Order parameter theory for Anderson localization

V. Dobrosavljević,[1] A.A. Pastor,[1] and Branislav K. Nikolić[2]
[1]*Department of Physics and National High Magnetic Field Laboratory Florida State University, Talahassee, FL 32306*
[2]*Department of Physics, Georgetown University, Washington, DC 20057-0995*
(Dated: May 16, 2002)

We present a self-consistent theory of Anderson localization, that identifies the *typical local density of states* as the fundamental order parameter. Both the escape rate of an electron from a given site, and the conductivity are shown to vanish in the insulating phase, which emerges for disorder strengths comparable to the electronic bandwidth. Due to the local character of our theory, it can easily be combined with standard dynamical mean-field approaches for strong electronic correlations, thus opening an attractive avenue for the study of the interplay of interactions and disorder.

PACS numbers: PACS Numbers: 71.30.+h, 72.15.Rn, 71.27.+a

After more than forty years of intense study, there remains little doubt that disorder-driven metal-insulator transitions (MITs) bear many similarities to more familiar critical phenomena. The basic physical process involved was identified by Anderson[1], who first discussed the localization of electronic wave functions as a driving force behind such MITs. Further theoretical progress has been slow, primarily due to ambiguities in identifying an appropriate order parameter for Anderson localization. Nevertheless, important information was obtained by using scaling approaches based on $2+\epsilon$ expansions [2], which were subsequently extended [3] to incorporate the interaction effects.

There are several reasons why the existing theories remain unsatisfactory. Most importantly, the MITs generically take place at *strong* disorder where the energy scales associated with both disorder and the interactions are comparable to the Fermi energy, in contrast to what happens in perturbative $2+\epsilon$-expansion approaches. As a result, well defined *precursors* of the MITs are seen even at very high temperatures, as experimentally demonstrated in many systems [4, 5]. These features include not only the scaling behavior of various quantities, but also the breakdown of the Matthiessen's rule and the Mooij correlation [4]. To understand such global behavior, a mean-field like formulation would be useful, but it should be one that can incorporate both the localization and the strong correlation effects on the same footing.

In this letter, we demonstrate how an appropriate local order parameter can be defined and self-consistently calculated, producing a mean-field like description of Anderson localization. This formulation is *not* restricted to either low temperatures or to Fermi liquid regimes, and in addition can be straightforwardly combined with well-known dynamical mean-field theories (DMFT) [6, 7] of strong correlation. In this way, our approach which we call the *typical medium theory* (TMT), opens an avenue for addressing questions difficult to tackle by any alternative formulation, but which are of crucial importance for many physical systems of current interest.

Our starting point is motivated by the original formulation of Anderson [1], which adopts a *local* point of view [8], and investigates the possibility for an electron to *delocalize* from a given site at large disorder. This is most easily accomplished by concentrating on the (unaveraged) local density of electronic states (LDOS)

$$\rho_i(\omega) = \sum_n \delta(\omega - \omega_n)|\psi_n(i)|^2. \qquad (1)$$

In contrast to the global (averaged) density of states (ADOS) which is not critical at the Anderson transition, LDOS undergoes a qualitative change upon localization, as first noted in Ref. [1]. This follows from the fact that LDOS directly measures the local amplitude of the electronic wavefunctions. When electrons localize, the local spectrum turns from a continuous to an essentially discrete one [1], but the *typical* value of LDOS vanishes. Just on the metallic side, but very close to the transition, these delta-function peaks turn into long-lived resonance states and thus acquire a finite *escape rate* from a given site. According to Fermi's golden rule, this escape rate can be estimated [1] as $\tau_{\rm esc}^{-1} \sim t^2\rho$, where t is the inter-site hopping element, and ρ is the density of local states of the immediate neighborhood of a given site.

The *typical* escape rate is thus determined by the typical local density of states (TDOS), so that TDOS directly determines the conductivity of the electrons. This simple argument strongly suggests that TDOS should be recognized as an appropriate order parameter for Anderson localization. Because the relevant distribution function for LDOS becomes increasingly broad as the transition is approached, the desired typical value is well represented by the *geometric average* $\rho_{\rm typ} = \exp\{\langle \ln \rho \rangle\}$, where $\langle \cdots \rangle$ represents the average over disorder. Interestingly, recent scaling analyses [11] of the multifractal behavior of electronic wavefunctions near the Anderson transition have independently arrived at the same conclusion, identifying TDOS as defined by the geometric average as the fundamental order parameter (somewhat related ideas have also been discussed earlier in Ref. [12]). These insights

make it possible to avoid a more complicated usage of the full LDOS distribution as "the order parameter function," an approach suggested in Ref. [13].

To formulate a self-consistent theory for our order parameter, we follow the "cavity method," a general strategy that we borrow from the DMFT [6]. In this approach, a given site is viewed as being embedded in an effective medium characterized by a local self energy function $\Sigma(\omega)$. For simplicity, we concentrate on a single band tight-binding model of noninteracting electrons with random site energies ε_i with a given distribution $P(\varepsilon_i)$. The corresponding local Green's function then takes the form

$$G(\omega, \varepsilon_i) = [\omega - \varepsilon_i - \Delta(\omega)]^{-1}. \tag{2}$$

Here, the "cavity function" is given by

$$\Delta(\omega) = \Delta_o(\omega - \Sigma(\omega)), \tag{3}$$

and

$$\Delta_o(\omega) = \omega - 1/G_o(\omega), \tag{4}$$

where the lattice Green's function

$$G_o(\omega) = \int_{-\infty}^{+\infty} d\omega' \ \frac{D(\omega')}{\omega - \omega'} \tag{5}$$

is the Hilbert transform of the bare density of states $D(\omega)$ which specifies the band structure.

Given the effective medium specified by a self-energy $\Sigma(\omega)$, we are now in the position to evaluate the order parameter, which we choose to be TDOS as given by

$$\rho_{\rm typ}(\omega) = \exp\left\{ \int d\varepsilon_i \ P(\varepsilon_i) \ \ln \rho(\omega, \varepsilon_i) \right\}, \tag{6}$$

where LDOS $\rho(\omega, \varepsilon_i) = -{\rm Im}G(\omega, \varepsilon_i)/\pi$, as defined by Eqs. (2-5). To obey causality, the Green's function corresponding to $\rho_{\rm typ}(\omega)$ must be specified by analytical continuation, which is performed by the Hilbert transform

$$G_{\rm typ}(\omega) = \int_{-\infty}^{+\infty} d\omega' \ \frac{\rho_{\rm typ}(\omega')}{\omega - \omega'}. \tag{7}$$

Finally, we close the self-consistency loop by setting the Green's functions of the effective medium to be equal to that corresponding to the local order parameter, so that

$$G_{\rm em}(\omega) = G_o(\omega - \Sigma(\omega)) = G_{\rm typ}(\omega). \tag{8}$$

It is important to emphasize that our procedure defined by Eqs. (2-8) is not specific to the problem at hand. The same strategy can be used in any theory characterized by a local self-energy. The only requirement specific to our problem is the definition of TDOS as a local order parameter given by Eq. (6). If we choose the *algebraic* instead of the geometric average of LDOS, our theory would reduce to the well-known coherent potential approximation (CPA) [14], which produces excellent results for the ADOS for any value of disorder, but finds no Anderson transition. Thus TMT is a theory having a character very similar to CPA, with a small but crucial difference — the choice of the correct order parameter for Anderson localization.

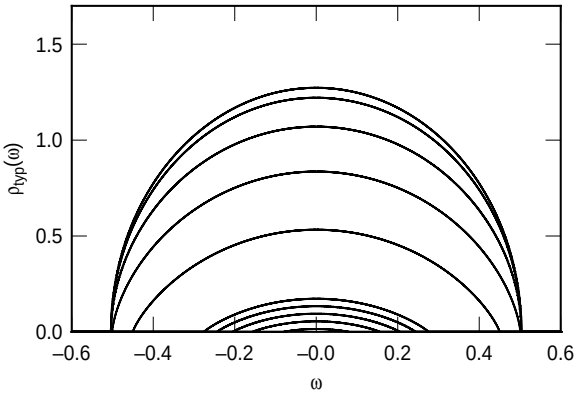

FIG. 1: Typical density of states for the SC model, for disorder values $W = 0$, 0.25, 0.5, 0.75, 1, 1.25, 1.275, 1.3, 1.325, 1.35. The entire band localizes for $W = W_c = e/2 \approx 1.359$.

In our formulation, as in DMFT, all the information about the electronic band structure is contained in the choice of the bare DOS $D(\omega)$. It is not difficult to solve Eqs. (2-8) numerically, which can be efficiently done using FFT methods [6]. We have done so for several model densities of states, and find that most of our qualitative conclusions do not depend on the specific choice of band structure. We illustrate these findings using a simple semicircular (SC) model for the bare DOS given by $D(\omega) = \frac{4}{\pi}\sqrt{1-(2\omega)^2}$, for which $\Delta_o(\omega) = G_o(\omega)/16$ [6]. Here and in the rest of the paper all the energies are expressed in units of the bandwidth, and the random site energies ε_i are uniformly distributed over the interval $[-W/2, W/2]$. The evolution of TDOS as a function of W is shown in Fig. 1. The TDOS is found to decrease and eventually vanish even at the band center for $W = W_c \approx 1.36$. When $W < W_c$, the part of the spectrum where TDOS remains finite corresponds to the region of extended states, and is found to shrink with disorder, indicating that the band tails begin to localize. The resulting phase diagram is presented in Fig. 2, showing the trajectories of the mobility edge (as given by the frequency where TDOS vanishes for a given W), and the band edge (where the ADOS calculated by CPA vanishes).

Further insight in the critical behavior is obtained by noting that near $W = W_c$ it proves possible to analytically solve Eqs. (2-8). Concentrating for simplicity on the band center ($\omega = 0$), we can expand Eqs. (2-8) in powers of the order parameter $\rho_o = \rho_{\rm typ}(0)$ giving

$$\rho_o = a\rho_o - b\rho_o^2 + \cdots, \tag{9}$$

where

$$a = \exp\left\{ -2 \int d\varepsilon P(\varepsilon) \ln|\varepsilon| \right\}; \quad b = 2aP(0). \tag{10}$$

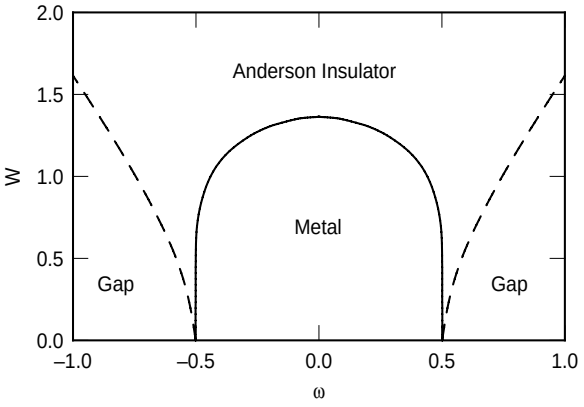

FIG. 2: Phase diagram for the SC model. The trajectories of the mobility edge (full line) and the CPA band edge (dashed line) are shown as a function the disorder strength W.

The transition where ρ_o vanishes is found at $a = 1$, giving $W = W_c = e/2 = 1.3591$, consistent with our numerical solution. Near the transition, to leading order

$$\rho_o(W) = \left(\frac{4}{\pi}\right)^2 (W_c - W), \tag{11}$$

so the order parameter exponent is $\beta = 1$.

The analytical solution is more difficult to obtain for arbitrary W. Still, the above approach can be extended to find a full frequency-dependent solution close to the critical value of disorder $W = W_c$. There it assumes a simple scaling form

$$\rho_{\rm typ}(\omega, W) = \rho_o(W) f\left(\omega/\omega_o(W)\right), \tag{12}$$

with $\omega_o(W) = \sqrt{\left(\frac{e}{4}\right)(W_c - W)}$ and the scaling function $f(x) = 1 - x^2$, again consistent in detail with the numerical solution of Fig. (1) (note that TDOS curves assume a simple *parabolic* shape close to $W = W_c$).

In order to gauge the quantitative accuracy of out theory, we have carried out exact numerical calculations for a three-dimensional cubic lattice with random site energies, using Green's functions for an open finite sample attached to two semi-infinite clean leads [15]. We have computed both the average and the typical DOS at the band center as a function of disorder, for cubes of sizes L =4, 5, 6, 7, 8, 9, 10, 11, and 12, and averages over 1000 sample realizations, in order to obtain reliable data by standard finite size scaling procedures. The TMT and CPA equations for the same model were also solved by using the appropriate bare DOS (as expressed in terms of elliptic integrals), and the results are presented in Fig. 3.

We find remarkable agreement between the numerical data and the self-consistent CPA calculations for the ADOS, but also a surprisingly good agreement between the numerical data and the TMT predictions for the TDOS order parameter. For a cubic lattice, the exact value is $W_c \approx 1.375$ [16], whereas TMT predicts a 20% smaller value $W_c \approx 1.1$. The most significant discrepancies are found in the critical region, since TMT predicts the order parameter exponent $\beta = 1$, whereas the exact value is believed to be $\beta \approx 1.58$ [17], consistent with our numerical data. Nevertheless, we conclude that TMT is as accurate as one can expect from a simple mean-field like formulation [19].

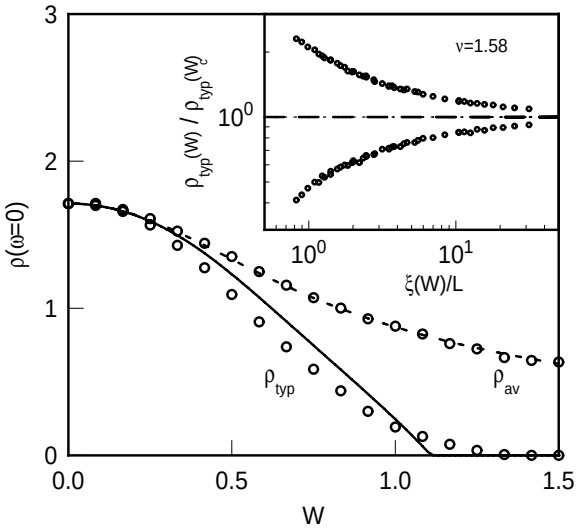

FIG. 3: Typical and average DOS as a function of disorder W, for a three dimensional cubic lattice at the band center ($\omega = 0$). Results from exact numerical calculations (circles) are compared to the predictions of TMT (for TDOS - full line) and CPA (for ADOS - dashed line). Finite size scaling of the numerical data in the critical region $W = 1.17-1.58$, and sizes $L = 4-12$ is shown in the inset, where $\rho_{\rm typ}(W, L)/\rho_{\rm typ}(W_c, L)$ is plotted as a function of $\xi(W)/L$, and $\xi(W) = 0.5|(W_c - W)/W_c|^{-\nu}$ is the correlation length in units of the lattice spacing. The numerical data are consistent with $\beta = \nu = 1.58$.

Next, we address the transport properties within TMT. The escape rate from a given site can be rigorously defined in terms of the cavity field (see Eq. (2)), and using our solution of the TMT equations, we find $\tau_{\rm esc}^{-1} = -{\rm Im}\Delta(0) \sim \rho_{\rm typ} \sim (W_c - W)$. To calculate the conductivity within our local approach, we follow a strategy introduced by Girvin and Jonson [21], who pointed out that close to the localization transition the conductivity can be expressed as $\sigma = \Lambda a_{12}$, where

$$a_{12} = \langle A_{12} A_{21} - A_{11} A_{22} \rangle, \tag{13}$$

$A_{ij} = -{\rm Im}G_{ij}$ is the spectral function corresponding to the nearest neighbor two-site cluster. We have computed a_{12} by examining two sites embedded in the effective medium defined by TMT, thus allowing for localization effects. The vertex function Λ remains *finite* at the localization transition [21], and thus can be computed

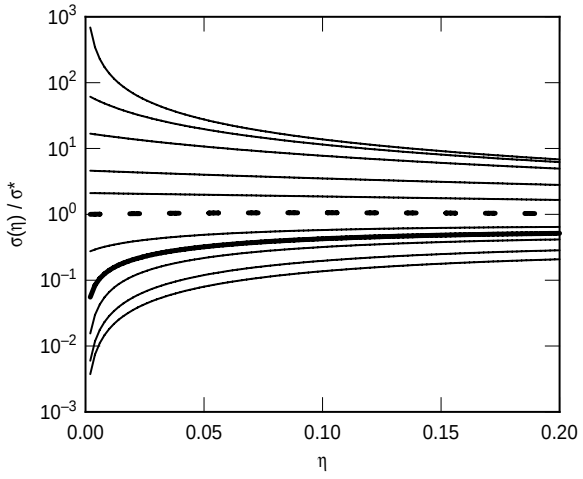

FIG. 4: Conductivity as a function of the inelastic scattering rate η for the SC model at the band center and $W = 0$, 0.125, 0.25, 0.5, 0.75, 1, 1.25, 1.36, 1.5, 1.75, 2. The "separatrix" ($\sigma = \sigma^*$ independent of η, i. e. temperature) is found at $W = W^* \approx 1$ (dashed line). The critical conductivity $\sigma_c(\eta) \sim \eta^{1/2}$ corresponds to $W = W_c = 1.36$ (heavy full line).

within CPA [22]. The resulting critical behavior of the $T = 0$ conductivity follows that of the order parameter, $\sigma \sim \rho_{\rm typ} \sim (W_c - W)$, giving the conductivity exponent μ equal to the order parameter exponent β, consistent with what is expected [17]. Finally, we examine the temperature dependence the conductivity as a function of W. Physically, the most important effect of finite temperatures is to introduce finite inelastic scattering due to interaction effects. At weak disorder, such inelastic scattering increases the resistance at higher temperatures, but in the localized phase it produces the opposite effect, since it suppresses interference processes and localization. To mimic these inelastic effects within our noninteracting calculation, we introduce by hand an additional scattering term in our self-energy, viz. $\Sigma \to \Sigma - i\eta$. The parameter η measures the inelastic scattering rate, and is generally expected to be a monotonically increasing function of temperature. The resulting behavior of the conductivity as a function of η and W is presented in Fig. 4. As η (i. e. temperature) is reduced, we find that the conductivity curves "fan out", as seen in many experiment close to the MIT [4, 5]. Note the emergence of a "separatrix" [4, 5] where the conductivity is temperature independent, which is found for $W \approx 1$, corresponding to $k_F \ell \sim 2$, consistent with some experiments [4]. At the MIT, we find $\sigma_c(\eta) \sim \rho_{\rm typ}(\eta) \sim \eta^{1/2}$.

In summary, we have formulated a local order parameter theory for disorder-driven MITs that in absence of interactions reproduces most of the expected features of the Anderson transition. In addition, the role of strong electronic correlations near disorder-driven MITs can be readily examined within the typical medium theory, since the local character of our approach offers a natural starting point for incorporating both the localization and the interaction effects using the DMFT framework.

We thank S. Chakravarty, S. Das Sarma, J. K. Freericks, D. A. Huse, G. Kotliar, E. Miranda, D. Popović, S. H. Simon, and S. Sondhi for useful discussions. This work was supported by the NSF grant DMR-9974311 and the National High Magnetic Field Laboratory (VD and AAP), and the ONR grant N00014- 99-1-0328 (BKN).

[1] P. W. Anderson, Phys. Rev. **109**, 1498 (1958).
[2] E. Abrahams *et al.*, Phys. Rev. Lett. **42**, 673 (1979); F. Wegner, Z. Phys. B **35**, 207 (1979).
[3] A. M. Finkel'shtein, Zh. Eksp. Teor. Fiz. **84**, 168 (1983); for a review see D. Belitz and T. T. Kirkpatrick, Rev. Mod. Phys. **66**, 261 (1994).
[4] P.A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).
[5] E. Abrahams *et al.*, Rev. Mod. Phys. **73**, 251 (2001).
[6] For a review see A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).
[7] V. Dobrosavljević and G. Kotliar, Phys. Rev. Lett. **71**, 3218 (1993); Phys. Rev. B **50**, 1430 (1994); Phys. Rev. Lett. 78, 3943 (1997).
[8] Ours is a diametrically opposite, but complementary approach to that of the weak localization theories [4], which investigate the stability of the metallic phase with respect to weak impurity scattering. The self-consistent theory of localization of Vollhardt and Wölfle [9] has a similar character, since it essentially represents a resummation of the most singular contributions at weak disorder near two dimensions. On the other hand, some recent experiments [5] indicate [10] that the observed quantum critical behavior may be dominated by the physics of the insulator, thus favoring the local picture.
[9] D. Vollhardt and P. Wölfle, Phys. Rev. Lett. **45**, 842 (1980).
[10] V. Dobrosavljević *et al.*, Phys. Rev. Lett. **79**, 455 (1997).
[11] M. Janssen, Phys. Rep. **295**, 1 (1998).
[12] D. E. Logan and P. G. Wolynes, Phys Rev B **36**, 4135 (1987).
[13] A.D. Mirlin and Y.V. Fyodorov, Phys. Rev. Lett. **72**, 526 (1994), and references therein.
[14] R. J. Elliot *at al.*, Rev. Mod. Phys. **46**, 465 (1974).
[15] B. K. Nikolić and P. B. Allen, Phys. Rev. B **63**, R020201 (2001).
[16] K. Slevin *at al.*, Phys. Rev. Lett. **86**, 3594 (2001).
[17] Arguments based on the multifractal scaling analysis [11], indicate that the conductivity exponent $\mu = (d-2)\nu$, and the order parameter exponent $\beta = (\alpha_o - d)\nu$, where ν is the correlation length exponent, and α_o characterizes the multifractal spectra of wavefunction amplitudes. In addition, numerical calculations find that in three dimensions, $\alpha_o \approx 4$ [18], and $\nu \approx 1.58$ [16], so that $\beta \approx \mu \approx 1.58$. The result $\beta = \mu = 1 + O(\varepsilon)$ is also found within the $2 + \epsilon$ approach [11].
[18] H. Grussbach and M. Schreiber, Phys. Rev. B **51**, 663 (1995).

[19] Within a mean-field like formulation such as ours, we do not expect the different symmetry classes (with respect to time-reversal or spin-rotation invariance) to result in different critical exponents. Although it is well known that these differences play a crucial role in the weak-localization regime [4], we note that recent numerical work [20] has found very similar critical behaviors in three dimensions in all cases.

[20] K. Slevin and H. Ohtsuki, Phys. Rev. Lett. **78**, 4083 (1997).

[21] S. M. Girvin and M. Jonson, Phys. Rev. B **22**, 3583 (1980).

[22] We have used the CPA approach to evaluate the vertex function as $\Lambda = \sigma_{cpa}/a_{12}^{cpa}$, where σ_{cpa} is the CPA conductivity [14], and a_{12}^{cpa} is the two-site correlation function embedded in the CPA effective medium. Since TMM coincides with CPA for weak disorder, our results reduce to the correct value at $W << W_c$, where the conductivity assumes the Drude-Boltzmann form.