Exact calculation of the two-electron interaction in the ground state of the Hubbard model

Liang Chen*
Department of Physics, University of Southern California, Los Angeles, California 90089-0484

Changjiang Mei†
Max-Planck-Institut für Festerkörperforschung, 7000 Stuttgart 80, Federal Republic of Germany
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The single-band Hubbard model has been studied in both the one-dimensional ring and two-dimensional torus. By the exact calculation of the pair correlation function $F(i,j)$ defined as the possibility of finding an electron at site j when there has been an electron at site i, it is shown that for two electrons, the interaction is always repulsive in the ground state for any positive value of the on-site Coulomb interaction U.

INTRODUCTION

Since the discovery of the high-T_c ceramic copper-oxide superconducting materials[1] there has been a great theoretical interest in the Hubbard model[2] which may provide a new mechanism for such phenomena. Up until now there has been much work[3-6] in this area. However, those calculations of correlation function of the full Hubbard model have been limited to small lattice sizes of the order of fifteen in one-dimension[4] (1D) and order 8×8 in 2D.[6] The finite-size effect, as is pointed out by Stollhoff,[7] calls for even larger size calculations to allow the true nature of the Hubbard model to be understood. Furthermore, as most of the calculations are either done in the large- or small-U limit, it is desirable to have an exact calculation for the whole range of U.

In this work we have been able to derive an exact formula for the ground state of two electrons in both one-dimensional Hubbard ring and two-dimensional Hubbard torus. Therefore, we can do the calculation for all on-site interactions U, and generally any size of lattice. Thus, the finite size effect is eliminated in our treatment. Here we will first discuss the formulation and then present the results. Finally, we will draw some conclusions.

FORMULATIONS

The single-band Hubbard Hamiltonian is written as

$$H=-t\left(\sum_{\langle i,j\rangle,\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.}\right)+U\sum_i n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

where $c_{i\sigma}^{\dagger}$, $c_{i\sigma}$, and $n_{i\sigma}$ are the creation, annihilation, and number operators, respectively, for an electron of spin σ in the Wannier state on the ith lattice site. $\langle i,j\rangle$ means that only nearest-neighbor site hoppings are allowed. One can easily show that the total spin and its z component commute with the Hamiltonian. Therefore, we can diagonalize the Hamiltonian simultaneously with the total spin S and S_z. In the following we will concentrate on the two-electron problem within the Hubbard Hamiltonian.

To give a brief illustration of our treatment, let us solve a simple two-site problem for the two-electron case. One can see that there is a total of six states: $|1\uparrow,1\downarrow\rangle$, $|2\uparrow,2\downarrow\rangle$, $|1\uparrow,2\uparrow\rangle$, $|1\downarrow,2\downarrow\rangle$, $|1\uparrow,2\downarrow\rangle$, $|1\downarrow,2\uparrow\rangle$. It is easy to show that the ground state is

$$|\psi_G\rangle=\frac{1}{2}\left[\frac{\sqrt{U^2+16t^2}-U}{\sqrt{U^2+16t^2}}\right]^{1/2}\{|1\uparrow,1\downarrow\rangle+|2\uparrow,2\downarrow\rangle\}$$
$$+\frac{1}{2}\left[\frac{\sqrt{U^2+16t^2}+U}{\sqrt{U^2+16t^2}}\right]^{1/2}\{|1\uparrow,2\downarrow\rangle-|1\downarrow,2\uparrow\rangle\}\,, \tag{2}$$

and the ground-state energy is

$$E_G=-\tfrac{1}{2}(\sqrt{U^2+16t^2}-U)\,. \tag{3}$$

The other energy eigenvalues are 0, U, $\frac{1}{2}(\sqrt{U^2+16t^2}+U)$. It may be seen that the ground state is a spin singlet. This is the most important feature in the construction of our correlated ground-state wave functions shown below.

One-dimensional ring

From the exact solution (2) of the two-site problem, we know that the ground state of the two-electron system is a spin singlet. Unlike the Gutzwiller ansatz, we write the correlated ground-state wave function in the form[8]

$$|\psi\rangle=\sum_{i\neq j}\chi(i,j)\{|i\uparrow,j\downarrow\rangle-|i\downarrow,j\uparrow\rangle\}$$
$$+\sum_i\chi(i,i)\,|i\uparrow,i\downarrow\rangle\,. \tag{4}$$

Here $|i\uparrow,j\downarrow\rangle$ means that one electron on lattice site i with spin up and the other electron on lattice site j with spin down. The $\chi(i,j)$ are variational parameters. Owing to the symmetry of the ring structure, it is obvious that $\chi(i,j)$ should be a function of $|i-j|$ only. From the statement above we can rewrite the wave function (4) as

$$|\psi\rangle=\sum_{l=0}^{k}x_l\,|\psi_l\rangle\,,\quad k=N/2 \text{ or } (N-1)/2\,, \tag{4'}$$

where

$$|\psi_0\rangle = \sum_{i=1}^{N} |i\uparrow, i\downarrow\rangle , \tag{5}$$

$$|\psi_l\rangle = \sum_{|i-j|=l} \{|i\uparrow, j\downarrow\rangle - |i\downarrow, j\uparrow\rangle\} , \tag{6}$$

and N is the number of lattice sites of the ring. We call $|\psi_l\rangle$ the state class l which consists of all the singlet states comprising two electrons separated by a distance of l units.

Let us treat the even lattice-site ring $N=2k$ $(k \geq 2)$ explicitly. First, all states are sorted in classes according to the separations. One can see that there is a total of $k+1$ classes of states with separations $l=0,1,\ldots,k$ units. All classes, except the one that is k units apart, have N singlet states in each. Whereas the remaining one includes $N/2$ singlet states. Therefore, we obtain

$$\langle\psi|\psi\rangle = N\left[x_0^2 + 2\sum_{l=1}^{k} x_l^2 - x_k^2\right], \quad N=2k . \tag{7}$$

After some algebra one obtains

$$\langle\psi|H|\psi\rangle = -8t\times N\left[\sum_{i=0}^{k-1} x_i x_{i+1}\right] + U\times N x_0^2 . \tag{8}$$

Then we have the variational ground-state energy expression

$$E_g = -4t\frac{2\sum_{i=0}^{k-1} x_i x_{i+1} - (U/4t)x_0^2}{x_0^2 + 2\sum_{i=1}^{k} x_i^2 - x_k^2}, \quad N=2k , \quad k \geq 2 . \tag{9}$$

By minimizing the expression (9) with respect to all the x_i's the ground-state energy can be obtained. From the known ground-state results of x_i's, the pair correlation function (PCF) can be obtained which is proportional to x_i^2.

Two-dimensional torus

In general, by considering the periodic boundary condition, the $M\times N$ square lattice will form a torus of $M\times N$ sites. Here we only treat the case of $M=N=2k-1$ explicitly. The clue which allows the treatment of $M=N=2k$ can be found in Ref. 8.

Let us take $k=6$ (i.e., 11×11 torus) as an example. As the first step, we have to classify the structure of the correlated ground-state wave function as we did in Eq. (4′). To do this, all states are sorted to classes according to the separations. The classification is shown in Fig. 1(a). Only unique ways of separations are shown, which are a total of $k(k+1)/2=21$. All different states can be obtained from states shown by considering periodic boundary conditions and translation invariance. In Fig. 1(a), numbers label different classes. For example, the number "0" stands for the class of singlet states of which the two electrons are on the same lattice site; while the number "2" represents the class of singlet states of which two electrons stay at diago-

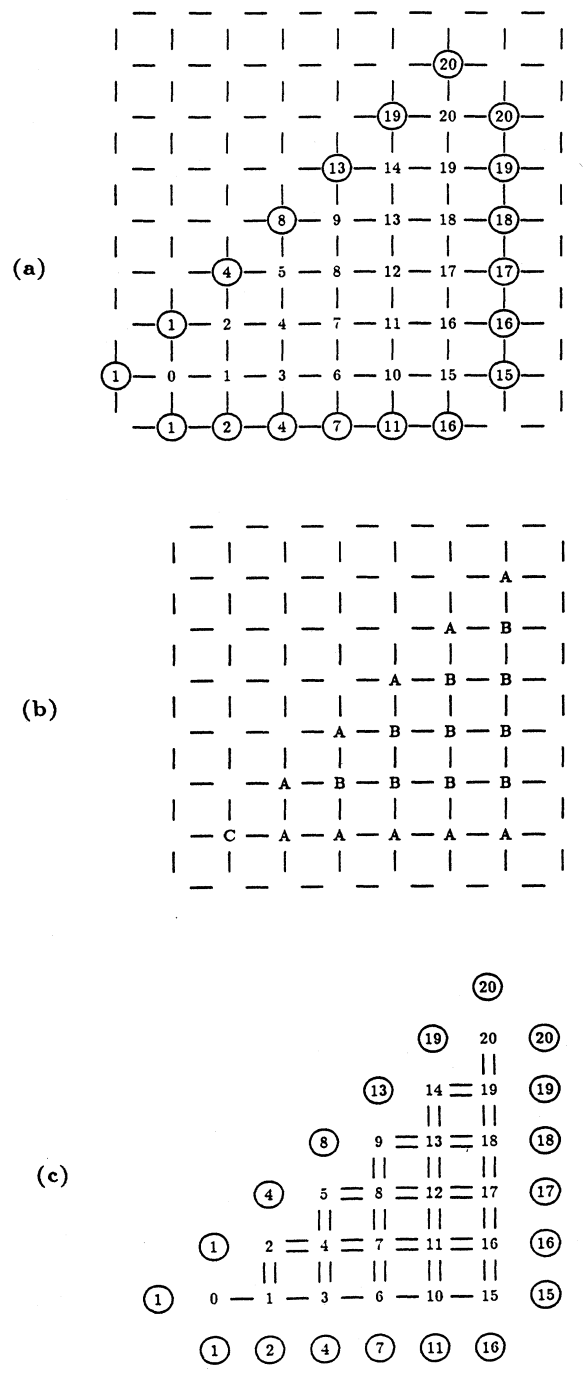

FIG. 1. (a) State classification for 11×11 square lattice in which one of the electrons stays at the origin (the point labeled "0"), and the other electron can be on any one of the numbered sites. The numbers are labels for different classes of singlet paired states. (b) According to the number of singlet states within each class, all classes are sorted into three different groups. Each class belonging to group A has $2\times(2k-1)^2$ singlet states, group B has $4(2k-1)^2$, and group C has $(2k-1)^2$. (c) The diagram for constructing function $F[x_i]$. Neighboring states, between which hoppings can occur, are connected either by double lines (= or ||) or by single line (− or |), according to the multiplicity of the hopping term, as described in the text.

nal lattice sites of the smallest square, etc. Therefore, we can write down the correlated ground-state wave function as

$$|\psi\rangle = \sum_{l=0}^{k(k+1)/2-1} x_l |\psi_l\rangle, \quad (2k-1)(2k-1), \quad \text{torus } k \geq 2. \quad (10)$$

Next we should find out how many different singlet states there are within each class, which can be computed by considering the symmetry of separation patterns and the corresponding multiplicities. The results are shown in Fig. 1(b) of which group A has $2(2k-1)^2$ states, group B has $4(2k-1)^2$ states, and group C has $(2k-1)^2$ states. By knowing the structure of the correlated ground-state wave function, it is then easy to obtain

$$\langle\psi|\psi\rangle = (2k-1)^2 G[x_i], \quad (11)$$

[refer to Fig. 1(b)]

$$G[x_i] = 4\sum_{i\in A} x_i^2 + 8\sum_{j\in B} x_j^2 + x_h^2 \in C, \quad (12)$$

and

$$\langle\psi|H|\psi = -(2k-1)^2 16tF[x_i] + (2k-1)^2 U x_0^2, \quad (13)$$

where [refer to Fig. 1(c) and Ref. 8]

$$F[x_i] = 2\sum_{i \text{ and } j \text{ connected by } =} x_i x_j - \tfrac{1}{2} x_{k^2(k-1)/2}^2 + \sum_{i \text{ and } j \text{ connected by } -} x_i x_j + \sum_{l=k(k-1)/2}^{[k(k+1)-2]/2} x_l^2. \quad (14)$$

Finally, we achieve the E_g for the $(2k-1)(2k-1)$ square lattice on the torus

$$E_g = -16t\frac{F[x_i] - (U/16t)x_0^2}{G[x_i]}. \quad (15)$$

RESULTS

Before we present the calculated results, it is interesting to discuss some of the limiting cases. First, in the case of $U=0$, one would expect that all the x_i's are the same. Indeed, this is what we have found. Second, in the case of $U=\infty$, i.e., the strongest correlation limit, one would expect there are some differences between 1D ring and 2D torus. In fact in the case of 1D, and under the open boundary condition, there is no way to exchange the positions of the two electrons. This makes the spin degrees of freedom irrelevant, i.e., in the 1D open end chain, the problem will be the same as that of the spinless fermion. On the other hand, if there are only two electrons in a ring, one *can* find a way of exchanging the positions between them, so one would expect that there will be a difference between open and periodic boundary conditions. However, once we put more than two electrons in the ring, all electrons become ordered in the $U=\infty$ limit, and their relative positions cannot exchange arbitrarily. Some spin degrees of freedom are lost. Making use of this fact, the arbitrarily filled 1D Hubbard model can be solved with the Bethe ansatz.[9,10] As soon as we go to the 2D case, the Bethe ansatz does not work any more because these restrictions do not apply. With our method, the two-electron problem can be solved in any dimension. We will demonstrate that the nature of the correlation within the Hubbard model depends on dimension.

Let us first discuss the 1D case. The minimization of Eq. (9) can be done for arbitrary size. To save computing time, it was carried out for a 80-site ring. Figure 2 shows the PCF and total energy of the ground state as a function of U. It has been calculated[8] that in the infinite-U limit, the total energy given by the Gutzwiller ansatz is $-4t(1-1/N)$, while that given by the correlated ground state in the large-U limit asymptotically is $-4t(1-5/N^2)$. So there is a significant deviation of the Gutzwiller ansatz for the kinetic energy in this limit. The PCF shows an even more dramatic change as a function of U, as being shown by Figs. 2(a)–2(f).

One can see from Fig. 2 that the PCF shows almost no changes for $U/4t > 1$, i.e., the "kink" at the center of the graph disappears. Therefore, one may safely treat the 1D Hubbard model as spinless fermion, i.e., as $U=\infty$, when $U/4t > 1$. However, one should be rather cautious when one performs the perturbation around an intermediate value of U ($0 < U/4t < 1$).

A similar calculation was carried out for the 2D lattice. Figure 3 shows the result for a 30×30 lattice on a torus. One can clearly see that as U increases the two electrons prefer to stay as far apart as possible, evidently it means that the effective interaction between them is repulsive. It is found also that the total energy given by Gutzwiller ansatz is $-8t(1-1/N^2)$, and that given by correlated ground state is $-8t(1-\alpha/N^2)$. Here $N\times N$ is the lattice size. α is found also N dependent, and is 0.618 for a 30×30 lattice, 0.631 for a 50×50 lattice, and 0.682 for a 100×100 lattice. So the result of Gutzwiller ansatz is only quantitatively wrong in the 2D contrary to its qualitatively wrong result in 1D before. It is worth noticing that despite the fact that there is only the on-site Coulomb repulsion U in the model, the PCF clearly shows that electrons feel a long-range repulsion through correlation effects. Again, from Fig. 3, one can see that PCF has very slight changes after $U/4t > 10$, i.e., it is a good approximation to treat the system as if $U=\infty$. However, in the range of physical interest (as in the case of a high-T_c material, where U/t is about 10), it is better to be cautious in using the infinite-U approximation. Of real importance is the difference between 1D and 2D in fluctuations. First, the on-site fluctuation in 2D is much larger than that in 1D, i.e., while no sizable double occupation occurs in 1D $U/4t > 1$, here it is found up to $U/4t \sim 10$. Second, for two electrons to come close, the probability is not as much reduced in 2D as in 1D. It is shown in Figs. 2(f) and 3(f) that the nearest-neighbor occupation in 1D drops off in a way similar to what the double occupation does, while it keeps a relatively larger value in 2D. This point can be easily seen from the asymptotic behavior of the correlation functions. The 1D correlation function varies like $1-\cos\alpha_1 r$, while in 2D, it behaves like $1-e^{-\alpha_2 r}$.

Finally, just for the completeness of the model itself, we have done a calculation for negative U for both 1D and 2D

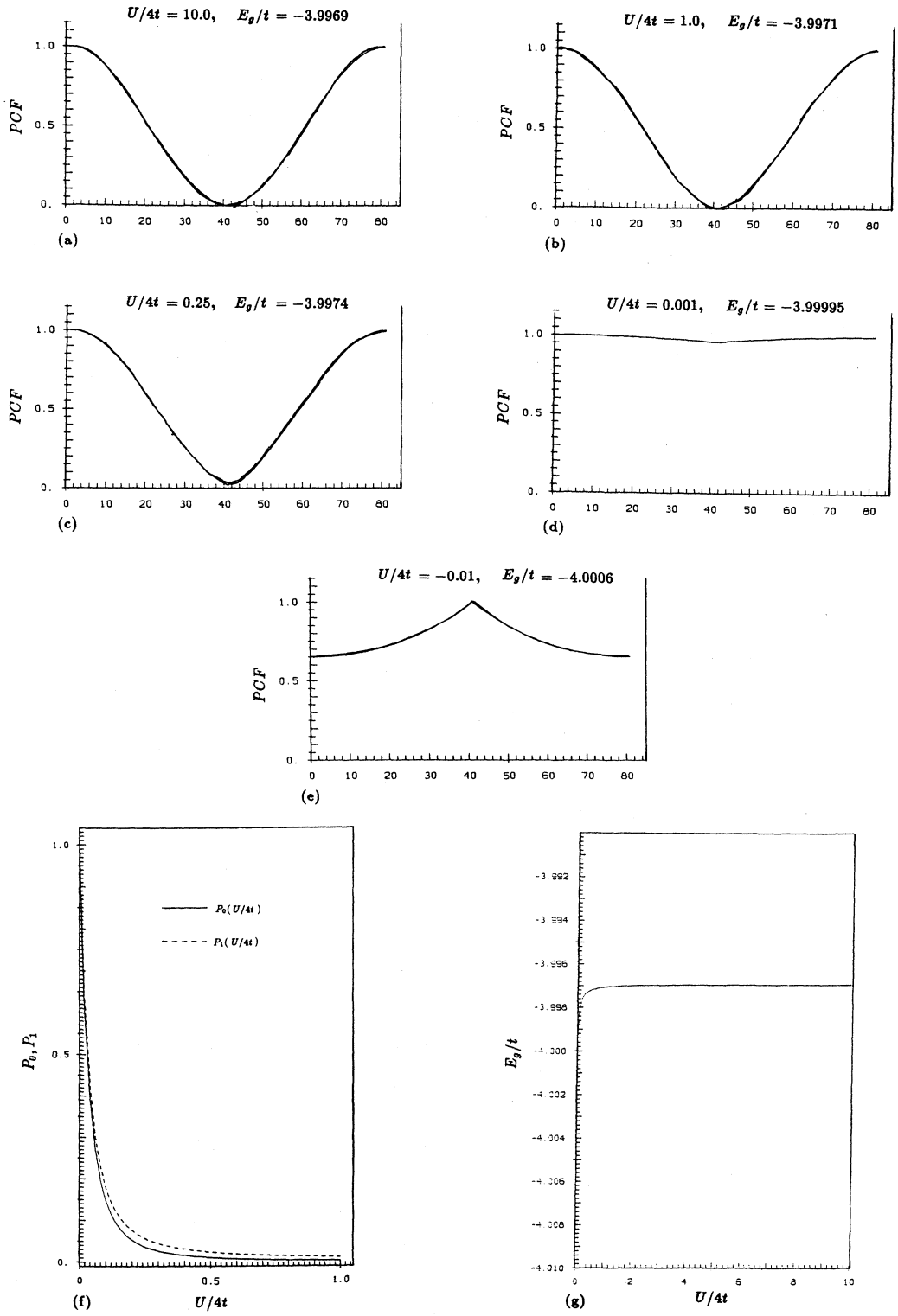

FIG. 2. (a)–(e) The 1D pair correlation functions (PCF's) for the 80 lattice ring as a function of $U/4t$, with $U/4t$ 10.0, 1.0, 0.25, 0.001, and -0.01, respectively. Here the PCF is defined as the possibility of finding an electron on a different site when one electron is supposed to be fixed at the middle, i.e., on site No. 41. The horizontal coordinate is the site label, and the vertical coordinate is the PCF. Their maximum value has been normalized to 1. (f) The double occupancy P_0 and nearest-neighbor occupancy P_1 as a function of $U/4t$, which have been defined as the possibility of two electrons on the same site or two electrons on nearest-neighbor sites, respectively. The $P_0(U=0)$ and $P_1(U=0)$ have been normalized to 1. (g) The total energy E_g/t of the correlated ground state as a function of $U/4t$.

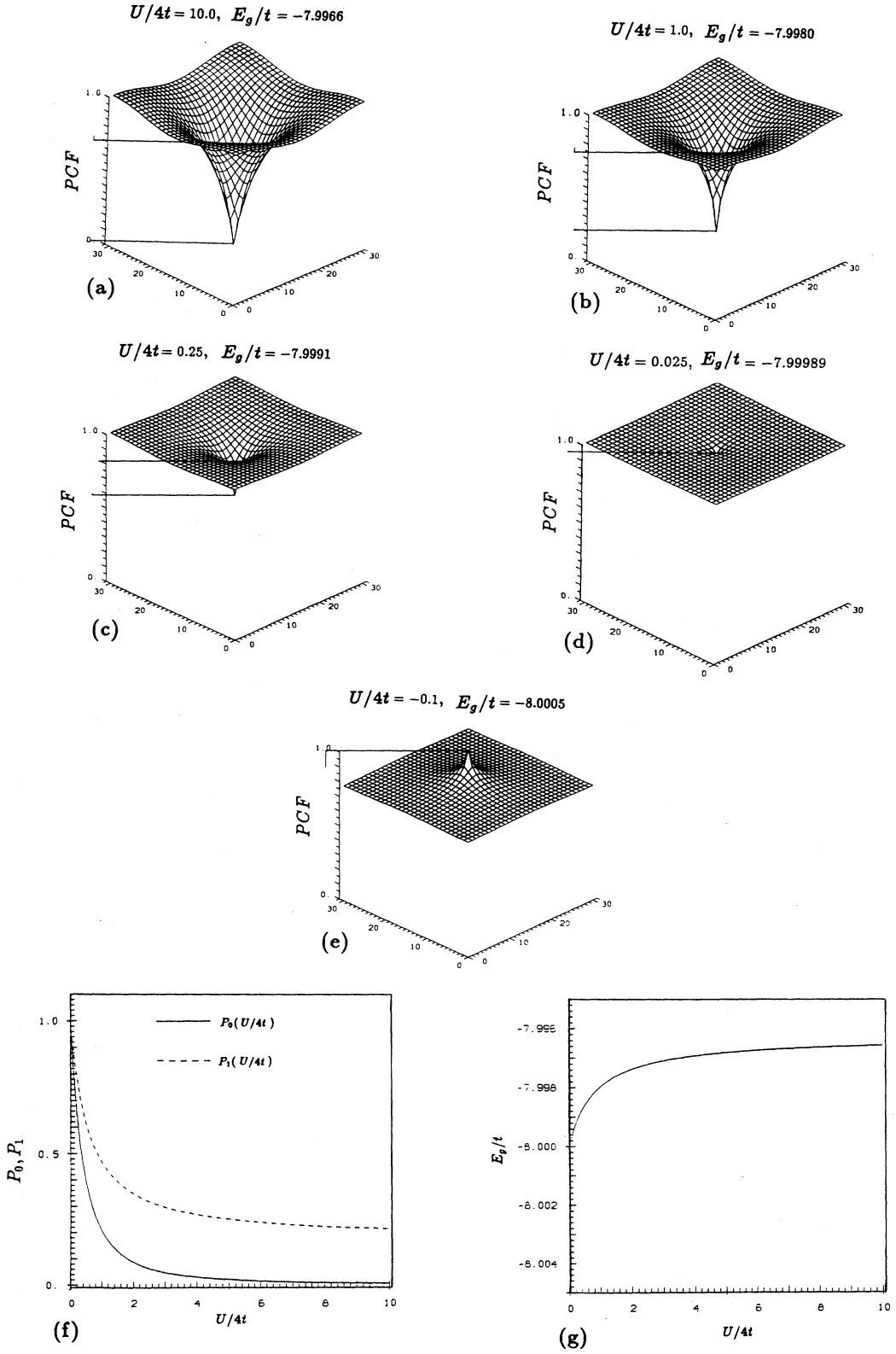

FIG. 3. (a)–(e) The 2D PCF's for the 30×30 lattice on torus as a function of $U/4t$, with $U/4t$ 10.0, 1.0, 0.25, 0.025, and −0.1, respectively. These are defined in a similar way to those above, with an electron supposed to be fixed on the site (15,15). Their maximum value has been normalized again to 1. (f) The double occupancy P_0 and nearest-neighbor occupancy P_1 as a function of $U/4t$, as defined in 1D. $P_0(U=0)$ and $P_1(U=0)$ have been normalized to 1. (g) is the total energy E_g/t of the correlated ground state as a function of $U/4t$.

problems. This time the electrons would prefer to remain close to each other to gain energy, as can be seen in the PCF of Figs. 2(e) and 3(e).

CONCLUSION

We have studied the two-electron problem in both the 1D and 2D Hubbard model. In 2D, our result shows that electrons behave differently than they do in 1D. The correlation behavior comes out to depend on dimension as does the quality of Gutzwiller ansatz. The fluctuations in 2D are much larger than those in 1D; the asymptotic form of the PCF is different. For any positive on-site interaction parameter U, it is shown from the PCF calculation that in the ground state, two electrons prefer to stay as far apart as possible to reach the lowest energy. This implies that the effective interactions between two electrons are repulsive. It should be noticed that the correlated ground-state wave functions constructed here are similar to that of the most generalized resonating-valence-bond state.[11] The method used here can be applied in principle in any dimension, so it might help to understand the nature of the Hubbard model in higher dimensions.

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*BITNET address: LIANGCHE@SC.
†BITNET address: MEI@DSOMPI 11.

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