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Variational studies of the 2D Hubbard model: less than half filled

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Abstract. We consider the variational Monte Carlo method of studying fermion systems in condensed matter physics. This method is a powerful tool for studying the properties of interacting electrons which are responsible for phenomena like the new high-T_c superconductors. Using our parallel algorithm for updating the determinants of large complex matrices on transputer arrays we study the energy and spin correlations for a 12×12 and a 22×22 lattice. Using the Hubbard model and the Gutzwiller projected wavefunction we have evaluated these quantities as functions of band filling and coupling constant. We find that although the Gutzwiller state is stable for densities near half filling it is not at low densities. For the stable states we find antiferromagnetic correlations. Statistically the thermodynamic limit is already attained with a 12×12 lattice.

1. Introduction

The field of computational physics has been instrumental in the advance of our understanding of complex many-body systems. It complements analytical investigations and the new insights gained often lead to further advances in analytical work. Parallel computing has been recognised for some time now as an efficient and cost effective way of doing large scale computations such as lattice gauge theory simulations.

Large scale computing is also necessary in the field of condensed matter where the problems are as demanding as those of high energy physics. Besides being computationally intensive the problems usually require large amounts of random access memory. With the advent of MIMD processors like the transputer, calculations on condensed matter systems are being gradually ported across to transputer networks. Most of these applications are parallelised using flood filling or farming techniques. There are, however, large classes of problems that cannot be farmed and one has to devise new algorithms to exploit the parallel structure of transputer arrays.

Monte Carlo techniques have been used in computational physics for quite a long time especially in the area of statistical mechanics. Recently these techniques have been extended to cover Fermi as well as Bose systems. However, the application of Monte Carlo techniques in the evaluation of the functional integrals in these statistical mechanics problems is computationally intensive and only very small systems can be handled.

More recently Monte Carlo techniques have been applied to variational calculations. The variational Monte Carlo (VMC) method was first successfully introduced by McMillan [1] for liquid ^{4}He and was extended to Fermi systems by Ceperley *et al* [2]. In this method one assumes certain states for the system and computes expectation values as functions of variational parameters. This method has recently been applied by

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Yokoyama and Shiba [3] to the investigation of the various phase changes in the one- and two-dimensional Hubbard model. However they studied relatively small lattices and did not investigate for two dimensions the very important effects of band filling on the stability of the various phases. Such band filling effects can only be studied for reasonably large lattices since experiments indicate that dramatic changes occur for very small changes near half band filling. Since they used a large sequential computer it is possible that they were limited by computational power.

In this paper we present results using a new parallel algorithm for updating large complex determinants so necessary for the VMC method mentioned above. This update algorithm uses the formulae developed by Ceperley *et al* [2]. This update method also gives rise to a new method of inverting a matrix which is different from the standard pivotal method. Our method, described in a previous paper [4] consists in slicing the matrix and storing each slice on a separate transputer. At each update each transputer requires only the information on its own slice and that of the current slice being updated. This implies that the size of matrix that can be inverted is determined by the total distributed memory of the transputer network.

The plan of this paper is as follows. In the following section we give some background about the Hubbard and related models and discuss several types of variational wavefunctions. We show that they may each be expressed as a product of a correlation factor and a reference wavefunction which is a determinant or a product of two determinants. Section three summarises the Ceperley, Chester and Kalos [2] formulae and our algorithm for updating the determinant and matrix inversion. A discussion of the physical results is presented in the last section.

2. Hubbard model

In the field of condensed matter physics phase transitions form one of the most important areas both from the technological and basic scientific points of view. The successful study of phase transitions involves the development and solution of models that describe the essential features of the phase changes. Phase changes are dependent on the system environment and the interactions of the various constituents of the system. Since we shall concentrate on solids in this paper the crystalline lattice environment will play a fundamental role in our model. The simplest model that contains both motion on a lattice and interactions between the electrons is the Hubbard model. This is defined by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow} \tag{1}$$

where $c_{i\sigma}$ destroys an electron localised at the site i with spin σ. $n_{i\sigma}$ is the corresponding number operator, t and U measure the band width and electron interaction respectively. The term $\langle ij \rangle$ denotes nearest neighbour sites i and j within the lattice.

Because of its conceptual simplicity the Hubbard model has been used for the investigation of metal–insulator phase transitions, magnetic phase transitions within the itinerant model, behaviour of heavy fermion systems and recently high-T_c superconductors. The exact solution in one dimension has been given by Lieb and Wu [5] in terms of the Bethe *ansatz* [6] solution originally developed for the one-dimensional Heisenberg model. There are no analytic solutions in two or three dimensions.

In two or higher dimensions we must therefore resort to approximate analytic methods or numerical methods. For small values of the ratio U/t (weak coupling regime) one can apply mean field or Hartree–Fock methods to obtain analytic results [7, 8]. In the strong coupling regime $U/t \gg 1$ the model goes over to the Heisenberg model and one can apply some of the approximate analytic methods appropriate to that model. In the intermediate regime and outside the regions of validity of the previously mentioned approximate methods one turns to numerical techniques.

Since there are four states on each site, for sufficiently small lattices one can set up basis states based on the atomic states on each site and then do a brute force diagonalisation of the Hamiltonian matrix constructed from these basis states. However, the number of basis states grows exponentially with the number of sites and therefore only very small systems can be studied with the present breed of supercomputers.

The variational Monte Carlo (VMC) approach is complementary to previous approaches. Given a knowledge obtained by the previous approaches of the various possible states that the Hubbard system can adopt, the emphasis of the VMC approach is to concentrate on a selected set of physically interesting states and to study how the properties of these states are influenced by the strength of the interaction, lattice symmetry and band filling. The stability or the likelihood of the various states is determined by the relative energies of the various trial states. The degree of long range ordering may be calculated via the correlation functions.

In a recent series of papers Yokoyama and Shiba [3] have discussed several types of physically interesting states. The simplest type of wavefunction is given by the Gutzwiller projected wavefunction

$$\psi = \prod_j [1 - (1-g)n_{j\uparrow}n_{j\downarrow}]\psi_F \tag{2}$$

where ψ_F is a reference Slater determinantal state. This function was originally introduced to study the correlations of the ground state of the Hubbard Hamiltonian. The variational parameter, which is the amplitude of the doubly occupied sites, highlights the effect of the Hubbard repulsion between electrons of opposite spin on the same site. Even for such a simple trial wavefunction exact analytic expectation values are only available in one dimension [10].

A second type of variational wavefunction is obtained by replacing the Fermi vacuum ψ_F by a spin density wave (SDW) state, ψ_{SDW}. This state corresponds to an itinerant antiferromagnetic state and has an additional parameter g_{AF} related to the staggered magnetic moment per site. With the current intense interest in high-T_c superconductors, a third type of trial wavefunction is obtained by replacing ψ_F in equation (2) by the Bardeen, Cooper and Schrieffer wavefunction ψ_{BCS}. In the limit of $g \to 0$ this form of the wave function corresponds to the resonating valence bond (RVB) state proposed by Anderson [11] for the explanation of high-T_c superconductivity. Recently Lee and Feng [12] have introduced a trial wavefunction which produces both an antiferromagnetic state and an RVB state.

The important feature of most trial wavefunctions used for the Hubbard model is that they are all projections of Slater determinants. This determinantal form of the wavefunction is crucial to our method of spreading the calculation on a network of transputers. Essentially the VMC method of calculating expectation values consists of summing over contributions for a series of random configurations. For a determinantal wave function each configuration is obtained from the previous one by the replacement

of one column in the determinant. As will be apparent in the next section this form of updating is eminently suited to parallelising over a network of computers.

The case for using a projected type of wavefunction has been made by Gutzwiller [13] and by Gros [14]. Essentially the parameter in the projection operator part of the wave function emphasises the correlations in the wavefunction that arise from the character of the Hubbard interaction. If we had used an extended Hubbard interaction or an Anderson type of Hamiltonian then we could have had a wider class of projection operators, which would be more akin to the Jastrow-type correlation factor used in ^{4}He calculations. Such modifications of the wavefunction via correlation factors are easily included in a VMC method.

In this paper we will consider only the Hubbard Hamiltonian. Recently, however, it has been argued that the behaviour of high-T_c superconductors requires an extended Hubbard Hamiltonian which includes the orbitals of both the oxygen and copper. Fortunately, however, in the energy region of interest one can transform the Hamiltonian into an effective one-band Hamiltonian called a $t-J$ Hamiltonian [15]

$$H = -tP\sum(c_{i\sigma}^{\dagger}c_{j\sigma} + \text{HC})P + \frac{1}{2}\sum_{\langle ij\rangle} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

where P projects out the doubly occupied states. For this Hamiltonian the previously mentioned trial states with $g = 0$ also apply.

To summarise this section we observe that many important areas of phase transitions in condensed matter are adequately described by a Hubbard or extended Hubbard Hamiltonian. Many of the interesting phases may be described by trial wavefunctions that are products of a Jastrow-type correlation factor and a reference state, which is either a single determinant or a pair of determinants. The expectation values of the relevant operators may be computed via a Monte Carlo method and because of the determinantal nature of the trial function the computation can be mapped over an array of transputers.

3. The variational Monte Carlo algorithm

We wish to summarise here the variational Monte Carlo (VMC) algorithm [4] we have developed for distribution across a network of transputers or other parallel processing elements. The method itself was first used for fermion systems by Ceperley *et al* [2], while a particular application of it for serial computers to the Hubbard model can be found in two informative papers by Yokoyama and Shiba [3].

The Hamiltonian for the simplest form of the Hubbard model has been given above in equation (1). It describes a set of electrons on a d-dimensional lattice with nearest neighbour hopping and a repulsive interaction between electrons on a doubly occupied site. It depends on only one parameter, the ratio U/t where U is the on-site repulsion energy and t is the hopping matrix element. A simple one-parameter variational wavefunction of singlet form can be written [3] as

$$\psi(\boldsymbol{R}) = \prod_j \left[1 - (1-g)n_{j\uparrow}n_{j\downarrow}\right] \Delta_{\uparrow}(\boldsymbol{R})\Delta_{\downarrow}(\boldsymbol{R}) \tag{3}$$

where g is the variational parameter, $\boldsymbol{R} = (\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)$ denotes the position space configuration of the N electrons and $\Delta_\sigma(\boldsymbol{R})$ denotes a single Slater determinant for the

electrons of spin σ

$$\Delta_\sigma(\boldsymbol{R}) = \det\ D_{\sigma pq}(\boldsymbol{R}).$$

The matrix $D_{\sigma pq}(\boldsymbol{R})$ has the form

$$D_{\sigma pq}(\boldsymbol{R}) = \phi_{\sigma p}(\boldsymbol{r}_q)$$

with $\phi_{\sigma p}(\boldsymbol{r}_q)$ a one-particle orbital of spin σ. In the singlet state we have equal numbers of spin-up ($\boldsymbol{r}_j$ for $j = 1,\ldots,N_e$) and spin-down ($\boldsymbol{r}_j$ for $j = N_e + 1,\ldots,2N_e$) electrons ($N = 2N_e$). As discussed in the previous section the one-particle orbitals can be chosen in different ways depending on one's intuition concerning the true ground state. In this paper we take simple plane waves

$$\phi_{\sigma p}(\boldsymbol{r}_q) = \exp(\mathrm{i}\boldsymbol{k}_p \cdot \boldsymbol{r}_q)$$

The essence of the VMC method is to estimate quantum expectation values by averaging over a finite ensemble of configurations generated by a random walk through the space of electron configurations. Each step in the walk corresponds to a randomly chosen electron attempting to move to a randomly chosen nearest neighbour site. Whether the move is acccepted or rejected is determined by the usual Metropolis algorithm [16], so the configurations generated during the walk form an ensemble with probability distribution

$$P(\boldsymbol{R}) = \frac{|\psi(\boldsymbol{R})|^2}{\sum_{\boldsymbol{R}'} |\psi(\boldsymbol{R}')|^2}.$$

An expectation value of an observable O can then be expressed as

$$\langle O \rangle = \sum_{\boldsymbol{R}} \frac{\psi^*(\boldsymbol{R}) O\psi(\boldsymbol{R})}{\sum_{\boldsymbol{R}'} |\psi(\boldsymbol{R}')|^2} = \sum_{\boldsymbol{R}} P(\boldsymbol{R}) \frac{O\psi(\boldsymbol{R})}{\psi(\boldsymbol{R})}$$

where $O\psi(\boldsymbol{R})/\psi(\boldsymbol{R})$ has a simple form for observables made up of sums of one- and two-body operators. We estimate the true quantum mechanical average by the average over the M configurations sampled by our random walk

$$\langle O \rangle \simeq \frac{1}{M} \sum_{i=1}^{M} \frac{O\psi(\boldsymbol{R}_i)}{\psi(\boldsymbol{R}_i)}.$$

In estimating averages this way there is always a statistical error associated with the fluctuations that occur in the sample of configurations taken. We have estimated this error in the standard way [14] by breaking up the full set of configurations generated into N subsets (typically $N \simeq 10$) and then treating the averages obtained within each subset as statistically independent in order to estimate a standard deviation. This error measure, which is shown in the figures by a vertical bar on the data points, gives an idea of the size of fluctuations in the averaging process.

In practice one determines each move by picking an electron, say the one at $\boldsymbol{r}_j$, at random. Then choose randomly one of its nearest neighbour sites as a trial position

$$\boldsymbol{r}_{j\,\mathrm{trial}} = \boldsymbol{r}_{j\,\mathrm{old}} + \boldsymbol{a}$$

where $\boldsymbol{a}$ is the appropriate lattice vector connecting the old site to the trial site. Next a random number ξ, uniformly distributed between zero and one, is chosen and the move is accepted if $\xi < P(\boldsymbol{R}_{\text{trial}})/P(\boldsymbol{R}_{\text{old}})$, and otherwise is rejected. If accepted, $\boldsymbol{R}_{\text{trial}}$ becomes the next configuration in the ensemble; if rejected, $\boldsymbol{R}_{\text{old}}$ is kept as the next configuration. For a determinantal wavefunction $\psi(\boldsymbol{R})$ of the form (3) the key numerical calculation is that of the ratio [3] of two determinants which differ from each other by a single altered column. Ceperley *et al* introduced a computationally efficient method of calculating such a ratio.

Based on this method we have developed an algorithm [4] with the following remarkable feature. To find the mth column of $\overline{\mathbf{D}}(\boldsymbol{R}_{\text{new}})$ we need only the mth column of $\overline{\mathbf{D}}(\boldsymbol{R}_{\text{old}})$ together with a scalar $Q_j(\boldsymbol{a})$, the jth column of $\overline{\mathbf{D}}(\boldsymbol{R}_{\text{old}})$ and the single particle wavefunctions $\phi_p(\boldsymbol{r}_j + \boldsymbol{a})$. The other columns of $\overline{\mathbf{D}}(\boldsymbol{R}_{\text{old}})$ are not required. This situation makes possible the distribution of the update algorithm over a parallel network of transputers or other processing elements. The matrix $\overline{\mathbf{D}}$ can be partitioned into *slices* each consisting of a subset of columns of $\overline{\mathbf{D}}$. Each slice can be kept permanently on a separate processor. During an update we need communicate only the scalar $Q_j(\boldsymbol{a})$ and a single column (the jth column of $\overline{\mathbf{D}}(\boldsymbol{R}_{\text{new}})$) to the different processors in order to update $\overline{\mathbf{D}}$. As the communication times are small compared with the time spent on floating point arithmetic, we can get a substantial improvement of the update speed by using a parallel machine rather than a single serial processor.

To start such a Monte Carlo calculation we begin from a standard configuration $\boldsymbol{R}_0$ (see later) and then the matrix $D_{\sigma pq}(\boldsymbol{R}_0)$ and the transpose of its inverse $\overline{D}_{\sigma lm}(\boldsymbol{R}_0)$ must be calculated before we can start the Monte Carlo steps. The matrix inversion is computationally expensive but we have observed that we can perform the matrix inversion by using the same update procedure as we use for the Monte Carlo steps.

Our algorithm may be implemented on any array of computers provided that the communications links have a reasonable speed. The calculations below were carried out with either our local physics department Meiko Computing Surface or with the largest domain of 132 transputers on the Edinburgh concurrent supercomputer (ECS) for the larger 22×22 lattice.

We reported in our previous paper [4] the remarkable feature that the times taken for computing grow linearly with the number of columns processed. This implies that our program is computationally intensive and that little time is used for communications across the network. Furthermore we found that the timings do not increase as the cube of the size of the matrix. Indeed a good fit shows that the timing goes as $N_e^{1.7}$. This indicates that our algorithm is far superior to the standard method whose timing goes as N_e^3.

4. Results and discussion

In this section we shall discuss some of the results obtained from the implementation of our algorithm in calculations of the energy for the Hubbard model. As explained above our calculations start with the electrons at a certain configuration $\boldsymbol{R}_0$. For simplicity we start with a configuration where the electrons are all clustered around the lattice origin at one per site in an alternating spin density wave (SDW) configuration. We generate a sufficient number of random configurations to 'thermalise' the electron distribution before we start counting configurations to use in the averaging process.

Since we are using a variational method we should start with a state that has a low energy. We start with a state characterised by a set of wavevectors, $\boldsymbol{k}$, which correspond to a filled Fermi sea in the paramagnetic state. The half-filled state corresponds to a square Fermi surface (contour). For less than half-filled states we chose to fill progressive square contours. This is not exactly the Fermi surface for the paramagnetic case but has the merit that it is easy to program. It should really make little difference to our final variational result. In order to avoid degeneracies of the variational wavefunction we have used [3] periodic and antiperiodic boundary conditions in the x and the y directions respectively in determining our wavevectors. This may introduce a finite size lattice error in our correlation functions in the sense that the x and y directions give us slightly different answers.

From the form of the Hubbard Hamiltonian (1) it is seen that the energy per site as a function of the variational parameter g may be written as

$$(1/t)E(g) = -S(g) + (U/t)P(g). \tag{4}$$

The score S is the negative of the kinetic energy per site (in units of t) and the pairs function P is the number of sites that are doubly occupied, normalised by the total number of sites.

In a previous paper [4] we concentrated exclusively on a 12×12 lattice since this size of lattice is most easily handled by conventional serial computers and on our local Meiko Computing Surface. Our new algorithm allows us to handle much bigger lattices whose size is limited only by the hardware and time allocation on the computer. In the simulation of large physical systems by small finite size lattices one needs to be convinced that the size of lattice used in the calculation is a good approximation to the thermodynamic limit. Therefore together with the 12×12 lattice results we did a series of runs for the 22×22 lattice which is bigger than lattices previously studied.

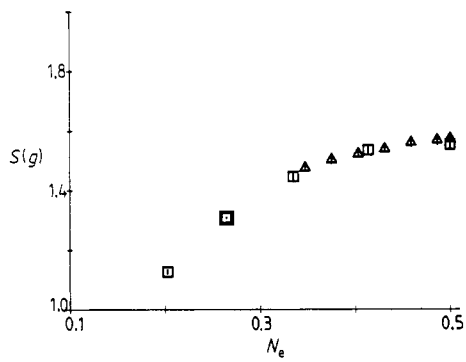

Figure 1. Plot of the function $S(g)$ (vertical axis) at $g = 0.7$ for a range of electron densities, N_e/(No of lattice sites), between 0.2 and 0.5 (half-filled). The triangles are data for a 12×12 lattice while the squares are for a 22×22 lattice.

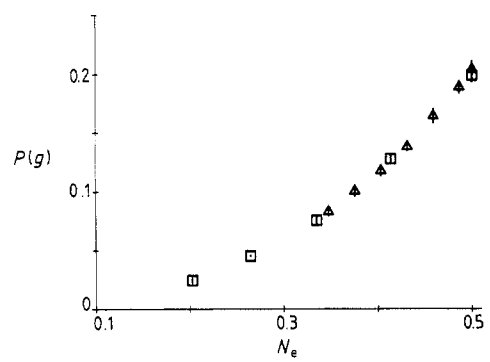

Figure 2. Plot of $P(g)$ (vertical axis) at $g = 0.7$ for a range of electron densities as in figure 1. Again triangles and squares refer to 12×12 and 22×22 lattices, respectively.

We show in figure 1 and figure 2 the score and the pairs function for both the 12×12 lattice and the 22×22 lattice over a range of electron fillings at a g value of 0.7. It is seen that the curves for the two lattices lie almost on top of each other. We

conclude that both of these lattices are sufficiently close to the thermodynamic limit that using larger lattices will not give any new information.

To get convergence of the energy averages we found that typically about 50 000 configurations will suffice. The acceptance ratio of electron moves ranged from about 50% at $g = 0.7$ (quarter-filled 22×22) to about 12% at $g = 0.3$ (half-filled 22×22). For the big 22×22 lattice it is not feasible to study the regime with $g < 0.3$ by the present technique because of the low acceptance ratio and the large number of initial configurations ($\simeq$ 15 000) which must be discarded before the starting configuration has been 'thermalised'. In this large coupling regime an alternative Hamiltonian and different variational wavefunctions may be used as mentioned elsewhere.

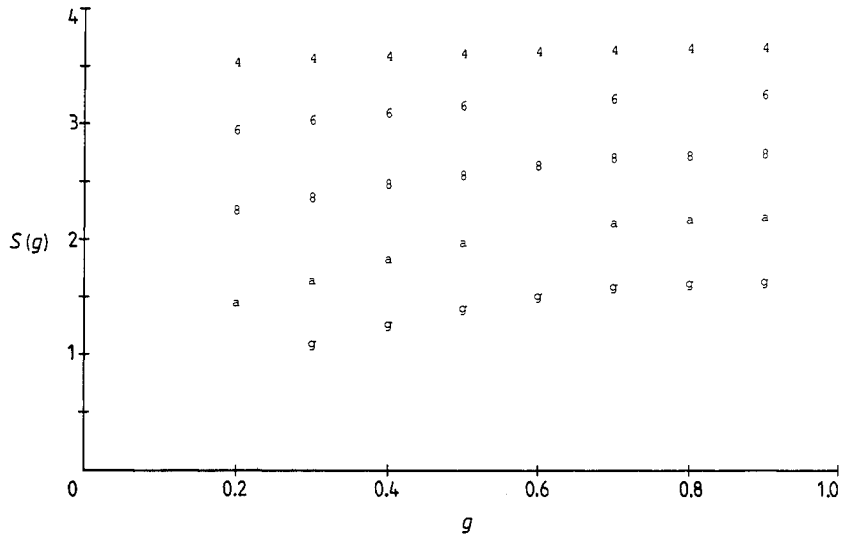

Figure 3. Values of $S(g)$ (vertical axis) as a function of g for a range of electron fillings on a 12×12 lattice. The alphanumeric coding of the points is the following: 4 denotes $N = 4^2$, 6 denotes $N = 6^2$, 8 denotes $N = 8^2$, a denotes $N = 10^2$, g denotes $N = 12^2$.

Figure 3 gives the dependence of the score on g for a range of fillings of a 12×12 lattice. The points are labelled by numbers or letters that correspond to the filling. For small fillings the electrons' score appears not to be affected by variation of g. The value of $1 - g$ is the amplitude of the projector of doubly occupied sites and therefore acts as a constraint to motion. For few particles on a large lattice this constraint is irrelevant and the electrons behave almost like free particles giving a kinetic energy that is linear in density. At large fillings the score changes more rapidly with g, with the largest kinetic energy occurring at the largest filling and smallest g. From figure 4 we see that for large fillings, N_e, the score deviates from its initial linear (free electron like) dependence on N_e.

The interaction energy is proportional to the pairs function, $P(g)$. Figure 5 shows the behaviour of P with respect to g at a fixed filling. It appears to be almost linear with a slight modulation. In figure 6 we note that for large g corresponding to nearly free electrons the number of pairs varies almost linearly with N_e. There are no pairs for $g = 0$ where all the pairs have been projected out. There seems to be some structure in the P versus N_e curves. This structure is especially pronounced for near half-filling.

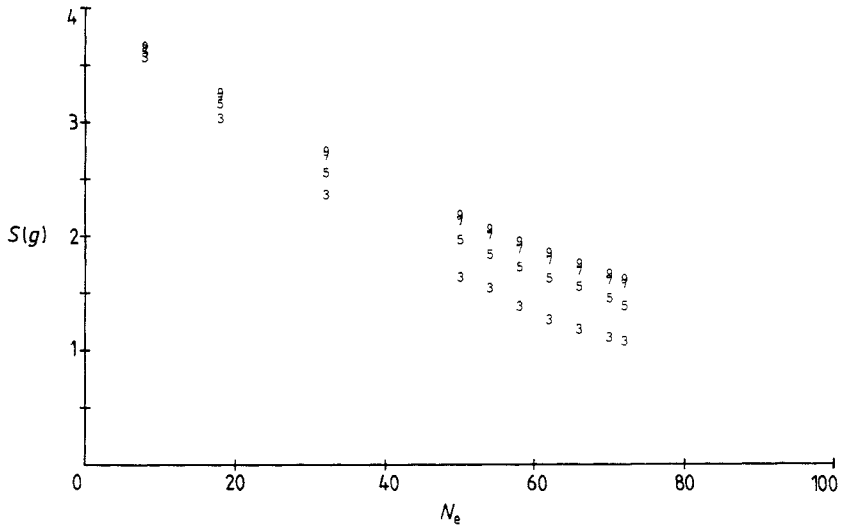

Figure 4. Values of $S(g)$ (vertical axis) as a function of N_e on a 12 × 12 lattice. The points are plotted with a number which is 10 times the Gutzwiller parameter g, e.g. points plotted with a 7 correspond to $g = 0.7$.

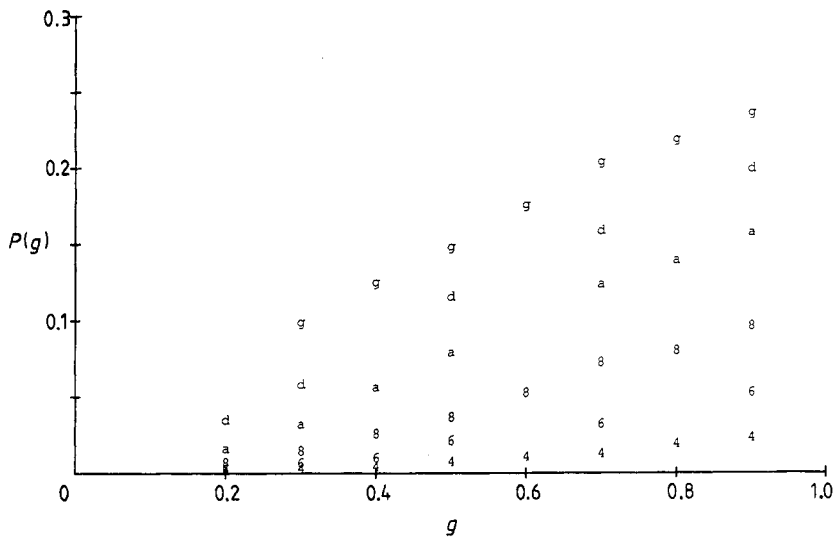

Figure 5. Values of the pairs function $P(g)$ (vertical axis) as a function of g for a range of fillings on a 12 × 12 lattice. The alphanumeric coding is the same as in figure 3 with the addition that d denotes $N = 124$.

The actual energy is obtained by minimising the total energy given above with respect to g. Given a value of U/t the minimum value occurs at $g_{\min}$ given by $S'(g_{\min})/P'(g_{\min}) = U/t$. From figures 3 and 5 we note that for small densities both S and P are almost linear over an appreciable range of g. This means that the value of $g_{\min}$ for a given value of U/t is poorly determined by the VMC method at low densities and that the projected Gutzwiller wavefunction is not a good one to use in this regime.

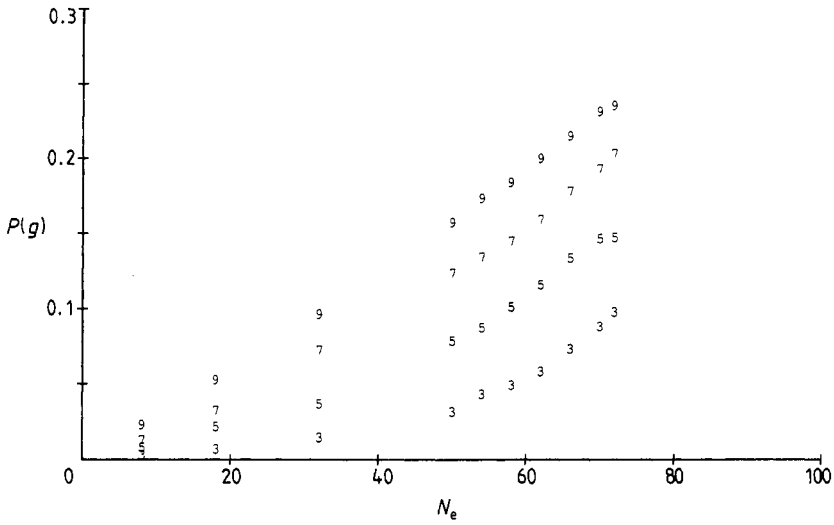

Figure 6. Values of the pairs function $P(g)$ (vertical axis) as a function of the electron number N_e on a 12×12 lattice. The numbers used to plot the points give the value of the Gutzwiller parameter as in figure 4.

In the region where the above equation gives a well defined solution we see that each value of g may be considered to correspond to a certain value of the coupling ratio U/t. Our figures 3 and 5 may be interpreted as curves of the score and pairs as a function of coupling constant.

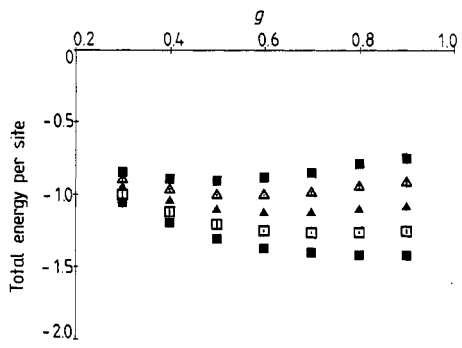

Figure 7. Total energy per site (vertical axis) as a function of g for 124 electrons ($N_e = 62$) on a 12×12 lattice at five values of the coupling ratio U/t. The lowest curve is for $U/t = 1$ and the curves above correspond, in order, to values 2, 3, 4, 5 (highest curve) for U/t.

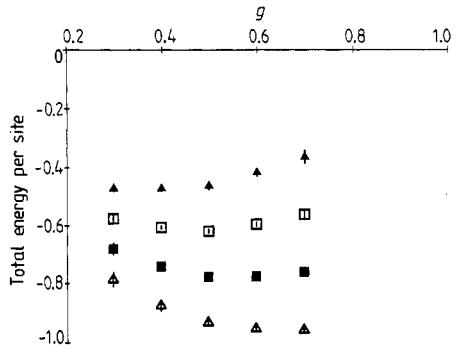

Figure 8. Total energy per site (vertical axis) as a function of g for a half-filled 22×22 lattice at four vaues of U/t. The lowest curve is for $U/t = 3$ with the curves above corresponding respectively to values 4, 5, 6 (highest curve) for U/t.

Figure 7 gives a plots of the total energy as a function of the variational parameter g for a particular density, 62/144, near to half-filled, for the 12×12 lattice. We give curves for a range of U/t; we note that there is a well defined minimum, $0 < g_{\min} < 1$, for ratios of the coupling constant > 3. For small ratios corresponding to large bandwidths or small Hubbard coupling the energy minimum moves to $g = 1$ which is

the free electron gas. However, for densities near to half-filled and for a largish value of U/t the Gutzwiller state is preferred to the free electron gas state. Figure 8 gives a set of curves of the energy versus g for the half filled 22×22 lattice for a range of coupling ratios.

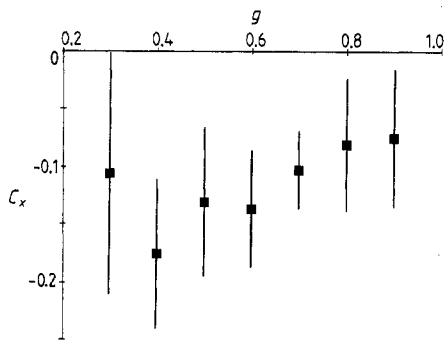

Figure 9. Nearest neighbour spin correlation function C_x (vertical axis) for 124 electrons ($N_e = 62$) on a 12×12 lattice plotted as a function of g. The error bars indicate the large statistical fluctuations in this quantity.

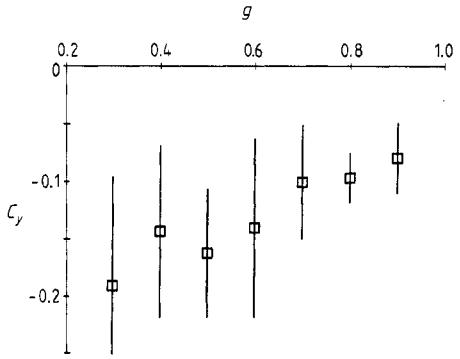

Figure 10. Nearest neighbour spin correlation function C_y (vertical axis) as a function of g for the same system as in figure 9. Again note the large fluctuations as well as the negative sign which indicates antiferromagnetic correlations as in figure 9.

For sufficiently large U/t the Hubbard Hamiltonian goes over to the antiferromagnetic Heisenberg Hamiltonian but for intermediate values of the coupling constant there may still be antiferromagnetic correlations. We have calculated the correlation functions $C_x = \langle S^z_{i_x+1,i_y} S^z_{i_x,i_y} \rangle$ and $C_y = \langle S^z_{i_x,i_y+1} S^z_{i_x,i_y} \rangle$, where $S^z_{i_x,i_y}$ denotes the z component of the spin on lattice site i_x, i_y. Whereas the kinetic energy and number of pairs are extensive quantities, the nearest neighbour spin–spin correlation function is not and thus shows much more statistical noise than do S and P. To try to reduce this noise we sampled the spin on several different nearest neighbour sites from each configuration. Since the spin correlations are short ranged this procedure can improve statistical convergence. Nevertheless much noise remains, as shown by the large error bars in figure 9 and figure 10 which give the correlation functions for the x and y directions. However, the antiferromagnetic nature of the correlations is clear. For values of g between 0.5 and 0.7 where the variational wavefunction gives a good minimum energy the x and y correlations agree within statistical error. It may be expected at first that because of the different boundary conditions used for the x and y directions these may be different. The boundary condition appears not to make too much difference. What is observed is that the correlation functions start with the values corresponding to the initial configuration and gradually tend to an equilibrium value. Starting from the SDW configuration corresponds to an initial value of $C_x = C_y = -1$. We used the relaxation of the correlation function towards the equilibrium average as a valuable marker of how many initial configurations to discard before starting to compute averages.

In summary then, our algorithm has enabled us to make variational calculations for the Hubbard model using Gutzwiller states for lattices larger than used previously. We are able to show that both the 12×12 and 22×22 lattices are good approximations to the thermodynamic limit. By investigating a range of fillings or electron densities we found that the Gutzwiller projected state gives a clear energy minimum for $0 < g_{\min} < 1$ for densities near half-filled and for large coupling-to-bandwidth ratio. For

parameters outside this range the energy minimum is poorly determined with this wavefunction. Within the useful range of parameters the lowest energy state has short range antiferromagnetic spin correlations.

It is known from the work of Yokoyama and Shiba [3] that the introduction of spin density wave correlations and an internal staggered field into the variational wavefunction can lower the energy significantly as compared with the states studied here. They did not study the less-than-half-filled regime nor the spin correlations, however. In future work we will use more correlated variational wavefunctions to explore the whole range of band fillings in the two-dimensional Hubbard model. Our use of periodic–antiperiodic boundary conditions means that we can go away from half-filling by removing electrons in groups of eight without losing the single-determinantal form of the wavefunction. With a large lattice (22×22) this means we can vary the filling factor in steps of less than 2% at a time thus getting a very detailed picture of how the ground state of the model depends on electron density.

In a recent paper Anderson *et al* [17] presented a whole new class of variational wave functions. This class of trial wavefunctions includes not only the wavefunctions discussed in section 2 but also wavefunctions corresponding to various flux phases. These flux phases are equivalent to mixtures of d and s pairing in the resonating valence bond model (RVB). The Anderson trial wavefunctions may be written in the form of three factors — a pair of Slater determinants and a Jastrow function. This is exactly the form of our trial wavefunction (3). Our algorithm will also be able to deal with this class of functions. We are in the process of doing a study of the comparative energetics of the various phases for the $t-J$ model for a range of fillings.

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