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H. Terletska, S.-X. Yang, Z. Y. Meng, J. Moreno, and M. Jarrell

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Dual Fermion Method for Disordered Electronic Systems

H. Terletska,[1,*] S.-X. Yang,[2,3] Z. Y. Meng,[2,3] J. Moreno,[2,3] and M. Jarrell[2,3]

[1] *Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA*

[2] *Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA*

[3] *Center for Computation and Technology, Louisiana State University, Baton Rouge, Louisiana 70803, USA*

While the coherent potential approximation (CPA) is the prevalent method for the study of disordered electronic systems, it fails to capture non-local correlations and Anderson localization. To incorporate such effects, we extend the dual fermion approach to disordered systems using the replica method. The developed method utilizes the exact mapping to the dual fermion variables, and includes inter-site scattering via diagrammatic perturbation theory in the dual variables. The CPA is recovered as a zeroth-order approximation. Results for single- and two- particle quantities show good agreement with a cluster extension of the CPA; moreover, weak localization is captured. As a natural extension of the CPA, our method presents an alternative to existing non-local cluster theories for disordered systems, and has potential applications in the study of disordered systems with electronic interactions.

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I. INTRODUCTION

Disorder, due to doping, impurities or structural defects, is universally present in electronic materials[1–9]. It introduces scattering of charge carriers and significantly affects their motion, and often plays a crucial role in determining the transport properties of materials. The most prominent example of such effects is the Anderson localization transition[1], where the scattering of electrons from random impurities prevents their propagation across the sample. To properly describe this phenomena, one needs to take into account quantum coherent multiple scattering effects of the charge carriers.

The simplest and the most commonly used theoretical method to study disordered systems is the coherent potential approximation (CPA)[10–12]. It is a single-site self-consistent mean field approximation, in which the real system is replaced by an effective medium described by a local coherent potential (momentum independent self-energy) which comprises the effects of the random potential on the motion of the electrons. While the CPA is a successful effective medium theory for the description of one-electron properties, especially in realistic calculations of random alloys[11–14], it is far from a complete theory for disordered systems. For example, its single-site nature leaves out disorder-induced non-local correlation effects involving different scatterers, which are responsible for finer details in the density of states. The most significant drawback of the CPA is, however, its failure to capture backscattering effects on the electron transport, and hence, electron localization.

A natural extension of a single-site theory is to use a finite sized cluster self-consistently embedded in the averaged effective medium. Cluster extensions of the CPA such as the Molecular CPA[15] or the Dynamical Cluster Approximation (DCA)[16] provide systematic improvements to the CPA, by capturing non-local correlations within the cluster[14]. For example, in the DCA, the self-energy acquires momentum dependence by taking into account multiple scattering effects within the cluster. As a result, the DCA captures fine structures and band tails in the density of states. It systematically restores some set of the maximally crossed diagrams known to be responsible for Anderson localization; however, it does not capture the transition itself[16].

The goal of this paper is to provide a systematic improvement upon the existing effective medium theories for disordered electronic systems, which will satisfy the following criteria: it recovers the CPA as a limiting case; like the DCA, it provides systematic non-local correction to the CPA; it properly describes the single-particle quantities with detailed structures in the density of states; unlike the CPA, it can provide finite vertex corrections from backscattering processes to the conductivity in low dimensions ($d \leq 2$); and it can also be used to study interacting disordered systems[17].

The method we pursue here is the Dual Fermion (DF) formalism [18–20], originally developed for interacting systems without disorder. It is complementary to existing non-local cluster approaches. It treats local correlations explicitly in the "impurity" solver, and non-local correlations perturbatively. So, if a geometric series of relevant diagrams is included, it has a potential to capture localization. Here we present such a DF method for disordered non-interacting systems, as an alternative effective medium theory which provides important non-local physics beyond the CPA.

The DF formalism is based on a set of auxiliary variables (dual fermions) which are introduced into the path integral representation of the lattice partition function via a canonical transformation[18,21,22]. It maps the lattice onto an impurity embedded in a self-consistently determined DF lattice. The DF lattice problem is treated via a perturbation theory involving the DF bare Green function, which is the difference between the lattice and impurity Green functions, and the impurity full vertex as the

effective bare DF interaction[23]. For systems with disorder, the DF mapping has to be done differently. In particular, as observables are calculated by taking derivatives of the free energy, the DF formalism for the disordered case needs to be constructed from the disorder-averaged free energy $\langle \ln Z \rangle_{av}$ instead of from the partition function Z as in References 18,19.

In this paper we employ the replica method [24] to deal with such averaging. We extend the DF method to systems with disorder, and construct the DF mapping directly on the Green function. We demonstrate that our method shows remarkable agreement for the single-particle Green function with the results obtained from large-cluster DCA calculations. It successfully accounts for weak localization in the conductivity with finite vertex corrections. The developed scheme presents a powerful non-local alternative to the existing cluster extensions of the CPA, with a broad venue of applications, including the possibility of treating both electron-electron interactions and disorder on equal footing, or even replacing the CPA in electronic structure calculations.

This paper is organized as follows. Section II outlines the model and the details of the replica based dual fermion formalism. Here we also discuss constraints the replica limit introduces on the topology of the single and two-particle diagrams. In section III we present and discuss our numerical results for the single-particle Green function, which are benchmarked with the CPA and DCA data. We then provide a conductivity calculation with finite v ertex corrections to the CPA. In section IV we present our conclusions and future perspectives.

II. FORMALISM

A. Replica method

We consider the Anderson model of non-interacting electrons subjected to a random diagonal disorder potential. It is described by the Hamiltonian

$$H = -\sum_{<ij>} t_{ij}(c_i^\dagger c_j + h.c.) + \sum_i v_i n_i, \qquad (1)$$

where t_{ij} is the electronic hopping probability ($4t = 1$ sets the unit of energy), $c_i^\dagger(c_i)$ is the creation (annihilation) operator for an electron on site i. The disorder is modeled by the local random potential v_i, a site-dependent random quantity, with a uniform ("box") disorder distribution, $p(v_i) = \frac{1}{W}\Theta(\frac{W}{2} - |v_i|)$, where W measures the strength of the disorder. We emphasize that the DF formalism developed here can be equally applied to other disorder distributions $P(v)$.

The disorder averaged lattice Green function is given by

$$\langle G_k(w_n)\rangle_{av} = -\frac{\delta}{\delta\eta_{wk}} \langle \ln Z(v_i, \eta_{wk})\rangle_{av} \,|_{\eta_{wk}=0}, \qquad (2)$$

with $\langle(...)\rangle_{av} = \int dv p(v)(...)$ indicating a disorder averaged quantity, and η_{wk} is a source field.

In the replica method, the relation $\ln Z = \lim_{m\to 0} \frac{Z^m - 1}{m}$ is employed, with m being the number of replicas[16,25,26]. Hence, the disorder-averaged Green function of Eq. (2) can be rewritten in terms of the m-th power of Z instead of a logarithm. As discussed in References 16,25, taking the replica limit, $m \to 0$, eliminates closed loop diagrams in the perturbation series expansion for the disorder averaged Green function. As a result, it properly accounts for the effect of the partition function in the denominator of the unreplicated theory.

Using Grassmann functional integrals for quantum averaging, and the replica method for disorder averaging, we rewrite Eq. (2) as

$$\langle G_k(w)\rangle_{av} = -\lim_{m\to 0}\frac{1}{m}\frac{\delta}{\delta\eta_{wk}} \left\langle \int \mathcal{D}\bar{c}\mathcal{D}c e^{-S[c^\alpha, \bar{c}^\alpha]} \right\rangle_{av} |_{\eta_{wk}=0}, \qquad (3)$$

where $\mathcal{D}c \equiv \prod_{wk\alpha} dc^\alpha_{wk}$, and α is the replica index. The lattice action

$$S = \sum_{wk\alpha} \bar{c}^\alpha_{wk}(-iw_n + \varepsilon_k - \mu + \eta_{wk})c^\alpha_{wk} + \sum_{i\alpha} v_i \int_0^\beta d\tau n_i^\alpha(\tau), \qquad (4)$$

where $w_n = (2n+1)\pi T$ are the Matsubara frequencies, ε_k is the lattice bare disperssion, and μ is the chemical potential. Averaging over the distribution $p(v)$ in Eq. (4), we obtain

$$S = \sum_{wk\alpha} \bar{c}^\alpha_{wk}(-iw_n + \varepsilon_k - \mu + \eta_{wk})c^\alpha_{wk} + \sum_i W(\tilde{n}_i), \qquad (5)$$

where $W(\tilde{n}_i)$ is the elastic, effective interaction between electrons of different replicas. It is local in space and non-local in time, and may be expressed through cumulants $< v^l >_c$ as[16]

$$\begin{aligned} e^{-W(\tilde{n}_i)} &= \int dv_i p(v_i) e^{-v_i \sum_\alpha \int d\tau n_i^\alpha(\tau)} \\ &= e^{-\sum_{l=2}^\infty \frac{1}{l!} < v^l >_c \left(\sum_\alpha \int d\tau n_i^\alpha(\tau)\right)^l}. \end{aligned} \qquad (6)$$

B. Dual fermion mapping

To construct the DF formalism for disordered electronic systems, we follow the original DF procedure[18]. The DF mapping is performed in three major steps.

First, we introduce an effective single-site impurity reference problem by formally rewriting the original action as

$$S = \sum_i S_{imp}[c^\alpha, \bar{c}^\alpha] - \sum_{wk\alpha} \bar{c}^\alpha_{wk}(\Delta_w - \varepsilon_k - \eta_{wk})c^\alpha_{wk}, \qquad (7)$$

with an effective impurity action (containing the disorder vertex, $W(\tilde{n}_i)$)

$$S_{imp} = \sum_{\alpha w} \bar{c}^\alpha_{iw}(-iw - \mu + \Delta_w)c^\alpha_{iw} + W(\tilde{n}_i). \qquad (8)$$

Here Δ_w is a local, and yet unknown, hybridization function describing the interaction of the impurity with the effective medium. As in the original DF formalism[18], it is assumed that all the properties of the impurity problem, i.e., the single-particle Green function

$$g_{imp}(w) = -\lim_{m\to 0}\frac{1}{m}\sum_{\alpha=1}^{m}\int \mathcal{D}\bar{c}\mathcal{D}c\, e^{-S_{imp}} c_w^\alpha \bar{c}_w^\alpha, \qquad (9)$$

and the two-particle Green functions

$$\chi_{imp}(w,w') = -\lim_{m\to 0}\frac{1}{m}\sum_{\alpha,\beta=1}^{m}\int \mathcal{D}\bar{c}\mathcal{D}c\, e^{-S_{imp}}\times c_w^\alpha c_{w'}^\beta \bar{c}_{w'}^\beta \bar{c}_w^\alpha \qquad (10)$$

can be calculated. In our case, these are local CPA quantities. Our task is to express the original lattice Green function and other properties via such quantities of the CPA impurity problem. What has been accomplished so far in Eq. (7) is that the local part of the lattice action has been moved to the effective impurity.

In the second step of the DF procedure, we introduce the auxiliary ("dual" fermions) degrees of freedom. In doing so, we transfer the non-local part of the action in Eq. (7) to the dual variables. As a result, the original real fermions carry information about the local part only. The transformation to dual fermions is done via a Gaussian transformation of the non-local part of Eq. (7),

$$e^{\bar{c}_{wk}^\alpha A_{wk}^2 c_{wk}^\alpha} = \frac{A_{wk}^2}{\lambda_w^2}\int \mathcal{D}\bar{f}\mathcal{D}f e^{-\lambda_w(\bar{c}_{wk}^\alpha f_{wk}^\alpha + \bar{f}_{wk}^\alpha c_{wk}^\alpha) - \frac{\lambda_w^2}{A_{wk}^2}\bar{f}_{wk}^\alpha f_{wk}^\alpha} \qquad (11)$$

with $A_{wk}^2 = (\Delta_w - \varepsilon_k - \eta_{wk})$, and λ_w yet to be specified.

With such a transformation, the lattice Green function of Eq. (3) can be rewritten as

$$\begin{aligned}\langle G_k(w)\rangle_{av} &= -\lim_{m\to 0}\frac{1}{m}\frac{\delta}{\delta\eta_{wk}}\frac{(\Delta_w-\varepsilon_k-\eta_{wk})}{\lambda_w^2}\\ &\times \int \mathcal{D}\bar{f}\mathcal{D}f\, e^{-\sum_{wk\alpha}\lambda_w^2\bar{f}_{wk}^\alpha(\Delta_w-\varepsilon_k-\eta_{wk})^{-1}f_{wk}^\alpha}\\ &\times \int \mathcal{D}\bar{c}\mathcal{D}c\, e^{-\sum_i S_{site}^i[\bar{c}_i^\alpha,c_i^\alpha;\bar{f}_i^\alpha,f_i^\alpha]}\big|_{\eta_{wk}=0}.\end{aligned} \qquad (12)$$

in which the replicated action for site i is of the form

$$S_{site}^i = S_{imp} + \sum_{\alpha w}\lambda_w\left(\bar{c}_{iw}^\alpha f_{iw}^\alpha + \bar{f}_{iw}^\alpha c_{iw}^\alpha\right). \qquad (13)$$

In Eq. (12) the inter-site coupling is transferred to a coupling between dual fermions.

In the third step of the DF mapping, we integrate out the real fermions from the local site action S_{site}^i for each site i separately, i.e.,

$$\begin{aligned}&\int\prod_{\alpha w} d\bar{c}_i^\alpha dc_i^\alpha e^{-S_{site}[\bar{c}_i^\alpha,c_i^\alpha;\bar{f}_i^\alpha,f_i^\alpha]}\\ &= Z_{imp}e^{-\sum_{w\alpha}\lambda_w^2 g_{imp}(w)\bar{f}_{iw}^\alpha f_{iw}^\alpha - V_{d,i}^{\alpha,\beta}[\bar{f}_i^\alpha,f_i^\beta]},\end{aligned} \qquad (14)$$

in which Z_{imp} is the partition function for the replicated impurity system. As in the clean case [18–20], formally this can be done up to infinite order, which makes the mapping to the DF variables exact. Choosing for convenience $\lambda_w = g_{imp}^{-1}(w)$, the lowest-order of the replicated DF potential $V_{d,i}^{\alpha,\beta}[\bar{f}_i^\alpha, f_i^\beta]$ (non-antisymmetrized) reads as

$$V_{d,i}^{\alpha,\beta}[\bar{f}_i^\alpha, f_i^\beta] = \frac{1}{2}\gamma(w,w')\bar{f}_{iw}^\alpha\bar{f}_{iw'}^\beta f_{iw'}^\beta f_{iw}^\alpha, \qquad (15)$$

where the CPA full vertex

$$\gamma(w,w') = -\frac{\chi_{imp}(w,w') - \chi_{0,imp}(w,w')}{g_{imp}(w)^2 g_{imp}(w')^2}, \qquad (16)$$

with $\chi_{0,imp}(w,w') = g_{imp}(w)g_{imp}(w')$. In general [18–20], the DF vertex $V_{d,i}^{\alpha,\beta}[\bar{f}_i^\alpha, f_i^\beta]$ contains n-body correlation terms introduced by disorder, but in the following discussion we will limit ourselves to the leading quartic term with four external DF fields only.

After taking the derivative with respect to the source field η_{wk}, the Green function of Eq. (12) reads as

$$\langle G_k(w)\rangle_{av} = (\Delta_w - \varepsilon_k)^{-1} + \frac{\langle G_{d,k}(w)\rangle_{av}}{(\Delta_w-\varepsilon_k)^2 g_{imp}(w)^2}, \qquad (17)$$

where we define the averaged DF Green function as

$$\begin{aligned}\langle G_{d,k}(w)\rangle_{av} &= -\lim_{m\to 0}\frac{1}{m}\sum_{\alpha'=1}^{m}\int \mathcal{D}\bar{f}\mathcal{D}f\, e^{-\sum_{wk\alpha}S_d^0}\\ &\times\ e^{-\sum_{i\alpha\beta w}V_{d,i}^{\alpha,\beta}[\bar{f}_i^\alpha,f_i^\beta]} f_{wk}^{\alpha'}\bar{f}_{wk}^{\alpha'},\end{aligned} \qquad (18)$$

and $S_d^0 = \bar{f}_{wk}^\alpha\left[-\frac{(\Delta_w-\varepsilon_k)^{-1}+g_{imp}(w)}{g_{imp}^2(w)}\right]f_{wk}^\alpha$ is the non-interacting DF action.

Notice, that for the case of non-interacting dual fermions when dual potential is zero, Eq. (17) reduces to the CPA solution for the lattice Green function with $\langle G_k(w)\rangle_{av} = \frac{1}{g_{imp}^{-1}+\Delta_w-\varepsilon_k}$. Hence, the CPA is the zeroth order approximation within our framework.

C. Dual fermion diagrammatics

While the local CPA solution is recovered as a zero-order approximation of the dual fermion potential, non-local corrections to the CPA self-energy require higher order corrections in $V_{d,i}^{\alpha,\beta}$. This is achieved with a standard diagrammatic perturbation expansion of the interacting part of the DF action in Eq. (18). The DF diagrams are constructed similarly to the standard Matsubara diagrams, except that now the lines are renormalized DF Green functions, and the vertex is approximated by the full CPA vertex.

Notice that a non-trivial and crucial difference between the disordered and clean cases is that here the interaction

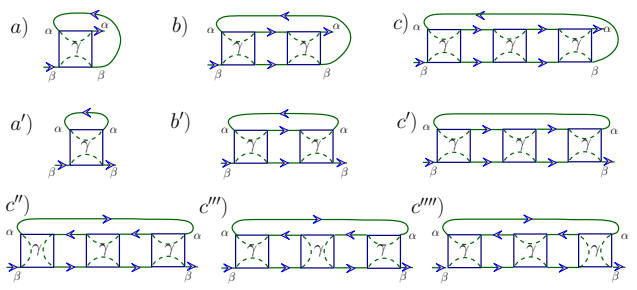

FIG. 1: (color online) The dual fermion self-energy diagrams up to the third order in the perturbation series. The replica limit imposes a constraint on the topology of the diagrams, i.e., all diagrams with closed electron loops, e.g., diagrams a'), b') and c' of Fig. 1) vanish in the replica limit. Here, γ is the CPA full vertex. Diagram a) is local, and vanishes to satisfy the DF self-consistency condition for determining the hybridization function Δ_w.

between replicas is off-diagonal, which puts certain constraints on the topology of the Green function graphs. In particular, all diagrams with closed fermion loops vanish (e.g., diagram a'), b') and c') of Fig. 1). This is because each closed fermion loop contains one free replica summation which gives an extra factor of m in Eq. (18), and thus equals to zero when $m \to 0$ [25].

III. RESULTS

A. Calculation procedure.

The calculation procedure we use here is similar to the clean DF case[18]. It is composed of two major steps. First, after solving the impurity (CPA) part, we obtain the averaged impurity Green function $g_{imp}(w) = \int dv p(v) \frac{1}{iw_n + \mu - \Delta(w) - v}$ and corresponding impurity vertex γ. These quantities are used in the second step to construct the input for the DF diagrammatic expansion. Here the DF self-energy is calculated self-consistently using standard diagrammatic perturbation theory. After this, the real lattice Green function from Eq. (17) is recalculated such that the non-local correlations are now included. Next, the new hybridization function $\Delta(w)$ is constructed to parametrize the impurity problem. This is repeated until self-consistency is reached, namely $\sum_k G_{d,k}(w) = 0$, with all local diagrams (e.g., diagram a) in Fig. 1) being zero.

B. Single-particle properties.

This section presents our main results. The diagram b) of Fig. 1 is the lowest non-vanishing contribution to the dual self-energy, with $\Sigma_d(w_n, k) = -\frac{T^2}{N_c^2} \sum_{q,k'} \gamma^2_{w_n,w_n} G^d(w_n, k+q) G^d(w_n, k'+q) \times G(w_n, k')$ It already provides some non-local corrections to the CPA solution. However, for our analysis we consider an infinite ladder diagram summation to capture quantum coherence effects from multiple impurity scatterings. In Fig. 2 we present results for the imaginary part of the local single-particle Green function of Matsubara frequency $\mathrm{Im}G_{\mathrm{loc}}(w_n)$ obtained from a fully self-consistent infinite ladder diagram summation, in both the particle-hole (p-h) and the particle-particle (p-p) channels for the DF self-energy.

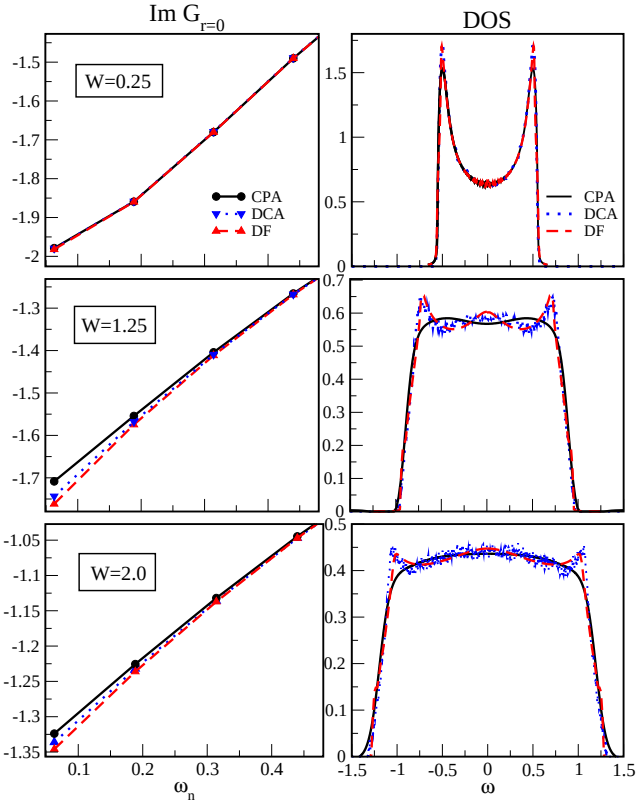

FIG. 2: (color online) The imaginary part of the local Matsubara Green function $\mathrm{Im}G_{r=0}(w_n)$ in $d = 1$ at $T = 0.02$ (left panel) and the total density of states (right panel) for different disorder strengths: $W = 0.25, 1.25, 2.0$ ($4t = 1$). For comparison, we present data obtained with the CPA, a finite cluster DCA ($N_c = 20$) and the DF methods. Inclusion of inter-site correlations leads to corrections to the CPA Green function (left panel) and the appearance of additional structures at larger disorder in the total density of states (right panel). In each case, the DF method captures the features of the DCA density of states and is in nearly exact agreement with DCA Green function.

To benchmark our results for the effect of non-local correlations to the CPA, we compare our DF data with CPA results and DCA results for cluster size $N_c = 20$. The DCA method has been extensively described in the literature, so here we only briefly outline its the main points. As mentioned already in the introduction, the DCA[16,27] is a non-local mean-field theory where the original lattice is mapped to the periodic cluster of size $N_c = L_c^d$

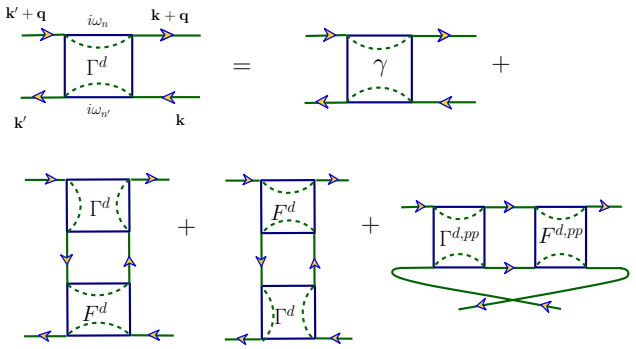

FIG. 3: (color online) Irreducible DF p-h horizontal vertex Γ^d calculated using the parquet equation with crossing contributions from the p-h "vertical" and p-p channels. The fully irreducible vertex is approximated by γ. $\Gamma^{d,pp}$ and $F^{d,pp}$ are the irreducible and full p-p vertices, respectively.

embedded in a self-consistently determined host. As a result, the coarse-grained lattice Green function and self-energy acquire a cluster resolved momentum dependence. Hence, in the DCA, multiple inter-site scattering effects which contribute nonlocal corrections to the self-energy are treated explicitly within the cluster, while the long-range effects are treated on a mean-field level. Notice, that for $N_c = 1$, the DCA reduces to the local CPA.

Our results for the local Matsubara Green function (left panel) and the local density of states (DOS) (right panel) calculated at $T = 0.02$ in one-dimension $d = 1$ with real and dual fermion lattice size $L = 100$ (large enough to reflect the thermodynamic limit) at various values of disorder strength $W = 0.25, 1.25, 2.0$ are shown in Fig. 2. The data for the local Matsubara Green function (left panel) of Fig. 2 show that inclusion of inter-site correlations leads to corrections to the CPA Green function. Both the DF and DCA results show good agreement at small and large disorder strength and differ from the CPA data in qualitatively the same way. The local DOS (right panel) also displays satisfactory agreement between the DF and DCA results. Indeed, for weak disorder ($W = 0.25$), the results from the CPA, DCA and DF calculations are practically the same. As the disorder strength increases, the non-local corrections become important (with finite momentum dependence of the self-energy) and the differences between the CPA and the DF density of states are more pronounced. The DF successfully captures such correlations by producing additional features[14] which are also in good agreement with the fully converged DCA result, especially for large disorder strength ($W = 2.0$).

C. Two-particle properties: nonlocal vertex corrections beyond CPA.

While the CPA provides a good qualitative description of the one-electron properties, it fails to capture backscattering effects on the transport of electrons[23,28]. In the CPA, the two-particle vertex is local and does not depend on the transfer momentum between incoming and outgoing particles. Hence, the CPA conductivity has contributions from the bare p-h bubble only. However, the vertex corrections are crucial for a proper calculation of the conductivity. In low dimensions, they lead to Anderson localization[23,28]. Thus, for a proper description of the disordered transport one needs to go beyond the CPA level in order to incorporate these backscattering contributions and spatial quantum coherence effects.

In our scheme, the full vertex is non-local, so we expect to obtain finite vertex corrections describing "weak" localization effects[3]. As our formalism is best converged on Matsubara frequencies, we calculate the low temperature dc conductivity σ_{dc} as[29,30]

$$\sigma_{dc} = \frac{\beta^2}{\pi}\Lambda_{xx}\left(\mathbf{q} = 0, \tau = \frac{\beta}{2}\right), \tag{19}$$

where $\beta = 1/k_BT$, the current-current correlation function $\Lambda_{xx}(\mathbf{q} = \mathbf{0}, \tau) =< j_x(\mathbf{q}, \tau) j_x(-\mathbf{q}, 0) >$ in x direction with the current density operator $j = \sum_k e n_{\mathbf{k}} v_x(\mathbf{k})$, and the electron group velocity $v_x = \partial\varepsilon(\mathbf{k})/\partial k_x$ is obtained from the bare dispersion $\varepsilon(\mathbf{k})$. To get such lattice density-density correlation functions, we need to calculate the DF two-particle Green function [18,20] $\chi^d = -\chi_0^d - \chi_0^d F^d \chi_0^d$, with $\chi_0^d = G^d G^d$. For the disordered case, one has to remember that in the DF vertex F^d all diagrams containing closed loops are zero due to the replica constraint.

As usual, the full dual fermion vertex F^d is obtained from the Bethe-Salpeter equation[20,23,31] $F^d = \Gamma^d + \Gamma^d \chi_0^d F^d$, where Γ^d is the irreducible DF vertex in the p-h horizontal channel (c.f. Fig. 3). To calculate this quantity, we use the parquet equation which accounts for the crossing contributions from the p-p and the "vertical" p-h channels[23]. Here, the fully irreducible vertex is approximated by the impurity full vertex γ. This procedure allows us to incorporate the important maximally-crossed diagrams[28] in our analysis. The resulting full conductivity can be decomposed into two parts, $\sigma = \sigma_0 + \Delta\sigma$, where σ_0 is the mean-field Drude conductivity coming from the bare bubble χ_0, and the second (two-particle contribution) part $\Delta\sigma$ incorporates the vertex corrections.

Our results for the CPA and DF dc conductivity σ_{dc} in dimensions $d = 1$ and $d = 2$ are presented in Fig. 4. Including finite vertex corrections, which vanish in the CPA, the data show that the disorder DF method is able to capture weak localization effects leading to a net decrease of the conductivity. In $d = 1$, as the disorder strength increases, the DF vertex corrections are more pronounced, while in $d = 2$ they are much weaker, as expected[3]. Hence, our disorder DF formalism is able to

improve upon another drawback of the CPA, i.e., it can incorporate the quantum coherence and backscattering

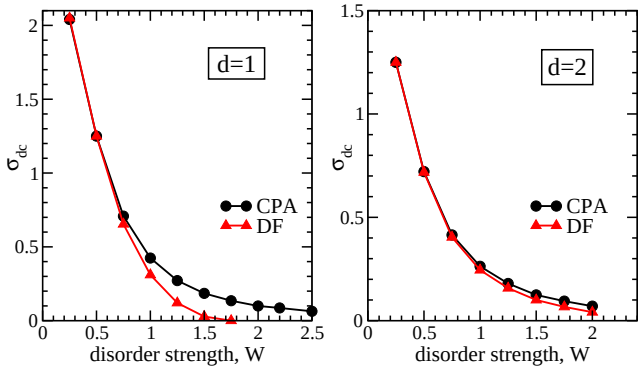

FIG. 4: (color online) Conductivity as function of the disorder strength using the CPA and DF methods. Results are shown for $d = 1$ and $d = 2$ at $T = 0.02$. Our results show that vertex corrections incorporated in the DF approach allow one to capture weak localization leading to the decrease of the conductivity.

IV. CONCLUSIONS

We present and extension of the dual fermion approach[18] for studying disordered electronic systems using the replica method. The developed disorder DF formalism is a non-local alternative to the existing cluster effective-medium theories beyond the local CPA level. In our approach, the nonlocal inter-site correlations are treated via diagrammatic perturbation theory of dual fermion system, and the CPA is recovered as a zero-order approximation for the DF potential. Our results for the single-particle Green function show that the disorder DF formalism provides significant corrections to the CPA results. Comparing our data with finite-cluster DCA results we find a rather good agreement. In particular, the disorder DF and DCA methods modify the CPA single-particle Green function in qualitatively the same fashion, and they both capture detailed structures in the local density of states. While in the DCA the multiple inter-site scattering effects are treated only within a finite cluster, our method allows one to treat spatial correlations on all length scales by summing a geometric series of dual fermion diagrams in the perturbation expansion.

Analysis of the two-particle quantities shows that our disorder DF formalism can successfully capture nonlocal vertex corrections, which are completely missed in the CPA scheme. Hence, the presented DF formalism is more appropriate for a proper description of transport in disordered electronic systems. In particular, we find that our method incorporates finite weak localization corrections from backscattering and spatial quantum coherence effects to the conductivity, the precursor effect of Anderson localization.

With all these findings, we believe that our DF disorder scheme is a promising tool for studying a wide variety of physical phenomena, including the interplay of weak localization effects and strong electron interactions, which may be treated on equal footing in our method. Work in this direction [17] and generalization to cluster cases[32] is in progress. As a possible candidate to replace CPA, its application to study non-local effects in electronic structure calculations is also envisioned.

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* Electronic address: terletska.hanna@gmail.com

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