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On the Mott formula for the a.c. conductivity and binary correlators in the strong localization regime of disordered systems

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Abstract

We present a method that allows us to find the asymptotic form of various characteristics of disordered systems in the strong localization regime, i.e., when either the random potential is big or the energy is close to a spectral edge. The method is based on the hypothesis that the relevant realizations of the random potential in the strong localization regime have the form of a collection of deep random wells that are uniformly and chaotically distributed in space with a sufficiently small density. Assuming this and using the density expansion, we show first that the density of wells coincides in leading order with the density of states. Thus the density of states is in fact the small parameter of the theory in the strong localization regime. Then we derive the Mott formula for the low frequency conductivity and the asymptotic formulas for certain two-point correlators when the difference of the respective energies is small.

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1 Introduction

It is widely accepted and proved rigorously in many cases that elementary excitations in disordered media are localized if the disorder is strong enough or/and the energy of the excitations is close enough to the band edges. The idea dates back to the famous paper [4] by P. Anderson who emphasized, in particular, the aspects related to the transition from localized to delocalized states. The idea was further developed by N. Mott and I. Lifshitz (see e.g. their review works [25, 20]). In particular, it was I. Lifshitz who singled out the regime of high disorder or low energy where the localization is most pronounced. This regime is now known as the strong localization regime. According to I. Lifshitz, in this case, the pertinent realizations of the random potential have the form of a collection of deep potential wells which are so rare and whose form is so irregular that the quantum

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mechanical probability for tunnelling through a macroscopic number of the localization wells vanishes.

The study of localization and relevant physical characteristics of disordered systems can be reduced to the study of moments of the density operator $\rho_E = \delta(E - H)$, where H is the (one-body) Hamiltonian of the system. By using the coordinate representation, we can write the l-th moment (l-th correlation function) as follows:

$$K_l(x_1, ..., x_l; y_1, ..., y_l; E_1, ..., E_l) = \langle \rho_{E_1}(x_1, y_1) ... \rho_{E_l}(x_l, y_l) \rangle, \tag{1.1}$$

where the $\langle ... \rangle$ denotes averaging with respect to the disorder.

The simplest case of the correlation function (1.1), corresponding to $l = 1$, $x_1 = y_1 = x$:

$$\rho(E) = \langle \rho_E(x, x) \rangle \tag{1.2}$$

i.e., to the average of the local density of states $\rho_E(x, x)$, is known as the density of states (DOS) of the system.

I. Lifshitz suggested a non-perturbative method of computing the asymptotic form of the DOS in the strong localization regime [19]. The above description of typical realizations of the random potential is implemented in this method by the assumption of independent quantization of a quantum particle in each localization well (see [20, 21, 7]), thus the complete localization of a particle in an exponential neighborhood of each well. A rigorous proof of the complete and exponential localization in the strong localization regime was given by J. Fröhlich and T. Spencer [9, 22, 27].

In both these important results of the localization theory the tunnelling between the localization wells plays no significant role. In Lifshitz's argument, other wells are simply ignored. The crucial ingredient in the rigorous proof of the complete localization in the strong localization regime is a rather sophisticated probabilistic extension of the Kolmogorov-Arnold-Moser theory (known as the multi-scale analysis) which allows one to verify that tunnelling between wells is strongly suppressed, and therefore does not change qualitatively the picture, suggested by the independent wells quantization assumption.

The DOS determines equilibrium properties of a disordered system in the one-body approximation, i.e., of the ideal Fermi gas in a random external field. The study of kinetic properties of the gas and of interaction effects requires the knowledge of higher moments (1.1) of the density operator ρ_E, especially the second moment K_2. Important quantities that can be expressed via K_2 are the density-density correlator and the current-current correlator [10, 21]. These correlators allow us to answer relevant questions concerning the nature of localization and the behavior of the conductivity and other physical characteristics.

The complete localization of states in a certain interval of energies implies that the zero temperature d.c. conductivity vanishes if the Fermi energy lies in this interval (see [2] for a proof and a discussion). On the other hand, since the energies of localized states are dense, the zero-temperature a.c. conductivity is expected to be non-zero for any non-zero frequency ν of the external field. It was N. Mott who first proposed "resonant" tunnelling between pairs of wells as a mechanism of the low frequency a.c. conductivity in localized systems [25]. According to Mott, one can view those states, resulting from independent quantization in each localization well (localization center in Mott's terminology), as a kind of "bare" states. They decay exponentially in the distance from the corresponding localization center. Two (several) bare states with widely spaced centers but with sufficiently close energies can "resonate". This leads to the two-center states (resp. multi

center states), whose energies are exponentially close in the separation between the centers. The condition for a pair of wells to be in resonance determines the distance between resonating wells, thereby determining the characteristic value of the dipole moment of two bare states of wells, and the square of the dipole moment is, in essence, the conductivity according to the linear response theory (see formula (3.4) below). This observation leads to the following asymptotic expression for the low frequency conductivity:

$$\sigma(\nu, E_F) = A\rho^2(E_F)\nu^2 \left(\log \frac{\nu_0}{\nu}\right)^{d+1} \tag{1.3}$$

in the case, where

$$T \ll \nu \ll E_F. \tag{1.4}$$

Here T is the temperature, ν the frequency of an alternating external field, E_F the Fermi energy (supposed to be in the localized spectrum). A and ν_0 are determined by the fundamental constants and by the random potential.

Formula (1.3) was discussed in many works (see e.g. [7, 8, 14, 10, 11, 21, 25, 15] and Section 5). However, a consistent "first principle" derivation of the formula is still not available in a general multi-dimensional case. We mean a derivation based on the Kubo formula (see formulas (3.2)–(3.4) below), in which the two-point correlation function is computed for a given random potential in the asymptotic regime (1.4).

The fact that such a derivation is still missing encourages us to present in this paper a heuristic method that allows us to obtain formula (1.3) and some other two-point correlation functions (i.e., (1.1) for $l = 2$ and $|E_1 - E_2| := \nu \ll |E_1|, |E_2|$), and that, we believe, clarifies Mott's initial arguments.

The method is based on the above hypothesis on the form of pertinent realizations of the random potential as systems of deep and rare localization wells. Viewing the density of wells as a small parameter of the theory, we apply a version of the virial expansion to compute the leading contribution to the moments K_l of (1.1) for $l = 1, 2$. In particular, by applying this procedure to the DOS, we find that its leading order is the density of the localization wells. This shows that the small parameter of the theory is the DOS itself, whose smallness is known to be an important condition for localization. Furthermore, we find that the leading order of the pair correlation functions, the a.c. conductivity in particular, is determined by two-center states, resulting from resonant tunnelling between a pair of localization wells, in agreement with Mott's ideas. This leads to formula (1.3) and, therefore, supports the idea of pair approximation in Mott's derivation of (1.3). Among our other results, we mention high peaks of some pair correlation functions (see (4.1) and (4.2) below), appearing in a neighborhood of the origin and on the "resonating" distance, determined by the frequency of the external field. Analogous peaks were found before in the one-dimensional case for strong localization [14] as well as in the weak localization regime [11]. However, in these cases, the peaks are of the order $\rho^2(E_F)$, while in the general d-dimensional case, the peaks are of the order $\rho^2(E_F)\,(\log \nu_0/\nu)^{d-1}$, i.e., much bigger in the regime (1.4) (see also [15] for a similar result).

The paper is organized as follows. In Section 2 we outline the method. In Section 3 the Mott formula (1.3) is derived. In Section 4 we derive asymptotic formulas for binary correlators and in Section 5 we comment on our results and on their relations to known results.

2 Method

2.1 Effective potential

It was already mentioned in the introduction that extensive studies of the strong localization regime show that the phenomenon is determined by realizations of the random potential, containing deep and rare potential wells. For a potential unbounded below (like the Poisson potential (2.6) below) the large parameter of the theory is the absolute value of the energy and/or the amplitude of the potential. These two cases of the strong localization regime are manifestations of the simplest mechanism of localization: capturing a quantum particle in strong and rare fluctuations of a random potential[1].

In other words, for an overwhelming majority of eigenfunctions ψ_j, corresponding to the strongly localized part of the spectrum, there exists a point ξ_j, the center of the localization well, such that ψ_j decays as $\exp\{-|x-\xi_j|/r_j\}$. Here r_j is the localization radius of ψ_j. The localization centers have to be uniformly and chaotically distributed in space and the distances between them have to be much bigger than the typical localization radii and than the radii of the localization wells. Hence, one has to expect an effective "decoupling" between the localization wells.

One obtains a simple form of this picture of the strong localization regime by replacing the random Schrödinger operator by the direct sum of operators, each of them defined in a certain cell, containing a single localization well. This procedure of independent quantization in isolated cells is supported by and even instrumental in studies of the density of states, the interband light absorption coefficient, and other spectral and physical characteristics of disordered systems (see e.g. [5, 7, 17, 21]), as well as of the probability distribution of spacings between adjacent energy levels (see [24, 23]) in the strong localization regime. However, the procedure is not appropriate in studies of transport properties of disordered systems. This is why we replace the procedure of independent quantization in isolated cells by the less restrictive assumption, according to which relevant properties of the strong localization regime can be described, assuming that any shortly correlated and smoothly distributed random potential can be replaced by an (effective) potential of the form:

$$V_{eff}(x) = \sum_j v_j(x-\xi_j). \tag{2.1}$$

Here $\{\xi_j\}$ are the Poisson random points of the density μ, modelling the centers of the localization wells, and the random functions $\{v_j\}$ are independent of each others and independent of the $\{\xi_j\}$. The $\{v_j\}$ model the shape of the localization wells. We assume that all v_j's have a finite range and the typical radius a of v_j's is related to the typical distance $\mu^{-1/d}$ between wells as

$$a \ll \mu^{-1/d}. \tag{2.2}$$

The density μ of the localization centers is not known and has to be found self-consistently. The density as well as the shapes of the wells may depend on the energy interval in question.

In other words, we believe that the strong localization regime possesses a certain robustness (insensitivity) with respect to a concrete form of random potential, provided

[1] We mention another localization mechanism : enhanced backscattering. The mechanism is responsible for localization at high energies in the one-dimensional case, and for weak localization effects in arbitrary dimensions.

that it is translation invariant in the mean, shortly correlated, and smoothly distributed (the last two properties facilitate the localization because they make it more unlikely that different localization wells are of the same shape, thereby suppressing tunnelling between different localization wells). One may say that our ansatz (2.1) replaces impenetrable walls between cells of the independent quantization procedure by a kind of "soft" walls, that strongly suppress particle mobility but do not exclude it completely.

To avoid technicalities, we will choose a simple form of the localization wells, setting

$$v_j(x) = g_j v\left(\sqrt{g_j}x\right), \tag{2.3}$$

where $v(x)$ is a finite range potential well and $\{g_j\}$ are independent identically distributed random variables, independent of $\{\xi_j\}$ and assuming arbitrary big positive values according to a smooth probability density $p(g)$.

Summarizing, we can write the following formula for the effective potential

$$V_{eff}(x) = \sum_j g_j v\left(\sqrt{g_j}(x-\xi_j)\right). \tag{2.4}$$

It should be noted that similar random functions are widely used in localization theory as "bare" random potentials in the Schrödinger equation (see e.g. [16, 21]). We mean the potentials of the form

$$V(x) = \sum_j \theta_j u(x-x_j), \tag{2.5}$$

where u is a non-positive function of a finite range (the single-impurity potential). In the case, where $\{\theta_j\}$ are independent identically distributed random variables and $\{x_j\}$ form a regular lattice, the potential models a substitutional alloy, and in the case, where $\theta_j = \theta = \text{const}$ for all j and $\{x_j\}$ are completely chaotic (Poisson) random points of the density c, the potential

$$V(x) = \sum_j \theta\, u(x-x_j), \tag{2.6}$$

models an amorphous medium. Assuming that c is large, θ is small but $c\theta^2 = D$ is fixed and shifting the energy by the mean value

$$c\theta \int u(y)dy$$

of the potential (2.6), we obtain a Gaussian random potential with zero mean and with the correlation function

$$D \int u(x-y)u(y)dy.$$

In a more general case, where the $\{x_j\}$ are completely chaotic and the $\{\theta_j\}$ are identically distributed random variables, independent of each others and of the $\{x_j\}$, (2.5) is a generalized Poisson potential.

We would like to stress here that while our effective potential (2.4) is similar to a generalized Poisson one (because of random g_j's), these two should not be identified. In particular, the density c of the impurity centers $\{x_j\}$ in (2.5) is not the density μ of the localization centers $\{\xi_j\}$ in (2.4) (μ is usually is much smaller than c), and the functions $\theta_j u$ in (2.5), modelling the single impurity potential, have little in common with the

functions v_j in (2.4), modelling the form of the localization wells. The latter are formed by sufficiently large and dense clusters of impurities in which the inter-impurity distances are much smaller than the typical distance $c^{-1/d}$ between impurities centers $\{x_j\}$. For example, if the "bare" random potential is given by (2.6), then it can be shown than the number of x_j's in a typical localization well is of the order $\log E/u(0) >> 1$ [21].

2.2 Density expansion

Recall that an important property of the effective potential is the small density μ of the localization centers (cf (2.2)). We describe now a technique that will allow us to use this property.

Let $\{F_l(x_1, ..., x_l)\}_{l\geq 0}$ be a system of functions of l d-dimensional variables $x_1, ..., x_l$ (F_0 is a constant). We denote the set $(x_1, ..., x_l)$ as X. Suppose that the system $\{F_l\}_{l\geq 0}$ satisfies the following conditions (we do not indicate explicitly the index l).

(i) Translation invariance: for any d-dimensional vector a

$$F(X) = F(X + a), \text{ where } X + a = (x_1 + a, ..., x_l + a).$$

(ii) Additive clustering:

$$F(X \cup (Y + a)) - [F(X) + F(Y)] \to 0, \text{ as } a \to \infty. \tag{2.7}$$

and the decay of the l.h.s. of (2.7) is fast enough (it will be exponential below).

For any system of functions, possessing these properties, we can write the combinatorial identity

$$F(X) = \sum_{Y\subset X} \sum_{Z\subset Y} (-1)^{N(Y\setminus Z)} F(Z), \tag{2.8}$$

where $N(X)$ is the number of points of X.

We will use this identity in the case, where X, Y, Z are the sets of random Poisson points $\{\xi_j\}$, entering in the effective potential (2.1). Recall that an infinite system $\{\xi_j\}$ of Poisson points of density μ in the d-dimensional space can be asymptotically described as a system of random points $\xi_1, ..., \xi_N$, uniformly distributed in a cube Λ, provided that the "thermodynamic" limit $N \to \infty$, $|\Lambda| \to \infty$ and $N/|\Lambda| \to \mu$ is carried out (we will denote this limiting transition by $\Lambda \to \infty$). By using this fact and identity (2.8), we can write that

$$\begin{aligned} \lim_{\Lambda\to\infty} |\Lambda|^{-1} \langle F_N(\xi_1, ..., \xi_N) - F_0\rangle &= \mu(F_1 - F_0) \\ &+ \frac{\mu^2}{2} \int [F_2(x) - 2F_1 + F_0] dx + ... \end{aligned} \tag{2.9}$$

where the symbol $\langle ... \rangle$ in the l.h.s. denotes averaging with respect to the Poisson points $\{\xi_j\}$.

In view of (2.4), we will need a more general formula in which the role of ξ_j's is played by pairs (ξ_j, g_j), where $\{g_j\}$ is a system of independent random variables of common density $p(g)$ which are also independent of the $\{\xi_j\}$. The corresponding formula can be

obtained from (2.9), written for fixed g_j's and subsequently integrated with respect to g_j's with the probability density $p(g)$. This yields

$$\lim_{\Lambda\to\infty} |\Lambda|^{-1}\langle F_N((\xi_1,g_1),...,(\xi_N,g_N)) - F_0\rangle = \int (F_1(g_1) - F_0)\mu(g_1)dg_1 \tag{2.10}$$
$$+ \frac{1}{2}\int [F_2(x;g_1,g_2) - F_1(g_1) - F_1(g_2) + F_0]\mu(g_1)\mu(g_2)dxdg_1dg_2 + ...,$$

where now the symbol $\langle ...\rangle$ in the l.h.s. of this formula denotes averaging with respect to $\{\xi_j\}$ and $\{g_j\}$ and

$$\mu(g) = \mu p(g). \tag{2.11}$$

2.3 Density expansion of the DOS

Now we apply the expansion described above to the density of states of the Schrödinger equation. We use the self-averaging property of the DOS, according to which [21]

$$\rho(E) = \lim_{\Lambda\to\infty} \langle |\Lambda|^{-1} \sum_{n\geq 1} \delta(E - E_n)\rangle, \tag{2.12}$$

where $\{E_n\}_{n\geq 1}$ are the energy levels of the Hamiltonian H_Λ defined by the Schrödinger equation with the potential (2.4) in the cube Λ.

Comparing the l.h.s. of (2.10) and the r.h.s. of (2.12), we conclude that in this case the role of F_l in (2.10) play

$$\sum_{n\geq 1} \delta(E - E_n^{(l)}((x_1,g_1),...,(x_l,g_l))),$$

where $\{E_n^{(l)}((x_1,g_1),...,(x_l,g_l))\}_{n\geq 1}$ is the negative spectrum of the l-wells Hamiltonian

$$H^{(l)} = -\Delta + \sum_{j=1}^{l} g_j v\left(\sqrt{g_j}(x - x_j)\right). \tag{2.13}$$

Thus, applying (2.10) to the DOS and taking into account that we are interested in negative energies of large absolute value and that $H^{(0)} = -\Delta$ has no negative spectrum, we find that the term $\rho^{(0)}(E)$ with $l = 0$ (the zero-well contribution) is absent in the expansion. Hence, the leading contribution in μ to the DOS is due to the one-well term of the expansion:

$$\rho^{(1)}(E) = \sum_{n\geq 1} \int \delta(E - E_n^{(1)})\mu(g)dg. \tag{2.14}$$

For the well of the form $gv\left(\sqrt{g}x\right)$ we have:

$$E_n^{(1)} = g\varepsilon_n, \tag{2.15}$$

where $\{\varepsilon_n\}_{n\geq 1}$ are the negative eigenvalues of the dimensionless operator $-\Delta + v(x)$. Thus

$$\rho^{(1)}(E) = \sum_{n\geq 1} \mu\left(\frac{E}{\varepsilon_n}\right)\frac{1}{|\varepsilon_n|}.$$

According to the spirit of our approach the density $p(g)$ should decay sufficiently fast as $g \to \infty$. Thus the leading contribution to $\rho^{(1)}(E)$ is due to the first term of the sum, i.e., we can use the approximation

$$\rho^{(1)}(E) \simeq \mu\left(\frac{E}{\varepsilon_1}\right)\frac{1}{|\varepsilon_1|}. \tag{2.16}$$

Normalizing the well v by the condition

$$\varepsilon_1 = -1, \tag{2.17}$$

we can write

$$\rho^{(1)}(E) \simeq \mu(-E). \tag{2.18}$$

The last formula is a version of the well known "classical" asymptotic formula for the DOS valid for smooth random potentials. By choosing as a randomizing parameter of the wells v_j in (2.1) their ground state energies, we can show that an analogue of (2.16) allows us to obtain also "quantum" versions of asymptotic formulas for the DOS valid for singular v's (see [21] for the respective terminology and results).

It can also be shown that the two-well contribution to the DOS is of the order $O(\mu^2)$. We postpone the corresponding argument to Section 5.1. Thus the two-well contribution is negligible with respect to the r.h.s. of (2.18). We conclude that the unknown (and small) function $\mu(g)$, determining our effective potential and having the sense of the probability density to find a well of amplitude lying between g and $g + dg$ with center in an infinitesimal neighborhood of a given x, coincides in our approximation with the DOS of the Schrödinger operator. This important conclusion makes our scheme self-consistent. It corresponds to the basic ingredient of the Lifshitz approach, according to which the DOS is the probability density of the localization wells, having the ground state energy E [20]. This interpretation of the DOS is widely used in the theory of disordered systems [7, 21]. In our approach it is a simple consequence of the ansatz (2.4) and of the expansion formulas of the previous section.

Let Δ be an interval of values of random variables g_j, lying in the strong localized spectrum with width much smaller than typical values of the g's under consideration. Then $\bar{\mu} = \int_\Delta \mu(g)dg$ will be the density per unit volume of wells, whose amplitudes are in Δ, and $\bar{\mu}^{-1/d}$ will be the typical distance between these wells. Our approach is based on the assumption that typical distances between wells are much larger than the typical radii of the localization wells (cf (1.4)). In the case of the effective potential (2.4), this assumption can be written as

$$g^{-1/2} \ll \bar{\mu}^{-1/d}. \tag{2.19}$$

3 A.C. Conductivity

3.1 Generalities

Recall that from the point of view of statistical physics, we are dealing with an ideal gas of electrons in the external random field $V(x)$ (one-body approximation). In this case, the linear response theory leads to the following formula for the tensor of the zero-temperature

a.c. conductivity of a macroscopic system of spinless electrons in an external spatially homogeneous electric field of the frequency ν at zero temperature:

$$\sigma_{\alpha\beta}(\nu, E_F) = \lim_{\Lambda\to\infty} \pi e^2 |\Lambda|^{-1} \sum_{m\neq n} \delta(E_F + \nu - E_m)\delta(E_F - E_n) V^{(\alpha)}_{mn} V^{(\beta)}_{nm},$$

where $V^{(\alpha)}_{mn}$ are the matrix elements of the velocity operator $i\nabla_\alpha$ between the states ψ_m and ψ_n of the system, confined to the box Λ. In the case of a random potential, homogeneous in mean and weakly correlated, the conductivity is self-averaging [21]. Thus we have in the thermodynamic limit, assuming for simplicity that the system is rotational invariant in mean:

$$\sigma_{\alpha\beta}(\nu, E_F) = \frac{\pi e^2}{d} \delta_{\alpha\beta} \sigma(\nu, E_F), \tag{3.1}$$

$$\sigma(\nu, E_F) = \lim_{\Lambda\to\infty} \left\langle |\Lambda|^{-1} \sum_{m\neq n} \delta(E_F + \nu - E_m)\delta(E_F - E_n) |V_{mn}|^2 \right\rangle, \tag{3.2}$$

where

$$|V_{mn}|^2 = \sum_{\alpha=1}^{d} |V^{(\alpha)}_{mn}|^2. \tag{3.3}$$

Since $V = i[H, X]$, where X is the coordinate operator, we have $|V^{(\alpha)}_{mn}| = |(E_m - E_n) X^{(\alpha)}_{mn}|$, and (3.2) can be written as

$$\sigma(\nu, E_F) = \nu^2 \lim_{\Lambda\to\infty} \langle |\Lambda|^{-1} \sum_{m\neq n} \delta(E_F + \nu - E_m)\delta(E_F - E_n) |X_{mn}|^2 \rangle. \tag{3.4}$$

where

$$|X_{mn}|^2 = \sum_{\alpha=1}^{d} |X^{(\alpha)}_{mn}|^2. \tag{3.5}$$

Note that we keep the frequency ν non-zero while making the thermodynamic limit $\Lambda \to \infty$ in the above formulas. This prescription is well known in kinetic theory and is reminiscent of keeping non-zero magnetic field while making the thermodynamic limit for a ferromagnetic system in order to obtain non-zero macroscopic spontaneous magnetization. Another way to obtain non-zero d.c. conductivity is to set $\nu = 0$ in (3.2) but to replace the δ-functions by a sharp function of width η (usually by the Lorenzian). This corresponds to an imaginary shift in energies instead of a real-valued shift ν (see e.g. [2], where the an imaginary shift is used). In this paper, we will use the formula (3.4), assuming always that the frequency is non-zero, but small compared to the Fermi energy, i.e., we will assume that inequality (1.4) holds.

3.2 Computation

Now we are going to apply the density expansion formula (2.10) to the a.c. conductivity. Comparing (3.4) and (2.10), we choose the functions F_l in this case as

$$\nu^2 \sum_{m\neq n} \delta(E_F + \nu - E^{(l)}_m)\delta(E_F - E^{(l)}_n) |X^{(l)}_{mn}|^2, \tag{3.6}$$

where $\{E_n^{(l)}\}_{n\geq 1}$ are negative levels of the l-wells Hamiltonian (2.13), and

$$X_{mn}^{(l)} = \int x\psi_m^{(l)}(x)\psi_n^{(l)}dx, \tag{3.7}$$

.Here the $\{\psi_n^{(l)}\}_{n\geq 1}$ are the bound states of (2.13). By the same reason as in the case of the DOS, the zero-well contribution $\sigma^{(0)}$ to the conductivity expansion is absent. Let us show that the one-well contribution $\sigma^{(1)}$ is also absent. Combining (3.6) for $l = 1$ and (2.15), we obtain

$$\sigma^{(1)}(\nu, E_F) = \nu^2 \sum_{m\neq n} \int \delta(E_F + \nu - g\varepsilon_m)\delta(E_F - g\varepsilon_n)|X_{mn}^{(1)}|^2\mu(g)dg.$$

where $\{E_n^{(1)}\}_{n\geq 1}$ are the bound state energies (2.15) of the one-well Hamiltonian $H^{(1)}(g) = -\Delta + gv(\sqrt{g}x)$, and $X_{mn}^{(1)}$ is the coordinate matrix element between the corresponding states $\{\psi_l^{(1)}\}$. Non-zero contributions to this expression are due to the pairs (m, n) such that

$$g\varepsilon_n = E_F,\ g\varepsilon_m = E_F + \nu \simeq E_F,\ g(\varepsilon_n - \varepsilon_m) = \nu. \tag{3.8}$$

Denoting by ε the typical value of the levels ε_n's of the potential well v and by $\delta\varepsilon$ the typical value of the spacings $|\varepsilon_{n+1} - \varepsilon_n|$, we see that the above conditions are incompatible if $g\delta\varepsilon \gg \nu$, i.e., if $E_F\delta\varepsilon/\varepsilon \gg \nu$. Since ε_n's are dimensionless, the last condition is just another form of our basic condition (1.4).

The two level contribution $\sigma^{(2)}(\nu, E_F)$ to the a.c. conductivity is (cf (2.10)):

$$\sigma^{(2)}(\nu, E_F) = \frac{\nu^2}{2} \sum_{m\neq n} \int \delta(E_F + \nu - E_m^{(2)})\delta(E_F - E_n^{(2)}) \tag{3.9}$$
$$\times |X_{mn}^{(2)}|^2\mu(g_1)\mu(g_2)dg_1dg_2dy,$$

where $\{E_n^{(2)}\}_{n\geq 1}$ are the bound state energies of the two-well Hamiltonian

$$H^{(2)}((x_1, g_1), (x_2, g_2)) = -\Delta + g_1v_1 + g_2v_2, \tag{3.10}$$

in which

$$v_k(x) = v\left(\sqrt{g_k}(x - x_k)\right),\ k = 1, 2,$$

$y = x_1 - x_2$, and $X_{mn}^{(2)}$ are the corresponding coordinate matrix elements.

In view of our basic condition (2.19), we have typically $|x_1 - x_2| \gg \max g_{1,2}^{-1/2}$. Hence, according to general principles of quantum mechanics, each level of (3.10) should be (exponentially) close to a certain level of one of infinite distant wells, and each eigenfunction is (exponentially) close either to an eigenfunction of one of the wells (non-resonant case) or to a linear combination of the eigenfunctions of the both wells with coefficients of the same order of magnitude (resonant case).

To make this description more quantitative, consider the one-well Hamiltonians

$$H_k^{(1)} = -\Delta + g_kv_k,\ k = 1, 2,$$

corresponding to (3.10). Normalize the potential well $v(x)$ by the same condition (2.17). Then the lowest eigenvalues of $H_k^{(1)}$, $k = 1, 2$ are $-g_k$, and the corresponding eigenfunctions are

$$\varphi_k(x) = g_k^{d/4}\varphi\left(\sqrt{g_k}(x - x_k)\right),\ k = 1, 2, \tag{3.11}$$

where $\varphi(x)$ is the ground state of the dimensionless operator $-\Delta + v(x)$. The function $\varphi(x)$ decays exponentially in x with rate 1. Hence

$$\varphi_k(x) \sim \exp\left(-\sqrt{g_k}|x - x_k|\right), \ |x - x_k| \gg g_k^{-1/2}. \tag{3.12}$$

Since we will be interested mostly in the resonant case, we assume that $g_{1,2} \simeq |E_F|$, i.e., the radii of the φ_k, $k = 1, 2$ in (3.11) are of the same order of magnitude

$$g_{1,2}^{-1/2} \simeq r_l = |E_F|^{-1/2}, \tag{3.13}$$

hence $r_l \ll |x_1 - x_2|$.

In this situation we can find the lowest eigenvalues of $H^{(2)}$ in the framework of the widely used approximation, in which $H^{(2)}$ is replaced by its projection on the span of the functions φ_1 and φ_2 [2]. The diagonal entries of this 2×2 matrix are

$$\begin{aligned}(\varphi_k, H^{(2)}\varphi_k) &= -g_k + g_{j\neq k} \int v_j(x)\varphi_k^2(x)dx \\ &= -g_k + O\left(\exp\left(-2|x_1 - x_2|/r_l\right)\right), \ |x_1 - x_2| >> r_l,\end{aligned}$$

and its off-diagonal entry is

$$(\varphi_1, H^{(2)}\varphi_2) = -g_1(\varphi_1, \varphi_2) + (\varphi_1, v_2\varphi_2).$$

Since v is of finite range, the first term here decays in $|x_1 - x_2|$ not faster than the second term. Hence, being interested in distances $|x_1 - x_2|$ that are much bigger than $g_{1,2}^{-1/2}$, we can neglect the second term, i.e., we can use as the off-diagonal entry of the matrix the quantity $-I(x_1 - x_2)$, where

$$I(x_1 - x_2) = g_1(\varphi_1, \varphi_2) \backsimeq g_2(\varphi_1, \varphi_2) \tag{3.14}$$

is known as the overlap integral, and in view of (3.11) and (3.13) we have

$$I(x) \simeq I_0 e^{-|x|/r_l}, \ |x| \gg r_l, \tag{3.15}$$

with

$$I_0 \simeq |E_F|. \tag{3.16}$$

We obtain that the two lowest eigenvalue of the two-well Hamiltonian $H^{(2)}$ can be found as the eigenvalues of the matrix

$$\begin{pmatrix} -g_1 & -I(x_1 - x_2) \\ -I(x_1 - x_2) & -g_2. \end{pmatrix}. \tag{3.17}$$

Assuming that $g_1 > g_2 > 0$, we obtain that the eigenvalues of this matrix are

$$E_k^{(2)} = -g - (-1)^{k-1}\sqrt{\delta^2 + I^2}, \ k = 1, 2, \tag{3.18}$$

[2] In the appendix, we compute exactly the negative spectrum of $H^{(2)}$ for $v(x) = -\delta(x)$ in the 1-dimensional case. The results for the conductivity, obtained from this spectrum, coincide with those found by using this approximation.

where

$$g = \frac{g_1 + g_2}{2}, \ \delta = \frac{g_1 - g_2}{2}, \tag{3.19}$$

and the corresponding eigenfunctions of the projection of $H^{(2)}$ are

$$\begin{aligned} \psi_1(x) &= \varphi_1(x)\cos\theta + \varphi_2(x)\sin\theta \\ \psi_2(x) &= -\varphi_1(x)\sin\theta + \varphi_2(x)\cos\theta, \end{aligned} \tag{3.20}$$

where

$$\tan\theta = \frac{I}{\delta + \sqrt{\delta^2 + I^2}}. \tag{3.21}$$

We are going to use these formulas in the r.h.s. of (3.9), keeping there only terms with $m, n = 1, 2$, i.e., in fact, the term, corresponding to $m = 1$, $n = 2$. It is easy to see that the equalities $E_F = E_1^{(2)}$, $E_F + \nu = E_2^{(2)}$ imply, in view of (3.18)–(3.19), that $\nu = 2\sqrt{I^2(y) + \delta^2}$, $y = x_2 - x_1$. Hence, by (3.15)–(3.16) and by the condition $\nu \ll |E_F|$, the values of y, contributing to (3.9), are bounded below by

$$r(\nu) = r_l \log \frac{2I_0}{\nu}, \tag{3.22}$$

and the values of $|\delta|$ do not exceed $\nu/2$. Under these conditions the coordinate matrix element $X_{12}^{(2)}$ in (3.9):

$$X_{12}^{(2)} = (x_1 - x_2)\frac{I}{2\sqrt{\delta^2 + I^2}} + (g_1^{-1/2} - g_2^{-1/2})\frac{I}{2\sqrt{\delta^2 + I^2}}\int x\varphi^2(x)dx \tag{3.23}$$

$$+ \frac{\delta}{\sqrt{\delta^2 + I^2}}\int x\varphi_1(x)\varphi_2(x)dx \tag{3.24}$$

between states (3.20) can be replaced by

$$X_{12}^{(2)} \simeq (x_1 - x_2)\frac{I}{2\sqrt{\delta^2 + I^2}}. \tag{3.25}$$

Indeed, the second term in (3.23) can be omitted because its ratio to the first term is of the order $\nu(|E_F|\log 2|E_F|/\nu)^{-1} \ll 1$. Besides, the term is zero if φ is even. The relative order of the third term is the same as the second one.

In view of the above we obtain that the two-well contribution (3.9) to the a.c. conductivity is

$$\sigma^{(2)}(\nu, E_F) = \nu \int \frac{|y|^2 I^2(y)}{\delta^2 + I^2(y)}\delta(E_F + \nu - E_2^{(2)})\delta(E_F - E_1^{(2)})\mu(g_1)\mu(g_2)dg_1dg_2dy. \tag{3.26}$$

We integrate first the product of two δ-functions with respect to g_1 and g_2, taking into account that $|g_1 - g_2| \lesssim \nu \ll |E_F| \sim g_{1,2}$. This allows us to replace $\mu(g_1)$ and $\mu(g_2)$ by $\mu(-E_F)$, to set

$$\delta = \frac{1}{2}\sqrt{\nu^2 - 4I^2(y)}, \tag{3.27}$$

and to obtain in view of (2.18)

$$\sigma^{(2)}(\nu, E_F) = \nu\rho^2(E_F)\int_{2|I(y)|\geq\nu} \frac{|y|^2 I^2(y)}{\sqrt{\nu^2 - 4I^2(y)}}dy. \tag{3.28}$$

Note that the restriction $2|I(y)| \geq \nu$ of the domain of integration in (3.28) is because of the presence of the two δ-functions in (3.26), i.e., in fact, because of energy conservation.

In view of the inequalities $0 < \nu << E_F$ and formulas (3.15)–(3.16), we can replace the condition $2|I(y)| \geq \nu$ by the condition $|y| \geq r(\nu)$, where $r(\nu)$ is defined in (3.22).

The integrand in (3.28) is divergent at the lower limit $|y| = r(\nu)$ and decays exponentially fast at infinity with the rate $2/r_l$ in view of (3.15). Thus the main contribution to the integral is due to a r_l-neighborhood of the lower integration limit. This leads to the asymptotic expression

$$\sigma^{(2)}(\nu, E_F) = \frac{\nu^2 \rho^2(E_F) S_d}{4} r_l^{d+2} \left(\log \frac{2I_0}{\nu} \right)^{d+1}. \tag{3.29}$$

where S_d is the area of the d-dimensional sphere. Taking into account relations (3.16), and (3.13), we obtain finally that

$$\sigma^{(2)}(\nu, E_F) = \frac{\nu^2 \rho^2(E_F) S_d}{4} |E_F|^{-(d+2)/2} \left(\log \frac{2|E_F|}{\nu} \right)^{d+1}. \tag{3.30}$$

In particular, we have for $d = 1$:

$$\sigma(\nu, E_F) = \frac{\nu^2 \rho^2(E_F)}{2} |E_F|^{-3/2} \left(\log \frac{2|E_F|}{\nu} \right)^{2}. \tag{3.31}$$

These are our versions of the Mott formula (1.3). They will be discussed in more details in Section 5.

4 Correlation Functions

4.1 Generalities

In this section we study the following two-point correlation functions:

$$C_1(x - y; \nu, E) = \langle \rho_E(x, y) \rho_{E+\nu}(y, x) \rangle, \tag{4.1}$$

and

$$C_2(x - y; \nu, E) = \langle \rho_E(x, x) \rho_{E+\nu}(y, y) \rangle, \tag{4.2}$$

In writing the above expressions, we took into account the translation invariance in coordinates of the correlation functions, following from the translation invariance in mean, a fundamental property of disordered systems.

The function C_1 of (4.1) is closely related to the a.c. conductivity. Indeed, recall the spectral theorem, according to which

$$\rho_E(x, y) = \int \delta(E - E') \psi_{E'}(x) \psi_{E'}(y) dE', \tag{4.3}$$

where the symbol $\int ...dE$ denotes both the integration over the continuous spectrum and the summation over the point spectrum.

Formulas (4.3), (3.4), and (4.1) imply that

$$\sigma(\nu, E) = -\frac{\nu^2}{2} \int |x|^2 C_1(x, E, \nu) dx. \tag{4.4}$$

The function C_2 of (4.2) is the local DOS–DOS correlator and is a characteristic of localization, providing information on correlations of eigenstates whose energy difference is ν and that are localized in spatial domains of distance $x-y$.

Comparing (1.1) for $l=2$ and (4.1) and (4.2), we obtain the equalities

$$\begin{aligned} C_1(x;\nu,E) &= K_2(0,x;x,0;E,E+\nu), \\ C_2(x;\nu,E) &= K_2(0,0;x,x;E,E+\nu). \end{aligned} \tag{4.5}$$

We list below certain properties of C_1 and C_2.

(i)

$$|C_1(x;\nu,E)| \le C_2(x;\nu,E). \tag{4.6}$$

The inequality follows from the inequality $|\rho_E(x,y)|^2 \le \rho_E(x,x)\rho_E(y,y)$ that is a simple consequence of the Schwarz inequality $\langle ab\rangle^2 \le \langle a^2\rangle \langle b^2\rangle$ and of the spectral theorem (4.3).

(ii)

$$\int C_1(x;\nu,E)dx = \delta(\nu)\rho(E). \tag{4.7}$$

This relation follows from (4.1) and (1.2) and can be interpreted as a weak form of the decay of the correlator C_1 at infinity.

(iii)

$$\lim_{\Lambda\to\infty} |\Lambda|^{-1} \int_\Lambda C_2(x;\nu,E)dx = \rho(E)\rho(E+\nu). \tag{4.8}$$

To prove this formula, we use the ergodic theorem for $\rho_E(x,x)$, implying the validity of the relation

$$\lim_{\Lambda\to\infty} |\Lambda|^{-1} \int_\Lambda \rho_E(x,x)dx = \langle \rho_E(0,0)\rangle \equiv \rho(E)$$

on almost all realizations of the random potential. Applicability of the ergodic theorem follows from the translation invariance in mean and the decay of the spatial correlation in disordered systems (see e.g. [21]).

Formula (4.8) expresses the decay of correlations between two density operators in (4.2) as $|x_1-x_2|\to\infty$. Indeed, its r.h.s. is the product of the averages of these two operators (see (1.2)), and its l.h.s. is a weak form of the relation $\lim_{x\to\infty} C_2(x,E,E+\nu) = \rho(E)\rho(E+\nu)$.

(iv) Assume that for a certain E

$$C_\alpha(x;\nu,E) = \delta(\nu)p_\alpha(x;E),\ \ \alpha=1,2. \tag{4.9}$$

Then

(a)

$$p_1(x;E) = p_2(x;E) = p(x;E) \ge 0;$$

(b)

$$p(x;E) = \left\langle \sum_{\rm loc} \delta(E-E_j)\psi_j^2(0)\psi_j^2(x) \right\rangle, \tag{4.10}$$

where the symbol $\sum_{\rm loc}$ denotes the summation over the localized states only;

(c) if one defines the density of localized states as

$$\rho_{loc}(E) = \int p(x;E)dx = \left\langle \sum_{\text{loc}} \delta(E-E_j)\psi_j^2(0) \right\rangle,$$

then

$$\rho_{\text{loc}}(E) \le \rho(E), \tag{4.11}$$

and the inequality $\rho_{\text{loc}}(E) > 0$ is equivalent to the existence of localized states in a neighborhood of E, and the equality $\rho_{\text{loc}}(E) = \rho(E)$ is equivalent to complete localization in a neighborhood of E.

The above properties follow from the spectral theorem (4.3). The functions $p_\alpha(x;E)$ of (4.9) are the "diagonal parts" of the r.h.s. of equalities (4.5), viewed as functions of two variables $E_1 = E$ and $E_2 = E + \nu$.

The property (iv) will not be used below. We presented this property to demonstrate usefulness of the correlators C_1 and C_2 in the theory of disordered system. In particular, in the classic paper by P. Anderson [4] the positivity of $\int p(0;E)dE$ was used as an indicator for localization. The quantum mechanical meaning of $\int p(0;E)dE$ is the probability for a particle to be in an infinitesimal neighborhood of the origin at time $t = \infty$, provided that at $t = 0$ it was at the origin (the return probability density)[21].

4.2 Computations.

To apply the density expansion formula (2.10) to the correlation functions (4.1) and (4.2), we write them in the form of extensive quantities per unit volume:

$$C_\alpha(x) = |\Lambda|^{-1}\Phi_\alpha(x),\ \alpha = 1,2, \tag{4.12}$$

where

$$\Phi_1(x) = \int_\Lambda C_1((x+a)-a)da = \int_\Lambda \langle \rho_E(a,x+a)\rho_{E+\nu}(x+a,a)\rangle da, \tag{4.13}$$

and

$$\Phi_2(x) = \int_\Lambda C_2((x+a)-a)da = \int_\Lambda \langle \rho_E(a,a)\rho_{E+\nu}(x+a,x+a)\rangle da, \tag{4.14}$$

Now it is clear that the role of the functions F_l in (2.10) for $C_\alpha$will play Φ_α, written for the l-well Hamiltonian (2.13).

By using these formulas, the zero-well and the one-well contributions to C_α, $\alpha = 1,2$ are absent by the same argument as for the conductivity. The two-well contribution $C_1^{(2)}$ to C_1 is (cf (3.9)):

$$\begin{aligned} C_1^{(2)}(x;\nu,E) = \frac{1}{2}\sum_{m,n}\int \delta(E+\nu-E_m)\delta(E-E_n) \\ \times \psi_m(a)\psi_m(a+x)\psi_n(a)\psi_n(a+x)\mu(g_1)\mu(g_2)dadydg_1dg_2, \end{aligned} \tag{4.15}$$

where y is the separation between two wells, implicit in $\psi_{m,n}$ and in $E_{m,n}$.

Since $\nu > 0$, the diagonal part $\sum_{m=n}$ of the double sum is zero. Moreover, as in the case of the conductivity, we restrict ourselves to the two lowest levels of the spectrum of $H^{(2)}$ of (3.10), found in the previous section in the framework of the projection method. This leaves the term $m = 1, n = 2$ in the double sum of (4.15). By using (3.18), we can integrate with respect to g_1 and g_2 the product of two δ-functions, fixing g_1 and g_2 by the relations $E + g + \sqrt{\delta^2 + I^2} = 0,\ E + g + \nu - \sqrt{\delta^2 + I^2} = 0$. In view of the condition $0 < \nu \ll E$ we obtain, replacing $\mu(-g_1)$ and $\mu(-g_1)$ by $\rho(E)$ in view of (2.18) (cf (3.28)):

$$C_1^{(2)}(x;\nu,E) = \rho^2(E)\nu \int da\psi_1(a)\psi_2(a) \times \int_{2|I(y)|\geq\nu} \psi_1(a+x)\psi_2(a+x)\frac{\nu}{\sqrt{\nu^2 - 4I^2(y)}}dy. \tag{4.16}$$

According to the previous section, if $\nu \ll E$, the restriction $2|I(y)| \geq \nu$ is equivalent to $|y| \geq r(\nu)$, where the resonant radius $r(\nu) \gg r_l$ is defined in (3.22). This and the form (3.20) of the functions $\psi_{1,2}$ imply the that if $|g_1 - g_2| \lesssim \nu \ll g \sim |E|$, then

$$\psi_1(a)\psi_2(a) = \cos\theta\sin\theta\left[\varphi^2(a) - \varphi^2(a+y)\right] + O\left(e^{-2r(\nu)/r_l}\right),$$

where $y = x_1 - x_2$. The formula and the analogous formula with a, replaced by $a+x$, lead to the following asymptotic expression for the two-well contribution $C_1^{(2)}$ to the correlator C_1:

$$C_1^{(2)}(x;\nu,E) = \frac{2\rho^2(E)}{\nu}\int \varphi^2(a)da \times \int_{|y|\geq r(\nu)} \frac{I^2(y)}{\sqrt{\nu^2 - 4I^2(y)}}\left[\varphi^2(a+x) - \varphi^2(a+x-y)\right]dy. \tag{4.17}$$

Similar arguments show that the two-well contribution

$$C_2^{(2)}(x;\nu,E) = \frac{1}{2}\sum_{m\neq n}\int \delta(E+\nu-E_m)\delta(E-E_n) \times \psi_m^2(a)\psi_m^2(a+x)\mu(g_1)\mu(g_2)dadg_1dg_2dy, \tag{4.18}$$

to the correlator C_2 is with the same accuracy:

$$C_2^{(2)}(x;\nu,E) = C_1^{(2)}(x;\nu,E) + \rho^2(E)\int \varphi^2(a)da\int_{|y|\geq r(\nu)} \frac{\nu}{\sqrt{\nu^2 - 4I^2(y)}}\varphi^2(a+x-y)dy. \tag{4.19}$$

We formulate now several properties of $C_1^{(2)}$ and $C_2^{(2)}$, following from (4.17)–(4.19).

According to (4.17)

$$\int C_1^{(2)}(x;\nu,E)dx = 0$$

This relation is in agreement with the exact sum rule (4.7), because formula (4.17) was obtained under the assumption that $\nu > 0$.

Likewise, we have the limiting relation

$$C_2^{(2)} \to \rho^2(E),\ x \to \infty, \tag{4.20}$$

which is in agreement with the exact sum rule (4.8).

It is also easy to see that $C_1^{(2)}(x;\nu,E)$:

(i) has a positive peak of order

$$\rho^2(E)\left(\log\frac{2I_0}{\nu}\right)^{d-1} \tag{4.21}$$

at the origin;

(ii) decays exponentially fast with the rate $2/r_l$ for $|x| \gg r_l$, and is exponentially small in the spatial domain $r_l \ll |x| \ll r(\nu) = r_l \log 2I_0/\nu \gg r_l$;

(iii) has a negative peak of the same order of magnitude (4.21) at a r_l-neighborhood of $|x| = r(\nu)$;

(iv) decays exponentially for $|x| \gg r(\nu)$ with the rate $2/r_l$, thereby complementing (4.8).

This behavior of $C_1^{(2)}$ allows us to obtain the Mott formula (3.29) from the relations (4.4) and (4.17).

The correlator $C_2^{(2)}$ has the same behavior as $C_1^{(2)}$ in x till $|x| \lesssim r(\nu)$, in particular it is exponentially small in x if $r_l \ll |x| \ll r(\nu)$. Then $C_1^{(2)}$ becomes asymptotically equal $\rho^2(E)$ in the domain $|x - r(\nu)| \lesssim r_l$ and it is equal to $\rho^2(E)$ for all x, $|x| \gg r(\nu)$ (see (4.20)). In view of spectral theorem one can expect $\rho_E(x,x)$ to be proportional to $\psi_E^2(x)$ in the strong localization regime (cf (5.18)). Then the factorization property (4.20) can be interpreted as the statistical independence of the localized states of energies close to each others with separation much bigger than $r(\nu)$. On the other hand, the exponential smallness of $C_{1,2}$ for $r_l \gg |x| \gg r(\nu)$ can be interpreted as a kind of strong correlation between states close in energy, that are not sufficiently well separated in space. These correlations can be viewed as a manifestation of a certain "repulsion" of nearby levels in the sense that the probability that nearby levels are close tends to zero as the level spacing tends to zero (see [12, 3]) for discussions of this property). Figures 1 and 2 show examples of graphs of $C_{1,2}$,

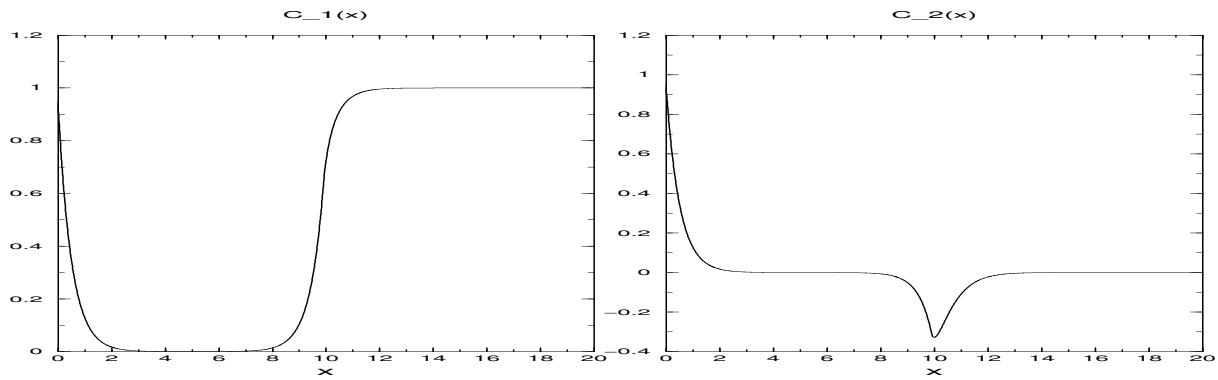

Figure 1: One dimensional correlation function $C_1(x)$ and $C_2(x)$ with $\nu = 10^{-4}$, $r_l = 1$ and $\rho(E) = 1$.

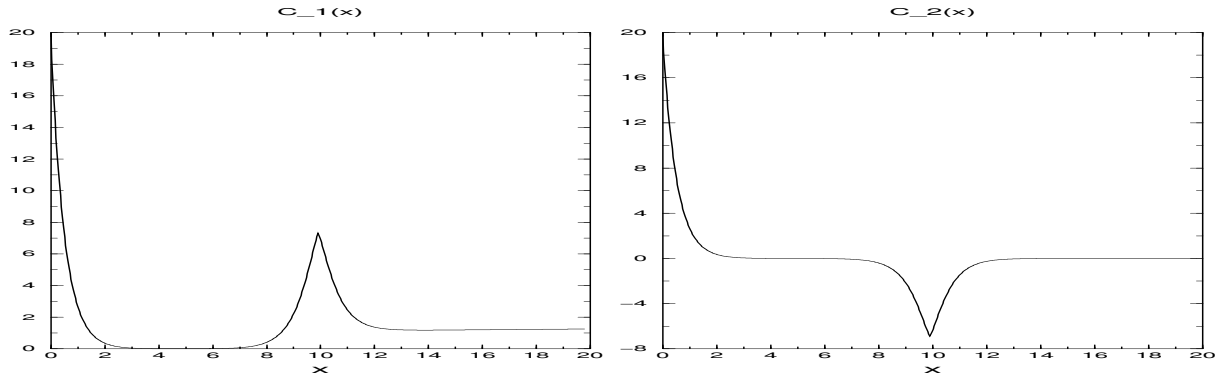

Figure 2: Two dimensional correlation function $C_1(x)$ and $C_2(x)$ with $\nu = 10^{-4}$, $r_l = 1$ and $\rho(E) = 1$.

Results similar to those outlined above were obtained as asymptotically exact ones in [14] in the one dimensional case of the strong localization regime and in [10, 11] in the one dimensional case of the weak localization regime (see the following section for more details). We see, however, that in dimension greater than 1 the characteristic value (4.21) of the peak of the correlation function (3.2) diverges as the difference of the energies tends to zero. Thus, unlike the conductivity that has the log-factor in all dimensions, the correlation functions $C_{1,2}$ are logarithmically big in the energy difference for $|x| \sim r(\nu)$ only in dimension bigger than 1. Similar results were obtained in [15] in the frameworks of the instanton approach (see Subsection 5.4).

The "two-hump" states (3.20) appear in our approach just as a computational tool, allowing us to find leading contributions to the low frequency conductivity and to the correlators $C_{1,2}$, by using the density expansion of Section 2.1, just as the "one-hump" states (3.11) are necessary to find the low energy asymptotic of the density of states in our approach (see also Section 2.3), in the optimal fluctuation method [20, 21, 7], and its version, known as the instanton approach (see Section 5.4, [15] and references therein). On the other hand, the development of localization theory of the last decades suggests that the "one-hump" states carry certain information on the structure of genuine localized states in disordered systems. This suggests the belief, that the "two-hump" states also reflect certain properties of genuine localized states. If this is true, we can interpret the above results on the spatial behavior of the correlators $C_{1,2}$ in the following way. The existence of the length scale $r(\nu)$ of (3.22), that determines drastic changes of the spatial behavior of the correlators $C_{1,2}$, is due to the "interaction" between close energy levels, and the interaction mechanism is the resonant tunnelling between the "bare" one-hump states, i.e., between different centers of genuine states. The parameter I_0 of (3.15) - (3.16) is the characteristic interaction energy, determining the level splitting (spacing), and $r(\nu)$ is the tunnelling distance, determined by the two energy scales ($E = (E_l + E_2)/2,\ v = |E_2 - E_1|,\ E >> \nu$). This inter-level interaction is a mechanism of a certain level repulsion, that prevents the spatial domains where the states are essentially non zero to be close and, as a result, leads to the exponentially small values of the two-point correlators for $r_l << |x| << r(\nu)$.

5 Discussion

5.1 Corrections

We comment now on the corrections (next terms of the density expansions) to our formulas of Sections 2–4. We are not able to prove the convergence of these expansions. We simply argue that they should be asymptotic, i.e., that their terms should be small in successive powers of $\rho(E)$. We will begin from the density of states itself.

It is easy to see that the next term in the expansion of the DOS has the form

$$\begin{aligned}\rho^{(2)}(E) &= \int \Big\{ \Big[\delta(E-E_1^{(2)}) - \delta(E-\varepsilon_1^{(2)})\Big] \\ &+ \Big[\delta(E-E_2^{(2)}) - \delta(E-\varepsilon_2^{(2)})\Big]\Big\} \mu(g_1)\mu(g_2) dy dg_1 dg_2.\end{aligned}$$

where $E_{1,2}^{(2)}$ are given by (3.18), and $\varepsilon_1^{(2)} = -\max(g_1, g_2)$, $\varepsilon_2^{(2)} = -\min(g_1, g_2)$. Recall that we assume that $\mu(g)$ is smooth enough and decays sufficiently fast for large g. Thus $\rho^{(2)}$ will be of the order $O(\mu^2)$ if the integral in the relative distance y between the wells will be convergent. This fact follows from the inequality $|E_k - \varepsilon_k^{(2)}| \leq (\sqrt{\delta^2 + I^2(y)} - |\delta|) \leq |I(y)|$, the exponential decay of $I(y)$ (see (3.15)), and the smoothness of $\mu(g)$, allowing us to transfer derivatives of delta-functions to the μ's.

In the general case of the correction of the order l the appropriate integrals in relative distances between wells will be convergent because of the subtractions of the functions F_k of lower orders $k < l$ from that of the order l in the lth term of the density expansion (2.10), the sufficiently fast splitting (additive clustering) of negative eigenvalues $E^{(l)}$ of the l-wells problem into the sums of negative eigenvalues $E^{(k)}$ of the k-wells problems $k < l$ and again because of the smoothness of $\mu(g)$.

The situation is less simple in the case of the conductivity as we have seen already for $l = 2$. This is because of the presence of families of tunnelling configurations for any number of wells (for example, for $l = 3$ there are two families: the equilateral triangles and the three equidistant points on a straight line). These configurations are responsible for the absence of decay (and even for the polynomial growth) in distances between wells of matrix elements $x_{ij}^{(l)}$ on the corresponding resonant sub-manifolds and for the appearance of extra powers of $\log \nu_0/\nu$ (where ν_0 can be different from that of formula (3.30)). However, since the dimension of these resonant manifolds grows slower than l, these powers of $\log \nu_0/\nu$ will be always multiplied by powers of ν, given by the dimensions of the manifolds transversal to the resonant ones. This is why the higher terms in the expansion of the low frequency conductivity should be small compared to the terms in Mott's formula (1.3).

In other words, it seems reasonable to believe that these higher resonant configurations will produce new peaks and new length scales in the higher terms of the density expansion of the correlators, but that the amplitudes of the peaks will be small relative to the amplitude (4.21) of the peak due to the resonant pairs. One can also speculate that for bigger densities of states (i.e., for energies closer to the mobility edge) higher resonant configurations will play a more significant role, leading eventually to the loss of the exponential decay of the correlators and to the delocalization transition according to the scenario, outlined in [20, 30]

5.2. Asymptotically exact one-dimensional results

The asymptotic behavior of the low frequency conductivity in the strong localization regime of the one-dimensional Gaussian white noise potential, defined by the relations

$$\langle V(x)\rangle = 0,\ \langle V(x)V(y)\rangle = 2D\delta(x-y), \tag{5.1}$$

was studied in [14]. The potential is often used in the theory of one-dimensional disordered systems (see [21] for results and references). In particular, the density of states $\rho(E)$ and the Lyapunov exponent $\gamma(E)$ of the Schrödinger equation with this potential can be found in quadratures. The strong localization regime corresponds to negative energies of large absolute value

$$D^{2/3} \ll |E|. \tag{5.2}$$

In this case we have the following asymptotic formulas [21]

$$\rho(E) = \frac{2|E|}{\pi D} e^{-4|E|^{4/3}/3D},\ \gamma(E) = |E|^{1/2}. \tag{5.3}$$

Moreover, the rate of the exponential decay of the eigenfunctions ψ_E is $\gamma(E)$, because we have with probability 1 [21, 27]:

$$\lim_{|x|\to\infty} |x|^{-1} \log\left(\psi_E^2(x) + \psi_E'^2(x)\right)^{1/2} = -\gamma(E) \tag{5.4}$$

Hence, the exact asymptotic form of (5.3) for the localization radius

$$r_l(E) = 1/\gamma(E). \tag{5.5}$$

coincides with our approximate formula (3.13).

In the paper [14] the low frequency conductivity was found using the Grassmann functional integral representation of the Green's function, which leads to an integral representation for the correlator C_1 of (4.1) (recall that the conductivity is related to the correlator via formula (4.4)). The condition (5.2) allowed the authors to apply the saddle point method to this integral representation. We will summarize the results of [14] in a form close to that of Sections 3 and 4.

The "two-hump" states, similar to (3.20) appear in [14] as the saddle points of the effective action for C_1. The states have in general a rather complicated (two-instanton) form, but in the low frequency limit $0 < \nu \ll |E|$ they can be written in the form (3.20), in which the role of the "bare" states play

$$\varphi_{1,2}(x) = \frac{1}{\sqrt{2r_l}\cosh\left(x \pm y/2\right)/r_l}, \tag{5.6}$$

where $y \geq y_0(\nu)$ and

$$y_0(\nu) = r_l \log 8|E|/\nu \tag{5.7}$$

(cf (3.11), (3.12), and (3.22)). As for the angle θ of (3.20), it is defined by the relation $e^{-y/r_l} = e^{-y_0/r_l}\sin 2\theta$, that can be written as

$$\tan\theta = \frac{e^{-y/r_l}}{e^{-y_0/r_l} + \sqrt{e^{-2y_0/r_l} - e^{-2y/r_l}}}. \tag{5.8}$$

Introduce $\widetilde{I}(y) = \widetilde{I}_0 e^{-y/r_l}$, where $\widetilde{I}_0 = 4|E|$. Then formula (5.7) can be written as $\widetilde{I}(y_0) = \nu/2$. These formulas have to be compared with (3.15), and (3.16). Furthermore, setting

$$\widetilde{\delta} = \sqrt{\nu^2/4 - \widetilde{I}^2(y)} = \sqrt{\widetilde{I}^2(y_0) - \widetilde{I}^2(y)}, \tag{5.9}$$

(cf (3.27)), we can write (5.8) in a form, analogous to that of (3.21).

According to [14], the correlator C_1 has the following asymptotically exact form for $0 < \nu \ll |E|$:

$$C_1(x;,E) = 2\rho^2(E) \int da \int_{y \geq y_0} \psi_1(a)\psi_1(a+x)\psi_2(a)\psi_2(a+x) \frac{e^{-y/r_l}}{\sqrt{e^{-2y_0/r_l} - e^{-2y/r_l}}} dy,$$

which can be written as (4.16) because, in view of the above notations, we can write the expression $e^{-y/r_l}\left(e^{-2y_0/r_l} - e^{-2y/r_l}\right)^{-1/2}$ in the last formula as $\nu\left(\nu^2 - 4\widetilde{I}^2(y)\right)^{-1/2}$.

Likewise, the asymptotically exact expression for the low frequency conductivity, obtained in [14], coincides with our formula (3.28), and the correlator C_2 has the form (4.19), after the replacement $E_F \to 4E_F$ under the log sign. The correlator C_2 was not considered in [14], however it can be found by using the techniques, developed in the paper.

We note a certain difference of these asymptotically exact results and our results. Namely, the role of the resonant distance $r(\nu)$ of (3.22) in the results of [14] plays (5.7) that differs from (3.22) by the factor 4 under the logarithm. A possible simple reason for this difference can be the fact that our estimate (3.16) for the amplitude I_0 of the overlap integral indicates only its order of magnitude, but not its precise value, or, more generally, that the projection method is not precise enough.

5.3. Weak localization regime in one dimension.

The case of the Gaussian white noise (5.1) in one dimension has also been studied in the weak localization regime of large positive energies

$$D^{2/3} \ll E \tag{5.10}$$

(see the works [6, 1, 21, 11, 10]). The density of states in this case is the free one $\rho_0(E) = (2\pi E)^{-1/2}$, and the localization radius is

$$r_l = \frac{4E}{D}. \tag{5.11}$$

The rate of the exponential decay of wave functions is $1/r_l$ with probability 1, as it was in the strong localization regime (see (5.4)).

There are several techniques that can be used in this case [6, 1, 21, 11], and yield the low frequency conductivity and the correlators C_1 and C_2 in quadratures. It turns out that these quantities have qualitatively the same spatial behavior as in the strong localization regime, provided that $2E_F$ (i.e., $2I_0$ according to (3.16)) in (3.31) is replaced by $(D/2E_F^{1/2})$. Note that $(D/2E_F^{1/2})^{-1}$ coincides with the relaxation time τ, well known from the kinetic theory [10]. According to [8], the quantities I_0 and τ^{-1} have the same meaning: they give the order of magnitude of the difference of the energies (spacing) of two localized states, whose centers are separated by a distance of the order of the localization radius. Similarly, the role of the resonant distance in the two-point correlators $C_{1,2}$ plays (cf (3.22) and (5.7)):

$$\widehat{r}(\nu) = r_l \log 8/\nu\tau, \tag{5.12}$$

and the rate of the exponential decay of the two-point correlators $C_{1,2}$ near the origin is $1/2r_l$. This rate is 4 times less than the rate $2/r_l$ of these correlators in the strong localization regime, found in Section 3 from the naive prediction, based on the spatial behavior of the envelope of the eigenfunctions with probability 1 (see (5.4)), and in [14] from an asymptotically exact analysis of the corresponding correlators. This difference can be related to the fact that eigenfunctions in the one dimensional case in the weak localization regime are much more spread out than in the strong localization regime. Hence, their behavior on almost all realizations can differ from the behavior of their moments, entering exact formulas (3.2), (4.1), and (4.2).

We stress that the basic properties of the strong localization regime and, in particular, those, motivated assumptions and techniques of this paper, are different in several important points from the basic properties of the weak localization regime in dimension 1, where the mechanism of localization is not trapping in deep and rare localization wells but the enhanced backscattering due to the destructive interference between incident and reflected waves from many defects. One of manifestations of this complex statistical structure of wave functions in the weak localization regime is the value of the rate of exponential decay of the correlators $C_{1,2}$, discussed above. Moreover, according to [11], the characteristic length scale of the correlators $C_{1,2}$ in the neighborhood of $r(\nu)$ is $\sqrt{r(\nu)r_l}$, i.e., is much bigger than the scale r_l in the neighborhood of the origin, while, according to our formulas and respective formulas of [14], in the strong localization regime this scale is r_l both near $r(\nu)$ and the origin.

5.4. Instanton approach.

This is a version of the variational method, proposed first by I. Lifshitz [20] to find the asymptotic form of the density of states and other characteristics of disordered systems in the strong localization regime (see e.g. [7]). The instanton approach was used to analyze the correlators $C_{1,2}$ and the low frequency conductivity for the white noise random potential in d dimensions in paper [15], in which the reader can find references on earlier applications of the approach. It is based on the assumption that in the strong localization regime the two-point correlators correspond to the two-well potential that minimizes the total probability distribution of the random potential under the constraints that $H(V)\psi_k = E_k\psi_k,\ k = 1, 2$ and that the well centers of the "optimal" potential are a distance $y = x_1 - x_2$ apart. This has to be compared with the DOS computation, where it is assumed that the optimal potential is a well for which $H(V)\psi = E\psi$ (see [21, 7]). The derivation of final formulas in [15] is rather involved because of existence of two energy scales and of collective modes, in particular those that correspond to the center of mass $(x_1 + x_2)/2$ of the optimal potential (it is an analogue of our parameter a in (4.12) - (4.14)). As a result, it is shown in [15] that in the strong localization regime (called the hydrodynamic regime in [15]) the correlator C_1 and the low frequency conductivity have qualitatively the same form as those found in Sections 3–4.

We note also that the 1-dimensional results for the white noise potential of [14] can be viewed as a justification of the instanton approach in the one-dimensional case, because it was shown in this paper that the two-well potential of a special from is indeed a saddle point of the respective functional integral.

5.5. Maryland model.

The most widely known signature of localization is the exponential decay of the localized states at infinity. However, the initial derivation of the Mott formula (1.3) as well as

the above derivation are based not only on the exponential localization, reflected in the exponential decay of "bare" states of the independent quantization in each localization well, but also on the weak correlation between the spectra of independent quantization, reflected in statistical independence of localization wells in our effective potential (2.1) and in appearance of the "two-hump" states in our calculations of Sections 3, and 4. The relevance of the last property becomes clearer if one recalls the results, obtained for an explicitly soluble model of an incommensurate system, known as the Maryland model [13, 26, 28]. This is a multi-dimensional tight binding model with an arbitrary short-range and translation invariant hopping and with the potential of the form

$$V(x) = g \tan \pi(\alpha \cdot x + \omega),\ x \in \mathbf{Z}^d, \tag{5.13}$$

where $g > 0$ is the coupling constant, α is a d-dimensional vector with incommensurate components, and $\omega \in [0, 1)$ is a phase, that plays the role of a randomizing parameter. It was found in the mentioned papers that if for some $C > 0$ and $\beta > d$ the vector α satisfies the Diophantine condition

$$|\alpha \cdot x + m| \geq C/|x|^\beta \tag{5.14}$$

for any integer m and $x \neq 0$, then all the states of the model are exponentially localized for any coupling constant, any energy, and arbitrary dimensionality d of the lattice $\mathbf{Z}^d$. Since the potential has arbitrary high peaks, the model can be viewed as an explicitly soluble model of the strong localization regime. The spectrum of the model consists of the solutions of the equation

$$N(E_t(\omega)) = \alpha \cdot t + \omega \ (\text{mod } 1), \tag{5.15}$$

where t is a lattice point, $N(E) = \int_{-\infty}^{E} \rho(E')dE'$,

$$\rho(E) = \frac{1}{\pi} \int_{\mathbf{T}^d} \frac{g}{(w(k) - E)^2 + g^2} dk,$$

is the density of states, in which $w(k)$ is the Fourier transform of the hopping coefficient, and $\mathbf{T}^d$ is the d-dimensional torus.

It is easy to show that for each point t of the d-dimensional lattice the equation has a unique solution, that if $E_{t_1}(\omega) = E_{t_2}(\omega)$, then $t_1 = t_2$, and that the set $\{E_t(\omega)\}_{t \in \mathbf{Z}^d}$ of eigenvalues is dense for any $\omega \in [0, 1)$.

The corresponding eigenfunctions $\psi_t,\ t \in \mathbf{Z}^d$ have the form

$$\psi_t(x) = \chi(x - t, E_t(\omega)), \tag{5.16}$$

where $\chi(x, E)$ decays exponentially in x:

$$|\chi(x, E)| \leq Ce^{-|x|/r_l} \tag{5.17}$$

with some positive $r_l(E)$. Formulas (5.15)–(5.17) seem fairly natural in the case of the strongly incommensurate potential (5.13), where due to the absence of any symmetry the only good quantum number to label levels and states is the "center" of localization well.

One can also say that Mott's notion of the localization centers is explicit here, because, according to (5.15) and (5.16), for any lattice point t there exists a unique eigenvalue E_t, whose eigenfunction is exponentially localized in a neighborhood of t. Thus the set

of localization centers coincides with the whole lattice and the density of localization centers, whose states have energies in a neighborhood of a given E is the density of states $\rho(E)$. This fact can be interpreted as the uniform distribution in space of the localization centers, corresponding to energy E, and is in qualitative agreement with our assumptions of Section 2, formula (2.18) in particular.

On the other hand, the low frequency conductivity and the correlators C_1 and C_2 for the potential (5.13) have a rather different structure than in the case of random potential discussed in Sections 3 and 4. This can be seen from the form of the kernel $\rho_E(x,y)$, following from (5.15) - (5.16):

$$\rho_E(x,y) = \sum_{t\in\mathbf{Z}^d} \delta(E - E_t(\omega))\chi(x-t, E_t(\omega))\chi(y-t, E_t(\omega)). \tag{5.18}$$

Consider first the correlator C_2. Plugging (5.18) into (4.2), and recalling that the averaging operation $\langle ... \rangle$ here is the integration with respect to the parameter $\omega \in [0,1)$ of (5.13), we find first of all that the correlator C_2 is not a regular function. Rather, there exists a dense set of special frequencies for which C_2 has δ-peaks. If, however, we are interested in the gross features of C_2, then we can apply a certain smoothing procedure, say $\nu^{-1}\int_0^\nu ...d\nu'$. Then we obtain that there exists the length scale

$$r_1(\nu) = \left(\frac{\nu_0(E)}{\nu}\right)^{1/\beta}, \;\; \nu_0(E) = C/\rho(E), \tag{5.19}$$

(here β and C are defined in (5.14)), such that $C_2(x;\nu,E)$ is of the order $e^{-r_1(\nu)/r_l}$ if $|x| \ll r_1(\nu)$, and $C_2(x;\nu,E)$ is $\rho^2(E)$ if $|x| >> r_1(\nu)$, and the transition from the first value to the second one is in the layer $|x - r_1(\nu)| \backsimeq r_l$, where r_l is defined in (5.17). We see that the qualitative form of the correlator C_2 for $|x| >> r_l$ is similar to that in the random case, however there is no peak at the origin and the length scale (5.19) is polynomial in ν (cf (3.22)). In addition, the length scale (5.19) has a different origin than (3.22): it is not due to the tunnelling for "soft" resonant pairs, but due to the Diophantine condition (5.14), which determines now the distance to the nearest localization well of an almost same energy. At low frequencies $r_1(\nu)$ is much bigger than the resonance tunnelling distance $r(\nu)$ of (3.22). This leads to the qualitative change of the form of the correlator C_1. Indeed, by using the same argument, we find that C_1 is of the order $e^{-2r_1(\nu)/r_l} \ll 1$ for all x. This and formula (4.4) imply that the low frequency conductivity is of a similar order [26]

$$\sigma(\nu, E_F) \backsimeq \exp\{-(\nu_1(E)/\nu)^{1/\beta}\}, \;\; \nu_1 = \frac{2^\beta \nu_0}{r_l^\beta}. \tag{5.20}$$

The significant difference between (5.20) and (1.3) can be related to the absence of long range tunnelling in the Maryland model. The spectrum of the model is too "rigid", the energy levels are too regularly distributed and small level spacing are too rare for the long-range tunnelling to happen. This illustrate the role of resonance tunnelling in obtaining the Mott formula as well as the range of applicability of the approach of this paper, based on ansatz (2.1) and on the density expansion. Besides, we see that the low frequency conductivity provides a physical distinction between the strong localization regimes of a random shortly correlated and smoothly distributed potential, and the incommensurate potential (5.13) (recall that the density of states and the Lyapunov exponent coincide for the Maryland model and for the random model in which the potential is a collection

of independent identically distributed Cauchy random variables, and in which we expect our approach to be applicable). Besides, recalling the structure of the localized states for smooth incommensurate potentials of large amplitude in one dimension [29], e.g. the potential $g\cos 2\pi(\alpha x+\omega)$, $g >> 1$, one may expect that these potentials will be closer to random potentials in the spatial behavior of two-point correlators and the low frequency asymptotics of the conductivity.

Appendix

One-dimensional case with delta potentials

To support the usage of the projection method by which the bound states of the two-well Hamiltonian in Section 3.2 were found, we will consider here the one-dimensional case with two delta-wells. The corresponding Hamiltonian is:

$$H^{(2)} = -\frac{d^2}{dx^2} - 2\sqrt{g_1}\delta(x-x_1) - 2\sqrt{g_2}\delta(x-x_2), \tag{A.1}$$

where $g_{1,2} > 0$. In this case each of two one-well Hamiltonians

$$-\frac{d^2}{dx^2} - 2\sqrt{g_{1,2}}\delta(x-x_{1,2})$$

has the unique bound state

$$\varphi_{1,2}(x) = g_{1,2}^{1/4}\varphi(\sqrt{g_{1,2}}x), \quad \varphi(x) = e^{-|x|}, \tag{A.2}$$

corresponding to the energy

$$E_{1,2}^{(1)} = -g_{1,2}. \tag{A.3}$$

Since the Hamiltonian $H^{(2)}$ is invariant under translation, we can replace x_1 by 0, and x_2 by y. It is easy to see that $H^{(2)}$ has two bound states:

$$\psi_{1,2}(x) = \left[\sqrt{g_1}\psi(0)\exp\left(-\sqrt{|E|}|x|\right) + \sqrt{g_2}\psi(y)\exp\left(-\sqrt{|E|}|x-y|\right)\right]\Big|_{E=E_{1,2}}, \tag{A.4}$$

where $E_{1,2}^{(2)}$ are the corresponding energies. They solve the equation:

$$(\sqrt{|E|}-\sqrt{g_1})(\sqrt{|E|}-\sqrt{g_2}) = \sqrt{g_1 g_2}\exp\left(-2\sqrt{|E|}|y|\right) \tag{A.5}$$

Assuming the same accuracy as in Section 3.2 ($|g_1 - g_2| \ll g_{1,2}$, $|y| >> g_{1,2}$), we find that the solutions $E_{1,2}^{(2)}$ of (A.5) have the form (3.18) in which $I(y) = 2ge^{-\sqrt{g}|y|}$ (cf (3.15) - (3.16)), and the eigenfunctions (A.2) have the form (3.20) - (3.21) in which $\varphi_{1,2}$ are given by (A.2).

Another way to act in this case is to plug the exact states and levels, given by (A.4) - (A.5), into the expressions (3.9), (4.15) and (4.18) for the two well contributions for the conductivity and the correlators C_1, and C_2. This leads to rather complicated formulas which, however, have the same asymptotic behavior as our formulas (3.28), (4.17), and (4.19) in the asymptotic regime $0 < \nu \ll |E|$.

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