Resonant-tunnelling conductance of a finite-size amorphous sample

Resonant-tunnelling conductance of a finite-size amorphous sample

Er'el Granot

School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences,
Tel-Aviv University, 69978 Ramat-Aviv, Israel

Abstract. The conductivity of an amorphous sample at low temperatures is calculated. While Mott's variable range hopping theory considers infinite samples, the proposed formalism treats finite ones. It turns out that this is a crucial difference. The model predicts a transition temperature (T_c) between two conductivity behaviours: $\ln(\sigma) \sim -(T_2^L/T)^{1/3}$ for $T < T_c$, and $\ln(\sigma) \sim -(T_2^H/T)^{1/2}$ for $T > T_c$ (the transition temperature, T_c, depends on the Fermi energy and on the sample's characteristics). The former resembles the simple two-dimensional Mott conductivity behaviour, while the latter resembles the Efrös and Shklovskiĭ conductivity theory. We also show a simple connection between these temperatures: $T_c = (T_2^H)^3/(T_2^L)^2$.

In 1969 Mott presented his variable range hopping (VRH) theory of an amorphous system [1]. The theory predicted that for a d-dimensional amorphous sample the electrical conductivity (σ) has the following temperature dependence: $\ln[\sigma(T)] \approx -T^{-1/(d+1)}$. This theory was found to be in good agreement with early experiments on three-dimensional (3D) [2] and on two-dimensional (2D) [3] systems, where Mott's theory predicts

$$\sigma_M \approx \exp[-(T_2/T)^{1/3}].\tag{1}$$

In 1975 Efrös and Shklovskiĭ (ES) introduced a model for VRH [4], which took into account the Coulomb interaction between localized electrons. Their model applied the phenomenon of the Coulomb gap (CG) within the density of states. They showed that the account of the CG leads to the following 2D VRH conductivity

$$\sigma_{ES} \approx \exp[-(T_2/T)^{1/2}]\tag{2}$$

which resembles the one-dimensional Mott conductivity.

This model also was found to be in good agreement with very low temperature experiments, where the CG cannot be ignored (see, for example, [5]. For experiments which predict a negligible CG, see [6]).

In this paper we present a rigorous calculation of the conductivity in the resonant tunnelling (RT) regime, i.e. in the regime where the coherence length is longer than the sample size, and in the absence of the Coulomb interactions. It should be emphasized that the Mott and ES theories assume an infinite sample. This paper shows that at very low temperatures the finite sizes of the samples have an important effect on the conductivity. The presented model exhibits a transition temperature T_c, above which ($T > T_c$) the temperature dependence behaves like (2), while when $T < T_c$ it behaves like (1). Despite the similarity between the present model and Mott and ES theories the presented model is based on resonant tunnelling and not on VRH as in the Mott and ES theories.
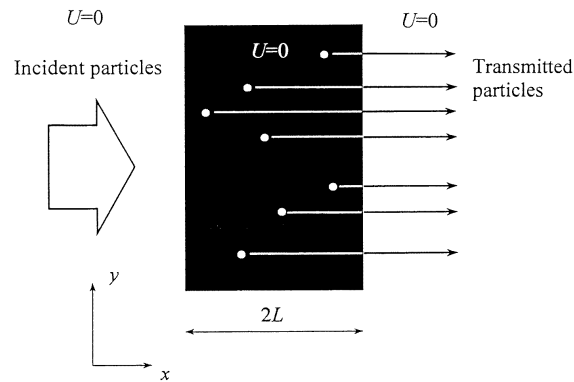
Figure 1. The substantial contribution to the current through the barrier comes from the resonant impurities, i.e. from the impurities whose energy is equal to the incoming electrons' energy. The white circles represent the resonance impurities.

Take a system where electrons are scattered over a large number of impurities (figure 1), which are uniformly placed in an opaque potential barrier.

The stationary-state Schrödinger equation can then be written as

$$\nabla^2\psi + (E - U)\psi = -\sum_i D(|r_i - r|)\psi. \tag{3}$$

Hereinafter, we use the units $\hbar = 2m = 1$ (Planck constant and the electron mass). ∇^2 is the 2D Laplacian, E is the incoming electron energy, U is the barrier potential:

$$U \equiv \begin{cases} V & \text{for } -L < x < L \\ 0 & \text{otherwise} \end{cases}$$

and the D are the impurity potentials, which are short range ones (see [7] and [8]).

V is a positive potential, and thus the electrons with energy $0 < E < V$ tunnel through the barrier. The exact form of the impurities' potentials (D) is unimportant as long as they are short-range ones, i.e. on atomic scales. Mathematically, they can be represented by the *impurity D function* (IDF—see [7]), which is infinitely shallower than the two-dimensional delta function (2DDF), but, unlike the 2DDF, it has an eigenvalue (say E_{i0}). Because of its infinitely small dimensions, the short-range potential can be fully determined by this single parameter (the eigenvalue). Thus, each impurity creates a resonance level $E_i \equiv V - E_{i0}$, to which the particles can tunnel. If the electrons energy equals the resonance energy of a specific impurity, the impurity presence will be felt in the conductance, since many electrons will tunnel through it. But if their energy does not match, the influence of the specific impurity will be negligible.

The solution $\psi(r)$ can be written as a summation over the contributions from each one of the impurities $\psi_i(r)$, i.e.

$$\psi(r) = \sum_i \psi_i(r, r_i). \tag{4}$$

For a specific incoming particle's energy, only the resonance impurities contribute considerably to ψ, the rest can be ignored since their contribution is exponentially smaller.

Therefore, one can evaluate $\psi(r)$ by assuming that only the impurities which are at resonance are present.

The contribution to $\psi(\mathbf{r})$ from a single impurity (for simplicity let us assume that $\mathbf{r}_i = 0$) in the case of a very opaque barrier (high and wide, for which $\sqrt{V}L \gg 1$) has the following form (within the leading approximation of r^{-1}):

$$\psi_i(\mathbf{r}) \cong f \frac{e^{ik|\mathbf{r}-\mathbf{L}|}}{\sqrt{r}} \tag{5a}$$

where $r \equiv |\mathbf{r}|$, $k = |\mathbf{k}| = \sqrt{E}$ and the scattering amplitude (f) has the following form [10]:

$$f(\theta, E) = C \frac{e^{-\sqrt{V-E\cos^2\theta}(L-x_i)-\sqrt{V-E}(L+x_i)}}{\frac{1}{2}\ln(\frac{V-E}{E_{0i}}) + i\Delta_i} \tag{5b}$$

where x_i and E_{0i} are the x location of the ith impurity and its resonance energy respectively. C changes slowly with the energy, θ is the (outgoing) scattering angle and $\Delta_i \sim \exp[-2\sqrt{V-E}(L-|x_i|)]$ is the resonance width. Notice that the homogenous solution of (3) is exponentially small, and thus is ignored in (4).

Hence, the contribution to the scattered wavefunction from the resonant impurities (those for which $E \cong V - E_{0i}$) is

$$\psi_i^{res} \sim \exp\left[-2\kappa|x_i| - \left(\sqrt{V-E\cos^2\theta} - \kappa\right)(L-x_i) + ikr\right] \tag{6}$$

where $\kappa \equiv \sqrt{V-E}$.

Notice that equation (5) and thus also equation (6) include intrinsically the finite width of the barrier. If the barrier was not finite (or if the coherence length was shorter than the barrier), such a resonant tunnelling conductance could not occur. For a wide barrier (wider than the coherence length) any transport mechanism must rely on hopping and not on resonant tunnelling.

Next, equation (6) will be substituted in (4) to evaluate the scattered wavefunction.

The conductivity in the two-terminal case can now be calculated. According to [9],

$$\sigma = 4i \sum_\lambda \frac{\partial f}{\partial \varepsilon} \int dy \left(\frac{\partial \psi_\lambda^*}{\partial x}\psi_\lambda - cc\right) \tag{7}$$

where: $f(\varepsilon_\lambda - \zeta)$ is the Fermi distribution function (ε_λ are the energy levels and ζ is the electrochemical potential); the summation over λ denotes summation over the quantum numbers (i.e. the energy levels E and the generalized momentum y-component k); the integration over y is over the width of the sample, and the asterisk stands for a complex conjugate (cc).

In equation 7 only a few impurities are at resonance and all the rest are out of resonance. Therefore, only these few make the major contribution to the conductivity (a resonant tunnelling current).

Now, suppose that the energies of the impurities are uniformly distributed. Then, instead of integrating over the energy, one may sum over the contributions (5a) or (6) from *all* the impurities.

$\partial f/\partial \varepsilon_\lambda$ behaves like a delta function around the Fermi level (ζ), and thus for a very low temperature (T) one can also use the following approximation:

$$\partial f/\partial \varepsilon_\lambda \xrightarrow[E-\zeta \gg T]{} T^{-1} e^{-|E-\zeta|/T}. \tag{8}$$

Then by substituting (6) and (8) in (7), and measuring the conductivity at x:

$$\sigma(x > L) \approx T^{-1} \int dy\, g(y) \tag{9}$$

where

$$g(y) = \sum_i \mathrm{e}^{-\frac{|E_i - \zeta|}{T}} \, \mathrm{e}^{-4\kappa_i |x_i| - 2(\sqrt{\kappa_i^2 + E_i (y - y_i)^2 / r_i^2} - \kappa)(L - x_i)}. \tag{9a}$$

E_i, x_i, y_i, r_i and κ_i are the resonance energy of the ith impurity, its x and y coordinates, $r_i^2 \equiv (x - x_i)^2 + (y - y_i)^2$ and $\sqrt{V - E_i}$ respectively. Notice the difference between E_{0i}, which characterizes only the impurity, and $E_i \equiv V - E_{0i}$, which depends also on the barrier (that is, $\kappa_i = \sqrt{E_{0i}}$).

In (9a) the summation is taken over all the impurities. The idea is the following.

Since one can assert that each one of the impurities has, more or less, a different resonance energy, and since the resonance width is always (for all the impurities) very narrow, it should be possible to do the following projection: every impurity i will be identified with its resonance energy E_{i0}. As a consequence, since the impurities' resonance energies are uniformly distributed, one can sum over the impurities (while taking their resonance contribution) instead of integrating over the energies. This is the basic idea that led to equation (9).

When $T = 0$, the main contribution to the conductivity comes from the impurities, whose resonance energy is equal to the Fermi energy (i.e. $E \cong V - E_{i0}$ as equation (5b) suggests). However, the probability that these impurities will be located at the centre of the barrier, i.e. at $x_i = 0$ is miniscule and by equation (5b) their contribution to the conductivity could be very small. When the temperature is finite ($T > 0$), the energy range of the incoming particles is finite and thus the prospect of finding resonant impurities in the vicinity of the centre of the barrier is larger. As a consequence the conductivity (the resonant tunnelling current) increases.

Because of the uniform distribution of the impurities inside the barrier, the number of impurities in a given region is proportional to its area. Therefore, in a given area $\tilde{A}$ the average difference between two energetically adjacent resonance levels is proportional to $\tilde{A}^{-1}$. Thus, the energy of the impurity, whose energy is the closest to ζ inside this area, maintains the relation $E_i - \zeta \approx \tilde{A}^{-1}$. Hence, if we measure the wave-function at a specific y (later on we integrate over this variable—see equation (9)) we can substitute in equation (9a) $E_i - \zeta \approx R^{-2}$ where $R^2 \equiv x_i^2 + (y_i - y)^2$.

Next, since the summation is taken over all the impurities, and since they are distributed uniformly within the barrier, we can replace the index i with two indices: one for the x-coordinate of the impurity and the other for its y-coordinate. This means that now every impurity will be identified by two indices (its coordinates) instead of one (i—which was related to its energy). In both cases we sum over all the impurities so the order of summation is not important.

Instead of calculating $g(y)$ for a specific y and then integrating over y, in our analysis we calculate the *average* $g(y)$ and then simply multiply it by the sample width.

The conductivity σ should be independent of x; however, since a few approximations were used one cannot substitute in (9a) any value for x. Instead, when the impurities are weak, i.e. $E_{0i} \ll \zeta$ (and thus $\kappa \ll k$), x should be taken as

$$x \approx L\sqrt{k/\kappa} \qquad (k = \sqrt{\zeta}, \kappa = \sqrt{V - \zeta}).$$

This is the only region which is consistent with the approximation that led to (5a), i.e. $x \gg L$ and with the demand that $|x_i| < L$ for every i.

Thus, by replacing the summation in (9a) with the summation over the impurities' components $\eta \equiv x_i$ and $\xi \equiv y_i - y$, it follows that

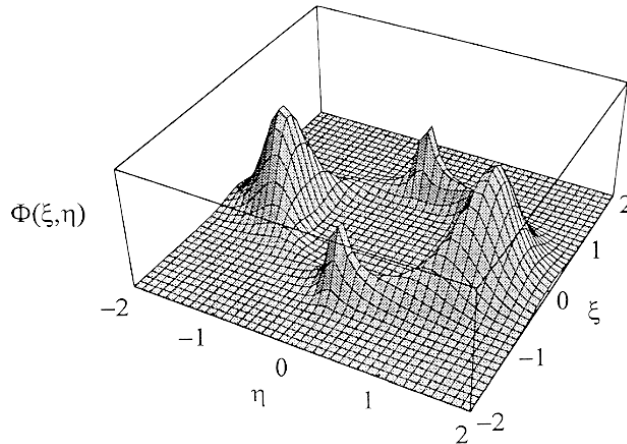$$\sigma \approx \sum_{\eta, \xi} \mathrm{e}^{-f(\eta, \xi)} \tag{10}$$

Figure 2. The surface graph of the function $\Phi(\eta, \xi) = e^{-f(\eta, \xi)}$. The maxima at $\eta = 0$ determine the $\sigma \approx \exp[-(T_2^H/T)^{1/2}]$ behaviour, while the maxima at $\xi = 0$ determine the $\sigma \approx \exp[-(T_2^L/T)^{1/3}]$ behaviour.

where

$$f(\eta, \xi) \equiv \frac{1}{(\eta^2 + \xi^2)NT} + 4\kappa|\eta| + \sqrt{\zeta}\left(\frac{\xi}{L}\right)^2 (L - \eta) \tag{10a}$$

N is the density of states at the Fermi energy, and we evaluated $E \approx \zeta$ for every η and ξ (and thus $\kappa \approx \sqrt{V - \zeta}$). We also used in the exponent the following approximation

$$\sqrt{\kappa^2 + E(\xi/r_i)^2} \cong \sqrt{\kappa^2 + E(\xi/x)^2} \cong \kappa + \tfrac{1}{2}\sqrt{\zeta}(\xi/L)^2. \tag{10b}$$

The second term in equation (10a) increases with the *absolute* value of η, and thus expresses the predominance of impurities, which are close to the centre of the barrier. The third term in (10a), which depends on the square of ξ, expresses the fact that particles 'prefer' to tunnel through the shortest path (see a discussion on this subject in [12]). These two parametric dependences emphasize the significance of the barrier geometry on the RT process.

In general, $f(\eta, \xi)$ has four minima of two kinds. However, when

$$T < T_c \equiv \frac{4}{3^6} \frac{\zeta^{3/2}}{N\kappa^4 L^3} \tag{11}$$

(in ordinary physical dimensions, i.e. when $2m$ and $\hbar$ are different from 1, the transition temperature is $k_B T_c = \hbar \zeta^{3/2}/[\sqrt{2m}N(V - \zeta)^2 L^3]$, where m is the electron mass inside the barrier).

The two dominant minima are at $\xi = 0$, $\eta = \pm(2\kappa NT)^{-1/3}$ and thus the conductivity can be evaluated:

$$\sigma \approx \exp\left[-3\left(\frac{4\kappa^2}{NT}\right)^{1/3}\right]. \tag{12}$$

This expression resembles the Mott temperature dependence of a 2D sample, i.e. $\sigma \sim \exp[-(T_2^L/T)^{1/3}]$ where $T_2^L = 108\kappa^2/N$, and in ordinary physical dimensions $k_B T_2^L = 216m(V - \zeta)/(N\hbar^2)$. The superscript '$L$' stands for low temperatures and the subscript '2' stands for 2D.

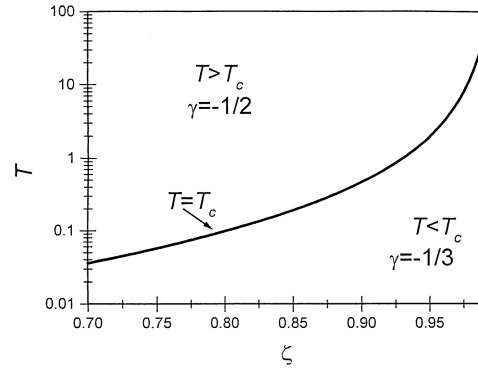On the other hand, when

$$T > T_c \tag{13}$$

Figure 3. The conductivity behaviour $\ln \sigma \approx -T^{\gamma}$ divides the T–ζ (temperature–electrochemical potential) diagram into two parts ('phases'): above the transition curve (high T) with $\gamma = -1/2$ and below the transition curve (low T) with $\gamma = -1/3$.

the conductivity is governed by the other two minima at $\xi = \pm(L/\sqrt{\zeta}NT)^{1/4}$, $\eta = 0$ (see figure 2). In this case, the conductivity can be evaluated as

$$\sigma \approx \exp\left[-2\left(\frac{\sqrt{\zeta}}{LNT}\right)^{1/2}\right].\tag{14}$$

This last result resembles Mott's VRH theory for 1D samples or the ES theory for 2D ones. Here $T_2^H = 4\sqrt{\zeta}/LN$, and in ordinary physical dimensions $k_B T_2^H = 4\sqrt{2m\zeta}/(LN\hbar)$. The superscript '$H$' stands for high temperatures. ζ is measured in units of V while T is measured in units of $1/(N\sqrt{V}L^3)$.

Thus, we conclude that the power in the exponent of the conductivity changes from $(-1/3)$ for low temperature to $(-1/2)$ for higher ones, while the transition temperature depends both on the chemical potential and on the barrier parameters. The transition can be seen in the 'phase diagram', which is presented in figure 3. A similar transition in the presence of a strong magnetic field has been anticipated elsewhere [11].

Although the temperature dependence is similar to the theories of Mott [1] and ES [4] the physics is quite different. In their theories the conductivity is governed by VRH. That is, they are based on thermal activation. Moreover, it is assumed that the coherence length is quite small and thus resonant tunnelling is totally ignored. In the presented model, however, the temperature is so low that the coherence length is larger than the sample dimensions, and thus non-activated resonant tunnelling is the main transport mechanism.

In order to observe the transition easily, one should demand both $T_c < T_2^L$ and $T_c < T_2^H$. However, it can easily be shown that this requirement can be achieved for a very wide barrier. In particular $\kappa L > \sqrt{\zeta}/\kappa$ will assert the two demands.

A straightforward calculation verifies a simple expression, which relates the transition temperature T_c to both T_2^L and T_2^H:

$$T_c = \frac{(T_2^H)^3}{(T_2^L)^2}.\tag{15}$$

The transition temperature depends on four parameters, and thus can vary considerably between one experiment and another.

Since in ordinary experiments $T_2^L/T_2^H = 10^2$–10^3 the transition temperature is extremely low, $T_c < (10^{-4}$–$10^{-6})T_2^H$. In particular, for a typical experiment with $T_2^H = 10^1$–10^2 K, the

transition temperature should be within the scope $T_c \approx (10^{-2}$–$10^{-5})$ K, which is quite a broad range of temperatures.

In general, a similar transition occurs in any dimensionality. For a d-dimensional sample within the low-temperature regime ($T < T_c$), the conductivity behaves like $\ln \sigma \sim -T^{-(d+1)^{-1}}$, while above the transition curve ($T > T_c$) one meets the following temperature dependence: $\ln \sigma \sim -T^{-(d/2+1)^{-2}}$.

To summarize, a model based on resonant tunnelling was presented in order to calculate the conductivity of an amorphous sample at low temperatures. Unlike the Mott and ES theories, the conductivity was calculated for a finite size sample, and this was found to have a crucial impact on the conductivity. The model demonstrates a temperature transition (for a general d-dimensional sample):

For $T > T_c$ the conductivity behaves like

$$\sigma \approx \exp[-(T_d^H/T)^{1/(d/2+1)}]$$

(when $d = 2$ it is similar to the ES theory or to the $d/2$-dimensional Mott VRH theory) while when $T < T_c$ it looks similar to the well known d-dimensional Mott conductivity

$$\sigma \approx \exp[-(T_d^L/T)^{1/(d+1)}].$$

Acknowledgments

I would like to thank Professor M Azbel for numerous valuable and stimulating discussions and Dr Y Glick for helping with the preparation of the manuscript.

References

[1] Mott N F 1969 *Phil. Mag.* **19** 835
    Mott N F 1969 *Festkörperprobleme* **9** 22
[2] See, for example, Clarck A H 1967 *Phys. Rev.* **154** 750
    Chopra K L and Bahl S K 1970 *Phys. Rev.* B **1** 2545
    Clarck A H 1970 *J. Non-Cryst. Solids* **2** 52
    Morgan M and Walley P A 1971 *Phil. Mag.* **23** 661
    Chittick R C 1970 *J. Non-Cryst. Solids* **3** 255
    Mott N F and Zinamon Z 1970 *Rep. Prog. Phys.* **33** 881
[3] See, for example, Nicholas R J, Stradling R A and Tidey R J 1971 *Solid State Commun.* **23** 341
    Störmer H L, Tsui D C and Gossard A C 1982 *Phys. Rev.* B **25** 1405
[4] Efrös A L and Shklovskiĭ B I 1975 *J. Phys. C: Solid State Phys.* **8** L49
[5] Tremblay F, Pepper M, Newbury R, Peacock C D, Frost J E F, Jones G A C and Hill G 1990 *J. Phys.: Condens. Matter* **2** 7367
[6] Timp G and Fowler A B 1986 *Phys. Rev.* B **33** 4392
    Shafarman W N and Castner T G 1986 *Phys. Rev.* B **33** 3570
    Timp G, Fowler A B, Hartstein A and Butcher P N 1986 *Phys. Rev.* B **33** 1499
[7] Azbel M Ya 1991 *Phys. Rev.* B **43** 2435
    Azbel M Ya 1991 *Phys. Rev.* B **43** 6717
[8] Landau L D and Lifshitz E M 1965 *Quantum Mechanics* (Oxford: Pergamon) ch VI, section 45, and problem therein
[9] Azbel M Ya 1993 *Phys. Rev.* B **47** 15 688
[10] Granot E and Azbel M Ya 1994 *Phys. Rev.* B **50** 8868
[11] Granot E 1997 *Phys. Rev.* B **55** 15 828
[12] Granot E and Azbel M Ya 1999 *J. Phys.: Condens. Matter* **11** 4031