Static screening and delocalization effects in the Hubbard-Anderson model

Peter Henseler and Johann Kroha

Physikalisches Institut, Universität Bonn, Nußallee 12, D-53115 Bonn, Germany

Boris Shapiro

Department of Physics, Technion-Israel Institute of Technology, Haifa 32000, Israel (Received 9 July 2007; revised manuscript received 10 October 2007; published 1 February 2008)

We study the suppression of electron localization due to the screening of disorder in a Hubbard-Anderson model. We focus on the change of the electron localization length at the Fermi level within a static picture, where interactions are absorbed into the redefinition of the random on-site energies. Two different approximations are presented, either one yielding a nonmonotonic dependence of the localization length on the interaction strength, with a pronounced maximum at an intermediate interaction strength. In spite of its simplicity, our approach is in good agreement with recent numerical results.

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I. INTRODUCTION

Understanding the interplay between disorder and electron-electron interactions remains one of the major challenges in modern condensed matter physics, experimental as well as theoretical. The research in this field has been stimulated by the possible metallic behavior in two-dimensional disordered interacting systems.¹ A metallic phase at zero temperature in two or less dimensions would be in contrast to the prediction of the scaling theory of Anderson localization.² The possible existence of a metallic phase, induced by interactions, is a long standing³ and still controversial problem, discussed by many authors during the last three decades.⁴

One of the ideas proposed and discussed by several authors is that interactions lead to a partial screening of the random potential and, thus, reduce the effect of localization. In particular, the 2d disordered Hubbard model (the Hubbard-Anderson model) has been studied, mostly numerically, and it was demonstrated that repulsive interactions can have a delocalizing effect.^{5–11}

In this paper, we present an analytical study of the screening effect, focusing on the case of strong disorder at zero temperature, when the Hubbard-Anderson model is in the regime of an Anderson insulator. Our approach is based on an exact treatment of the atomic limit, followed by "switching on" the intersite hopping t, under the assumption that the atomic-limit occupation numbers do not change. Let us emphasize that in our static approach, the interactions only change the original on-site energies. Therefore, we are left with a single-particle Anderson Hamiltonian, and the question is how the localized single-particle states may change due to the new, renormalized probability distribution of the on-site energies. In this sense, the approach is close, although not identical, to the Hartree-Fock treatment. A comparison of both methods will be presented. Although this approach is formulated for an arbitrary filling factor, it becomes inadequate close to half filling where magnetic effects dominate¹² (such effects are not considered in our work).

Furthermore, we will show that, for fixed disorder, the localization length ξ is a nonmonotonic function of the Hubbard interaction energy U, with a maximum for some inter-

mediate value of U. This is because for strong interactions, the Mott-Hubbard physics of interaction-suppressed hopping dominates, leading to the formation of two disorder broadened Hubbard bands with a reduced average density of states at the Fermi level and, as a consequence, increasing effectively the disorder strength. In spite of the simplicity of the approach, the results are in good agreement with recent numerical studies,^{5,7–10,13,14} in the appropriate range of parameters.

The evaluation of the localization length within our present study is limited to one dimension. However, since the competition of screening on the one hand and Mott-Hubbard physics on the other hand operates in any dimension, the nonmonotonic dependence of ξ on U should also hold in two and three dimensions, as argued below.

II. ATOMIC-LIMIT APPROXIMATION

In this paper, we consider the Hubbard-Anderson model, with on-site repulsion and on-site disorder, at zero temperature. The corresponding Hamiltonian

$$H = H_0 + H_{\rm kin} + H_{\rm e-e}$$

= $\sum_{i,\sigma} (\varepsilon_i - \mu) c^{\dagger}_{i\sigma} c_{i\sigma} - t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}.$ (1)

As usual, $c_{i\sigma}^{\dagger}(c_{i\sigma})$ denote fermion creation (destruction) operators of an electron at site *i* with spin σ , $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, *t* is the nearest-neighbor hopping amplitude, *U* is the on-site repulsion, μ is the chemical potential, and $\{\varepsilon_i\}$ are the on-site energies. The latter are assumed to be independent and uniformly distributed over the interval $\left[-\frac{\Delta}{2}, \frac{\Delta}{2}\right]$, with the disorder parameter Δ . To focus on the screening effect in the case of strong localization, i.e., $\Delta \gg t$, the interaction term will be absorbed into the on-site energies, yielding a renormalized distribution of the ε_i . This results in an effective single-particle problem with a probability function $p_A(\varepsilon_i)$ which is derived as follows.

In the atomic limit (*t*=0), the ground state of the system can be solved exactly for an arbitrary filling factor $\rho = \frac{N_e}{N}$, where N_e , N are the numbers of electrons and lattice sites,

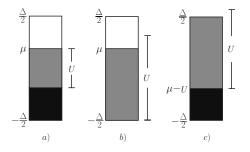


FIG. 1. Site occupation in the atomic ground state with doubly occupied (black), singly occupied (gray), and empty states (white). (a) Weak interaction, (b) strong interaction for less than half filling (i.e., $\rho < 1$), and (c) strong interaction for more than half filling ($\rho > 1$).

respectively.⁹ The chemical potential μ and the sitedependent occupation numbers $\langle n_i \rangle_0$ can be expressed as functions of ρ , Δ , and U: All sites with on-site energies below $\mu - U$ are doubly occupied, all sites within $[\mu - U, \mu]$ are singly occupied, and all other sites are empty (see Fig. 1). Thus, the total occupation number of site *i* and the chemical potential are, respectively,

$$\langle n_i \rangle_0 = \begin{cases} 2 & \text{if } \varepsilon_i \leq \mu - U \\ 1 & \text{if } \mu - U < \varepsilon_i \leq \mu \\ 0 & \text{if } \varepsilon_i > \mu \end{cases}$$
(2)

 and^{15}

$$\varepsilon_{i} \mapsto \begin{cases} \varepsilon_{i} + U & \text{if } \varepsilon_{i} \leq \mu - U \\ \varepsilon_{i} + U & \\ \varepsilon_{i} & \text{if } \mu - U < \varepsilon_{i} \leq \mu \\ \varepsilon_{i} & \\ \varepsilon_{i} & \text{if } \varepsilon_{i} > \mu. \end{cases}$$

$$\mu = \begin{cases} \frac{1}{2}(\Delta\rho - \Delta + U) & \text{if } \rho < 1, \quad U < \Delta\rho \\ \Delta(\rho - \frac{1}{2}) & \text{if } \rho < 1, \quad U \ge \Delta\rho \\ \frac{1}{2}(\Delta\rho - \Delta + U) & \text{if } \rho \ge 1, \quad U < 2\Delta - \Delta\rho \\ \Delta(\rho - \frac{3}{2}) + U & \text{if } \rho \ge 1, \quad U \ge 2\Delta - \Delta\rho. \end{cases}$$
(3)

The renormalized site energies depend on the site occupation numbers and can be read off from the poles of the (timeordered) single-particle propagator,

$$G_{i\sigma}(\omega) = \frac{\langle n_{i,\sigma} \rangle_0 \langle n_{i,-\sigma} \rangle_0}{\omega - (\varepsilon_i - \mu + U) - i0^+} + \frac{\langle n_{i,\sigma} \rangle_0 (1 - \langle n_{i,-\sigma} \rangle_0)}{\omega - (\varepsilon_i - \mu) - i0^+} + \frac{(1 - \langle n_{i,\sigma} \rangle_0) \langle n_{i,-\sigma} \rangle_0}{\omega - (\varepsilon_i - \mu + U) + i0^+} + \frac{(1 - \langle n_{i,\sigma} \rangle_0) (1 - \langle n_{i,-\sigma} \rangle_0)}{\omega - (\varepsilon_i - \mu) + i0^+}.$$
 (4)

The first term in Eq. (4) corresponds to the doubly occupied sites showing that these on-site energies are shifted by U. The next two terms correspond to singly occupied sites. In the absence of spin polarization, $\langle n_{i,\sigma} \rangle_0 = \langle n_{i,-\sigma} \rangle_0$, half of these on-site energies are again shifted by U whereas the other half remain unchanged. Finally, the last term corresponds to the unoccupied sites, whose energies also remain unchanged. Combining Eqs. (3) and (4), the rule for replacing the bare site energy ε_i by a renormalized one is

(each with probability of
$$\frac{1}{2}$$
) (5)

For a weak to intermediate repulsion U, these shifts lead to a raise of the lowest lying on-site energies toward the Fermi level μ resulting in a renormalized probability function $p_A(\varepsilon)$ with a reduced width and modified shape [see Fig. 2(a)].

In the atomic-limit approximation, the Hamiltonian [Eq. (1)] is replaced by the effective single-particle Anderson Hamiltonian,

$$H = \sum_{i\sigma} (\varepsilon_i - \mu) c_{i\sigma}^{\dagger} c_{i\sigma} - t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma}, \qquad (6)$$

with on-site energy probability function $p_A(\varepsilon)$, where the two-particle interaction U enters only as a (screening) parameter in $p_A(\varepsilon)$. Note that, due to the asymmetry of $p_A(\varepsilon)$, the average value of the renormalized on-site energies is

$$\langle \varepsilon \rangle_{\rm A} = \int p_{\rm A}(\varepsilon) \varepsilon d\varepsilon = \frac{1}{2} \rho U.$$
 (7)

In deriving Eq. (6), it was assumed that in the case of strong disorder, the occupation numbers in the atomic ground state [Eq. (2)] are close to the occupation numbers $\langle n_i \rangle$ in the true ground state, with finite hopping amplitude *t*. This assumption is based on the results from the single-particle theory of localization,¹⁶ where it is known that for strong disorder, an electron, once located at any site *i*, will stay at that site with high probability. More precisely, the change of the occupation number of site *i*, $\delta \langle n_i \rangle \equiv \langle n_i \rangle - \langle n_i \rangle_0$, is of order t^2/Δ . The same estimate holds if one considers hopping of a single electron on the background of the other electrons, which are assumed to be immobile. Furthermore, for strong disorder, a perturbative expansion in *t*, around the atomic ground state of Eq. (1), is possible.¹⁷ Thus, with the same reasoning as in

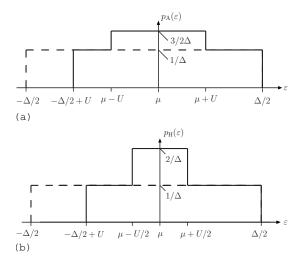


FIG. 2. The renormalized on-site energy probability functions (solid line) for weak repulsion U: (a) atomic-limit approximation and (b) Hartree-Fock approximation. For comparison, also the original function is shown (dashed lines).

the noninteracting case, the leading self-energy corrections are again only of second order.

One measure of localization is the localization length ξ which governs the exponential decay of the single-particle wave functions $\psi(r)$ at distances far away from its localization center. It can be calculated from the probability for a transition from site *i* to site *j* as¹⁸

$$-\frac{1}{\xi(E)} = \lim_{|x_i - x_j| \to \infty} \frac{\log\langle |G_{ij}^{\kappa}(E)|^2 \rangle}{2|x_i - x_j|},\tag{8}$$

where $G_{ij}^{\text{R}}(E)$ is the retarded propagator for a particle with energy *E* from site *j* to site *i*. In general, it is not possible to deduce ξ from the probability distribution analytically, but in case of a one-dimensional lattice, there exists a relatively simple relation¹⁸ between ξ and $\langle D(\omega) \rangle$, the disorder averaged density of states,

$$\xi^{-1}(E) = \int_{-\infty}^{\infty} \langle D(\varepsilon) \rangle \log |E - \varepsilon| d\varepsilon.$$
(9)

(Here and in the following, we choose units where t=1 and measure ξ in units of the lattice spacing.)

In the strong disorder limit, $\langle D(\varepsilon) \rangle$ can be replaced by $p_{\rm A}(\varepsilon + \mu)$, so that the inverse localization length at the Fermi level (*E*=0) is given by

$$\xi^{-1} = \int_{-\infty}^{\infty} p_{\rm A}(\varepsilon) \log |\varepsilon - \mu| d\varepsilon.$$
 (10)

A plot of ξ as a function of U and ρ , for fixed disorder strength $\Delta = 15$, is shown in Fig. 3(a). It can be seen that for each given filling factor, the localization length exhibits a pronounced maximum. This maximum can be calculated to appear at

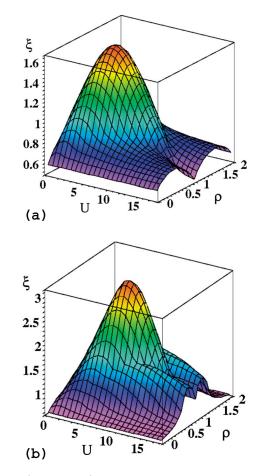


FIG. 3. (Color online) Localization length ξ at the Fermi level as a function of repulsion U and lattice filling ρ for $\Delta = 15$: (a) atomic-limit approximation and (b) Hartree-Fock approximation.

$$U_{\xi}^{A} = \frac{\Delta}{3} (\sqrt{1 + 3\rho(2 - \rho)} - 1) \approx \frac{\Delta}{2} \rho(2 - \rho) + \mathcal{O}[\rho^{2}(2 - \rho)^{2}].$$
(11)

The reason for this nonmonotonic behavior is simple: A weak to intermediate repulsion U changes the on-site energy distribution from a rectangular distribution to a narrower one by shifting low site energies toward the Fermi level (screening) [see Fig. 2(a)]. In contrast, a very strong on-site repulsion enhances the localization by a large broadening of the probability density. Therefore, in between, there will be some value U_{ξ}^{A} for which the screening is optimal and the localization length acquires a maximum. Such behavior is expected, since a strong repulsion effectively suppresses hopping processes and leads to an accumulation of spectral weight in the upper Hubbard band.

In Fig. 4(a), the localization length ξ is shown as a function of U for $\rho = \frac{1}{2}$ (quarter filling). A similar, nonmonotonic behavior was also found in recent quantum Monte Carlo simulations^{5,9,13,14} and a most recent statistical dynamical mean field theory evaluation¹⁰ of the problem, where the conductivity and the inverse participation ratio⁷ of a finite system were calculated, respectively. Identifying a maximum of conductivity with a maximum of localization length, we

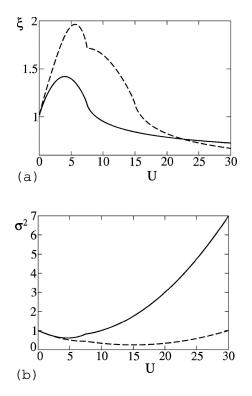


FIG. 4. (a) Localization length ξ at the Fermi level, normalized by its noninteracting value, as a function of the on-site repulsion U for $\Delta = 15$ and $\rho = \frac{1}{2}$. (b) Variance of the renormalized on-site energy distribution, also normalized by its noninteracting value. The solid curves show the results for the atomic-limit approximation and the dashed curves are the Hartree-Fock results.

find in all cases a good qualitative agreement with our results. Furthermore, we even find a reasonable quantitative agreement with our results for the points of maximal delocalization, U_{ξ}^{A} , Eq. (11), and U_{ξ}^{H} , defined in Eq. (17) below. Thus, there is a strong correlation between the degree of screening and the conductivity: optimal screening corresponds to maximal conductivity. In addition, our analytical results indicate that much of this physics of the nonmonotonic behavior can already be understood on the level of a static screening approximation.

Our result appears to be at odds with the statement⁹ that screening alone cannot account for the nonmonotonic behavior of the conductivity. We will discuss this point in the next section. For that discussion, we need the variance of the renormalized on-site energies which is given by

$$\sigma_{\rm A}^{2} \equiv \langle \varepsilon^{2} \rangle_{\rm A} - \langle \varepsilon \rangle_{\rm A}^{2} \\ = \frac{\Delta^{2}}{12} \begin{cases} 1 - \hat{\rho}\hat{U} + \hat{\rho}\hat{U}^{2} + 3\hat{U}^{3}, \quad \rho < 1, \quad \hat{U} < \rho \\ 1 - 2\rho'\hat{U} + \hat{\rho}\hat{U}^{2}, \quad \rho < 1, \quad \hat{U} \ge \rho \\ 1 - \hat{\rho}\hat{U} + \hat{\rho}\hat{U}^{2} + 3\hat{U}^{3}, \quad \rho \ge 1, \quad \hat{U} < 2 - \rho \\ 1 - 2\tilde{\rho}\hat{U} + \hat{\rho}\hat{U}^{2}, \quad \rho \ge 1, \quad \hat{U} \ge 2 - \rho, \end{cases}$$
(12)

$$\hat{U} = U/\Delta, \quad \hat{\rho} = 3\rho(2-\rho), \quad \rho' = 3\rho(1-\rho), \tilde{\rho} = 3\left[\frac{1}{4} - \left(\rho - \frac{3}{2}\right)^2\right].$$
(13)

Here, σ_A^2 has a minimum at

$$U_{\sigma}^{A} = \begin{cases} \frac{\Delta}{9} (\sqrt{\hat{\rho}^{2} + 9\hat{\rho}} - \hat{\rho}) & \text{for } \frac{1}{3} \leq \rho \leq \frac{5}{3} \\ \Delta \frac{|1 - \rho|}{1 + |1 - \rho|} & \text{otherwise,} \end{cases}$$
(14)

which can be seen in Fig. 4(b) for $\rho = \frac{1}{2}$ and $\Delta = 15$.

So far, our calculations were restricted to one dimension because a generalization of relation (9) to two or three dimensions is, in general, not possible. However, in the limit of strong disorder, $G_{ij}(E)$ can be calculated in good approximation by taking into account only the direct path¹⁹ from *i* to *j*. Therefore, Eq. (8) can be considered as a one-dimensional problem, leading again to Eqs. (9) and (10), respectively. Hence, we conjecture that the general result, i.e., the nonmonotonic behavior of localization, holds also in two and three dimensions.

III. SITE-DEPENDENT HARTREE-FOCK APPROXIMATION

The second model which will be discussed in this paper is the site-dependent Hartree-Fock approximation.^{6,9} In this single-particle approximation, each site has a single renormalized energy level, given by

$$\varepsilon_i \mapsto \varepsilon_i + \frac{U}{2} \langle n_i \rangle_0,$$
 (15)

which in Eq. (1) corresponds to the replacement,

$$Un_{i\uparrow}n_{i\downarrow} \to U(\langle n_{i\uparrow}\rangle n_{i\downarrow} + \langle n_{i\downarrow}\rangle n_{i\uparrow}) \to \frac{U}{2} \langle n_i\rangle (n_{i\downarrow} + n_{i\uparrow})$$

$$\approx \frac{U}{2} \langle n_i\rangle_0 (n_{i\downarrow} + n_{i\uparrow}). \tag{16}$$

Here, the absence of any kind of magnetization was assumed. Note that for a local, energy independent interaction U, the Hartree and the Hartree-Fock approximations are identical. The average on-site occupation $\langle n_i \rangle$ was taken to be the one of the atomic ground state, $\langle n_i \rangle_0$ [Eq. (2)], according to the assumption of a stable atomic configuration.

As in the atomic-limit approximation, the shift of the occupied on-site energies leads to a renormalized distribution, with probability function $p_{\rm H}(\varepsilon)$ [Fig. 2(b)]. The screening effect now is even more pronounced because all singly occupied states are shifted by $\frac{U}{2}$ yielding a smaller width and a stronger increase of the probability to find a state around the Fermi level. The resulting effective single-particle Hamiltonian is again given by Eq. (6), however, with the probability function $p_{\rm H}(\varepsilon)$.

The corresponding plots for the localization length in Hartree-Fock approximation are shown in Figs. 3(b) and 4(a), respectively. Again, a pronounced maximum of ξ arises. In this case, it is found at the value

with

$$U_{\xi}^{\mathrm{H}} = \frac{\Delta}{2}\rho(2-\rho), \qquad (17)$$

which up to order $\mathcal{O}\left[\rho^2(2-\rho)^2\right]$ coincides with the result from the atomic-limit approximation [Eq. (11)]. The increase of the localization length is considerably more pronounced in the Hartree-Fock approximation due to its narrower probability distribution and especially its larger probability density around the Fermi level. In both approaches, the effect of screening becomes stronger with decreasing disorder. However, for small values of Δ , the stability of the atomic ground state becomes doubtful.

The average and the variance of the renormalized on-site energy distribution are, respectively,

$$\langle \varepsilon \rangle_{\rm H} = \langle \varepsilon \rangle_{\rm A} = \frac{1}{2} \rho U,$$
 (18)
=
$$\frac{\Delta^2}{12} \begin{cases} 1 - \hat{\rho} \hat{U} + \hat{\rho} \hat{U}^2, & \rho < 1, & \hat{U} < \rho \\ 1 - 2\rho' \hat{U} + \rho' \hat{U}^2, & \rho < 1, & \hat{U} \ge \rho \\ 1 - \hat{\rho} \hat{U} + \hat{\rho} \hat{U}^2, & \rho \ge 1, & \hat{U} < 2 - \rho \\ 1 - 2\tilde{\rho} \hat{U} + \tilde{\rho} \hat{U}^2, & \rho \ge 1, & \hat{U} \ge 2 - \rho, \end{cases}$$

with the same abbreviations as in Eq. (13). Its minimum is found at the value

 $\sigma_{\rm H}^2$

$$U_{\sigma}^{\mathrm{H}} = \begin{cases} \Delta/2 & \text{if } \frac{2}{3} < \rho < \frac{4}{3} \\ \Delta & \text{else.} \end{cases}$$
(20)

(19)

As mentioned above, it was argued in Ref. 9 that the picture of screening would be too primitive to explain the nonmonotonic behavior and the evidence for a metallic state found in the conductivity simulations by varying the repulsion strength U. The argumentation was based on the observation, which the variance was a featureless, monotonically decreasing function of U around the transition point. Our results show that this reasoning is generally not conclusive. Although the static, single-particle treatment does not allow for the occurrence of a metallic state, we find a strong enhancement and nonmonotonic behavior of the localization length ξ as function of U, whereas the variance is also only a monotonically decreasing function around the point of maximal delocalization. For strong disorder and a distribution which is not characterized by a single parameter (like in the present case, cf. Fig. 2), there is no simple relation between ξ and the variance σ^2 . Especially for lower fillings, our results, Eqs. (11), (14) and (17), (20), respectively, show that the values of U for which the maximum of ξ and the minimum of σ^2 occur, can be separated systematically. Moreover, we find that the atomic-limit approximation and the Hartree-Fock approximation do yield close values of ξ , although the variances can differ strongly (see Fig. 4).

In Ref. ^{8,13}, the inverse participation ratio was calculated as a function of the disorder strength Δ , and a nonmonotonic behavior with evidence for a metallic state was found. It was argued there that the screening picture would necessarily pre-

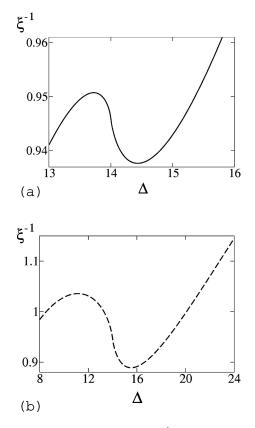


FIG. 5. Inverse localization length ξ^{-1} as a function of Δ for $\rho = \frac{1}{2}$ and (a) U=7 in the atomic-limit approximation and (b) U=14 in the Hartree-Fock approximation, respectively.

dict a monotonic increase of the inverse participation ratio with increasing Δ , excluding screening as a possible explanation. Our model, contrary to that statement, exhibits such nonmonotonic behavior as well, as shown in Fig. 5, where ξ^{-1} is plotted as a function of the disorder strength Δ , for some fixed values of ρ and U. This nonmonotonicity is caused by the crossover from the regime of disorder screening by interaction, $\Delta \ge U$, to the regime of interactionreduced hopping, $\Delta \ll U$, which is controlled by the parameter U/Δ . However, the exact position of the nonmonotonicity depends also on t/Δ , ρ , and the probability function.

IV. CONCLUSION

We examined the effect of static disorder screening by on-site repulsion in the one-dimensional Hubbard-Anderson model for strong disorder. We presented two different approximation schemes by absorbing the interactions into a redefinition of the single-particle on-site energies. In both approaches, a renormalized probability distribution with an enhanced probability of finding site energies close to the Fermi level was obtained. We calculated the localization length at the Fermi energy for these single-particle problems and found a pronounced maximum of the localization length for some intermediate value of the repulsion strength. This can be understood as a consequence of the fact that the increase of the localization length ξ for small U ($U < U_{\xi}$) and the decrease of ξ for large $U(U > U_{\xi})$ have different physical origins, namely, disorder screening and reduced hopping, respectively. Similarly, a change of the "bare" disorder Δ , for fixed repulsion, resulted in a nontrivial, nonmonotic dependence of the localization length on the disorder strength. In contrast to the case of weak disorder, we found no significant correlation between the variance of the effective on-site energy distribution and the localization length. Our results, especially in the case of the Hartree-Fock approximation, are in qualitative and to some degree even quantitative agreement with recent numerical studies. By our analytic approach, it was possible to investigate the static screening effects separately from dynamical (inelastic) processes.

We gave an argument that the same behavior should also be found for strong disorder in two and three dimensions.²⁰ In three dimensions, there might be an interesting possibility of an interaction induced metal-insulator transition. Such a possibility is based on the assumption that our results, obtained in the strongly localized regime, can be extrapolated up to the mobility edge. Under this assumption, a noninteracting Anderson-localized system, whose Fermi energy is sufficiently close to the mobility edge, will become metallic upon switching on interactions by shifting the mobility edge across the Fermi level. Furthermore, when the interactions exceed a certain strength, the system would reenter the insulating phase in analogy to the nonmonotonic behavior of the localization length in one dimension.²¹ (Let us emphasize that throughout this paper, we do not discuss the case of half filling, with its characteristic Mott's physics.^{12,22}) A similar, and experimentally more relevant, effect could also happen under a change of the bare disorder Δ , as suggested by Fig. 5, since the relevant dimensionless parameter is U/Δ .

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