

Coupled-cluster method applied to the motion of a single hole in a Hubbard antiferromagnet

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(Received 15 July 1993)

The coupled-cluster method has recently proved to be efficient in calculating the ground state of strongly interacting spins or fermions on lattices. We apply it to the ground state of one hole in the half-filled Hubbard model on a two-dimensional square lattice. In a wide range for the interaction $10 \lesssim U/t \lesssim 80$, the ground-state energy of a hole is fitted by a simple function $\epsilon/t \approx -3.40 + 8.9(t/U)^{0.70}$, in good agreement with the results obtained through exact diagonalizations on small clusters. The effective mass of a hole $m^* = 8t/W$ (W represents the bandwidth) is proportional to U/t ($m^* \approx 0.845U/t$) for $5 \lesssim U/t \lesssim 20$ and saturates to a constant value $m^* \approx 84$ for large U/t .

I. INTRODUCTION

Over the last two decades, the coupled-cluster method (CCM) has met with great success in calculating ground-state energies for a variety of strongly interacting systems from quantum chemistry to condensed matter physics.¹ It has more recently been extended to strongly interacting spins or fermions on lattices.²⁻⁴

The CCM generally starts with a ground state of independent particles $|0\rangle$ (usually from a mean field or Hartree-Fock theory) and develops a better approximation of the form $|\Psi\rangle = \exp(S)|0\rangle$. The correlation operator $S = S_2 + S_3 + S_4 \dots$ consists of two-body, three-body, four-body, ..., raising operators, and $|\Psi\rangle$ converges to the exact result as more terms are included in S .⁵

In the so-called "SUB- n " coupled-cluster approximation, S is generally truncated at the S_n level.¹ For the lattice problem, more efficient approximation schemes have been proposed.^{2,3} These are utilized in the following.

II. CCM APPLIED TO THE HALF-FILLED HUBBARD HAMILTONIAN

We consider the one-band Hubbard Hamiltonian on a square lattice:

$$H = t \sum_{i,j,\alpha} a_{i\alpha}^\dagger a_{j\alpha} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (2.1)$$

The $a_{i\alpha}^\dagger$ ($a_{i\alpha}$) create (destroy) a fermion of spin α on site i , and $n_{i\alpha} = a_{i\alpha}^\dagger a_{i\alpha}$. The first sum is restricted to nearest neighbors. In the half-filled case, this Hamiltonian reduces at large U to an effective antiferromagnetic Heisenberg Hamiltonian acting on the subspace of singly occupied sites.⁶ Let us start from the two-sublattice Néel state with one fermion per site:

$$|0\rangle = |\uparrow, \downarrow, \uparrow, \downarrow, \dots\rangle, \quad (2.2)$$

where spins \uparrow are on sublattice A and spins \downarrow on sublattice B . It is convenient to perform successively (i) a

rotation of the spin axes of π on sublattice B and (ii) an electron-hole transformation for the fermions with spins \uparrow in the new local spin axes. In that way, $|0\rangle$ appears now as the vacuum state for the new fermion operators defined as $c_{i\uparrow}^\dagger = a_{i\uparrow}^\dagger$, $c_{i\uparrow} = a_{i\uparrow}$, $c_{i\downarrow}^\dagger = a_{i\downarrow}^\dagger$, $c_{i\downarrow} = a_{i\downarrow}$ for the sublattice A and $c_{j\uparrow}^\dagger = a_{j\downarrow}^\dagger$, $c_{j\uparrow} = a_{j\downarrow}$, $c_{j\downarrow}^\dagger = a_{j\uparrow}^\dagger$, $c_{j\downarrow} = a_{j\uparrow}$ for the sublattice B . In terms of these new operators, the Hamiltonian is

$$H = t \sum_{i,j} (c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger + c_{i\uparrow} c_{j\downarrow}) + U \sum_i c_{i\uparrow} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\downarrow}. \quad (2.3)$$

Provided that $|0\rangle$ is not orthogonal to the ground state $|\Psi\rangle$, we can write $|\Psi\rangle = \exp(S)|0\rangle$.⁵ The Schrödinger equation is

$$H \exp(S)|0\rangle = E_0 \exp(S)|0\rangle, \quad (2.4)$$

i.e.,

$$\tilde{H}|0\rangle = E_0|0\rangle \quad \text{with} \quad \tilde{H} = \exp(-S)H\exp(S). \quad (2.5)$$

Using the property $\tilde{A}\tilde{B} = \tilde{A}\tilde{B}$ we obtain \tilde{H} from the elementary transformations

$$\tilde{c}_{i\alpha} = c_{i\alpha} + [c_{i\alpha}, S] \quad \text{and} \quad \tilde{c}_{i\alpha}^\dagger = c_{i\alpha}^\dagger, \quad (2.6)$$

where $[A, B] = AB - BA$ is the usual commutator.

After moving all annihilation operators to the right, we obtain

$$\tilde{H}|0\rangle = \mathcal{C}|0\rangle, \quad (2.7)$$

where the operator \mathcal{C} contains exclusively creation operators.

At the lowest level we only retain in S the terms

$$S^{(1)} = \alpha \sum_{i,j} c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger \quad (i, j \text{ first neighbors}) \quad (2.8)$$

from the kinetic part of the Hamiltonian, which create a double occupancy leaving one neighboring site empty.

After simple algebra, we obtain

$$\begin{aligned}
 C = 4\alpha Nt &+ [t(1 - 9\alpha^2) + \alpha U] \sum_{i,j}^{(1)} c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger \\
 &- 3\alpha^2 t \sum_{i,j}^{(4)} c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger - \alpha^2 t \sum_{i,j}^{(6)} c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger \\
 &- \alpha^2 U \sum_{i,k,l} c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{k\uparrow}^\dagger. \quad (2.9)
 \end{aligned}$$

The three first sums are restricted respectively to pairs of first, fourth, and sixth neighbors. The last sum is restricted to triplets such that k and l (possibly equal) are first neighbors of i .

The parameter α introduced in S is obtained by setting the second term to zero. The constant term $E_0 = 4\alpha Nt$ gives the energy $E_0/N = \frac{2}{9}[U - (U^2 + 36t^2)^{1/2}]$, which is identical to the Hartree-Fock (HF) approximation in the large U limit. The last three terms cannot be set to zero. Hence we now reintroduce in S the terms necessary to cancel these remaining terms. This gives a scheme for successive approximations. There are five new terms to introduce in S at the next level, and the algebra is a little more tedious; the parameters introduced in S are a solution of a coupled system of six nonlinear equations.² At large U , the most important among these new terms is that which exchange first-neighbor spins: $\sum_{i,j} c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger$; the others are of higher order in t/U .² Hence let us simply take here

$$S^{(2)} = \alpha \sum_{i,j} c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger + \frac{1}{2} \chi_E \sum_{i,j} c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger, \quad (2.10)$$

with (i, j) first neighbors. After straightforward algebra, we obtain

$$\begin{aligned}
 C = 4\alpha Nt &+ [t(1 - 9\alpha^2 + \chi_E) + \alpha U] \sum_{i,j} c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger \\
 &- [8\chi_E \alpha t + \alpha^2 U] \sum_{i,j} c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger + \dots \quad (2.11)
 \end{aligned}$$

Setting the coefficients of the first and second sum to zero gives α and χ_E as a solution of a second order equation. The constant term provides a simple but reliable approximation of the energy

$$E_0/N = \frac{2}{9} \left\{ 7U/8 - \left[(7U/8)^2 + 36t^2 \right]^{1/2} \right\}, \quad (2.12)$$

which for U larger than the bandwidth $8t$ is only $\approx 2\%$ above the best estimates through quantum Monte Carlo (QMC) calculations⁷⁻⁹ (see Fig. 1). Since, in that range, the HF approximation is roughly 10% higher, we conclude that this simple χ_E terms takes $\approx 80\%$ of the correlation energy into account. We shall stay at this elementary step in the following.

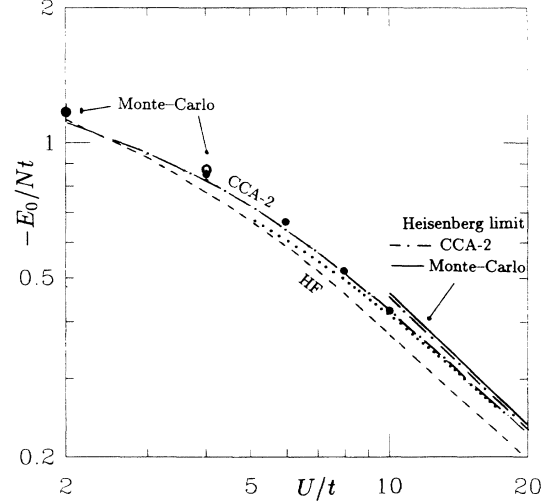


FIG. 1. Ground-state energy for the half-filled Hubbard model. The simple approximation corresponding to Eq. (2.12) (dotted curve) is compared to the more accurate “CCA-2” approximation of Ref. 2 (dash-dotted curve), the Hartree-Fock approximation (dashed curve), and quantum Monte Carlo calculations from Refs. 7 (\circ) and 8 (\bullet). The straight lines indicate the Heisenberg limit [solid line, QMC (Ref. 9); dash-dotted line, leading term in t/U of Eq. (2.12)].

III. THE SINGLE-HOLE PROBLEM

In contrast to this approach, most of the works on this subject have focused not on the Hubbard Hamiltonian [Eq. (2.1)] but on its large U effective limit: the “ t - t' - J ” (Ref. 6) model, often reduced to the “ t - J ” or “ t - J_z ” part. In the t - J_z model which only takes into account the Ising part of the antiferromagnetic Heisenberg interaction between first neighbors, a hole is localized. Starting from a Néel state, a hole after n nearest-neighbor hops leaves n spins overturned and $2n + 1$ frustrated J_z links that correspond to a “string” potential. Its ground-state energy behaves as^{10,11}

$$\epsilon/t \approx -2\sqrt{3} + 6.90(t/U)^{2/3}. \quad (3.1)$$

Trugman¹² has pointed out that if a hole travels around a plaquette one and a half times it unwinds the string and find itself translated to a next-nearest-neighbor site with the background spins undisturbed. Nevertheless such intricate paths lead to a high effective mass.

In a t - J model, the $J\sigma_i^+ \sigma_j^-$ terms can flip two neighboring spins and restore the original antiferromagnetic order after two vacancy hops. In a t - t' - J model the t' terms induce direct hops of the hole to the second or third neighbors. Since $t' = J = t/U$, both effects contribute at t/U to the bandwidth and vanish for $U \rightarrow \infty$. In both t - J and t - t' - J models, the fluctuations of the ground state with respect to the Néel state can also contribute to the coherent motion of the hole. The CCM offers a simple picture for this effect since the χ_E terms introduced in S flip two neighboring spins and can also restore the correct antiferromagnetic order after two hops.

This contribution does not vanish at large U .

In the presence of one hole, the wave function is written

$$|\Psi\rangle_L = T \exp(S)|0\rangle = \exp(S)T|0\rangle, \quad (3.2)$$

where T represents some quasiparticle operator associated with one vacancy. Since T contains exclusively creation operators, it commutes with $\exp(S)$. The Schrödinger equation is

$$\tilde{H}T|0\rangle = (E_0 + \epsilon)T|0\rangle. \quad (3.3)$$

The left hand side can be split into two parts:

$$\mathcal{L}|0\rangle = \left\{ -\alpha\gamma^2(\mathbf{k}) \sum_i a_i^\dagger \exp(i\mathbf{k} \cdot \mathbf{R}_i) + \sum_\tau [\alpha U + \chi_E \gamma(\mathbf{k}) \exp(i\mathbf{k} \cdot \boldsymbol{\tau})] a_{i\downarrow}^\dagger a_{i\uparrow}^\dagger a_{i+\tau,\uparrow}^\dagger \exp(i\mathbf{k} \cdot \mathbf{R}_i) \right\} |0\rangle, \quad (3.7)$$

with $\gamma(\mathbf{k}) = \sum_\tau \exp(i\mathbf{k} \cdot \boldsymbol{\tau})$; $\tau \in \{\pm\mathbf{x}, \pm\mathbf{y}\}$ joins two nearest neighbors. The prefactor of the first sum gives the zeroth order approximation for the energy of one hole. The second sum cannot be set to zero. It represents nearest-neighbor hops of the vacancy. At the next level, to cancel these terms, we take

$$T_1 = \sum_i \left(a_{i\uparrow}^\dagger + \sum_\tau u_\tau a_{i\downarrow}^\dagger a_{i\uparrow}^\dagger a_{i+\tau,\uparrow}^\dagger \exp(i\mathbf{k} \cdot \mathbf{R}_i) \right). \quad (3.8)$$

From Eq. (3.5), the u_τ appear as a solution of a linear eigensystem with lowest eigenvalue ϵ_1 , representing the ground-state energy of a hole.

The most important terms to reintroduce in T at the next step to cancel the remaining terms are those describing two successive nearest-neighbor hops of the vacancy:

$$T_2 = \sum_{\tau, \tau' \neq -\tau} w_{\tau, \tau'} a_{i\downarrow}^\dagger a_{i\uparrow}^\dagger a_{i+\tau,\downarrow}^\dagger a_{i+\tau,\uparrow}^\dagger a_{i+\tau+\tau',\uparrow}^\dagger \exp(i\mathbf{k} \cdot \mathbf{R}_i) + T_1. \quad (3.9)$$

We shall neglect other more intricate terms which are of higher order in t/U or appear with various phases and are expected to cancel partly. For the same reasons, at the step T_3 , we shall only add terms corresponding to three successive hops, etc. In that way, the successive approximations $T_1|0\rangle, T_2|0\rangle, T_3|0\rangle \dots$, with one, two, three, ... hops strictly correspond to the states retained by Trugman.¹² However, these states are improved here by the $\exp(S)$ operator which through the χ_E terms takes into account the most important part of the quantum fluctuations. In the infinite U limit, if we set χ_E to zero, our formalism is strictly equivalent to Trugman's. The construction of the operators T_1, T_2, T_3, \dots is similar to that proposed, within a more general framework, by Dagotto and Schrieffer to describe the behavior of quasiparticles in the t - J model.¹³

These quasiparticle operators lead to an accurate description of the single-hole wave function, which is completely different from that proposed by Lo *et al.*¹⁴ through a more intricate coupled-cluster approximation scheme.

Figure 2 represents the minimum energies $\epsilon_1, \epsilon_2, \epsilon_3$, corresponding to T_1, T_2, T_3 . For any U , the minimum occurs at $\mathbf{k} = (\pi/2, \pi/2)$ and the maximum at $\mathbf{k} = (0, 0)$.

$$\tilde{H}T|0\rangle = CT|0\rangle + \mathcal{L}|0\rangle, \quad (3.4)$$

where \mathcal{C} represents the terms obtained in the half-filled case [Eq. (2.7)], with $CT|0\rangle = TC|0\rangle = E_0T|0\rangle$. We thus have to solve

$$\mathcal{L}|0\rangle = \epsilon T|0\rangle. \quad (3.5)$$

Let us take a simple Bloch wave as a first approximation for T :

$$T_0 = \sum_i a_{i\uparrow}^\dagger \exp(i\mathbf{k} \cdot \mathbf{R}_i). \quad (3.6)$$

We obtain

In the infinite U limit, and setting $\chi_E = 0$ the results are identical to those obtained through the first moments of order 2,4,6 within the retraceable path approximation, if we neglect the “one and a half cycle” of Trugman. In that case Heritier¹⁵ has shown that a linear extrapolation of $1/\epsilon_n^2$ as a function of $1/(2n-1)$ is relevant. Although there is no theoretical support for that with finite U and $\chi_E \neq 0$ the points representing $1/\epsilon_n^2$ as a function of $1/(2n-1)$ remain approximatively aligned (cf. inset). For every U , we deduced from such plots the extrapolated dotted line. As shown in Fig. 3, this extrapolated energy can be fit in a wide range $10 < U/t < 80$ through a simple function

$$\epsilon/t = \epsilon_\infty/t + \delta(t/U)^\nu, \quad (3.10)$$

with $\epsilon = -3.40$, $\delta = 8.9$, and $\nu = 0.70$, in good agreement with results obtained for the t - J model, through exact diagonalization and finite-size scaling on small clusters up to 26 sites.^{16,17} Comparing with Eq. (3.1), we confirm by a completely different approach the idea that the “string scenario” keeps some relevance for the Hubbard Hamiltonian in spite of the strong quantum fluctuations.

The effective mass defined from the inverse bandwidth,

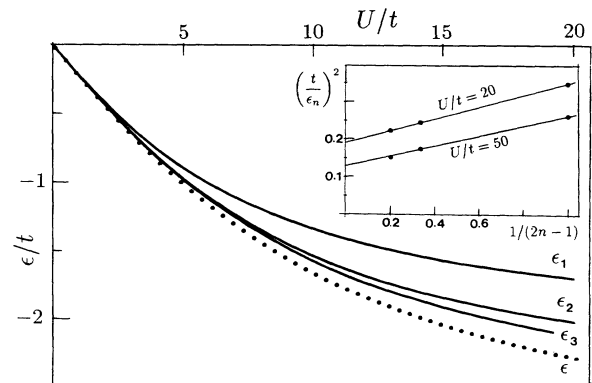


FIG. 2. Successive approximations of the minimum energy at $\mathbf{k} = (\pi/2, \pi/2)$ of one hole, with one, two, and three hops (solid curves). The extrapolation (dotted line) is obtained as shown in the inset.

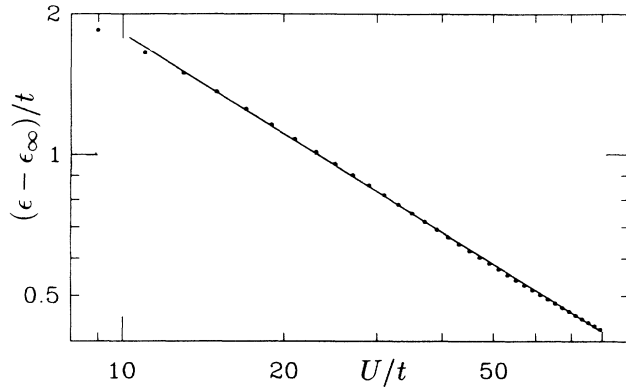


FIG. 3. Log-log plot of the extrapolated energy (dotted line of Fig. 2). A linear fit to $\ln[(\epsilon - \epsilon_\infty)/t]$ as a function of $\ln(U/t)$ is made. The value $\epsilon_\infty = -3.40$ is then adjusted to minimize the mean-square deviation.

$m^* = 8t/W$ with $W = \epsilon_{\mathbf{k}=(\pi/2, \pi/2)} - \epsilon_{\mathbf{k}=(0,0)}$, and obtained with T_3 (three hops) is represented in Fig. 4. In the range $5 < U/t < 20$, it is roughly proportional to U/t : $m^* \approx 0.845U/t$ in agreement with Refs. 11, 16, and 18. In the "string picture," the mean excursion of the hole is $l = 1.9(4t/U)^{1/2}$, giving $l < 3$ for $U < 16$. Hence we expect our approximation with three hops to be quite accurate in that range.

For $U \rightarrow \infty$, the effective mass saturates to a constant value m_∞^* . The quantum fluctuations around the Néel state (χ_E terms) have an important contribution to this limit. At the successive steps T_1, T_2, T_3 , we obtain respectively $m_\infty^* = 12.8, 23.3, 84.0$. Such a drastic increase has two origins: (i) The χ_E terms contribute essentially to the coherent motion to next-nearest neighbors. More complex paths included in T_2, T_3 decrease their relative weight. (ii) At the last step T_3 , the "one and a half cycle" around a plaquette contributes to the

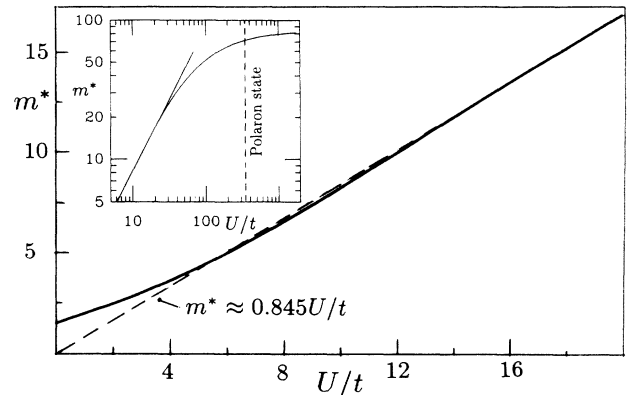


FIG. 4. Effective mass of a hole.

bandwidth. However, this contribution gives a minimum energy at $\mathbf{k} = (0, 0)$,¹² whereas the χ_E terms give a maximum at $\mathbf{k} = (0, 0)$. Since the effect of the χ_E term is more important, the global minimum energy remains at $\mathbf{k} = (\pi/2, \pi/2)$; however, both effects partly cancel and the effective mass is enhanced. We should go further in our approximation scheme to conclude definitively. However, we can say that the asymptotic value m_∞ is high and it is reached for values of U/t which are beyond the transition to the polaron regime $U/t \approx 350$ (Ref. 16) (see inset of Fig. 4).

The same approach has been applied to the two-vacancy problem. No binding has been observed over the whole range of U . The details will be reported elsewhere.

ACKNOWLEDGMENTS

We thank S. Perrier (student from Ecole Polytechnique) for an important contribution to the preliminaries of this work during a stay at Saclay.

* Also at Ecole Polytechnique, 91128 Palaiseau Cedex, France.

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