Application of the Locally Self-Consistent Embedding Approach to the Anderson Model with Non-Uniform Random Distributions

K.-M.Tam[a,b], Y. Zhang[c], H. Terletska[d], Y. Wang[e], M. Eisenbach[f], L. Chioncel[g], J. Moreno[a,b]

[a]*Department of Physics & Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA*
[b]*Center for Computation & Technology, Louisiana State University, Baton Rouge, LA 70803, USA*
[c]*Kavli Institute for Theoretical Sciences, University of the Chinese Academy of Sciences, Beijing, 100190, China*
[d]*Department of Physics and Astronomy, Computational Science Program, Middle Tennessee State University, Murfreesboro, Tennessee 37132, USA*
[e]*Pittsburgh Supercomputing Center, Carnegie Mellon University, PA 15213, USA*
[f]*Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*
[g]*Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, and Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany*

Abstract

We apply the recently developed embedding scheme for the locally self-consistent method to random disorder electrons systems. The method is based on the locally self-consistent multiple scattering theory and the typical medium theory. The locally self-consistent multiple scattering theory divides a system into many small designated local interaction zones. The subsystem within each local interaction zone is embedded in a self-consistent field from the typical medium theory. This approximation allows the study of random systems with large numbers of sites. We present results for the three dimensional Anderson model with different random disorder potential distributions. Using the typical density of states as an indicator of Anderson localization, we find that the method can capture the localization for commonly studied disorder potentials. These include the uniform distribution, the Gaussian distribution, and even the unbounded Cauchy distribution.

Keywords: Anderson Localization, Typical Medium Theory, Locally Self-Consistent Multiple Scattering

1. Introduction

The seminal work by Anderson highlights the importance of random disorder. Instead of a small perturbation on the otherwise metallic system, strong random disorder can lead to the absence of diffusion [1]. This remarkable result has triggered a tremendous amount of fascinating research over the past six decades [2, 3, 4].

The advances in computational condensed matter physics have led to rather accurate descriptions of materials, often from first principles. However, even with improvements in methodology and computer power, simulations of systems with random disorder remain one of the most challenging topics in materials science. One of the major obstacles is the large unit cell required for the study of disorder systems. This problem is particularly acute for materials which hold promising device applications where the density of impurities is rather low, such as doped semiconductors.

One route to subdue the challenges for first principle simulations of disorder materials is to consider methods not based on the conventional plane wave expansion of the Kohn-Sham equations. A promising candidate is the multiple scattering method, the Korringa–Kohn–Rostoker (KKR) method. Instead of finding the eigenvalues and eigenstates of the Kohn-Sham equation, the KKR method directly finds the Green function by the multiple scattering approach [5, 6, 7, 8]. This allows the modeling of systems with larger unit cells. Combined with the coherent potential approximation (CPA) [9, 10, 11, 12, 13], the KKR method has been applied to many systems, such as binary alloys, and more recently high entropy alloys, in which multiple species are present in a well mixed system [14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29].

Even with its success in the study of alloys, the KKR method still suffers from the limitation of the system size. An insightful idea is to limit the range of the electronic couplings: for the portion of the system within a cutoff distance, the coupling is treated by the density functional theory; outside of the cutoff distance, the system is replaced by a vacuum. This approximation, coined as locally self consistent multiple scattering (LSMS) method, renders the calculations to be order-N with respect to the system size [30, 31]. Tens of thousands of atoms can be studied by this method. In addition, the method can readily be parallelized in distributed memory computing clusters. The main class of materials targeted by LSMS are alloys. Rather detailed studies have been conducted on binary alloys, and its capability to handle larger systems has been demonstrated [30].

An intuitive step to improve the method is to consider the system embedded in some form of self-consistently determined bath in the same spirit as that of the CPA or the dynamical mean field theory [9, 32, 13]. While this approach should improve the quality of the approximation, the effects of localization are absent in the CPA and its cluster extensions, such as the dynamical cluster approximation (DCA)[33, 34].

The failure to capture the Anderson localization transition is apparently due to the fact that these mean field methods are based on the average of a single particle quantity, which does not become critical around the critical disorder strength. One may naively expect that the local density of states can serve as an indicator of localization transition. However, this is not the case because a small number of itinerant states dominates the average value of the local density of states which remains finite [35]. For this reason, the averaged local density of states fails as an order parameter of the localization transition.

The typical medium theory (TMT) employs the concept of the typical density of states to generalize the CPA [36, 37, 38]. Instead of using the average density of states to compute the self-consistent mean field bath, the typical density of states is used. Large numerical simulations using the kernel polynomials method have shown that the typical density of states does become critical near the localization transition in the three dimensional Anderson model [39]. It has been further demonstrated that the local density of states has a log normal distribution near the localization transition [39].

The TMT replaces the arithmetic averaging method in the CPA by the geometric average. Note that the geometric average is equal to the typical value for the log normal distribution. One can show that the typical density of states decreases as the disorder strength increases and eventually vanishes as the disorder reaches the critical value. The TMT thus represents a mean field theory of localization which is not admissible by the CPA [37].

The typical medium dynamical cluster approximation (TMDCA) extends the TMT to a cluster theory in line with the development of the DCA [38]. Over the past few years, the TMDCA has been applied on the three dimensional Anderson model [40, 41], off-diagonal disorder, [42], phonon localization [43], multi-orbital models [44], and materials studies [45, 46, 47]. In particular, it has been shown that the re-entrance effect because of non-local scattering in the three dimensional Anderson model, which is absent in the TMT single site theory, is captured by the TMDCA [41].

The locally self-consistent embedding approach uses the locally self-consistent multiple scattering (LSMS) method to study each subsystem within the local interaction zone, but unlike the LSMS the local interaction zone is embedded in a mean field bath [48]. Similar to that of the TMT method, the mean field bath is calculated using the geometric average of the Green functions from disorder realizations rather than the linear average, as in the conventional CPA method.

The embedding method is not an altogether unfamiliar concept by itself, it has been extensively used in the study of strongly correlated systems under the name of quantum cluster theory [33]. It has also been applied for the study of random disorder systems [38]. The objective for the embedded typical medium theory is not to construct a dynamical cluster approximation [49, 23, 38], a cellular dynamical mean field theory [50], nor a real space supercell effective medium approximation [51, 52], but to build up a linearly scaling method which generalizes the concept of LSMS and TMT to study lattice models, and to capture the localization transition [48]. The method should also be readily pertinent to the KKR method for materials studies [48].

The goal of the present paper is to further benchmark the locally self-consistent embedding approach by studying the three dimensional Anderson model with different random disorder distributions. The paper is organized as follows. In section II, we provide a short overview of the method. In section III, we present and discuss the results for the three dimensional Anderson model with uniform, Gaussian, and Cauchy (Lorentzian) distributions. We conclude and provide a discussion of the prospect of the method in the last section.

2. Typical Medium Theory and Embedding Method

The central idea of the embedding method is to consider a small system coupled to an environment. The simplest example is the Weiss mean field theory of the Ising model, in which a single spin is coupled to a mean magnetization. For a fermionic system the coupling between the system and the environment can be embodied in the self-energy.

The LSMS is based on the approximation which divides the system into many smaller subsystems. Each subsystem can be studied by accurate but computational expensive methods. Within the multiple scattering theory, each site or ion in the system is encircled by the so-called local interaction zone (LIZ). The original LSMS treats the LIZ embedded in a vacuum.

In the following we describe the embedding of the LIZ in a self-consistently determined dynamical mean field. Consider a one dimensional system with a four-site supercell (Fig. 1). We denote the number of sites in a supercell as N_c. Each site in the supercell has its own LIZ, we denote the size of the LIZ as N_{LIZ}. Fig. 1 shows an example of $N_c = 4$ and $N_{LIZ} = 3$. In practical calculations N_{LIZ} is smaller, often much smaller, than N_c. For the four sites supercell, there are four different LIZ. The top row of Fig. 1 displays the supercell of the system. The next four rows are the LIZ for the four different sites, the site in consideration is painted in red, and the LIZ is represented by an empty rectangle.

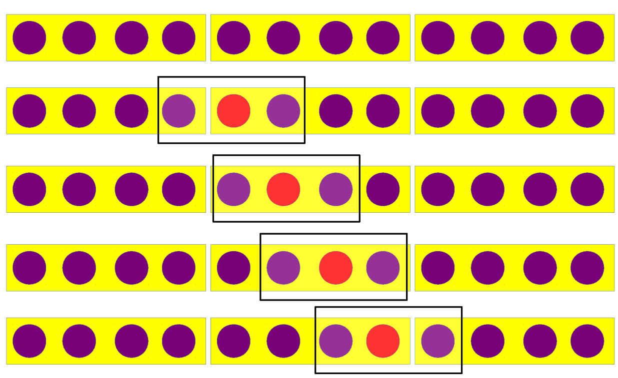

Figure 1: An example of the local interaction zone (LIZ) for a one dimensional system with a four-site supercell. The top row shows the supercells. The next four rows display the LIZ for the four sites in a supercell. The site in consideration is painted in red, and the LIZ is represented by an empty rectangle.

Consider the Fourier transform of the Green function $\bar{G}(\omega, K)$:

$$\bar{G}_{IJ}(\omega) = \frac{1}{N_c} \sum_K e^{iK \cdot R_{IJ}} \bar{G}(\omega, K), \tag{1}$$

where K is the wavenumber, N_c the number of sites, and (I, J) the coordinates of the supercell sites [53]. The LIZ Green function is obtained simply by restricting the indices (I, J) to the given LIZ.

$$\bar{G}^{\text{LIZ}}_{IJ}(\omega) = \frac{1}{N_c} \sum_K e^{iK\cdot R_{IJ}} \bar{G}(\omega, K), \quad (I, J) \in \text{LIZ}. \tag{2}$$

$\bar{G}(\omega, K)$ is defined through the coarse-graining procedure as

$$\bar{G}(\omega, K) = \frac{N_c}{N} \sum_{\tilde{k}} \frac{1}{\omega - \epsilon(K + \tilde{k}) - \Sigma(\omega)}, \tag{3}$$

where the local effective self-energy is denoted by $\Sigma(\omega)$ and $\epsilon(K + \tilde{k})$ is the lattice dispersion. The supercell wavenumbers K correspond to the N_c cells as prescribed by the dynamical cluster approximation [54, 53, 49]. $\tilde{k}$ labels the wavenumbers surrounding K within each patch in the Brillouin zone.

The LIZ excluded Green function can be obtained as,

$$\underline{\mathcal{G}}^{-1}(\omega) = \left(\underline{\bar{G}}^{\text{LIZ}}(\omega)\right)^{-1} + \Sigma(\omega) \cdot \underline{\mathbb{I}}, \tag{4}$$

where $\underline{\mathcal{G}}(\omega)$ is the real space Green function within a LIZ in the absence of disorder. The underline denotes the quantities are $N_{LIZ} \times N_{LIZ}$ matrices. Note that for a translational invariant system $\underline{\mathcal{G}}(\omega)$ is the same for all possible LIZs obtained by running the center of the LIZ (I_c) through each sites of the supercell [48].

Within a supercell the cluster Green function with the disorder potential can be obtained for each site for solving the real space cluster Green function of the corresponding LIZ centered around the site I_c:

$$\left(\underline{G}^{\text{LIZ}}(\omega, V, I_c)\right)^{-1} = \underline{\mathcal{G}}^{-1}(\omega) - \underline{V}(I_c), \tag{5}$$

where $\underline{V}(I_c)$ is a diagonal matrix of size $N_{LIZ} \times N_{LIZ}$. The index I_c (the center of the LIZ) serves also as an additional label indicating the presence of disorder at that specific site. N_r number of random realizations are solved for each LIZ.

The cluster Green function averaged over disorder realizations and the sites within the supercell can be obtained as $\underline{G}^{\text{LIZ}}_{ave}(\omega) = \frac{1}{N_r N_c} \sum_{I_c, V} \underline{G}^{\text{LIZ}}(\omega, V, I_c)$. As we discussed above, the linear average of the Green function fails to capture the localization transition. We thus follow the TMT to promote the linear average to geometric average (typical average for log-normal distribution) as follow [37],

$$\underline{G}^{\text{LIZ}}_{ave(typ)}(\omega) = e^{\frac{1}{N_c}\sum_{I_c}\langle \ln(\rho_{I_c I_c}(\omega, V, I_c))\rangle_V} \times \frac{1}{N_c} \sum_{I_c} \left\langle \frac{\underline{G}^{\text{LIZ}}(\omega, V, I_c)}{\rho_{I_c I_c}(\omega, V, I_c)} \right\rangle_V, \tag{6}$$

where $\rho_{I_c I_c}(\omega, V, I_c)$ is the local density of state at the center of the LIZ defined as

$$\rho_{I_c I_c}(\omega, V, I_c) = -\frac{1}{\pi} \text{Im}(\underline{G}^{\text{LIZ}}(\omega, V, I_c))_{I_c, I_c}. \tag{7}$$

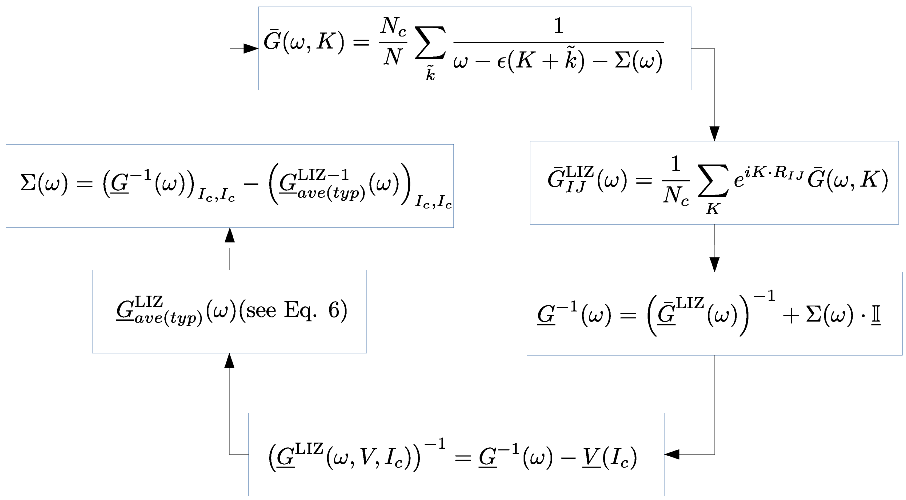

Figure 2: The self-consistency loop for the TMT embedding method. It can be broken down into the following steps. 1. Starting from the top of the figure, the lattice Green function is obtained by coarse-graining over each patch labelled by K in the Brillouin zone. 2. The Green function within the LIZ in real space is obtained by Fourier transforming the lattice Green function. 3. The bath Green function is obtained by the cluster excluded Green function using the Dyson equation. 4. The impurity cluster Green function within the LIZ is obtained by solving the system exactly within the LIZ. 5. The typical averaged Green function is obtained by solving the impurity cluster Green function over many random realizations. 6. The self-energy is obtained via the Dyson equation. 7. Repeat from the initial step until the self energy is converged.

With the averaged cluster Green function, we update the self-energy via the Dyson equation as follow,

$$\Sigma(\omega) = \left(\underline{\mathcal{G}}^{-1}(\omega)\right)_{I_c, I_c} - \left(\underline{G}^{\mathrm{LIZ}-1}_{ave(typ)}(\omega)\right)_{I_c, I_c}, \tag{8}$$

where $\underline{G}^{\mathrm{LIZ}}_{ave(typ)}(\omega)$ is the disorder averaged $\underline{G}^{\mathrm{LIZ}}(\omega, V, I_c)$ via geometric averaging. The algorithm is summarized in Fig. 2.

3. Results

In the present study we focus on the standard Anderson model in a simple cubic lattice.

$$H = -t \sum_{<i,j>,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + H.c.) + \sum_{i\sigma} V_i n_{i\sigma}, \tag{9}$$

where $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are the creation and annihilation operators, respectively, for electrons at site i and spin σ. $n_{i,\sigma}$ is the number operator for site i, spin σ, t is the hopping parameter between nearest neighbors, and the local random disorder is given by V_i. We set $t = 1$ to serve as the energy scale.

Three vastly different disorder distributions are studied:

1. The bounded uniform distribution, also called box disorder. The disorder distribution function is $P(V) = \frac{1}{W}\Theta(|W/2 - V|)$, where the disorder strength is characterized by W.

2. The Gaussian distribution with distribution function given as $P(V) = \frac{\sqrt{6/\pi}}{W^2} exp(-\frac{6V^2}{W^2})$.

3. The Cauchy distribution or the Lorentzian distribution which is an unbounded distribution. The distribution is given as $P(V) = \frac{W^2}{\pi(V^2+W^2)}$.

We use the TMT embedding algorithm to study the three dimensional Anderson model for the above three random distributions. We only study the case for zero energy. Most of the studies in the literature are also focused at zero energy and very accurate data is available [3, 55, 56]. There are interesting physics at non-zero energy, a prominent feature is the reentrance of the metallic phase as disorder is increased at high energies. Since there are not many studies on this issue and our purpose is benchmarking our approach for different disorder distributions, we reserve the study at high energies for future work.

In the simulations, we use 1,000 random realizations for disorder averaging. The supercell size is chosen to be $N_c = 8 \times 8 \times 8$, and the LIZ size is chosen to be $N_{LIZ} = 3 \times 3 \times 3$. According to the TMT, the indicator or 'order parameter' for the localization transition can be represented by the geometric averaged local density of states, $\rho_{typ}(\omega)$. After the self-consistency for the self energy is attained, we calculate $\rho_{typ}(w) = exp[\frac{1}{N_c}\sum_{I_c} \langle \ln(\rho_{I_c I_c}(\omega, V, I_c))\rangle_V]$.

From Fig. 3, one can observe that the typical density of states decreases as the disorder strength increases. It approaches zero above a certain value of disorder, which can be identified as the critical disorder strength for the localization transition [37]. The three random distributions we consider have very different values of the critical disorder. From the highly accurate transfer matrix calculation, the critical disorder strengths are $16.536, 21, 293, 4.2707$ for the box, Gaussian, and Cauchy distributions, respectively [56].

The critical disorder strengths calculated by the present method follow roughly the values predicted by the transfer matrix calculations, but our values are overestimated for all three distributions (Fig. 3). Note that the results presented are for a fixed LIZ size and a supercell size. A rather accurate estimate for critical disorder can be obtained for proper scaling of the typical density of state as a function of LIZ size and supercell size [48]. The present results show the trend that the typical density of state drops appreciably near the expected critical disorder strength.

4. Conclusion

We use the embedding locally self-consistent method to study the Anderson model in three dimensions with different disorder distributions. The method provides a path for the study of random disorder systems without solving a large lattice or cluster problem. The computational cost scales with the third power of the size of the local interaction zone but only linearly with the system size.

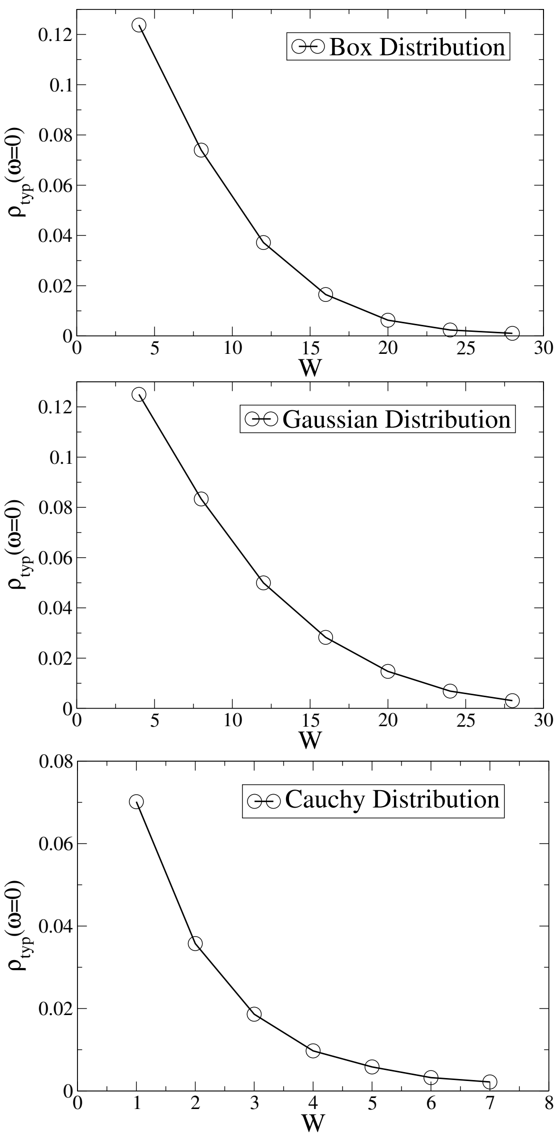

Figure 3: Geometric averaged local density of states at zero energy, $\rho_{typ}(\omega = 0)$, as a function of disorder strength for a $8 \times 8 \times 8$ supercell, and $3 \times 3 \times 3$ local interaction zone. Upper Panel: $\rho_{typ}(\omega = 0)$ for the box distribution. Middle Panel: $\rho_{typ}(\omega = 0)$ for the Gaussian distribution. Lower Panel: $\rho_{typ}(\omega = 0)$ for the Cauchy distribution.

The approximation being used renders it to be a linearly scaling method as that of the locally self-consistent multiple scattering theory; moreover, the method can be easily parallelized to run in distributed memory computer clusters [30]. The present results on the single band model with local random potentials are encouraging for the prospect of its application in other models and materials study.

We emphasize that the purpose of the present method is to construct an order-N theory for the study of random disorder systems, particularly for capturing localization transition so that it can be used to generalize the locally self-consistent multiple scattering theory [30]. For the Anderson model in three dimensions, accurate embedding methods which are not an order-N method are available, such as the well studied typical medium dynamical cluster approximation [38]. The real space supercell effective medium approximation is another possible proposal [51, 52].

The immediate future work for the present method is to investigate the scaling of the typical density of state as a function of supercell size and the LIZ size. The next step will be to employ the present scheme with the KKR multiple scattering theory [57, 46] for disorder materials such as high entropy alloys and doped semiconductors. This method, in principle, can also be used to calculate two particle quantities [58], which allows the access of physically relevant quantities such as the conductivity. Combining with the ab initio KKR multiple scattering method, this approach thus provides a route for the investigation of the effect of localization in weakly interacting materials [59].

5. Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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