Comparison of two-quantum-cluster approximations

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We provide microscopic diagrammatic derivations of the molecular coherent potential approximation (MCA) and dynamical cluster approximation (DCA) and show that both are Φ derivable. The MCA (DCA) maps the lattice onto a self-consistently embedded cluster with open (periodic) boundary conditions, and therefore violates (preserves) the translational symmetry of the original lattice. As a consequence of the boundary conditions, the MCA (DCA) converges slowly (quickly) with corrections $\mathcal{O}(1/L_c)$ $[\mathcal{O}(1/L_c^2)]$, where L_c is the linear size of the cluster. These analytical results are demonstrated numerically for the one-dimensional symmetric Falicov-Kimball model.

I. INTRODUCTION

One of the most active areas in condensed matter physics is the search for new methods to treat disordered and correlated systems. In these systems, especially in three dimensions or higher, approximations which neglect long ranged correlations are generally thought to provide a reasonable first approximation for many properties.

Perhaps the most successful of these methods are the coherent potential approximation[1] (CPA) and the dynamical mean-field approximation (DMFA),[2–5] for disordered and correlated systems, respectively. Although these approximations have different origins, they share a common microscopic definition. Both the DMFA (Ref. 3) and the CPA (Ref. 6) may be defined as theories which completely neglect momentum conservation at all internal diagrammatic vertices. When this principle is applied, the diagrammatic expansion for the irreducible quantities in each approximation collapse onto that of a self-consistently embedded impurity problem.

Many researchers have actively searched for a technique to restore nonlocal corrections to these approaches. Here, we discuss just two approaches which are fully causal and self-consistent: the molecular coherent potential approximation[7,8] (MCA) and the dynamical cluster approximation (DCA).[10–12,6] Recently the cellular dynamical mean-field approach[9] was proposed for ordered correlated systems, while the molecular coherent potential approximation has traditionally been applied to disordered systems. Since both methods share a common microscopic definition we use the term MCA to refer to both techniques in the following.

While the MCA is traditionally defined in the real space of the lattice, the DCA is traditionally defined in its reciprocal space. In the MCA, the system lattice is split into a series of identical molecules. Interactions between the molecules are treated in a mean-field approximation, while interactions within the molecule are explicitly accounted for. In the DCA, the reciprocal space of the lattice is split into cells, and momentum conservation is neglected for momentum transfers within each cell while it is (partially) conserved for transfers between the cells. These approximations share many features in common: they both map the lattice problem onto that of a self-consistently embedded cluster problem. Both recover the single site approximation (CPA or DMFA) when the cluster

size reduces to one and become exact as the cluster size diverges. Both are fully causal,[7,11] and provided that the clusters are chosen correctly,[6] they maintain the point group symmetry of the original lattice problem. Here, we provide a microscopic diagrammatic derivation of both the MCA and the DCA, and explore their convergence with increasing cluster size.

II. FORMALISM

For simple Hubbardlike models, momentum conservation at each vertex is completely described by the Laue function

$$\Delta = \sum_{\mathbf{x}} e^{i\mathbf{x}\cdot(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)} = N\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}, \qquad (1)$$

where $\mathbf{k}_1, \mathbf{k}_2$ ($\mathbf{k}_3, \mathbf{k}_4$) are the momenta entering (leaving) the vertex. Müller-Hartmann[3] showed that the DMF theory may be derived by completely ignoring momentum conservation at each internal vertex by setting $\Delta = 1$. Then, one may freely sum over all of the internal momentum labels, and the graphs for the generating functional Φ and its irreducible derivatives, contain only local propagators.

The DCA and MCA techniques may also be defined by their respective Laue functions. Since our object is to define cluster methods we divide the original lattice of N sites into N/N_c clusters (molecules), each composed of $N_c = L_c^D$ sites, where D is the dimensionality. We use the coordinate $\tilde{\mathbf{x}}$ to label the origin of the clusters and $\mathbf{X}$ to label the N_c sites within a cluster, so that the site indices of the original lattice $\mathbf{x} = \mathbf{X} + \tilde{\mathbf{x}}$. The points $\tilde{\mathbf{x}}$ form a lattice with a reciprocal space labeled by $\tilde{\mathbf{k}}$. The reciprocal space corresponding to the sites $\mathbf{X}$ within a cluster shall be labeled $\mathbf{K}$, with $K_\alpha = n_\alpha 2\pi/L_c$ and integer n_α. Then $\mathbf{k} = \mathbf{K} + \tilde{\mathbf{k}}$. Note that $e^{i\mathbf{K}\cdot\tilde{\mathbf{x}}} = 1$ since a component of $\tilde{\mathbf{x}}$ must take the form $m_\alpha L_c$ with integer m_α.

In the MCA, we approximate the Laue function by

$$\Delta_{MC} = \sum_{\mathbf{X}} e^{i\mathbf{X}\cdot(\mathbf{K}_1+\mathbf{K}_2-\mathbf{K}_3-\mathbf{K}_4+\tilde{\mathbf{k}}_1+\tilde{\mathbf{k}}_2-\tilde{\mathbf{k}}_3-\tilde{\mathbf{k}}_4)}. \qquad (2)$$

Thus the MCA omits the phase factors $e^{i\tilde{\mathbf{k}}\cdot\tilde{\mathbf{x}}}$ resulting from the position of the cluster in the original lattice but retains

the (far less important) phase factors $e^{i\tilde{\mathbf{k}}\cdot\mathbf{X}}$ associated with the position within a cluster. In the DCA we also omit the phase factors $e^{i\tilde{\mathbf{k}}\cdot\mathbf{X}}$, so that

$$\Delta_{DC} = N_c \delta_{\mathbf{K}_1+\mathbf{K}_2,\mathbf{K}_3+\mathbf{K}_4}. \tag{3}$$

Both the MCA and DCA Laue functions recover the exact result when $N_c \to \infty$ and the DMFA result, $\Delta=1$, when $N_c =1$.

If we apply the MCA Laue function Eq. (2) to diagrams in Φ, then each Green function leg is replaced by the MCA coarse-grained Green function

$$\bar{G}(\mathbf{X}_1,\mathbf{X}_2;\tilde{\mathbf{x}}=0)$$

$$=\frac{1}{N^2}\sum_{\substack{\mathbf{K}_1,\mathbf{K}_2 \\ \tilde{\mathbf{k}}_1,\tilde{\mathbf{k}}_2}} e^{i(\mathbf{K}_1+\tilde{\mathbf{k}}_1)\cdot\mathbf{X}_1} G(\mathbf{K}_1,\mathbf{K}_2;\tilde{\mathbf{k}}_1-\tilde{\mathbf{k}}_2) e^{-i(\mathbf{K}_2+\tilde{\mathbf{k}}_2)\cdot\mathbf{X}_2}$$

$$=\frac{N_c^2}{N^2}\sum_{\tilde{\mathbf{k}}_1,\tilde{\mathbf{k}}_2} G(\mathbf{X}_1,\mathbf{X}_2,\tilde{\mathbf{k}}_1-\tilde{\mathbf{k}}_2), \tag{4}$$

or in matrix notation for the cluster sites $\mathbf{X}_1$ and $\mathbf{X}_2$

$$\hat{\bar{G}} = \frac{N_c}{N}\sum_{\tilde{\mathbf{k}}} \hat{G}(\tilde{\mathbf{k}}). \tag{5}$$

(We have dropped the frequency dependence for notational convenience.) The summations of the cluster sites $\mathbf{X}$ remain to be performed. Note that the inclusion of the phase factors $e^{i\tilde{\mathbf{k}}\cdot\mathbf{X}}$ in the MCA Laue-function Eq. (2) leads directly to a cluster approach formulated in real space that violates translational invariance. Therefore the Green function is a function of two cluster momenta $\mathbf{K}_1,\mathbf{K}_2$ or two sites $\mathbf{X}_1,\mathbf{X}_2$, respectively.

If we apply the DCA Laue function Eq. (3), Green function legs in Φ are replaced by the DCA coarse grained Green function

$$\bar{G}(\mathbf{K}) = \frac{N_c}{N}\sum_{\tilde{\mathbf{k}}} G(\mathbf{K},\tilde{\mathbf{k}}), \tag{6}$$

since Green functions can be freely summed over the $\tilde{\mathbf{k}}$ vectors within a cell about the cluster momentum $\mathbf{K}$. As a result, Φ is a functional of the coarse grained Green function $\bar{G}(\mathbf{K})$ and thus depends on the cluster momenta $\mathbf{K}$ only.

To establish a connection between the cluster and the lattice we minimize the lattice free energy

$$F = -k_B T(\Phi_c - \text{tr}[\mathbf{\Sigma}\mathbf{G}] + \text{tr}\ln[\mathbf{G}]), \tag{7}$$

where Φ_c is the generating functional calculated with the coarse-grained propagators, $\mathbf{\Sigma}$ is the lattice self-energy, and $\mathbf{G}$ is the full lattice Green function. The trace indicates summation over frequency, momentum and spin. As we have discussed elsewhere, only the compact part of the free energy, Φ, is coarse grained. F is stationary with respect to $\mathbf{G}$ when $\delta F/\delta G=0$. This happens for the MCA if we estimate the lattice self energy as

$$\Sigma(\mathbf{K}_1,\mathbf{K}_2;\tilde{\mathbf{k}}_1-\tilde{\mathbf{k}}_2)$$

$$=\sum_{\mathbf{X}_1,\mathbf{X}_2} e^{-i(\mathbf{K}_1+\tilde{\mathbf{k}}_1)\cdot\mathbf{X}_1} \Sigma_{MC}(\mathbf{X}_1,\mathbf{X}_2) e^{i(\mathbf{K}_2+\tilde{\mathbf{k}}_2)\cdot\mathbf{X}_2}. \tag{8}$$

Thus the corresponding lattice single-particle propagator reads in matrix notation

$$\hat{G}(\tilde{\mathbf{k}},z) = [zI - \hat{\epsilon}(\tilde{\mathbf{k}}) - \hat{\Sigma}_{MC}(z)]^{-1}, \tag{9}$$

where the dispersion $\hat{\epsilon}(\tilde{\mathbf{k}})$ and self-energy $\hat{\Sigma}_{MC}(z)$ are matrices in cluster real space with

$$[\hat{\epsilon}(\tilde{\mathbf{k}})]_{\mathbf{X}_1\mathbf{X}_2} = \epsilon(\mathbf{X}_1-\mathbf{X}_2,\tilde{\mathbf{k}}) = \frac{1}{N_c}\sum_{\mathbf{K}} e^{i(\mathbf{K}+\tilde{\mathbf{k}})(\mathbf{X}1-\mathbf{X}2)} \epsilon_{\mathbf{K}+\tilde{\mathbf{k}}} \tag{10}$$

being the intracluster Fourier transform of the dispersion. For the DCA, $\Sigma(\mathbf{k}) = \Sigma_{DC}(\mathbf{K})$ is the proper approximation for the lattice self energy corresponding to Φ_{DC}. The corresponding lattice single-particle propagator is then given by

$$G(\mathbf{K},\tilde{\mathbf{k}};z) = \frac{1}{z-\epsilon_{\mathbf{K}+\tilde{\mathbf{k}}}-\Sigma_{DC}(\mathbf{K},z)}. \tag{11}$$

Both the MCA and DCA are optimized when we equate the lattice and cluster self energies. A similar relation holds for two-particle quantities. Thus with few exceptions,[13] only the irreducible quantities on the cluster and lattice correspond one-to-one.

The MCA (DCA) algorithm follows directly: We first make an initial guess for the cluster self-energy matrix Σ. This is used with Eqs. (5) and (9) [(6) and (11)] to calculate the coarse-grained Green function $\bar{G}$. The cluster excluded Green function $\hat{\mathcal{G}} = [\hat{\bar{G}}^{-1} + \hat{\Sigma}_{MC}]^{-1}$ ($\mathcal{G}(\mathbf{K}) = [\bar{G}(\mathbf{K})^{-1} + \Sigma_{DC}(\mathbf{K})]^{-1}$) is defined to avoid overcounting self-energy corrections on the cluster. It is used to compute a new estimate for the cluster self-energy which is used to reinitialize the process. Once convergence is reached, the irreducible quantities on the cluster may be used to calculate the corresponding lattice quantities.

In order to compare the character of the two different cluster approaches as a function of the cluster size N_c it is instructive to rewrite the corresponding coarse grained Green functions Eqs. (5) and (6) to suitable forms by making use of the independence of the self-energy Σ on the integration variable $\tilde{\mathbf{k}}$. For the MCA coarse grained Green function we find

$$\hat{\bar{G}}(z) = [zI - \hat{\epsilon}_o - \hat{\Sigma}_{MC}(z) - \hat{\Gamma}_{MC}(z)]^{-1}, \tag{12}$$

with the "cluster-local" energy $\hat{\epsilon}_o = N_c/N\sum_{\tilde{\mathbf{k}}}\hat{\epsilon}(\tilde{\mathbf{k}})$. For the DCA we obtain a similar expression

$$\bar{G}(\mathbf{K},z) = [z - \bar{\epsilon}_{\mathbf{K}} - \Sigma_{DC}(\mathbf{K},z) - \Gamma_{DC}(\mathbf{K},z)]^{-1}, \tag{13}$$

with the coarse grained average $\bar{\epsilon}_{\mathbf{K}} = N_c/N\Sigma_{\tilde{\mathbf{k}}}\epsilon(\mathbf{K},\tilde{\mathbf{k}})$. The hybridization functions $\hat{\Gamma}_{MC/DC}(z)$ describe the coupling of the cluster to the mean field representing the remainder of the system.

The behavior of Γ for large N_c is important. For the MCA, Γ averaged over the cluster and frequency

$$\bar{\Gamma}_{MC} = \frac{1}{N_c} \sum_{\mathbf{X}_1,\mathbf{X}_2} \Gamma_{MC}(\mathbf{X}_1,\mathbf{X}_2) \sim \mathcal{O}\left(\frac{2D}{L_c}\right), \qquad (14)$$

where $L_c = N_c^{1/D}$ is the linear cluster size. A detailed derivation of this form will be published elsewhere. However, since in the MCA the cluster is defined in real space with open boundary conditions, this form is evident since only the sites on the surface $\propto 2D \cdot L_c^{D-1}$ of the cluster couple to the effective medium. For the DCA we have previously shown[12] that $\Gamma(\mathbf{K}) \sim \mathcal{O}(1/N_c^{2/D})$ so that we obtain for the average hybridization of the DCA cluster to the effective medium

$$\bar{\Gamma}_{DC} = \frac{1}{N_c} \sum_{\mathbf{K}} \Gamma_{DC}(\mathbf{K}) \sim \mathcal{O}\left(\frac{1}{L_c^2}\right). \qquad (15)$$

The DCA coarse graining results in a cluster in $\mathbf{K}$ space; thus, the corresponding real space cluster has periodic boundary conditions, and each site in the cluster has the same hybridization strength $\bar{\Gamma}$ with the host.

In both the MCA and the DCA, the average hybridization strength acts as the small parameter. The approximation performed by the MCA (DCA) is to replace the lattice Green function $\hat{G}(\tilde{\mathbf{k}}) = [zI - \hat{\epsilon}(\tilde{\mathbf{k}}) - \hat{\Sigma}(\tilde{\mathbf{k}},z)]^{-1}$ $(G(\mathbf{K},\tilde{\mathbf{k}},z) = [z - \epsilon_{\mathbf{K}+\tilde{\mathbf{k}}} - \Sigma(\mathbf{K},\tilde{\mathbf{k}},z)]^{-1})$ by its coarse grained quantity $\hat{\bar{G}}$ $[\bar{G}(\mathbf{K})]$ in diagrams for the self-energy Σ. Once the sums over $\tilde{\mathbf{k}}$ are performed, all terms which are lower order in $1/L_c$ than Γ vanish. Thus the MCA (DCA) is an approximation with corrections of order $\bar{\Gamma} \sim \mathcal{O}(1/L_c)$ $(\sim \mathcal{O}(1/L_c^2))$.

III. NUMERICAL RESULTS

To illustrate the differences in convergence with cluster size N_c we performed MCA and DCA simulations for the symmetric one-dimensional (1D) Falicov-Kimball model (FKM). At half filling the FKM Hamiltonian reads as

$$H = -t\sum_i (d_i^\dagger d_{i+1} + \text{h.c.}) + U\sum_i (n_i^d - 1/2)(n_i^f - 1/2), \qquad (16)$$

with the number operators $n_i^d = d_i^\dagger d_i$ and $n_i^f = f_i^\dagger f_i$ and the Coulomb repulsion U between d and f electrons residing on the same site. The FKM can be considered as a simplified Hubbard model with only one spin-species (d) being allowed to hop. However it still shows a complex phase diagram including a Mott transition and Ising-like charge ordering with the corresponding transition temperature T_c being zero in one dimension (1D). The dispersion in (1D) $\epsilon_k = 2t\cos k$; thus for $t = 1/4$ the bandwidth $W = 1$ which we use as unit of
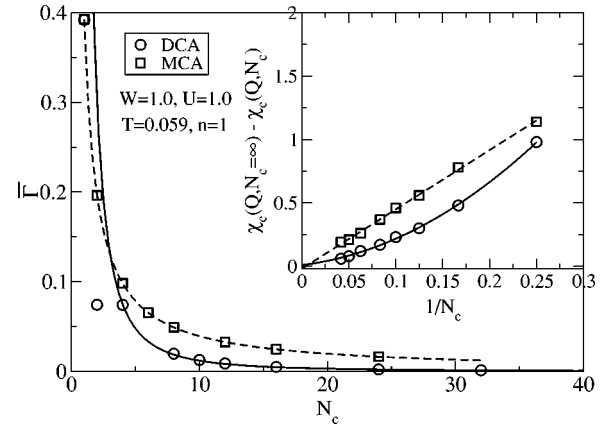

FIG. 1. The average integrated hybridization strengths $\bar{\Gamma}$ of the MCA (squares) and DCA (circles) versus the cluster size N_c when $\beta = 17$ and $U = W = 1$. The solid and dashed lines represent the fits $1.1946/N_c^2$ and $0.3361/N_c$, respectively. Inset: Convergence of the cluster charge susceptibility for $Q = \pi$. The solid and dashed lines are quadratic and linear fits, respectively.

energy. To simulate the effective cluster models of the MCA an the DCA we use a quantum Monte Carlo (QMC) approach described in Ref. 11.

To check the scaling relations, Eqs. (14) and 15, we show in Fig. 1 the average hybridization functions $\bar{\Gamma}_{MC}$ and $\bar{\Gamma}_{DC}$ for the MCA and DCA, respectively, at the inverse temperature $\beta = 17$ for $U = W = 1$. For $N_c = 1$ both approaches are equivalent to the DMFA and thus $\bar{\Gamma}_{MC} = \bar{\Gamma}_{DC}$. For increasing N_c, $\bar{\Gamma}_{MC}$ can be fitted by $0.3361/N_c$ and $\bar{\Gamma}_{DC}$ by $1.1946/N_c^2$ when $N_c > 2$. Cluster quantities, such as the self energy and cluster susceptibilities, are expected to converge with increasing N_c like $\bar{\Gamma}$. This is illustrated in the inset for the staggered ($Q = \pi$) charge susceptibility $\chi_c(\mathbf{Q})$ of the cluster.

Since only the compact parts represented by Φ of the lattice free energy [Eq. (7)] are coarse grained, this scaling is expected to break down when lattice quantities, such as the lattice charge susceptibility, are calculated. The susceptibility of the cluster $\chi_c(Q)$ cannot diverge for any finite N_c; whereas the lattice $\chi(Q)$ diverges at the transition temperature T_c to the charge ordered phase. Note that the residual mean field character of both methods can result in finite transition temperatures $T_c > 0$ for finite $N_c < \infty$. However as N_c increases, this residual mean field character decreases gradually and thus increased fluctuations should drive the solution to the exact result $T_c = 0$.

In the DCA (Ref. 11), $\chi(Q)$ is calculated by first extracting the corresponding vertex function from the cluster simulation. This is then used in a Bethe-Salpeter equation to calculate $\chi(Q)$. T_c is calculated by extrapolating $\chi(Q)^{-1}$ to zero using the function $\chi(Q)^{-1} \propto (T - T_c)^\gamma$ (see inset to Fig. 2). This procedure is difficult, if not impossible, in the MCA due to the lack of translational invarance. Here, we calculate the order parameter $m(T) = 1/N_c \Sigma_i (-1)^i \langle n_i^d \rangle$ in the symmetry broken phase. T_c is then obtained from extrapolating $m(T)$ to zero using the function $m(T) \propto (T_c - T)^\beta$. For the DCA this extrapolation is shown by the solid line in the
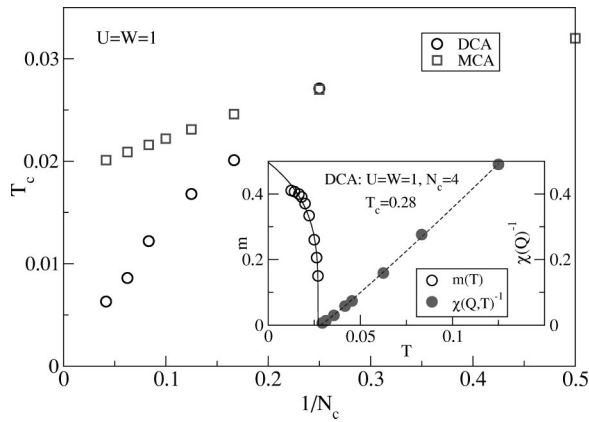
FIG. 2. The transition temperature T_c for the DCA (circles) and MCA (squares) when $U=W=1$ versus the cluster size N_c. For all values of N_c the DCA prediction is closer to the exact result ($T_c=0$). Inset: Order parameter $m(T)$ and inverse charge susceptibility $\chi(Q)^{-1}$ versus temperature. The solid (dashed) line represents a fit to the functions $m(T) \propto (T_c-T)^\beta$ with $\beta=0.245$ [$\chi(T) \propto (T-T_c)^{-\gamma}$ with $\gamma=1.07$].

inset to Fig. 2 for $N_c=4$. The values for T_c obtained from the calculation in the symmetry broken phase and in the unbroken phase must agree, since as we have shown above, both the DCA and MCA are Φ derivable. This is illustrated in Fig. 2 for the DCA.

A comparison of the DCA and MCA estimate of T_c is presented in Fig. 2. T_c obtained from MCA (squares) is larger than T_c obtained from DCA (circles). Moreover we find that the DCA result seems to scale to zero almost linearly in $1/N_c$ (for large enough N_c), whereas the MCA does not show any scaling form and, in fact, seems to tend to a finite value for T_c as $N_c \rightarrow \infty$. This striking difference of the two methods can be attributed to the different boundary conditions. The open boundary conditions of the MCA cluster result in a large surface contribution so that $\bar{\Gamma}_{MC} > \bar{\Gamma}_{DC}$. This engenders pronounced mean field behavior that stabilizes the finite temperature transition for the cluster sizes treated here. For larger clusters we expect the bulk contribution to the MCA free energy to dominate so that T_c should fall to zero.

Complementary results are found in simulations of *finite-sized* systems. In general, systems with open boundary conditions are expected to have a surface contribution in the free energy of order $\mathcal{O}(1/L_c)$.[14] This term is absent in systems with periodic boundary conditions. As a result, simulations of finite-sized systems with periodic boundary conditions converge much more quickly than those with open boundary conditions.[15]

IV. SUMMARY

By defining appropriate Laue functions, we provide microscopic diagrammatic derivations of the MCA and DCA. We show that they are Φ derivable, and that the lattice free energy is optimized by equating the irreducible quantities on the lattice to those on the cluster. The MCA maps the lattice to a cluster with open boundaries and consequently, the cluster violates translational invariance. In contrast, the DCA cluster has periodic boundary conditions, and therefore preserves the translational invariance of the lattice. This difference in the boundary conditions translates directly to different asymptotic behaviors for large clusters N_c. As we find analytically as well as numerically, the surface contributions in the MCA lead to an average hybridization $\bar{\Gamma}$ of the cluster to the mean field that scales like $1/L_c$ as compared to the $1/L_c^2$ scaling of the DCA. Since $\bar{\Gamma}$ acts as the small parameter for these approximation schemes, the DCA converges much more quickly than the MCA. These effects are more pronounced near a transition, where the large surface contribution of the MCA stabilizes the mean-field character of the transition. Consequently, the DCA result for the transition temperature T_c of the 1D symmetric FKM model scales almost like $1/N_c$ to the exact result $T_c=0$, whereas the MCA result converges very slowly. Since the origin of this difference lies in the different boundary conditions we expect this primacy of the DCA over the MCA to hold generally for any model of electrons moving on a lattice.

ACKNOWLEDGMENTS

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