d/2}}\right]^{2/(d+1)} \left(\frac{2\alpha}{d}\right)^{2d/(d+1)} \left[\frac{\partial \ln D_0(\varepsilon)}{\partial \varepsilon}\right]_{\varepsilon=\mu} (k_B T)^{(d-1)/(d+1)} \tag{19}$$

so that S does indeed vary as $T^{(d-1)/(d+1)}$. Thus for three dimensions the thermopower tends to zero with a square root dependence and for the two-dimensional case it approaches zero as the cube root of temperature. In all cases where $d > 1$, $S \rightarrow 0$ as $T \rightarrow 0$ and for $d = 1$ the thermopower should be a constant.

The thermopower in the Efros model can be calculated for very low temperatures ($T < T_c$) in a manner similar to the Mott case, resulting in

$$S(T) = \frac{(E_h)^2}{2k_B T}\left[\frac{\partial \ln D_0(\varepsilon)}{\partial \varepsilon}\right]_{\varepsilon=\mu} \tag{20}$$

which using equation (8) becomes

$$S(T)(\text{Efros}) = \frac{k_B e}{K}\alpha\left[\frac{\partial \ln D_0(\varepsilon)}{\partial \varepsilon}\right]_{\varepsilon=\mu} \equiv S'. \tag{21}$$

A comparison between equations (9), (19) and (21) shows

$$S(T)(\text{Mott}) = \frac{1}{d}\left(\frac{T}{T_c}\right)^{(d-1)/(d+1)} S' \tag{22}$$

for the Mott non-interacting model and the Efros model for $T > T_c$.

Therefore, in the interacting system as interpreted by Efros, as the temperature of the system is lowered from infinity, the thermopower should decrease with decreasing temperature in the same manner as in the non-interacting (Mott) model. At the same time as the thermopower is following equation (22), the conductivity of the system (in both models) should follow equation (1). As T drops below T_c, while in the non-interacting model the thermopower will continue decreasing with decreasing temperature, in the interacting (Efros) model the states within the 'soft' gap begin to play an important role and the conductivity should change over to equation (10). As was shown above, the thermopower, which at $T = T_c$ has dropped to $(1/d)S'$, should now start to increase with decreasing temperature until at $T \ll T_c$, when it should level off to a non-zero constant, going as $S \rightarrow S'$ as $T \rightarrow 0$ rather than $S \rightarrow 0$ as $T \rightarrow 0$ as in the Mott case. This behaviour is illustrated in figure 1 for two and three dimensions. The full lines in figure 1 represent a purely Mott behaviour while the broken curves show the low-temperature deviation from the Mott model which an Efros-type system should display. The important point to note is that, according to an Efros-type description, if the change-over in behaviours occurs at T_c, then at no point below T_c (which is where Efros would say the two models disagree) does the thermopower in the Efros case decrease with decreasing temperature, while in a Mott model, at no point does the thermopower increase with decreasing temperature.

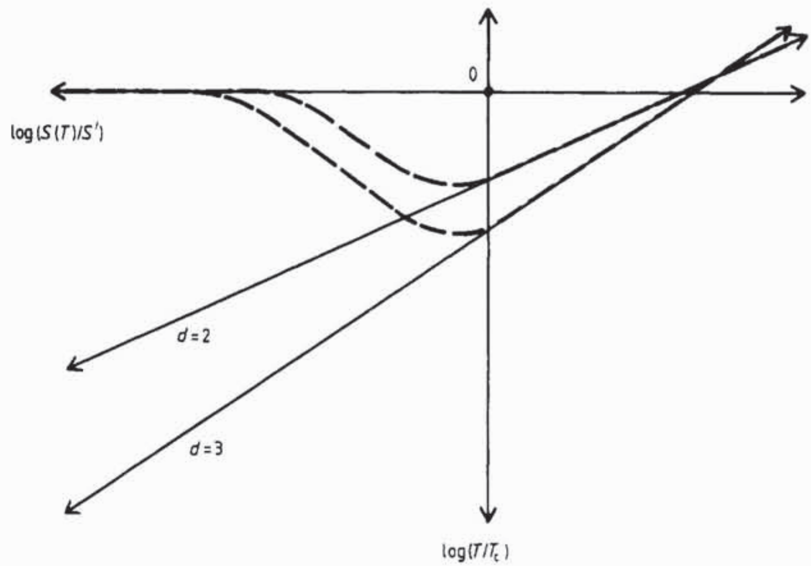

Figure 1. Thermopower as a function of temperature in variable-range hopping systems in two and three dimensions. Full lines show the non-interacting (Mott) model; broken curves show the deviation for the interacting-electron (Efros) model below T_c, assuming the states in the 'soft' gap become important only below T_c. S' is the thermopower in the interacting-electron picture at $T = 0$. At no point below T_c, which is the region where the Efros model conductivity should follow $\log(\sigma) \propto T^{-1/2}$, should the thermopower decrease with decreasing temperature.

Equation (6) describes the point when Mott-type hopping definitely breaks down in the presence of interactions and the states within the 'soft' gap can no longer be ignored. The calculations for the Efros model are all in limits of $T \gg T_c$ and $T \ll T_c$, with the change-over between behaviours occurring when

$$E_{\text{hop}}(\text{Mott}) = \Delta \tag{23}$$

which may actually represent a lower bound for the change-over in behaviours. We note that the change-over from Mott to Efros behaviour in the interacting model occurs when equation (23) is satisfied. The states within the gap may actually begin to play a role as early as when the two hopping activation energies are equal, i.e.

$$E_{\text{hop}}(\text{Mott}) = E_{\text{hop}}(\text{Efros})$$

which occurs at a temperature T_c' given by

$$T_c' = (d)^{(2d-1)/(d-1)}\, T_c.$$

Equation (22) can then be expressed in terms of T_c' as

$$S(T)(\text{Mott}) = (d)^{(d-2)/(d+1)} \left(\frac{T}{T_c'}\right)^{(d-1)/(d+1)} S'. \tag{24}$$

If the interactions manifest themselves at T_c' rather than T_c then as the temperature is lowered from infinity, the thermopower should decrease with decreasing temperature in the same manner as in the non-interacting (Mott) model. At the same time, the conductivity in both models should follow equation (1) as before; however, as T drops

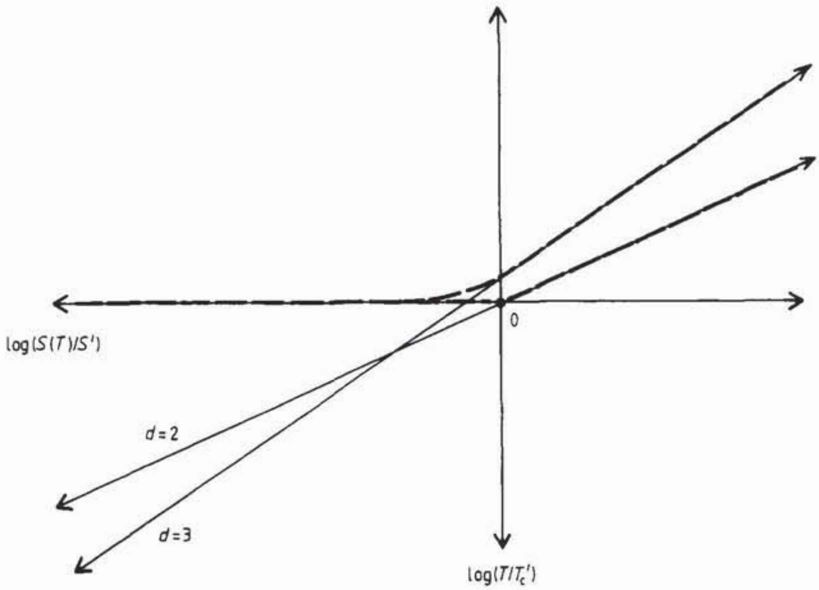

Figure 2. Same as figure 1, only assuming the states within the 'soft' gap influence the transport properties when the 'Efros' and 'Mott' hopping energies become comparable, which occurs at T_c'. S' is the thermopower in the interacting electron picture at $T = 0$.

below T_c', the thermopower in the Efros model should gradually level off (to $S(0) = S'$) as illustrated in figure 2, with $S(T_c') \sim 1.3\, S'$ for three dimensions and $S(T_c') \sim S'$ in two dimensions, while in the non-interacting model the thermopower will continue decreasing towards zero as the temperature is lowered. As T drops below T_c', the conductivity in the interacting system should change over to equation (10).

In conclusion, we have shown that the temperature dependence of the thermopower in a disordered system is much more sensitive to the presence of a 'soft' gap in the single-particle density of states than is the conductivity. While the use of the conductivity to determine the presence of electron–electron interactions requires the precise determination of a power law exponent which resides inside an exponential, to use the thermopower to gain the same information requires only the determination of whether or not it is a decreasing function of temperature at low temperatures.

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