Extension of Anderson’s Localization Theory to Interacting Systems.

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Abstract. The paper adapts Anderson’s original paper on localization to include interaction. For that purpose his perturbation expansion is extended to a many-body Rayleigh Schrödinger perturbation expansion. Two systems are compared which are similar except that one does and the other does not include Coulomb interactions. The latter is assumed to have all states localized. It is shown that interactions have two opposing effects – one enhancing localization, the other delocalization. Deep in the Anderson localization regime the first effect prevails, close to the Anderson transition the latter prevails.

1. Introduction
Anderson’s original paper [1] argued on the basis of a perturbation expansion that under large enough disorder conditions a particle could not propagate over a macroscopic distance. The criterion for localization in this approach is the convergence of the perturbation series. Such a convergence indicates that as higher order terms add local functions at more remote sites to the eigenfunction their amplitude keeps decreasing. In contrast, a divergent series indicates that amplitudes at very remote sites are still important, implying a delocalized wave function.

Since Coulomb interactions are important in most disordered systems their effect on Anderson localization has been of interest for some decades. Early arguments held that interactions in disordered systems are a source of additional disorder energy so they should enhance localization. Such arguments are basically Hartree type. An extension to Hartree-Fock [2] also found that interactions enhance localization. Neither of these include correlation effects and it was argued [3] that these act in favor of enhancing delocalization. More recent works on the subject found that short range interactions preserve localization [4] but long range interactions can induce delocalization [5,6].

This paper adapts [1] to include many-body effects, using a many-body Rayleigh-Schrödinger (RS) perturbation expansion which allows for studying effects of interaction. The paper takes of on previous work [7]. To evaluate the effect of interaction on localization the perturbation series are compared for an interacting and a non-interacting system.

As in [1], the basis set is taken to be the set of N local functions located around N sites. Slater determinants formed of these constitute the many-particle basis set into which the perturbation series is expanded. Interaction increases both the numerators and the denominators in the expansion thus indicating two diverse effects of interactions on localization. Arguments based on RS perturbation theory are presented that close to the Anderson transition interactions can cause delocalization where a similar non-interacting system is still fully localized. The said delocalization is of a collective nature.
2. Physical Considerations

The one-particle RS expansion is stated in (1). For the purpose of this paper, the set of functions $|m_0\rangle$ are local functions, say 1s functions centered on sites $m$.

$$\langle m_0| V |n_0 \rangle = t_{mn} \approx r_{mn}^{-1} \exp(-r_{mn}/\xi)$$

are the transfer energies between sites $m,n$, $\xi$ is the localization length, $r_{mn}$ is the distance between sites $m,n$ and $\epsilon_m$ is the random energy (distributed over an energy range $W$) of site $m$. For simplicity of notation the charge of the electron and the dielectric constant were taken to have the values 1. In the one-electron localization theory the important parameter is $t/W$ where $t$ is taken to be the value corresponding to the average nearest neighbour distance. The critical value of $t/W$ where the Anderson transition occurs in 3D is not known precisely but is close to 1/20. The equation differs from the original Anderson perturbation expansion in that his expansion was for the time-dependent Schrödinger equation while (1) is for the stationary Schrödinger equation. Since at question is the nature of the eigenfunction (localized or delocalized), the latter is more convenient here. The expansion of (1) can be visualized as shown in figure 1. The dots represent sites and the lines of different colours represent successive terms in the perturbation series. When the successive terms become sufficiently smaller than their preceding terms the series converges. The wave function centred on $j$ then cannot extend to infinity except with infinitesimal amplitude, so the eigenstate is localized. In the opposite case the series diverges, the amplitude at infinity is comparable to the amplitude at $i$ and the particle is delocalized. As is well known, the possibility of forming loops puts a caveat on the former statement. However this appears to only affect the point at which the divergence occurs, not the divergence per se.

![Figure 1. Aid to visualize equation 1. The dots represent sites in a disordered system. The lines represent the successive terms in the equation as indicated in the figure. Each term adds a local function with amplitude corresponding to the value of the term to the eigenfunction. The higher the order of the term the further the eigenfunction can spread.](image)

To be able to deal with interactions the expansion is written below in a form to accommodate many-electron wave-functions.
\[ |I_i\rangle = |I_0\rangle + \sum_{J \neq I} \langle J | V | J_0 \rangle |J_0\rangle + \sum_{J \neq I} \langle J | V | J_0 \rangle \langle J | V | I \rangle |I_0\rangle + \sum_{J \neq I} \langle J | V | J_0 \rangle \langle J | V | I \rangle \langle I | V | I_0 \rangle \langle I_0 | L_0 \rangle + \ldots \]  

(2)  

(2)  

(2) \langle X_0 \rangle (and the dots in the figure 1) are now Slater determinants (configurations) so the space in the figure becomes the phase space (or Fock space).

Both the interacting and the non-interacting case can be expressed in this form and compared with each other. For that purpose, the basis set is the same in both cases, namely the set of local functions as described above. The many-body basis set is the set of all Slater determinants formed of these local states.

To compare “apples with apples” one needs to compare similar situations, except for interactions, in both cases. In particular both systems should have the same ratio of electrons to sites \( N \), say \( n/N = \frac{1}{2} \). The interactions are strongest for such a ratio - for a smaller ratio the density of particles is smaller, for a larger ratio one can consider the holes as the interacting particles. In order to deal with a neutral system a positive charge \( +|e| \) is placed on each site as is customary. To see whether interactions can enhance delocalization, assume that without interactions all states are localized and examine whether interactions can cause the RS series to diverge.

There is a formal problem with the expansion (2). In the thermodynamic limit the number of sites \( N \) goes to infinity so already the first sum in (2) has an infinite number of terms, each of which may be finite. The series therefore may diverge even when the numerators are very small. But the meaning of it merely is that \( |I_0\rangle \) is connected to an infinite number of Slater determinants. One could argue that the system is delocalized in Fock space. But the question of interest whether the system is delocalized in real space. In real space the first sum in (2), even if infinite, merely signifies that the wave function extends from each of the \( N \) sites to only nearby sites in real space. In that sense the inclusion of the term accounts only for an extension of the wave function through a short distance. Whether it extends over a microscopic distance is determined by the magnitude of the high order terms. The reasonable approach thus is to begin with a single site in \( |I_0\rangle \) and examine the probability \( P \) that the amplitude of the high order terms connected to that site through all the lower order terms is comparable to the amplitude on this site. Since there are \( N \) sites in \( |I_0\rangle \) the wave function will be delocalized in space if \( P \approx 1/n \).

Since it is known that in three dimensions there is a transition in the absence of interactions, we need not actually execute such an expansion but merely see whether, in comparison with the non-interacting system the expansion for the interacting system enhances or diminishes \( P \).

As will be shown below, interactions introduce two effects, one favoring enhancement of localization, the other enhancement of delocalization. The former involves the denominators, the latter the numerators.

Note at this point that in the case of Coulomb interactions there is a relation between \( t \) and \( E_C \), defined as the Coulomb energy over an average nearest neighbor distance \( \langle r \rangle \):

\[ t = \langle r \rangle^{-1} \exp(-\langle r \rangle / \xi) = E_C \exp(-\langle r \rangle / \xi) \]  

(3)  

with \( t \approx W/20 \) (in 3 dimensions) one has near the Anderson transition \( W \approx E_C \). The importance of this relation will become clear later on.

Starting with the denominators, without interactions when \( I, J \) differ only in the occupation of two sites (i.e. an electron occupying a different site in \( I \) and in \( J \) \( E_I-E_J \) is just the difference in the random energies \( \epsilon_i - \epsilon_j \). \( i, j \) are, respectively, the two sites in \( I, J \) that differ in occupation. In the presence of interactions the site energies include also interactions with all the other sites. Considering such interaction as an additional random energy (due to random spatial distribution), the effect of interactions on the denominators in (2) is to increase them - the spread of \( E_k \) is larger than the spread of the random energies \( \epsilon_k \). (It turns out that \( E_I-E_J \) is determined by the energies \( E_k \) of the sites \( k \) that differ in \( I \) and in \( J \)) This basically corresponds to the old argument that interactions enhance localization. It should be remarked in passing that the definition of \( E_k \) here differs somewhat from the definition of Efros and Shklovskii [8]. Although in their definition and in the present definition \( E_k \) includes both the random and the interaction energies, in [8] \( E_k \) for an unoccupied site relates to an.
n+1 electron system but in the present definition it always refers to an n-electron system, whether k is occupied or not.

Turning now to the effect of interaction on the numerators, without interaction V is a 1-particle operator so \( \langle X_0 | V | Y_0 \rangle \) is non-zero only for \( Y_0 \neq X_0 \) differing in the occupation of two sites. For a two-electron transition (involving four sites) \( \langle X_0 | V | Y_0 \rangle \) includes terms with coefficients of the form
\[
\int \alpha(x_i) \beta(x_j) V(x_i) \gamma(x_j) \delta(x_i) d(x_i) d(x_j) = \langle \alpha | V | \gamma \rangle \langle \beta | \delta \rangle = 0
\]
where \( \alpha \) (say) is the local function centered on site \( \alpha \). (3) vanishes because \( \langle \beta | \delta \rangle \) is a dot product of two orthogonal functions. The integral of the product of all other electron coordinates in \( \langle X_0 | V | Y_0 \rangle \) is \( \prod_x \langle \nu | \nu \rangle = 1 \). All exchange terms vanish, again because of orthogonality.

In the presence of interactions V is a two-particle operator so the terms corresponding to (4) involving \( V(x_i,x_j) \) do not vanish: \( \int \alpha(x_i) \beta(x_j) V(x_i,x_j) \gamma(x_j) \delta(x_i) d(x_i) d(x_j) \neq 0 \). Thus, interactions add a large number of terms to the perturbation expansion (2). Furthermore, the Coulomb interaction between near neighbors amplifies this effect: due to electron-electron repulsion near neighbor pairs are likely to be singly occupied. This is particularly so near the Anderson transition where the disorder energy \( W \approx E_C \).

Figure 2 illustrates the point: there are about twice as many possible transitions from \( k \) in \( K \) to some \( l \) in \( L \) with than without interactions. Furthermore, each such transition can be either a one-electron or a part of a two-electron transition. Thus, a large number of terms in each sum in (2) vanishes without interaction that do not vanish with interaction. This can be visualized in figure 2 as an increase in the numerators therefore is to favor delocalization,

In summary, interaction increases both the numerators and the denominators. Bringing on divergence depends on whether there is a sufficient number of new paths introduced by interaction which do not decay rapidly with the perturbation order. The ratios \( \sum_L \langle K_0 | V | L_0 \rangle / E_K - E_L \) can increase or decrease with interaction – an increase in their value enhances divergence, i.e. delocalization and a decrease enhances localization.

When the interactions are of Coulomb type the values of the transition matrix elements are
\[
\langle I_0 | V | J_0 \rangle = r_{ij} \left[ 1 + W_{ij} \sum (r_{kl}^{-1} - r_{kl}^{-1}) \right] \exp(-r_{ij} / \xi)
\]
when \( I_0 \) and \( J_0 \) differ in two sites and
\[
\langle I_0 | V | J_0 \rangle = r_{ij} \left[ 1 + W_{ij} \sum (r_{kl}^{-1} + r_{kl}^{-1} - r_{kl}^{-1} - r_{kl}^{-1}) \right] \exp(-r_{ij} / \xi) \exp(-r_{ij} / \xi)
\]
when they differ in four sites. In (4) and (5) \( i \) is a site in \( I_0 \), \( j \) in \( J_0 \), \( k \) runs over all other sites identically occupied in \( I_0 \) and \( J_0 \) and \( W_{ij} = e^{-r_{ij} / \eta} \). In (5) \( k \in I_0 \) and \( l \in J_0 \).

3. Quantitative consideration.

Two limits are considered here
- when the non-interacting system is just localized
- when the non-interacting system is strongly localized

In the first case a necessary and sufficient condition for interaction to induce delocalization is
\[
\sum_L \langle K | V | L \rangle (E_I - E_L)_{\text{int}} > \sum_L \langle K | V | L \rangle (E_I - E_L)_{\text{non-int}}
\]
for the delocalizing effect of the numerators to prevail over the localizing effect of the denominators.

The difference between the denominators in the two expression in (7) arises because of the interaction energy of a site with other sites in the system. Considering the interactions on a site as a
random energy and the relation $W/E_c \approx 1$ associated with incipient localization, the denominators differ by a factor of 2.

The numerators are responsible primarily for a difference in the number of terms in the summation. For the condition of incipient localization there are about twice as many one-electron paths originating at a site in the interacting system as there are in the non-interacting system (see figure 2). This is true in 3D and as well as in 2D. In addition, each such path can be traversed by a two-electron transition or a one-electron transition. So a good estimate is that there are four times the possible paths in the interacting system as in the non-interacting system, i.e. four times as many non-vanishing terms in the sum. This is actually a conservative estimate since there is a large number of two electron transitions containing each one-electron transition to $l$ indicated in figure 2 (sites for the second electron transition are outside the figure). However, even with the conservative estimate (6) is clearly satisfied indicating that interactions can induce delocalization when the non-interacting system would still be localized.

In the case of strong localization $W >> E_C$. As a result the near neighbor correlation portrayed by figure 2 is very weak so interaction hardly changes the number of terms in the sum $\sum_{l} \langle K_0 | V | L_{0} \rangle$. In addition, the effect of the interaction energies on the random energy is also very small, $W + E_C \approx W$. The total effect of interaction on localization in this regime is therefore very small.

4. Conclusions.

Interaction affects Anderson localization in two ways. One is to enhance localization the other to enhance delocalization. The first can be traced physically to an effective increase of the disorder energy, the latter to a correlation in the occupation and to a correlated motion of electrons. Near the Anderson transition the correlation effects prevail and interaction can cause delocalization of some states. The motion of the electrons is however highly collective so one can expect strong collective slowing of motion implying that conductivity at $T=0$ can be immeasurably small. If the energy regime of delocalized electron reaches the lowest energies, they can however, act as a thermal bath.

The reasoning leading to the conclusion that interactions can cause delocalization did not differentiate qualitatively between 2D and 3D. It is widely accepted that in the absence of interactions no truly delocalized states exist in the thermodynamic limit [9]. However, the states can be localized weakly. One can thus conclude that in such cases interaction should bring about delocalization.

Finally, it should be stressed that the considerations in this paper rest heavily on the Rayleigh Schrödinger perturbation expansion which is not an exact theory. The conclusions thus are not totally irrefutable.

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