

A many-body theory of conduction in electron glasses

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An analytic theory is developed for conduction in electron glasses that includes all the important correlations arising from many-body effects. The theory yields the same functional dependence of the conductance on temperature as the widely used Efros-Shklovskii (ES) theory where many body are neglected. The degree to which the present theory differs quantitatively from ES cannot be at present evaluated analytically.

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1. Introduction

In disordered electronic systems on the localized side of the Anderson transition [1] the basic transport mechanism consists of thermally induced transitions between localized electronic states. When electron-electron interactions are negligible, the conductivity is described by the well known Mott law [2].

A well established theory for transport in Anderson localized systems is the percolation theory [3] where one finds the path in which the most difficult transitions to traverse are as easy as possible. The difficulty of the transitions (constituting the bonds in percolation theory) is quantified by the so-called Miller-Abrahams (MA) resistances

$$\rho_{ij} \propto \exp(E_{ij}/kT) \exp(2r_{ij}/a) \quad (1)$$

where a is the localization radius, $E_{ij}(\varepsilon_i, \varepsilon_j) = \max(|\varepsilon_i|, |\varepsilon_j|)$ when i, j are on the same side of the Fermi level and $E_{ij}(\varepsilon_i, \varepsilon_j) = |\varepsilon_i - \varepsilon_j|$ when they are on opposite sides. ε_k is the random energy on site k . The largest ρ_{ij} in the least resistive macroscopic path is referred to as the critical or maximal resistance ρ_m . Because of the exponential dependence of the MA resistances on the random variables E_{ij} , r_{ij} the ρ_m is much larger than all the other resistances in the current path so that the macroscopic resistivity is characterized by ρ_m . The important feature in the percolation method is the relative magnitude of the bond strengths. Since the exponential is a monotonic function of its argument one may more conveniently adopt the logarithm of (1) $\ln \rho_{ij} \equiv \xi_{ij} = E_{ij}/kT + 2r_{ij}/a$, as the bond strength.

An alternative theory that yields the same results as the percolation theory is a scaling theory [4] that also justifies the original optimization method Mott used in his original derivation of the Mott law.

These theories apply when interactions between electrons are negligible. When they are important (an electron glass, alias a Coulomb glass) they strongly affect

physical properties. There is much experimental evidence [5] that the conductivity in the electron glass behaves as

$$\sigma = \sigma_0 \exp[-(T_0/T)^{1/2}]. \quad (2)$$

Such a behavior was predicted by Efros and Shklovskii (ES). In their theory, ES derive the interaction-modified energy dependence of the one-particle density of states and use it in a percolation theory to obtain (1). ES has been questioned because by using a one-particle density of states it excludes many body effects and with it dynamic[6] and other [7] correlations. Here an alternative derivation of (1) is presented that does account for these effects.

2. Theory

The commonly used model for the electron glass is defined by its Hamiltonian

$$H = \sum_i \varepsilon_i n_i + \sum_{j,i \neq j} n_i n_j / 2r_{ij}, \quad (3)$$

where n_i is the occupation number of site i and r_{ij} the distance between sites i and j . The occupation numbers are restricted to the values $n_k = 0, 1$. This makes the model applicable to the strong localization region where intra-site interaction energies are very large and inter-site hopping energies (and thus also exchange energies) very small. The states K of the system are defined by a set $\{n_i^K\}$ of occupation numbers with i ranging from 1 to the total number of sites N . The energy of configuration K is

$$E^K = \sum_i \varepsilon_i n_i^K + \sum_{j,i \neq j} n_i^K n_j^K / 2r_{ij} \quad (3a)$$

Site energies are defined to include the random energies as well as the interaction energies with all other sites,

$$E_i^K = \varepsilon_i n_i^K + \sum_{j \neq i} n_i^K n_j^K / 2r_{ij} \quad (4)$$

An important effect of the interaction term is to modify the one-particle density of states from $n(\varepsilon_i)$ to $n(E_i)$ by depleting states near the Fermi level. The physical reason for the depletion is that an invasion of an electron into a region of space already occupied by other electrons *per force* leads to a repulsion energy that distances the electron from the Fermi level. Since conduction occurs near the Fermi level interactions clearly reduce the conductivity. However, the reduction in conductivity can be alleviated in part by a collective motion of electrons (collective correlations) or by an electron waiting for a favorable fluctuation of other electrons to enter their space (sequential correlations). These many-body processes are not accountable for by a single particle density of states nor can they be incorporated in the percolation theory developed for the non-interacting systems. However, a percolation theory suitable for the interacting systems was developed [8]. Instead of generating bonds between sites in real space in accordance with (1) it generates bonds between configurations [8] in the configuration space in accordance with

$$\rho_{IJ} \propto \gamma^{m-1} \exp(E_{IJ}/kT) \exp(2\sum r_{ij}/a) \quad (5)$$

Equation (5) is an expression [9] for (direct) transition times between configurations I and J . Here

$$E_{IJ} = \max(E_i, E_j), \quad (5a)$$

E_K is the energy of configuration K as given by (4), and \sum designates the minimal sum, with respect to exchange [9], of distances of the electrons transferred between I and J , m is the number of electrons transferred between the two configurations, γ is a measure of the importance of interaction energy in the m electron transition: $\gamma=0$ when interactions vanish (i.e. when the electrons participating in the transition are distant from each other) and γ is of the order of 1 when interactions are important (when the electrons are nearby). Notice that when $\gamma=0$ only 1-electron transitions exist. Many-particle transitions can allow electrons to avoid each other and thus lower E_{IJ} , making the transition easier [10], while increasing $\sum r_{ij}$ makes the transition more difficult. Whether a collective transition is favored thus depends on whether the gain in lowering E_{IJ} wins over the increase of $\sum r_{ij}$.

In the percolation procedure γ can always be taken to be 1 since for small γ the drop in E_{IJ} is small but the increase in $\sum r_{ij}$ is substantial. Thus, even if γ for a transition is small but made to be 1, the percolation procedure will always pick the less resistive sequence of distant single-particle transitions over the more resistive many-particle transition (for a fuller explanation see [8]). Setting γ to 1 simplifies (5) to

$$\rho_{IJ} \propto \exp(E_{IJ}/kT) \exp(2\sum r_{ij}/a) \equiv \exp(E_{IJ}/kT) \exp(R_{IJ}/a) \quad (6)$$

Percolation in configuration space accounts for collective as well as sequential correlations: collective because a transition between two configuration generally involves a transition of more than one electron and sequential because different sequences of the same transitions take the path through a different intermediate state. This is illustrated in figure 1 by a very simple example of four sites and two electrons.

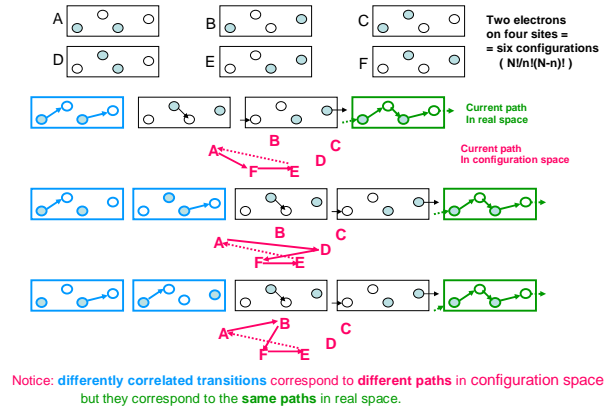


Fig. 1. Transport in a tiny electron glass. Notice that the same current path (green) results from differently correlated transitions with different resistances. (top blue, collectively correlated, following blue, sequentially correlated). In configuration space (red) the paths are distinct. Insertion and extraction of an electron from the “electrodes” returns the configuration to status quo ante and allows for the current to keep flowing. In the configuration space this corresponds to $E \Rightarrow A$. The factorial expression in the upper right indicates the number of configurations for N sites and n electrons.

Recent work on computer simulation of percolation in configuration space demonstrates that collective correlations are very important at low temperatures [8].

Turning now to the scaling theory we first briefly outline the method of [4], developed for non-interacting systems. One scales all the distances between sites by a factor c . When the original distribution is a random distribution then the scaled version will also represent a random distribution. Since large random systems are expected to exhibit properties independent of a specific realization, it is immaterial that scaling is done on a particular realization. The scaling of distances corresponds to a change of concentration. There is clearly a one-to-one correspondence between a path in the scaled and in the unscaled system. Since the resistance of a path depends primarily on its largest resistance it is easy to identify the critical resistance in the scaled system when the critical resistance is known in the unscaled system. One can similarly scale the random energies. Again there will be a one-to-one correspondence between paths in the scaled and in the unscaled systems. Now clearly changing the temperature changes the energy range in which transport occurs and this in turn changes the effective concentration of the active sites in transport. To obtain a realistic

dependence on temperature one needs of course to scale the energy range and the concentration together, in accordance with the existing density of states. This still leaves one degree of freedom in the scaling. The scaled critical paths are possible paths at the desired temperature but the desired critical path will be the one where the critical resistance is the smallest. It turns out [9] that the procedure to obtain the minimal critical resistance corresponds exactly to Mott's optimization method and also gives results identical to those obtained by percolation theory.

Let us now apply the scaling method to the configuration space in an interacting system. The bonds to be scaled are given by (6) where we need to scale the energies and the distances. Some complication arises with the scaling of the energies $E_{IJ} = \max(E_I, E_J)$ which now according to (4) depends both on the random energies and on distances via the Coulomb interactions. However, this problem can be simplified by focusing on the low temperature regime where only sites in the vicinity of the Fermi level can participate in transport of carriers. Further from the Fermi level electrons and holes are frozen on their sites and cannot participate in conduction. Occupation on sites close to the Fermi level is determined predominantly by interaction [6,11]. Thus the term $\sum_i \varepsilon_i n_i$, important only on frozen sites, is constant at low temperatures for all configurations and can be taken out of the problem. Then from (3a) E_{IJ} acquires the following form

$$E_{IJ}^K \approx \sum_{i,j \neq I} n_i^K n_j^K / 2r_{ij} \quad (3b)$$

Where $K=I$ or $K=J$ in accordance with (5a). Notice that at low temperature both the energy terms E and the tunneling terms R of the resistances ρ_{IJ} in (6) are determined by the random variables r_{ij} . The energy term involves distances to sites that change occupation in the transition and the tunneling term, $2\sum r_{ij}/a \equiv R_{IJ}/a$, involves the minimized sum of hopping distances of electrons that change position between I and J .

Using the scaling method, the r_{ij} in the bonds in the configuration space at T' (say), $\xi(T') = E_{IJ}/kT' + 2R_{IJ}/a$ are to be scaled by c , so the scaled bonds in the configuration space become

$$\xi(T') = (E_{IJ})_{T'}/kT' + (R_{IJ})_{T'}/a \Rightarrow (1/c)(E_{IJ})_{T'}/kT + c(R_{IJ})_{T'}/a \quad (7)$$

The subscripts T' indicate values appropriate for ξ at the temperature T' . We are interested primarily in the bonds ξ_m corresponding to the maximal resistances. To avoid unnecessarily cumbersome notation (7) will be taken below to represent these bonds: the left hand side is then $\xi_m(T')$ while the right hand side with the appropriate c becomes $\xi_m(T)$. The scaling parameter c is to be adjusted such that the scaled maximal resistances are as small as possible, i.e.

$$d/dc[(1/c)(E_{IJ})_{T'}/kT + c(R_{IJ})_{T'}/a] = 0 = -(1/c^2)(E_{IJ})_{T'}/kT + (R_{IJ})_{T'}/a,$$

$$c = [(E_{IJ})_{T'}/(R_{IJ})_{T'}]^{1/2}/(a/kT)^{1/2} \quad (8)$$

Substituting c into the right hand side of (7) yields for each of the two terms $[(E_{IJ})_{T'}(R_{IJ})_{T'}]^{1/2}/(akT)^{1/2}$. Thus the scaled maximal bonds become

$$\xi_m(T) = 2[(E_{IJ})_{T'}(R_{IJ})_{T'}]^{1/2}/(akT)^{1/2} = (E_{IJ})_{T'}/kT + (R_{IJ})_{T'}/a \quad (9)$$

It is interesting to examine the maximal energy E_{IJ} and the maximal total hopping distance R_{IJ} . In a slightly rewritten form,

$$[(E_{IJ})_{T'}(R_{IJ})_{T'}/a]^{1/2} (kT)^{1/2} = (E_{IJ})_{T'}$$

$$[(E_{IJ})_{T'}(R_{IJ})_{T'}/a]^{1/2} (kT)^{-1/2} = (R_{IJ})_{T'}$$

Thus, as in variable range hopping, the hopping energy decreases with decreasing T while the (total) hopping distance increases with decreasing T . Here, in configuration space, the increase of the total hopping distance with decreasing T incorporates both variable range and variable number hopping. As a corollary of the above two equations we can conclude that the product $E_{IJ}R_{IJ}$ is temperature independent. Since T' is just another temperature, we can drop the subscripts T' from (9) and observe that $\xi_m(T)$ depends only on the temperature T and not on T' . It must be pointed out that there exists a spectrum of combinations $\{(E_{IJ}), (R_{IJ})\}$ that produce the same ξ_m in accordance with (7). One should average $E_{IJ}R_{IJ}$ over all such values, i.e. integrate over the surface $\xi_m = \text{const}$. To execute such an integration one must have better knowledge of the geometry of the configuration space so here we merely write $\langle E_{IJ}R_{IJ} \rangle$ for the appropriate average without evaluating it. We can then rewrite (9) to finally obtain

$$\xi_m(T) = 2\langle E_{IJ}R_{IJ} \rangle^{1/2}/(akT)^{1/2} \equiv (T_0/T)^{1/2},$$

or

$$\sigma = \sigma_0 \exp[-(T_0/T)^{1/2}]. \quad (10)$$

which corresponds exactly to (2). For the reason stated above, it is impossible at present to calculate analytically $T_0 = 2(\langle E_{IJ}R_{IJ} \rangle/ak)^{1/2}$

3. Summary and discussion

With (10) we showed that the many-body calculation of the conductance of an electron glass results, at low temperatures, in the same functional dependence derived by ES with neglect of the many-body effects. While ES calculate T_0 from the one-particle density of states, a many body theory does not connect the one-particle density of states to conductance. Thus, for reasons stated above, it is impossible at present to calculate T_0 here. Computer simulation is at present the only way to do so. To my knowledge, the most thorough many-body computer simulation of conductance in the electron glass is done in [8] for a two dimensional system. There it was found that

the conductance does follow (10). While collective correlations are found in [8] to be very important at low temperatures, the value of T_0 is found to have a mildly smaller value than the ES value.

It should be stressed that like most hopping transport theories the theory presented here is restricted to the strongly localized regime, i.e. deep in the insulator side of the Anderson-Mott metal-insulator transition (MIT). On the other hand, most of the experimental works showing the $T^{-1/2}$ conductance are performed not very far from the MIT. The practical reason probably is that deep in the insulator regime the resistance is too high to measure at the temperatures of interest. Several important aspects (not all independent of each other) of the conduction close to MIT were neglected here – the intra-site repulsion is not very large, the localized states are not confined to single sites and the localization lengths are not uniform, and the inter-site tunneling energy is not negligible. Further work to ascertain whether (2) and (10) can be justified closer to the MIT transition will thus be required.

Acknowledgement

It is a rare pleasure to have the opportunity to contribute to a celebratory volume in honor of Professor Radu Grigorovici, one of the pioneering researchers in the field of disordered systems. I consider Professor Grigorovici to be one of the founders of the field. His contributions to structural, optical and electrical properties of granular metal films, chalcogenide glasses and amorphous group IV semiconductors had an undeniable impact on the evolution of the physics of disorder. My sincere best wishes to Professor Grigorovici on the occasion of his 95th birthday.

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