Parametrized canonical transformation for the Hubbard model at arbitrary interaction strength

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The $t-J$ and Heisenberg models are truncated expansions of a canonically transformed Hubbard model coinciding with it at $U \to \infty$. We show that a modified canonical transformation applied to the Hubbard model leads to alternative models of similar form but whose convergence properties with respect to the expansion are more favorable, resulting in a good description of the half-filled ground state even at $0 < U \leq 1$. We investigate the transformed Hamiltonian and observables for metallic and insulating variational wave functions.

The Hubbard model[1–4] and its descendants have contributed greatly to our understanding of strongly correlated systems[5–7] and, in particular, the metal-insulator transition[5] (MIT) exhibited by these systems. Early attempts[4,8] to explain the MIT were based on the use of a projected wave function due to Gutzwiller (GW). An approximate variational calculation based on the Gutzwiller approximation (GA) (Ref. 4) for the GW in the general case predicts a MIT (Ref. 8) between a paramagnetic metal and an insulator (Brinkman-Rice transition). The order parameter for the Brinkman-Rice transition is the fraction of doubly occupied sites that goes to zero at the critical $U = U_c$. A shortcoming of the GA is that second-order hopping processes are not included, i.e., double occupations that arise as a result of second-order hoppings [which give rise to antiferromagnetic (AFM) coupling] are entirely absent. Thus the number of double occupations is not a valid order parameter for the actual MIT. In one dimension, the exact solution for the Hubbard model[9] indicates insulating behavior for all finite values of the interaction whereas the exact solution for the GW (Ref. 10) for the same system is always metallic.

The importance of higher-order hopping processes is made obvious by a canonical transformation of the Hubbard model, which eliminates those first-order hopping processes that increase (decrease) the number of doubly occupied sites $[H_t^+(H_t^-)]$.[11–16] Expansion and truncation of the transformed Hamiltonian leads to the well known $t-J$ and spin $-\frac{1}{2}$ antiferromagnetic Heisenberg models, which coincide with the Hubbard model in the strong-coupling limit in which it leads to antiferromagnetism.[15,17]

The effective Hamiltonians derived from the Hubbard model have other applications as well. In the resonating valence bond (RVB) method,[18–20] the expectation value of the $t-J$ Hamiltonian is evaluated over a fully Gutzwiller projected wave function.[3,4] The RVB wave function has recently been applied to the problem of high-temperature superconductivity and many experimentally observed features of the relevant materials have been reproduced.[20–22]

In the present study the unitary operator that transforms the Hubbard model into the $t-J$ or Heisenberg models is parametrized so that the number of double occupations, as a function of the transformation, can be minimized. The effect of our procedure is similar to that of the original transformation. The difference is that H_t^+ and H_t^- are not *canceled* from the Hamiltonian as in the standard case but instead *con-*

strained so that their expectation values are zero. In contrast, the $t-J$ and spin-$\frac{1}{2}$ Heisenberg models will, in general, give finite expectation values for H_t^+ and H_t^-. In our approach first-order double occupations are eliminated at the wave-function level as opposed to the operator (Hamiltonian) level. The optimized transformation can be applied at any value of the interaction and not only in the strongly interacting limit. We diagonalize the transformed Hamiltonians for systems of up to 12 lattice sites and it is shown that the optimized expansion converges much faster than the standard one. Convergence is also demonstrated for $U \leq 1$.

We also investigate the behavior of the optimally transformed double occupation operator using two different variational wave functions: the GW (Ref. 4) and Baeriswyl[23] (BW) wave functions, and compare them to the exact result.

The Hubbard model Hamiltonian can be written as

$$H = \overbrace{-t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma}}^{H_t} + \overbrace{UD}^{H_U},$$

(1)

where $D = \sum_i n_{i\uparrow} n_{i\downarrow}$ and where the operator $c_{i\sigma}^\dagger (c_{i\sigma})$ creates (destroys) a particle at site i with spin σ, and $n_{i\sigma}$ is the density operator at site i for particles of spin σ. In deriving the canonically transformed Hamiltonian, it is helpful to break up the kinetic-energy operator into terms consisting of different types of hoppings:[7]

$$H_t = H_t^+ + H_t^- + H_t^0,$$

(2)

where

$$H_t^+ = -t \sum_{\langle i,j \rangle \sigma} n_{i-\sigma} c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j-\sigma}),$$

$$H_t^0 = -t \sum_{\langle i,j \rangle \sigma} n_{i-\sigma} c_{i\sigma}^\dagger c_{j\sigma} n_{j-\sigma} - t \sum_{\langle i,j \rangle \sigma} (1 - n_{i-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j-\sigma}),$$

$$H_t^- = -t \sum_{\langle i,j \rangle \sigma} (1 - n_{i-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} n_{j-\sigma}.$$

(3)

$H_t^+(H_t^-)$ include only hopping processes that increase (decrease) the number of double occupations and H_t^0 includes only those that leave the number of double occupations unchanged. The Hermitian operator, defined as

$$S = -\frac{i}{U}(H_t^+ - H_t^-), \qquad (4)$$

is useful in defining the transformation

$$H_S = e^{iS}He^{-iS} = H + i[S,H] + \frac{i^2}{2}[S,[S,H]] + \dots. \qquad (5)$$

The series can be viewed as a power series in $\frac{t}{U}$. It can be shown that

$$i[S,H_U] = -(H_t^+ + H_t^-), \qquad (6)$$

and thus, up to first order, hoppings that change the number of double occupations are canceled from the transformed Hamiltonian [Eq. (5)]. The $t-J$ and Heisenberg models, which are used as effective models in the large U limit, can be derived by explicitly evaluating the terms of Eq. (5) up to second order in t/U,

$$H_S \approx H_t^0 + H_U + J\sum_{\langle i,j \rangle}\left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4}\right) + \text{three site terms}, \qquad (7)$$

where $J=4t^2/U$.

We now consider a similar transformed Hamiltonian derived using the modified operator $e^{i\alpha S}$, which leads to

$$H_{\alpha S} = e^{i\alpha S}He^{-i\alpha S} = H + i\alpha[S,H] + \frac{i^2\alpha^2}{2}[S,[S,H]] + \dots, \qquad (8)$$

where α is a parameter to be determined. If for a particular state the transformed number of double occupations,

$$\langle \Psi | D_{\alpha S} | \Psi \rangle = \langle \Psi | e^{i\alpha S}De^{-i\alpha S} | \Psi \rangle, \qquad (9)$$

is minimized as a function of α, then it holds that

$$\langle \Psi | e^{i\alpha S}[S,D]e^{-i\alpha S} | \Psi \rangle = 0, \qquad (10)$$

which with Eq. (6) is equivalent to

$$\langle \Psi | e^{i\alpha S}(H_t^+ + H_t^-)e^{-i\alpha S} | \Psi \rangle = 0. \qquad (11)$$

Thus, double occupations up to first order can be excluded via a transformation that sets the expectation value of the sum of the operators $H_t^+ + H_t^-$ to zero. The main difference between the Hamiltonians in Eqs. (5) and (8) is that in the latter the *expectation value* of the sum of the operators that change the number of double occupations is zero, as opposed to being canceled by another term equal but opposite in sign at the operator level.

If Φ is the ground state of the Hubbard Hamiltonian, then

$$\langle \Phi | H | \Phi \rangle = \langle \Phi_{\alpha S} | H_{\alpha S} | \Phi_{\alpha S} \rangle, \qquad (12)$$

where the transformed wave function $|\Phi_{\alpha S}\rangle = e^{i\alpha S}|\Phi\rangle$ is the ground state of the transformed Hamiltonian $H_{\alpha S}$. While the optimization procedure can be carried out on any state, in the rest of this work we deal exclusively with the ground state at half filling.

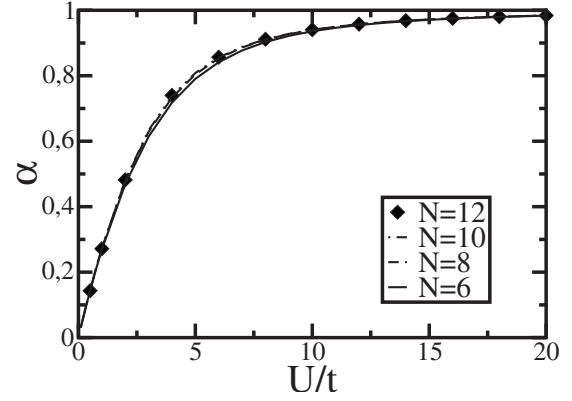The analogous derivation that leads to the $t-J$ model leads in this case [Eq. (8)] to

FIG. 1. Optimal α as a function of U for systems with different sizes.

$$H_{\alpha S} \approx H_t^0 + H_U + J_{\alpha S}\sum_{\langle i,j \rangle}\left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4}\right) + \text{three site terms}, \qquad (13)$$

where $J_{\alpha S}$ denotes a modified coupling constant satisfying

$$J_{\alpha S} = (2\alpha - \alpha^2)J. \qquad (14)$$

The first-order term in α originates from the transformed H_t^+ and H_t^-.

The size of the parameter α determines the convergence of the expansion [Eq. (8)]. In Fig. 1 the results of power-method type calculations[24] are shown for systems of various sizes at half filling. Antiperiodic (periodic) boundary conditions were applied for system sizes with odd (even) multiples of two.[25,26] The parameter α, which minimizes Eq. (9) [and satisfies Eqs. (10) and (11)] and is closest to the origin, is calculated as a function of the interaction parameter U. We find that convergence is achieved for all U considered. As expected, H_S is recovered for large U. The size dependence of α is negligible. Interestingly, as U approaches 0, α/U converges to a finite value of ~ 0.3, whereas in the standard case this ratio diverges.

In Table I we compare energies calculated using the standard transformation [Eq. (5)] and those resulting from the transformation with optimized α [Eq. (8) and Fig. 1]. The optimal value of α was obtained from exact diagonalization. In these calculations periodic boundary conditions were used. Subsequently, α was used in the expansion [Eq. (8)]. In order to investigate the convergence, the expansion of the Hamiltonian was carried out to second, fourth, and sixth orders in α, and then diagonalized. The optimized transformation gives energies closer to the exact result in all cases and the convergence is also better when the expansion of the Hamiltonian is carried out to higher orders. The advantage is more pronounced at lower values of U; in particular our transformation is even applicable for $U \leq 1$ where the standard expansion fails due to slow convergence. The second-order results with optimal α (similar to the $t-J$ model) are in considerably better agreement with the exact results than the standard ($\alpha=1$) second-order ones; therefore the $t-J$ model

TABLE I. Comparison of ground-state energies calculated for a lattice composed of six sites. The upper (lower) half shows results for the transformed Hamiltonian with $\alpha=1$ (optimized α). The rightmost column shows the exact results. The expansion is in the parameter α.

Hamiltonian	U	second order	fourth order	sixth order	Exact
$e^{iS}He^{-iS}$	0.5	−395.505	−4613.096	−35947.499	−7.275
	1.0	−99.211	−270.19	−495.743	−6.601
	2.0	−24.713	−10.3987	−7.6983	−5.409
	5.0	−4.557	−2.974	−3.092	−3.088
	10.0	−1.824	−1.661	−1.664	−1.664
$e^{i\alpha S}He^{-i\alpha S}$	0.5	−11.084	−6.695	−7.328	−7.275
	1.0	−9.850	−6.159	−6.634	−6.601
	2.0	−7.742	−5.158	−5.421	−5.409
	5.0	−3.819	−3.047	−3.088	−3.088
	10.0	−1.792	−1.662	−1.664	−1.664

is, in this sense, applicable even at $U \leq 1$ but with a modified coupling.

In Fig. 2 the expectation value of the transformed inter-action energy is shown. The expansion is carried out to second and sixth orders (inset) for $\alpha=1$ and for optimized α, i.e. the Hamiltonian is calculated up to a given order, and diagonalized. The observable is also transformed and truncated at the given order. Optimized α gives quantitative agreement for the whole range of U shown, whereas the standard ($\alpha=1$) gives agreement only for large U for both second and sixth order expansions.

The $t-J$ type model derived herein is not as easy to derive as the standard one. At a particular U the normal $t-J$ model can easily be derived to any order. Our modified model depends on a parameter, α, which is a function of the ground-state solution. For a particular U one can obtain α by expanding the transformed Hamiltonian [Eq. (8)], solving for its ground state, and varying α to satisfy the condition in Eq. (10). It also appears possible to apply our formalism using the generalized version of the canonical transformation of Ref. 16.
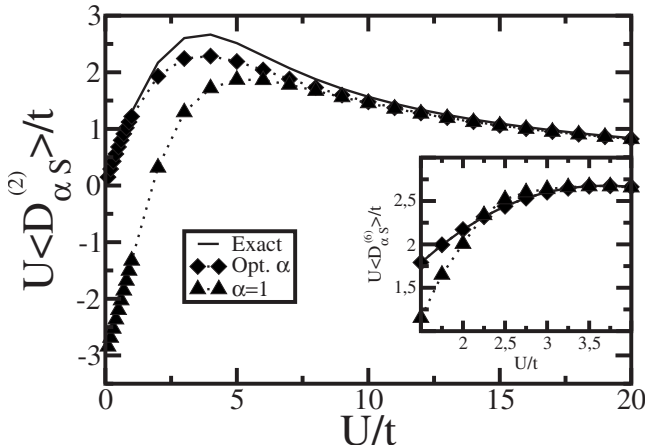
We have also investigated our scheme for different variational wave functions. For our studies we have chosen the BW and GW wave functions. The properties of these wave functions are well known. In particular it has been shown by Millis and Coppersmith[27] that the Drude weight of the GW is always finite in the thermodynamic limit; hence the GW is metallic. This property can be attributed to the lack of explicit phase dependence of the GW. The BW has been shown to consist of rotating dipoles formed of empty and doubly occupied sites, and to be in general an insulating wave function.[28]

In Fig. 3 we present a comparison of the ratio

$$\Omega = \frac{\langle\Psi|D_{\alpha S}|\Psi\rangle}{\langle\Psi|D|\Psi\rangle} \qquad (15)$$

for systems with different sizes calculated exactly. As U increases, Ω decreases sharply. The inset of Fig. 3 shows a comparison for the system of size 12 between the exact result, and two variational wave functions BW and GW. An interesting feature is that in the large U limit, the GW tends

FIG. 2. Ground state expectation value of the transformed inter-action $U\langle D_{\alpha S}\rangle/t$ for the standard expansion and the optimized one compared to the exact results for a model with six sites. The transformed $D_{\alpha S}$ was expanded to second order in α in the main plot and sixth order in the inset.
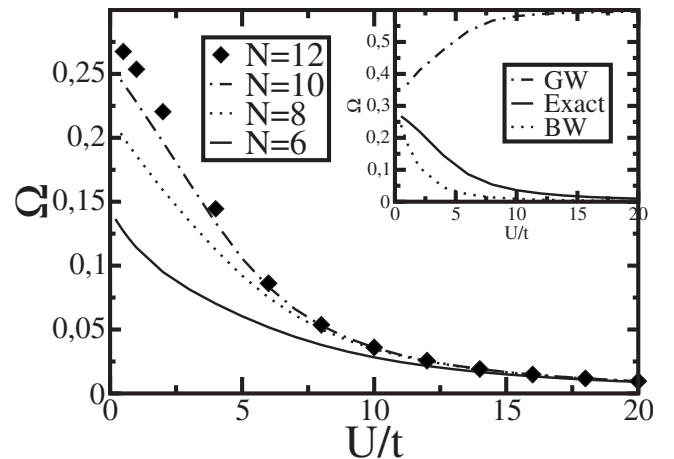

FIG. 3. Ratio Ω [defined in Eq. (15)], calculated exactly for different system sizes. The inset shows a comparison between the exact result and two different variational wave functions (BW and GW) for the system with 12 lattice sites.
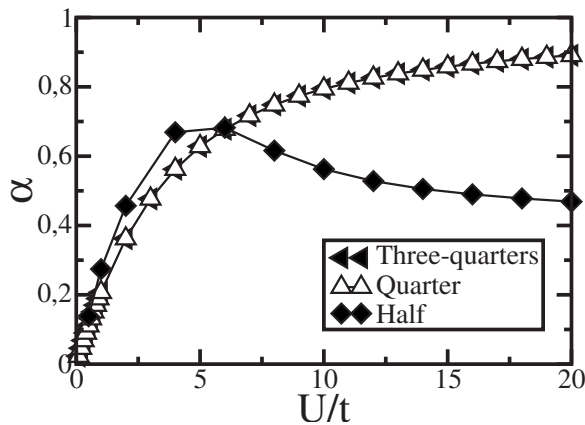
FIG. 4. Optimal α as a function of U for the Gutzwiller wave function with 12 sites for different fillings.

to a finite value unlike the exact or the BW result. These qualitative tendencies persist away from half filling (results not shown). Hence the GW tending to a finite limit is not due to metallicity.

In Fig. 4 we show the optimum α at three different fillings for the GW. At half filling, the behavior is qualitatively different from the other fillings investigated and different from the behavior found for the exact case (Fig. 1). At large U α appears to be bounded below for half filling, where GW is expected to be in error since it is a metallic wave function. Away from half filling, the α obtained from GW is monotonically increasing. We have also investigated the BW and found the qualitative tendencies (monotonic increase, upper bound of $\alpha=1$) to be the same as for the exact calculation.

In conclusion we have shown that the standard canonical transformation, which when applied to the Hubbard model gives the $t-J$ model at large interaction strength, can be optimized to give a $t-J$-like model applicable for the whole range of the interaction strength. In particular convergence of the expanded Hamiltonian is achieved for interaction strength close to zero where the standard transformation leads to slow convergence.

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