Parametrized canonical transformation for the Hubbard-model at arbitrary interaction strength

Balázs Hetényi and Hans Gerd Evertz

Institut für Theoretische Physik, TU Graz, 8010 Graz, Austria

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 favourable, 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.

PACS numbers: 71.10.Fd,71.30+h

The Hubbard model [1,2,3,4] and its descendants have contributed greatly to our understanding of strongly correlated systems [5,6,7] and in particular the metal-insulator transition (MIT) exhibited by these systems. Early attempts [4,8] to explain the MIT were based on the use of a projected wavefunction due to Gutzwiller (GW). An approximate variational calculation based on the Gutzwiller approximation (GA) [4] for the GW in the general case predicts a MIT [8] between a paramagnetic metal and an insulator (Brinkman-Rice transition). The order parameter for the Brinkman-Rice transition is the density operator at site $i$, which is the number of double occupations that arise as a result of second-order hoppings (which give rise to anti-ferromagnetic (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 [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 that eliminates those first-order hopping processes which increase(decrease) the number of doubly occupied sites ($H_i^\dagger (H_i^-)$) [11,12,13,14,15,16]. Expansion and truncation of the transformed Hamiltonian leads to the well-known $t-J$ (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 wavefunctions the Gutzwiller [4] (GW) and Baeriswyl [22] (BW) wavefunctions and compare them to the exact result.

The Hubbard model Hamiltonian can be written as

$$ H = -t \sum_{(i,j)\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U D $$

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 $\sigma$, and $n_{i\sigma}$ is the density operator at site $i$ for particles of spin $\sigma$. 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]:

$$ H_t = H_i^\dagger + H_i^- + H_i^0, $$

The effective Hamiltonians derived from the resonating valence bond (RVB) method [18,19,20] the expectation value of the $t-J$ Hamiltonian is evaluated over a fully Gutzwiller projected wavefunction [3,4]. The RVB wavefunction has recently been applied to the problem of high temperature superconductivity, and many experimentally observed features of the relevant materials have been reproduced. [20,21,22]
where
\[ H_t^+ = -t \sum_{\langle i,j \rangle} n_{i-\sigma} c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j-\sigma}) \]  
\[ H_t^0 = -t \sum_{\langle i,j \rangle} n_{i-\sigma} c_{i\sigma}^\dagger c_{j\sigma} n_{j-\sigma} \]
\[ -t \sum_{\langle i,j \rangle} (1 - n_{i-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} (1 - n_{j-\sigma}) \]
\[ H_t^- = -t \sum_{\langle i,j \rangle} (1 - n_{i-\sigma}) c_{i\sigma}^\dagger c_{j\sigma} n_{j-\sigma}. \]

\( H_t^+ (H_t^-) \) include only hopping processes which increase(decrease) the number of double occupations, and \( H_t^0 \) includes only those which leave the number of double occupations unchanged. The Hermitian operator defined as
\[ S = -\frac{i}{U}(H_t^+ - H_t^-) \]  
(4)
is useful in defining the transformation
\[ H_S = e^{iS} H e^{-iS} = H + i[S, H] + \frac{i^2}{2} [S, [S, H]] + ... \]  
(5)
The series can be viewed as a power series in \( \frac{t}{U} \). It can be shown that
\[ i[S, H_U] = -(H_t^+ + H_t^-), \]  
(6)
and thus, up to first order, hoppings that change the number of double occupations are cancelled 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 \( t/U \),
\[ H_S \approx H_t^0 + H_U + J \sum_{\langle i,j \rangle} (S_i \cdot S_j - \frac{n_{i\sigma} n_{j\sigma}}{4}) \]  
(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
\[ H_{\alpha S} = e^{i\alpha S} H e^{-i\alpha S} \]
\[ = H + i\alpha [S, H] + \frac{i^2 \alpha^2}{2} [S, [S, H]] + ..., \]  
(8)
where \( \alpha \) is a parameter to be determined. If for a particular state the transformed number of double occupations
\[ \langle \Psi | D_{\alpha S} | \Psi \rangle = \langle \Psi | e^{i\alpha S} D e^{-i\alpha S} | \Psi \rangle, \]  
(9)
is minimized as a function of \( \alpha \), then it holds that
\[ \langle \Psi | e^{i\alpha S} [S, D] e^{-i\alpha S} | \Psi \rangle = 0, \]  
(10)
which with Eq. (8) is equivalent to
\[ \langle \Psi | e^{i\alpha S} (H_t^+ + H_t^-) e^{-i\alpha S} | \Psi \rangle = 0. \]  
(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 Eq. (5) and Eq. (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 cancelled by another term equal but opposite in sign at the operator level.

If \( \Phi \) is the ground state of the Hubbard Hamiltonian, then
\[ \langle \Phi | H | \Phi \rangle = \langle \Phi_{\alpha S} | H_{\alpha S} | \Phi_{\alpha S} \rangle, \]  
(12)
where the transformed wavefunction \( | \Phi_{\alpha S} \rangle = e^{i\alpha S} | \Phi \rangle \) 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 analog derivation that leads to the \( t - J \) model...
applied to Eq. (8) results in
\[ H_{aS} = H_0^t + H_U + J_{aS} \sum_{\langle i,j \rangle} (S_i \cdot S_j - \frac{n_{ij}}{4}) \] (13)
+ 3-site terms,

where \( J_{aS} \) denotes a modified coupling constant satisfying

\[ J_{aS} = (2\alpha - \alpha^2) J. \] (14)

The first-order term in \( \alpha \) originates from the transformed \( H_0^p \) and \( H_0^-- \).

The size of the parameter \( \alpha \) 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. Anti-periodic(periodic) boundary conditions were applied for system sizes with odd(even) multiples of two \( ^{27,28} \).

The parameter \( \alpha \) 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 \( \alpha \) is negligible. Interestingly, as \( U \) approaches zero \( \alpha/U \) converges to \( \approx 0.3 \), whereas in the standard case \( 1/U \) diverges.

![FIG. 2: Ground state expectation value of the transformed interaction energy](image)

In Table 1 we compare energies calculated using the standard transformation (Eq. (5)), and those resulting from the transformation with optimized \( \alpha \) (Eq. (8) and Fig. 1). The optimal value of \( \alpha \) was obtained from exact diagonalization. In these calculations periodic boundary conditions were used. Subsequently, \( \alpha \) was used in the expansion, Eq. (5). In order to investigate the convergence, the expansion of the Hamiltonian was carried out to second, fourth, and sixth orders in \( \alpha \), 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 \( \alpha \) (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 is, in this sense, applicable even at \( U \leq 1 \), but with a modified coupling.

![FIG. 3: Ratio \( \Omega \) (defined in Eq. (15)) calculated exactly for different system sizes. Inset shows a comparison between the exact result and two different variational wavefunctions (Baeriswyl (BW) and Gutzwiller (GW)) for the system with 12 lattice sites.](image)

In Fig. 2 the expectation value of the transformed interaction energy is shown. The expansion is carried out to second and sixth order (inset) for \( \alpha = 1 \) and for optimized \( \alpha \), 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 \( \alpha \) gives quantitative agreement with the exact result even at second order (\( t-J \) like model), whereas the standard version is not in agreement with the exact results at second order, and even when the expansion is carried out to sixth order, agreement is only reached when \( U \) is large.

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, \( \alpha \), which is a function of the ground state solution. For a particular \( U \) one can obtain \( \alpha \) by expanding the transformed Hamiltonian (Eq. (5)), solving for its ground state, and varying \( \alpha \) 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 wavefunctions. For our studies we have chosen...
the Baeriswyl and Gutzwiller wavefunctions (BW and GW respectively). The properties of these wavefunctions are well-known. In particular it has been shown by Millis and Coppersmith [24] 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 wavefunction [25].

In Fig. 3 we present a comparison of the ratio

$$\Omega = \frac{\langle \Psi | D_{\alpha S} | \Psi \rangle}{\langle \Psi | D | \Psi \rangle}$$

(15)

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

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.

Beneficial discussions with E. Arrigoni and W. von der Linden are gratefully acknowledged.

[1] J. Hubbard, Proc. Roy. Soc. A276 238 (1963).
[2] J. Kanamori, Prog. Theoret. Phys. 30 275 (1963).
[3] M. C. Gutzwiller, Phys. Rev. Lett. 20 1445 (1963).
[4] M. C. Gutzwiller, Phys. Rev. 137 A1726 (1965).
[5] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. 70 1039 (1998).
[6] A. Auerbach, Interacting Electrons and Quantum Magnetism, Springer (1998).
[7] P. Fazekas, Lecture Notes on Electron Correlation and Magnetism, World Scientific (1999).
[8] W. F. Brinkman and T. M. Rice, Phys. Rev. B, 2 4302 (1970).
[9] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett., 20 1445 (1968).
[10] W. Metzner and D. Vollhardt, Phys. Rev. Lett., 59 121 (1987).
[11] W. Kohn, Phys. Rev., 133 A171 (1964).
[12] A. B. Harris and R. V. Lange, Phys. Rev. 157 295 (1967).
[13] V. J. Emery, Phys. Rev. B, 14 1989 (1976).
[14] K. A. Chao, J. Spaëk, and A. M. Oles, Phys. Rev. B 18 3453 (1978).
[15] C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B, 36 381 (1987).
[16] A. H. MacDonald, S. M. Girvin, and D. Yoshioka, Phys. Rev. B, 37 9753 (1988).
[17] D. J. Scalapino, Handbook of High-Temperature Superconductivity, Eds. J. R. Schrieffer and J. S. Brooks, Springer, (2007). (arXiv:cond-mat/0610710v1)
[18] P. W. Anderson, Mater. Res. Bull., 8 153 (1973).
[19] P. Fazekas and P. W. Anderson, Philos. Mag., 30 432 (1974).
[20] P. W. Anderson, P. A. Lee, M. Randeria, T. M. Rice, N. Trivedi, and F. C. Zhang J. Phys. Cond. Mat., 16 R75 (2004).
[21] A. Paramekanti, M. Randeria, and N. Trivedi, Phys. Rev. Lett., 87 217002 (2001).
[22] B. Edegger, V. N. Muthukumar, C. Gros, and P. W. Anderson, Phys. Rev. Lett., 96 207002 (2006).
[23] D. Baeriswyl in Nonlinearity in Condensed Matter, Ed. A. R. Bishop, D. K. Campbell, D. Kumar, and S. E. Trullinger, Springer-Verlag (1986).
[24] A. J. Millis and S. N. Coppersmith, Phys. Rev. B, 43 13770 (1991).
[25] D. Baeriswyl, Found. Physics, 30 2033 (2000).
[26] B. Hetényi, H. G. Evertz, and W. von der Linden, in preparation.
[27] C. A. Stafford, A. J. Millis and B. S. Shastry, Phys. Rev. B, 43 13660 (1991).
[28] R. M. Fye, M. J. Martins, D. J. Scalapino, J. Wagner, and W. Hanke, Phys. Rev. B, 44 6909 (1991).