Self-consistent study of Anderson localization in the Anderson-Hubbard model in two and three dimensions

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(Received 27 August 2008; revised manuscript received 26 October 2008; published 12 December 2008)

We consider the change in electron localization due to the presence of electron-electron repulsion in the Anderson-Hubbard model. Taking into account local Mott-Hubbard physics and static screening of the disorder potential, the system is mapped onto an effective single-particle Anderson model, which is studied within the self-consistent theory of electron localization. We find rich nonmonotonic behavior of the localization length ξ in two-dimensional systems, including an interaction-induced exponential enhancement of ξ for small and intermediate disorders although ξ remains finite. In three dimensions we identify for half filling a Mott-Hubbard-assisted Anderson localized phase existing between the metallic and the Mott-Hubbard-gapped phases. For small U there is re-entrant behavior from the Anderson localized phase to the metallic phase.

DOI: 10.1103/PhysRevB.78.235116 PACS number(s): 71.10.Fd, 73.20.Fz, 72.15.Rn, 71.30.+h

I. INTRODUCTION

The research on interacting disordered systems is one of the central topics in today's condensed-matter physics. In particular, the experimental signatures of a two-dimensional (2D) metal-insulator transition in dilute disordered electron systems,[1] absent in the single-particle theory of Anderson localization,[2,3] have triggered many theoretical research activities. As a prototype model for the interplay of strong correlations and randomness, the Anderson-Hubbard model has been intensely studied.[4–13] While in electron systems the bare Coulomb interaction is long ranged, inducing the additional question of the range of the effective interaction in a disordered system, the Anderson-Hubbard model assumes an on-site interaction which may grasp many of the salient features of the electron-electron interaction. Disordered many-body systems with tailor-cut short-range interactions have most recently been realized experimentally as cold atomic gases in random potentials.[14] Despite these efforts, even in systems with short-range interaction the existence of a metallic ground state in $d \leq 2$ dimensions has remained elusive. Recent numerical works showed that the presence of interactions can at least suppress significantly the localizing effect of the disorder.[4–9,15]

One of the ideas proposed to explain the delocalizing effect is screening of the random potential by the interaction, discussed controversially in the literature. A detailed analysis of this screening effect is the subject of this paper. For that purpose, our approach starts from the atomic limit of the Anderson-Hubbard model. In the presence of a Hubbard interaction U, the on-site energy of a particle depends on whether this site is occupied by another particle or not, leading to an interaction-induced renormalization of the distribution of on-site energy levels. Below we argue that this effective disorder distribution of the atomic limit will still provide a good description of the static interaction effects when a finite hopping amplitude is included in the full Anderson-Hubbard model as long as the fluctuations of the on-site energy levels are large compared to the kinetic band energy (hopping amplitude). In particular, this will hold for arbitrarily large Hubbard interaction even when the localization length becomes large. As seen below, the latter may occur even for relatively strong disorder near the Anderson transition in three dimensions and as an interaction effect in two dimensions. By this reasoning, the Anderson-Hubbard model is reduced to an effective single-particle Anderson disorder model[2] with renormalized level distribution, for which we calculate ensemble-averaged single-particle and transport properties at temperature $T=0$. Clearly, inelastic as well as virtual interaction effects are neglected by this approach. For the present purpose they may, however, be unimportant due to the vanishing quasiparticle relaxation rate[16] at the Fermi energy in 2D and three-dimensional (3D) disordered systems for $T=0$.

In a previous work,[17] we already presented an analytical study of this approach, exploiting an exact relation[18] between the localization length and the ensemble-averaged single-particle density of states (DOS) in one dimension. In accordance with numerical results obtained for the Anderson-Hubbard model,[4–8] we could demonstrate that weak interaction reduces the effective disorder (screening) while a strong interaction effectively enhances the localization, corresponding to a hopping suppression by interaction (Mott-Hubbard physics).

In this paper, we extend our analysis by applying the self-consistent theory of Anderson localization,[19–21] which allows for a quantitative analysis of the effective single-particle Anderson disorder model in a broad parameter regime, particularly in two and three dimensions. Despite the simplifications made in our approach, we find good agreement with recent numerical studies, especially in the Anderson localized regime of one and two dimensions. Our analytical approach therefore allows for a critical assessment of some of the conclusions drawn from the numerical results. Our results indicate that screening of the disorder seems to be the

most relevant physical mechanism for the interaction-induced delocalization effect in the disorder localized regime of the Anderson-Hubbard model.

II. ATOMIC-LIMIT APPROXIMATION

We consider the Anderson-Hubbard model for fermions at zero temperature on a hypercubic lattice in d dimensions with lattice spacing a. It is described by the Hamiltonian

$$H = H_0 + H_{\text{kin}} + H_{\text{e-e}} = \sum_{i,\sigma} (\varepsilon_i - \mu) c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle i,j\rangle,\sigma} c_{i,\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

$c_{i\sigma}^\dagger$ ($c_{i\sigma}$) are creation (destruction) operators of a fermion at site i with spin σ and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. t is the nearest-neighbor hopping amplitude, $U > 0$ is the on-site repulsion, and μ is the chemical potential. The on-site energies $\{\varepsilon_i\}$ are assumed to be independent random variables with a box probability distribution $p(\varepsilon) = \Theta(\Delta/2 - |\varepsilon|)/\Delta$, where the disorder strength is parametrized by the width Δ. The lattice filling, i.e., the average particle number per lattice site (summed over spin), will be denoted by ρ.

In the atomic limit, $t = 0$, the energy of a particle on site i depends on the occupation number n_i of that site and can be obtained in the paramagnetic phase by shifting the bare on-site energy ε_i according to[17]

$$\varepsilon_i \mapsto \begin{cases} \varepsilon_i + U & \text{if } \varepsilon_i \le \mu - U \\ \varepsilon_i + U & \\ & \text{if } \mu - U < \varepsilon_i \le \mu \\ \varepsilon_i & \\ \varepsilon_i & \text{if } \varepsilon_i > \mu. \end{cases} \quad \left(\text{each with probability of } \tfrac{1}{2}\right) \quad (2)$$

The probability distribution $p_A(\varepsilon)$ of these renormalized energy levels is, hence, identical to the (averaged) spectral density of the Hubbard two-pole Green's function in the atomic limit (shifted by the chemical potential). Examples of this renormalized distribution are given in Fig. 1 and in Ref. 17. There it was shown that for $U \ll \Delta$ the variance of $p_A(\varepsilon)$ as compared to $p(\varepsilon)$ is reduced. On the other hand, it is evident from Eq. (2) that for $U \ge \Delta$ the support of the distribution $p_A(\varepsilon)$ splits into two disconnected intervals, leading eventually to a Mott-Hubbard gap in the averaged DOS of the model [Eq. (3)] below.

When a finite hopping amplitude $t > 0$ is switched on, the particles become delocalized from a single site (with finite or infinite localization length ξ). The hopping induces quantum fluctuations of the occupation numbers n_i, and the on-site energies are renormalized by self-energy corrections of leading relative order $O[(t/\Delta)^2]$. However, since the average occupation number on each site is essentially determined by the minimization of the local electrostatic energy, the atomic limit approximation will still capture the essential *static* physics of the Anderson-Hubbard model (disorder screening and Mott-Hubbard physics), as long as $t \ll \Delta$, for arbitrary U.[22] In particular, this remains valid even for arbitrary localization length ξ (Ref. 23) since the charge density may vary on the scale of a lattice spacing, independently of the size of ξ. With these assumptions the Anderson-Hubbard model is mapped onto an effective single-particle Anderson disorder model,

$$H = \sum_{i\sigma} (\varepsilon_i - \mu) c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle i,j\rangle\sigma} c_{i\sigma}^\dagger c_{j\sigma}, \quad (3)$$

with the renormalized on-site energy distribution $p_A(\varepsilon)$.

In $d = 1, 2$ dimensions, as well as in $d = 3$ dimensions for sufficiently strong disorder, all particles described by Hamiltonian (3) are exponentially localized.[3] The decay of their wave functions $\psi(r)$, in the limit $r \to \infty$, is governed by the localization length ξ. To analyze the effect of the repulsive interaction on the localization, we study the U dependence of ξ. For a first qualitative estimate we used in Ref. 17 the relation[18] (from now on we choose units where $a = t = 1$)

$$\xi_1^{-1} = \int_{-\infty}^{\infty} N(\varepsilon) \log|E - \varepsilon| d\varepsilon \approx \int_{-\infty}^{\infty} p_A(\varepsilon) \log|E - \varepsilon + \mu| d\varepsilon, \quad (4)$$

valid in one dimension, where ξ_1 is the wave-function decay length, $N(\varepsilon)$ denotes the disorder-averaged DOS, and E is the

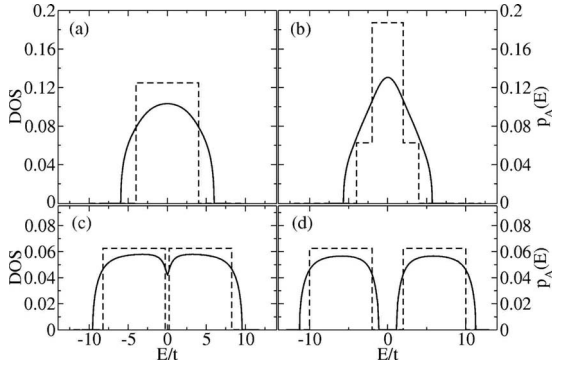

FIG. 1. CPA density of states (solid lines) and renormalized site-energy distribution $p_A(\varepsilon)$ (dotted lines) in $d = 2$ at half filling for $\Delta/t = 8$ and (a) $U/t = 0$, (b) 4, (c) 8.5, and (d) 12. Energies are measured relative to the Fermi level.

particle energy measured relative to the chemical potential. The second approximate equality in Eq. (4) holds for $\Delta \gg t$. For sufficiently large disorder, Eq. (4) becomes also a good approximation in $d>1$ dimensions.[24] In Ref. 17 we found that for all lattice fillings ρ the localization length of a particle at the Fermi level, ξ_1, is a nonmonotonic function of U with a pronounced maximum at intermediate U.

III. SELF-CONSISTENT TRANSPORT THEORY

In order to extend our analysis of the effective single-particle system [Eq. (3)] to two- and three-dimensional systems as well as to parameter regimes with large localization lengths and to the calculation of general transport properties, one must go beyond the restrictions of one dimension and strong disorder implied by Eq. (4). Therefore, we study the system within the self-consistent theory of Anderson localization.[19–21] This theory constitutes a resummation of the most divergent (Cooperon) contributions to the irreducible particle-hole vertex, leading to a self-consistent equation for the dynamical diffusion coefficient. The theory was originally developed for weak disorder and was extended to arbitrary disorder later on.[21,25,26] By comparison with direct numerical diagonalization results,[27] it was demonstrated that for the noninteracting Anderson model this theory yields quantitatively correct results for the phase diagram of Anderson localization in $d=3$ and for the localization length in $d=1,2,3$ dimensions (with exception of the critical regime).

For the interacting case with short-range instantaneous interaction U, it is believed on general grounds that Fermi-liquid theory remains valid in the presence of disorder. Then the diffusion pole structure of the density propagator is preserved for particles at the Fermi energy ($E=0$) for temperature $T=0$. This was recently shown with the use of Ward identities[13] to hold strictly at least when disorder- and interaction-induced self-energy contributions may be taken to be additive.

In the formulation of Refs. 25 and 26 the self-consistent equation for the diffusion coefficient $D(\omega,E)$ reads

$$D(\omega,E) = D_0(E) + \frac{2\ \mathrm{Im}\ \Sigma(E)}{[\mathrm{Im}\ G(E)]^2 D_0(E)} \int \frac{d^d k}{(2\pi)^d} \times \int \frac{d^d k'}{(2\pi)^d} (\mathbf{v}_\mathbf{k} \cdot \hat{\mathbf{q}}) \frac{\mathrm{Im}\ G_\mathbf{k}(E)[\mathrm{Im}\ G_{\mathbf{k}'}(E)]^2}{(\mathbf{k}+\mathbf{k}')_p^2 - i\omega/D(\omega,E)} (\mathbf{v}_{\mathbf{k}'} \cdot \hat{\mathbf{q}}), \tag{5}$$

where $D_0(E)$ is the bare diffusion constant,

$$D_0(E) = -\frac{1}{\mathrm{Im}\ G(E)} \int \frac{d^d k}{(2\pi)^d} (\mathbf{v}_\mathbf{k} \cdot \hat{\mathbf{q}})^2 [\mathrm{Im}\ G_\mathbf{k}(E)]^2 \tag{6}$$

and $\hat{q}$ is the unit vector in the direction of the transport. The disorder-averaged retarded single-particle propagators are given in terms of the self-energy $\Sigma(E)$ as

$$G_\mathbf{k}(E) = [E + \mu - \varepsilon_\mathbf{k} - \Sigma(E)]^{-1}, \tag{7}$$

and $G(E) = \int \frac{d^d k}{(2\pi)^d} G_\mathbf{k}(E)$. $\varepsilon_k = -2\Sigma_{i=1}^d \cos(k_i)$ is the dispersion and $\mathbf{v}_\mathbf{k} = \nabla_\mathbf{k} \varepsilon_\mathbf{k}$ is the group velocity.

In Eq. (5) the diffusion pole structure of the integral kernel holds strictly for $Q = |\mathbf{k}+\mathbf{k}'| \ll 2\pi/\ell$, where ℓ is the elastic mean-free path. For larger Q the integral kernel does not vanish but behaves in a nonsingular way. Therefore, the momentum integrals in Eq. (5) must not be cut off for $Q > 2\pi/\ell$ but extend over the complete first Brillouin zone of the lattice.[25,26] Furthermore, one has to keep in mind that not only the single-particle Green's function but also the particle-hole propagator obey lattice periodicity with respect to their momentum arguments. In particular, the particle-hole propagator, which enters into the integral kernel of Eq. (5),[20,26] is lattice periodic with respect to the center-of-mass momentum of the particle-hole pair. However, in Eq. (5) this periodicity is not explicit since the diffusion pole form of the kernel arises from a hydrodynamic expansion for small Q and ω. To restore the lattice periodicity in the transport properties, the subscript p in the denominator of the kernel of Eq. (5) implies a shift by a reciprocal-lattice vector so as to keep the momentum argument $\mathbf{k}+\mathbf{k}'$ within the first Brillouin zone.

The localization length ξ for particles at the Fermi energy is defined as the exponential decay length of the density correlation function in the static limit,[20,28]

$$\xi = \lim_{\omega \to 0} \sqrt{\frac{D(\omega,0)}{-i\omega}}, \tag{8}$$

where in the localized phase the diffusion coefficient is purely imaginary to first order in ω and vanishes linearly for $\omega \to 0$.

For the evaluation of the theory, we first calculate the disorder-averaged single-particle quantities, i.e., the self-energy $\Sigma(E)$ and the local Green's function $G(E)$, within the well-known coherent-potential approximation[29] (CPA). The CPA is known to interpolate disorder-averaged single-particle quantities correctly between the limits of weak and strong disorder, neglecting only exponentially rare disorder configurations (Lifshitz tails of the DOS), and provides quantitatively reliable results for disorder-averaged single-particle quantities over the complete parameter range.[26] It is defined in connection with Eq. (7) and the renormalized level distribution $p_A(\varepsilon)$ by the self-consistent relation,

$$\int d\varepsilon p_A(\varepsilon) \frac{\varepsilon - \Sigma(E)}{1 - [\varepsilon - \Sigma(E)] G(E)} = 0. \tag{9}$$

After the single-particle quantities are determined, the diffusion coefficient $D(\omega \to 0,0)$ or the localization length ξ, respectively, is calculated by solving numerically Eqs. (5) and (6) with Eq. (8). The two static interaction effects, disorder screening and Mott-Hubbard gap formation, are incorporated in the single-particle transport theory through the quantities $G_\mathbf{k}(E=0)$ and $\Sigma(E=0)$, determined by the renormalized distribution $p_A(\varepsilon)$.

In our static treatment of the interaction term, the hopping of a particle at the Fermi level was assumed to happen on a background of immobile particles. In the case of singly occupied sites, the spin of these particles was considered to be randomly distributed. Therefore, in the absence of the site-energy disorder, i.e., $\Delta \to 0$, Eq. (9) reduces to the Hubbard

III approximation[30,31] and, consequently, can be understood as an average over both spin and site-energy disorder. Implications and restrictions on the applicability of our approach will be mentioned in the discussion of our results in the following sections.

In $d>1$, the evaluation of the 2D integrals in Eq. (5) is numerically costly. Taking advantage of the periodicity of the integrands, this problem can be overcome by rewriting the factors in the integrand as Fourier series and using the convolution theorem. While for weak disorder the evaluation of the Fourier series is numerically still somewhat costly because of the pronounced peak structure of the Green's functions, the Fourier series converges quickly for larger disorder. The solution of the self-consistent [Eq. (5)] is easily performed on a single desktop computer.

IV. RESULTS AND DISCUSSION

The transport theory described above allows one to analyze in detail the static disorder screening effect of the Hubbard repulsion U in the Anderson-Hubbard model in arbitrary dimensions.

A. Two-dimensional systems

Figure 1 shows the 2D DOS $N(E)$, computed within CPA from Eq. (9), for a fixed disorder strength Δ and different values of the repulsion U. The figure clearly exhibits the regime of interaction-induced screening of disorder for small values of U, characterized by a narrowing of the disorder-averaged DOS with increasing U [Figs. 1(a) and 1(b)]. It also shows the regime of hopping suppression for large U, where the Mott-Hubbard gap gradually develops with increasing U [Figs. 1(b)–1(d)]. The crossover between the two regimes occurs roughly at $U\approx\Delta$. Note that the present static approximation does not describe the Kondo-like quasiparticle resonance at the Fermi level that would be induced by dynamical processes in high dimensions near half filling.[32] Therefore, it does not capture the typical many-body effects at the metal-insulator transition and inside the correlated metallic phase, known to be important when $\Delta\to 0$.

Figure 2 shows the generic behavior of the localization length at the Fermi level, $\xi(U)$, as a function of the repulsion U for (a) strong and (b) intermediate disorders Δ. The most salient feature seen in Fig. 2 is the nonmonotonic behavior of the localization length with a pronounced maximum at an intermediate value $0\le U_\xi\le\Delta$. Within the one-dimensional (1D) or strong disorder[24] approximation [Eq. (4)], U_ξ can be calculated as $U_\xi\approx U_\xi^{(1D)}=\Delta[\sqrt{1+3\rho(2-\rho)}-1]/3$.[17] As seen in Fig. 2, this provides even in $d=2$ an excellent quantitative estimate for the results of the self-consistent theory not only for large disorder, as expected, but also for intermediate disorder. The nonmonotonic behavior is reproduced by numerical methods for finite-size systems, i.e., by quantum Monte Carlo (QMC) simulations[4,7] and statistical dynamical mean-field theory (DMFT),[8] with the maximum of $\xi(U)$ occurring almost precisely at $U_\xi^{(1D)}$. In the case of the QMC results[7] the nonmonotonicity can be inferred from the dependence of the finite-temperature conductivity on U. In Ref. 8 the on-site

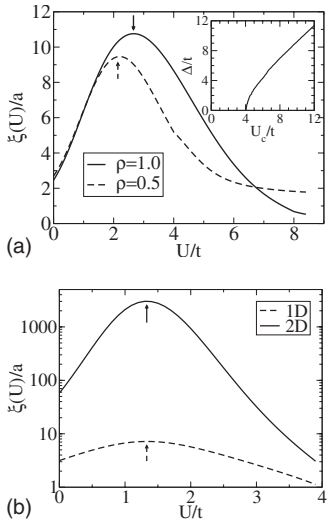

FIG. 2. (a) Localization length ξ at the Fermi level ($E=0$) in $d=2$ as a function of U for $\Delta/t=8$ and two different band fillings. The arrows indicate the positions of the maximum of ξ as obtained from Eq. (4) for a 1D system (Ref. 17). At the Mott transition for $\rho=1$ [vanishing $N(0)$ due to Mott-Hubbard gap formation], $\xi(U)$ vanishes exponentially as $\ln\xi(U)\simeq -1/2N(0)$ because of the logarithmic divergence of the Cooperon integral in Eq. (5) in $d=2$. The inset shows the critical interaction strength, $U_c(\Delta)$, for the Mott transition at half filling. (b) Localization length ξ at the Fermi level as a function of U in $d=1$ and 2 at half filling, $\rho=1$, for $\Delta/t=4$. The exponential enhancement of $\xi_{2D}(U)\sim\exp[1/\Delta_{\rm eff}^2]$ in $d=2$ due to interactions is clearly seen while in $d=1$ the dependence is comparatively weak (Refs. 20 and 26), $\xi_{1D}\sim[\Delta_{\rm eff}(U)]^{-1/2}$ (see text).

energies were calculated as poles of the atomic limit Green's function of the Anderson-Hubbard Hamiltonian, resulting in precisely the same Hamiltonian as our effective model [Eqs. (2) and (3)]. In Ref. 8 this Hamiltonian was then diagonalized numerically exactly for finite-size systems according to the statistical DMFT approach, and the localization length was extracted from the disorder-averaged inverse participation ratio (IPR) using the definition

$$\xi := (\mathrm{IPR})^{-1/d}. \tag{10}$$

We find good agreement with the results of Ref. 8 for all parameter values available up to a factor of order unity. This factor might be attributed to the slight difference in their and our definitions of ξ [Eqs. (8) and (10)], respectively. This agreement lends additional support to the quantitative correctness of the results of the self-consistent transport theory within the atomic limit approximation.

In our semianalytic theory the nonmonotonic behavior of ξ is easily traced back to the two competing interaction-induced effects: screening of the random potential and DOS suppression due to a Mott-Hubbard gap. Both effects are already incorporated in the effective distribution $p_A(\varepsilon)$, as seen in Fig. 1: under an increase in U, the effective disorder is initially reduced, leading to an increase in ξ. For large U, however, the formation of a Mott-Hubbard gap implies a reduction in the DOS at the Fermi level and a broadening of

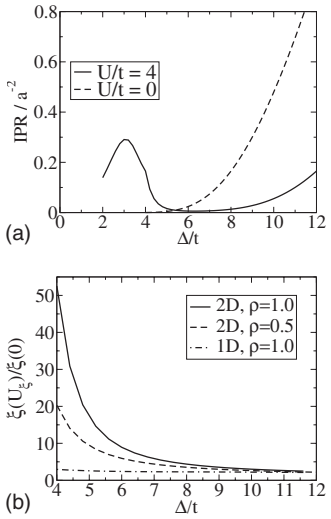

FIG. 3. (a) Inverse participation ratio ξ^{-2} as a function of the disorder strength Δ in $d=2$ for $U/t=4$ at half filling ($\rho=1$). The exponential suppression of the IPR for small disorder and the absence of the nonmonotonic behavior in the noninteracting case ($U=0$) are also shown (dashed line). (b) Magnitude of the delocalization effect as a function of disorder strength in $d=1$ and 2.

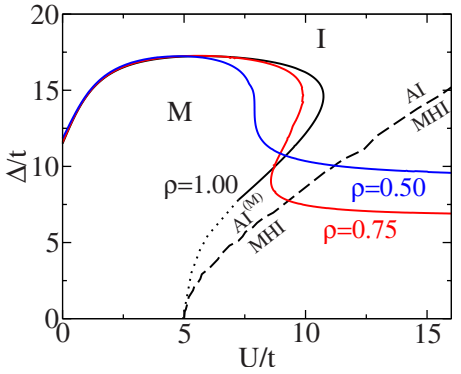

FIG. 4. (Color online) 3D phase diagram in the (U,Δ) plane for different lattice fillings ρ. The metallic phase (M) is to the lower left while the insulating phase (I) is to the upper right of the solid mobility edge curves for $\rho=1.00$, 0.75, and 0.50, respectively. The dashed curve shows the critical interaction strength for the Mott transition at half filling. The dotted line is an extrapolation of the mobility edge for $\rho=1$ toward small disorder, where the evaluation of the self-consistent Eq. (5) becomes numerically costly. The corresponding Anderson, Mott-Hubbard, and Mott-Hubbard assisted Anderson insulating regions at half filling are marked by AI, MHI, and $AI^{(M)}$, respectively.

the disorder distribution and, hence, a reduction in ξ with increasing U [Fig. 2(a)].

In Ref. 5 the interaction strength was fixed and the IPR as a function of the disorder strength was studied. That work was based on a local unrestricted Hartree-Fock treatment of the interaction and subsequent exact diagonalization of the resulting effective disordered single-particle Hamiltonian. Our results show a nonmonotonic behavior of the IPR with a pronounced suppression (i.e., increase in ξ) for intermediate disorder, as seen in Fig. 3(a), in good agreement with the finite-size data of Ref. 5.[33] Our theory indicates that this results from an intricate competition of Anderson localization and correlation-induced disorder screening effects: for small increasing Δ the IPR increases from zero due to Anderson localization in $d=2$ for arbitrarily weak disorder. As Δ increases further to intermediate values, the effective disorder potential, derived from Eq. (2), is *reduced* by the screening effect until $\Delta \approx U$, resulting in a suppression of the IPR. Finally, when $\Delta > U$, the on-site repulsion U cannot induce a further significant change in local occupation numbers as Δ grows; hence the effective disorder potential and the IPR increase.

Because of the logarithmic divergence of the Cooperon integral in Eq. (5) for $d=2$, the disorder screening effect can induce an exponentially large effect as seen in Fig. 2(b). To demonstrate this screening-induced delocalization effect quantitatively, we show in Fig. 3(b) the ratio $\xi(U_\xi)/\xi(U=0)$ of the maximal interaction-enhanced localization length and its noninteracting value. The effect is especially strong for weak disorder in $d=2$, where ξ depends exponentially on the screening-reduced disorder strength Δ_{eff} of the effective Anderson model [Eqs. (2) and (3)] $\xi \sim \exp[1/\Delta_{\text{eff}}^2]$.[34]

In Refs. 5 and 7 also the observation of a metallic phase was reported. The existence of such a phase is not possible in an effective single-particle model[3] and would consequently be beyond our approach. However, the good agreement of our results with the finite-size data of these works and the observation of the exponentially enlarged localization length, which exceeds the largest system size used in the numerics, suggests strongly that the infinite-size extrapolations erroneously indicated a true metallic state in $d=2$.[35]

The remarkable quantitative agreement of our theory with the results of numerical calculations wherever comparison is possible suggests that the essential physics of localization in the 2D Anderson-Hubbard model is captured by the assumptions of static disorder screening and Mott-Hubbard gap formation.

B. Three-dimensional systems

In $d>2$, the noninteracting Anderson model describes a disorder induced metal-insulator transition, where extended and localized states are separated by the mobility edge.[3] Hence, the question about a possible disorder reduction by interaction gets even more relevant. We have calculated the phase diagram of localization in $d=3$ using the atomic limit approximation [Eqs. (2) and (3)] with the self-consistent transport theory of Anderson localization [Eqs. (5)–(9); see Fig. 4].

The figure shows, for different values of the lattice filling ρ, the disorder screening effect: above the critical disorder value for Anderson localization without interaction[36] $\Delta_c/t \approx 11.7$, the increase in interaction leads to a re-entrance from the Anderson insulating into the metallic phase, i.e., the metallic phase is extended to larger values of Δ. This behavior was also observed in a recent DMFT study[12] of the Anderson-Hubbard model where a site-dependent self-energy correction was used. Contrarily, generalized DMFT studies based on site-independent averaged self-energy corrections do not describe the screening effect.[13]

For the half-filled case ($\rho=1$) a further increase in U eventually leads to a suppression of the averaged DOS at the Fermi level, $N(0)$, because of the gradual formation of a Mott-Hubbard gap (dashed line). Consequently the system undergoes first a transition from the metallic phase to a (Mott-Hubbard assisted) Anderson insulator with a reduced but finite $N(0)$ just before the DOS vanishes at the dashed line and the Mott-Hubbard insulating phase is entered. This intermediate phase is not likely to be seen in DMFT studies of the problem[12,13] because within DMFT the formation of a Kondo resonance and the concatenated unitarity sum rule for $N(0)$ in the metallic state prevent a Mott-Hubbard-induced suppression of $N(0)$ and lead to a complete screening of the disorder potential.[12,13] It remains to be seen whether in the physical 3D disordered systems Kondo physics or pseudogap formation dominates.

Away from half filling, a pure Mott-Hubbard transition is not possible because $N(0)$ remains nonzero. Therefore, for weak disorder the metallic phase extends out to arbitrarily large U. However, for large U ($U/t \gtrsim 10$) increasing disorder Δ does induce an Anderson metal-insulator transition, and this transition occurs at a substantially smaller value of Δ than for small and intermediate $U/t \lesssim 7$ because of a Mott-Hubbard reduced DOS at the Fermi level (pseudogap). It is interesting to note that this interplay of Anderson localization and Mott-Hubbard physics away from half filling leads to a steplike behavior of the phase boundary, as seen in Fig. 4, connecting smoothly to the phase boundary of the half-filled case.

V. CONCLUSION

We have presented a self-consistent study of the static disorder screening effect and of Mott-Hubbard gap formation, induced by the local repulsion in the Anderson-Hubbard model. Both of these effects are represented by an interaction-induced renormalization of the effective distribution of on-site energy levels and a subsequent mapping of the Anderson-Hubbard model onto a single-particle Anderson model. While this mapping is exact in the atomic limit, we have argued that it still provides a good description of the static screening effect for finite hopping amplitude even when the localization length ξ is large. The localization properties of the effective single-particle Anderson model were then treated by the self-consistent theory of Anderson localization.[19,26] We found rich behavior of the localization length in two dimensions and of the phase diagram in three dimensions due to an intricate interplay of disorder screening and Mott-Hubbard physics in the different regions of parameter space.

Despite the technical simplicity of our approach, it yields good agreement with numerical studies[4–8] of the same problem for two-dimensional finite-size systems, including the nonmonotonic dependence of ξ on both the interaction strength U and the disorder Δ. At the same time, we found in $d=2$ an exponential interaction-induced enhancement of ξ for weak and intermediate values of Δ although a true metallic state is not possible within our effective single-particle theory. The good agreement of our results with the numerical finite-size calculations and, simultaneously, our prediction of a large but finite localization length show that the indications of a true metallic state, found in some works by infinite-size extrapolations of the numerical data, are not conclusive. These indications might rather be due to the fact that the largest system sizes were still smaller than the localization length of the infinite system.

For three-dimensional systems we found that for weak Hubbard interaction U the disorder screening effect results in a re-entrant behavior from the insulating to the metallic phase, while for large U disorder and Hubbard interaction cooperate to form a Mott-Hubbard assisted Anderson insulating phase (with finite density of states at the Fermi level), which exists in a finite range between the metallic phase and the Mott-Hubbard-gapped phase present for half filling.

ACKNOWLEDGMENTS

This work was supported in part by the Deutsche Forschungsgemeinschaft through SFB 608.

[1] For a review, see S. V. Kravchenko and M. P. Sarachik, Rep. Prog. Phys. **67**, 1 (2004).
[2] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[3] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).
[4] B. Srinivasan, G. Benenti, and D. L. Shepelyansky, Phys. Rev. B **67**, 205112 (2003).
[5] D. Heidarian and N. Trivedi, Phys. Rev. Lett. **93**, 126401 (2004).
[6] K. Kobayashi, B. Lee, and N. Trivedi, arXiv:0807.3372 (unpublished).
[7] P. B. Chakraborty, P. J. H. Denteneer, and R. T. Scalettar, Phys. Rev. B **75**, 125117 (2007).
[8] Y. Song, R. Wortis, and W. A. Atkinson, Phys. Rev. B **77**, 054202 (2008).
[9] I. F. Herbut, Phys. Rev. B **63**, 113102 (2001).
[10] D. Tanaskovic, V. Dobrosavljevic, E. Abrahams, and G. Kotliar, Phys. Rev. Lett. **91**, 066603 (2003).
[11] M. C. O. Aguiar, V. Dobrosavljevic, E. Abrahams, and G. Kotliar, Physica B **403**, 1417 (2008).
[12] K. Byczuk, W. Hofstetter, and D. Vollhardt, Phys. Rev. Lett. **94**, 056404 (2005).
[13] E. Z. Kuchinskii, I. A. Nekrasov, and M. V. Sadovskii, JETP **106**, 581 (2008).
[14] For recent references on that topic, see, e.g., D. Clement, P. Bouyer, A. Aspect, and L. Sanchez-Palencia, Phys. Rev. A **77**, 033631 (2008); L. Fallani, C. Fort, and M. Inguscio, arXiv:0804.2888, Adv. At., Mol., Opt. Phys. (to be published).
[15] Such an effect has also been observed in models with long-range Coulomb interactions. See Z. A. Nemeth and J.-L. Pichard, Eur.

Phys. J. B **45**, 111 (2005), and references therein.
[16] B. L. Altshuler and A. G. Aronov, in *Electron-Electron Interactions in Disordered Systems*, edited by A. L. Efros and M. Pollak (North Holland, Amsterdam, 1985), p. 1.
[17] P. Henseler, J. Kroha, and B. Shapiro, Phys. Rev. B **77**, 075101 (2008).
[18] D. J. Thouless, J. Phys. C **5**, 77 (1972).
[19] D. Vollhardt and P. Wölfle, Phys. Rev. Lett. **45**, 842 (1980); Phys. Rev. B **22**, 4666 (1980); Phys. Rev. Lett. **48**, 699 (1982).
[20] D. Vollhardt and P. Wölfle, in *Electronic Phase Transitions*, edited by W. Hanke and Y. V. Kopaev (Elsevier Science, Amsterdam, 1992), p. 1.
[21] T. Kopp, J. Phys. C **17**, 1897 (1984); **17**, 1919 (1984).
[22] A recent DMRG study of the 1D Anderson-Hubbard model supports this assumption. See M. Okumura, S. Yamada, N. Taniguchi, and M. Machida, Phys. Rev. Lett. **101**, 016407 (2008).
[23] Note that in $d=3$ ξ diverges at the Anderson transition, and in $d=2$ it can become large even for $\Delta/t \sim O(10) \gg 1$, as seen in Sec. IV.
[24] E. Medina and M. Kardar, Phys. Rev. B **46**, 9984 (1992).
[25] J. Kroha, T. Kopp, and P. Wölfle, Phys. Rev. B **41**, 888 (1990).
[26] J. Kroha, Physica A **167**, 231 (1990).
[27] B. Bulka, M. Schreiber, and B. Kramer, Z. Phys. B: Condens. Matter **66**, 21 (1987).
[28] Note the relative factor of 2 in the definitions of the decay length of the wave function and of the density correlations, $\xi_1 = 2\xi$.
[29] F. Yonezawa and K. Morigaki, Prog. Theor. Phys. **53**, 1 (1973).
[30] J. Hubbard, Proc. R. Soc. London, Ser. A **281**, 401 (1964).
[31] B. Velicky, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. **175**, 747 (1968).
[32] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[33] Note the factor of 1/2 in the definitions of the disorder parameter in Ref. 5 and the present study, $V = \Delta/2$.
[34] P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).
[35] For a similar discussion in the case of a long-ranged interaction, see, e.g., G. Fleury and X. Waintal, arXiv:0807.3433 (unpublished).
[36] This value is somewhat smaller than the one obtained in Ref. 26, because there the lattice periodicity of the particle-hole propagator in the center-of-mass momentum Q was not considered.