THE GRAND CANONICAL PARTITION FUNCTION
OF A 2-DIMENSIONAL HUBBARD MODEL

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Abstract

We present a new technique for a numerical analysis of the phase structure of the 2D Hubbard model as a function of the hole chemical potential. The grand canonical partition function for the model is obtained via Monte Carlo simulations. The dependence of the hole occupation number on the chemical potential and the temperature is evaluated. These calculations, together with a study of the Yang-Lee zeros of the grand canonical partition function, show evidence of a phase transition at zero temperature and particle density below half-filling. The binding energy of a pair of holes is calculated in the low temperature regime and the possibility for pairing is explored.
1. Introduction

For many years the Hubbard model, and other related systems with a finite density of electrons, has attracted much attention in the field of numerical simulations [1],[2]. The main interest in these simulations arose from the suggested relation between the planar Hubbard model and high T_c superconductivity (HTSC) [3],[4],[5]. Since the model is non-relativistic, its analysis avoids some of the problems associated with relativistic fermions, such as fermion doubling [2]. However, the inherent difficulties of simulating fermions at finite density remain: integration over the fermionic degrees of freedom leads to a non-positive integration measure in the path integrals. This arises from the determinant of the fermion matrix being non-positive definite and any importance sampling based on a partition function proportional to this determinant loses its normal meaning.

In the Hubbard model, this problem manifests itself via the so-called sign problem of the partition function. The partition function of the half-filled Hubbard model (one electron per lattice site) is always positive, being a product of a determinant of a matrix and its hermitian conjugate. However, if one introduces a finite real chemical potential for the impurities (holes), then this positivity is lost, and configurations with real determinants, but
with negative signs can occur. Unfortunately, the finite density of holes is the case of greatest physical interest, as the impurities play an essential role in the superconducting transition \[ 6 \].

In this paper we propose an analysis of the Hubbard model which treats the fermion dynamics in a rigorous manner. This method is similar to one applied to the chiral phase transition at finite density QCD, and is based on a study of the zeros of the grand canonical partition function in the complex fugacity \( e^{\beta \mu} \) plane \[ 7 \], \[ 8 \]. Here we simulate the configurations of the Hubbard-Stratonovich (HS) fields (given by Ising variables) at half-filling, as well as at finite doping fraction and expand the grand canonical partition function (GCPF) as a polynomial in \( e^{\beta \mu} \) (or equivalently in \( e^{\beta \mu} + e^{-\beta \mu} \)) \[ 3 \]. The coefficients of this polynomial are averaged over an equilibrated ensemble of configurations. The distribution of the zeros of this polynomial in the neighbourhood of the physical region, \( \mu \) real, can indicate a phase transition. In particular, their scaling behaviour with respect to the lattice size can indicate if real zeros can occur in the infinite lattice limit. Such zeros would correspond to divergences within the theory at the corresponding values of the fugacity.

The simulation is performed on a 2D spatial square lattice with the third
euclidean time dimension corresponding to the inverse temperature $\beta$. The updating procedure is the one described by White et al. [4].

As we show below, the evaluation of the partition function as an explicit polynomial in the fugacity variable permits analysis of the superconducting properties of the model for various values of the hole density.

In Section 2 we describe the construction of the partition function of the Hubbard model as a polynomial in the fugacity variable. Section 3 summarizes the simulation procedure and the measurements, and in Section 4 we present the preliminary numerical results for the critical value of the chemical potential.

2. Finite-temperature partition function

The original Hubbard hamiltonian is given by:

$$H = -t \sum_{i,j,\sigma} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_{i} (n_{i+} - \frac{1}{2})(n_{i-} - \frac{1}{2}) - \mu \sum_{i} (n_{i+} + n_{i-})$$

(1)

where the $i,j$ denote the nearest neighbour spatial lattice sites, $\sigma$ is the spin degree of freedom and $n_{i\sigma}$ is the electron number operator $c_{i\sigma}^{\dagger} c_{i\sigma}$. The constants $t$ and $U$ correspond to the hopping parameter and the on-site Coulomb repulsion respectively. The chemical potential $\mu$ is introduced such that $\mu = 0$ corresponds to half-filling.
The finite temperature grand canonical partition function (GCPF) is given by:

$$Z = Tr(e^{-\beta H})$$

(2)

where $\beta$ is the inverse temperature.

The finite temperature is represented on the lattice by extending the spatial lattice in the imaginary-time direction and relating the inverse temperature $\beta$ to the length of the time dimension $n_\tau$ by $\beta = n_\tau dt$, where $dt$ is the length of the time step. Following Hirsch and White et al. we rewrite the partition function as:

$$Z = Tr(e^{-dtV}e^{-dtK}e^{dt\mu})^{n_\tau}$$

(3)

where $K$ corresponds to the nearest neighbour hopping term in the Hubbard hamiltonian and $V$ to the onsite interaction including quartic products of fermion fields. This decomposition, based on the Trotter formula, introduces a systematic error proportional to $dt^2$. The quartic interaction can be rewritten in terms of Ising fields $s_{i,l}$ using the discrete Hubbard-Stratonovich transformation:

$$e^{-dtV} = e^{-\frac{dt^2}{4}} \sum_{s_{i,l} = \pm 1} e^{-dt\lambda s_{i,l}(n_{i+} - n_{i-})}$$

(4)
where \( i, l \) is the space-time index of a lattice site and the coupling \( \lambda \) is related to the original on-site repulsion constant by:

\[
\cosh (dt \lambda) = \exp \left( \frac{dtU}{2} \right).
\]  

This linearization of the interaction enables one to integrate out the fermionic degrees of freedom and the resulting partition function is written as an ensemble average of a product of two determinants:

\[
Z = \sum_{s_{i,j} = \pm 1} \tilde{z} = \sum_{s_{i,l} = \pm 1} \text{det}(M^+) \text{det}(M^-)
\]  

such that

\[
M^\pm = (I + P^\pm) = (I + \prod_{l=1}^{n_x} B_l^\pm)
\]  

where the matrices \( B_l^\pm \) are defined as

\[
B_l^\pm = e^{-(\pm dtV)} e^{-dtK} e^{dt\mu}
\]

with \( V_{ij} = \delta_{ij} s_{i,l} \) and \( K \) the matrix connecting nearest-neighbours sites with the hopping parameter \( t = 1 \). The matrices in (7) and (8) are of size \((n_xn_y) \times (n_xn_y)\), corresponding to the spatial size of the lattice. However, \( \text{det}(M^\pm) \) can be represented as a determinant of an \((n_xn_yn_z)\) square matrix of the
form \[2\]:

\[ I + A^\pm = \begin{pmatrix}
I & 0 & \ldots & B_i^\pm \\
-B_2^\pm & I & \ldots & 0 \\
0 & \ldots & \ldots & \ldots \\
\ldots & \ldots & \ldots & 0 \\
0 & \ldots & -B_n^\pm & I \\
\end{pmatrix}, \quad (9) \]

a fact which is exploited below in the evaluation of the partition function \( Z \).

The expectation value of a physical observable at chemical potential \( \mu \),
\(< O >_{\mu} \), is given by:

\[ < O >_{\mu} = \frac{\int O \tilde{z}(\mu)}{\int \tilde{z}(\mu)} \quad (10) \]

where the sum over the configurations of Ising fields is denoted by an integral

Since \( \tilde{z}(\mu) \) is not positive definite for \( \text{Re}(\mu) \neq 0 \) we weight the ensemble of

configurations by the absolute value of \( \tilde{z}(\mu) \) at some \( \mu = \mu_0 \). Thus

\[ < O >_{\mu} = \frac{\int \frac{O \tilde{z}(\mu)}{|\tilde{z}(\mu_0)|} |\tilde{z}(\mu_0)|}{\int \frac{\tilde{z}(\mu)}{|\tilde{z}(\mu_0)|} |\tilde{z}(\mu_0)|} = \frac{< O \tilde{z}(\mu) >_{\mu_0}}{< \tilde{z}(\mu) >_{\mu_0}} \quad (11) \]

The partition function \( Z(\mu) \) is given by

\[ Z(\mu) \propto < \frac{\tilde{z}(\mu)}{|\tilde{z}(\mu_0)|} >_{\mu_0}. \quad (12) \]

The normalization of the GCPF is irrelevant as can be seen from eq.(11).

The particle-hole transformation \[1\],\[10\]

\[ d_{i\sigma} = (-1)^i c_{i\sigma}^\dagger \quad (13) \]
is equivalent to the unitary transformation
\[ B_i^+ \rightarrow \begin{pmatrix} i & 0 & \ldots & 0 \\ 0 & -i & 0 & \ldots \\ 0 & 0 & i & \ldots \\ 0 & \ldots & 0 & -i \end{pmatrix} B_i^+ \begin{pmatrix} -i & 0 & \ldots & 0 \\ 0 & i & 0 & \ldots \\ 0 & 0 & -i & \ldots \\ 0 & \ldots & 0 & i \end{pmatrix} \] (14)

which reverses the sign of the hopping term \( K \). Hence on an even sized lattice the determinant of \( e^{dtK} \) is 1. Applying this transformation to the statistical weight gives:
\[ \tilde{z} = \det(Ie^{-\beta \mu} + P|_{\mu=0}^-)\det(Ie^{\beta \mu} + (P|_{\mu=0}^-)^\dagger) e^{\mu n_x n_y \beta} e^{\chi \sum_{i,t} s_{i,t}} . \] (15)

Equation (15) suggests two different ways of expansion of the partition function. The first one based on
\[ \tilde{z}(\mu) = \frac{\prod \lambda_i((e^{\mu \beta} + e^{-\mu \beta}) + (\lambda_i + \frac{1}{\lambda_i})) \times e^{\mu n_x n_y \beta}}{\prod \lambda_i(e^{\mu \alpha \beta} + e^{-\mu \alpha \beta} + \lambda_i + \frac{1}{\lambda_i})} \sum_{n=0}^{n_x n_y} a_n (e^{\mu \beta} + e^{-\mu \beta})^n \] (16)

and the second on:
\[ \tilde{z}(\mu) = \frac{\prod \lambda_i(e^{-\mu \beta} + \lambda_i)(e^{-\mu \beta} + \frac{1}{\lambda_i})) \times e^{2\mu n_x n_y \beta}}{\prod \lambda_i(e^{-\mu \alpha \beta} + \lambda_i)(e^{-\mu \alpha \beta} + \frac{1}{\lambda_i})} \sum_{n=-n_x n_y}^{n_x n_y} b_n e^{n \mu \beta} . \] (17)

where the \( \lambda_i \) are the eigenvalues of the matrix \( P|_{\mu=0}^- \). Note that the expansion coefficients \( b_n \) are the canonical partition functions of the \( n \)-electron excitations above half-filling, (with \( n < 0 \) corresponding to holes). We note here
that eqns. (16), (17) follow from the fact that the eigenvalues of $P_{\mu=0}^-$ are either real or appear in complex conjugate pairs. The coefficients of the characteristic polynomials, namely $\{a_n\}$ and $\{b_n\}$, are obtained from (16), (17) by the recursion procedure described in [11]. The sign problem manifests itself in the fluctuating signs of these coefficients from configuration to configuration of equilibrated Ising fields. The expansion coefficients for a grand canonical partition function (GCPF) are then obtained by averaging the coefficients of each of these polynomials over the ensemble of configurations. A similar procedure has been applied in the study of the chiral phase transition in finite density lattice QCD and in the evaluation of the critical mass in lattice QCD [11].

At $\mu_0 = 0$ (and at any imaginary chemical potential [3]) $\tilde{z}(\mu_0)$ is clearly positive. With alternative choice of the updating $\mu_0$ the GCPF, $\tilde{Z}(\mu_0)$, is equal to the average sign of the weight function $\tilde{z}(\mu_0)$ [12], [13]. We have performed calculations using updating at half-filling and at $\mu_0 \neq 0$. The latter choice of the updating chemical potential is important for simulations performed at low temperatures. We will show below that it provides results consistent with the half-filling updating at relatively high temperatures ($\beta \leq 5$) while at higher values of $\beta$ it provides better numerical stability in
obtaining the expansion coefficients of the GCPF, corresponding to the finite hole occupation.

As the temperature is lowered the bounds on the eigenvalues of the matrix $P_{\mu=0}^{-}$, which are found via the Lanczos algorithm, become very large. Simulating configurations at $\beta = 10$, $dt = 0.125$ we need to handle a lattice with $n_\tau = 80$. For this set of parameters we find that the eigenvalues vary between $10^{23}$ and $10^{-23}$ on a $10^2$ lattice which damages severely the efficiency and the accuracy of the whole calculation. However, the characteristic polynomial can be also obtained from the determinant of the the $(n_\tau n_x n_y) \times (n_\tau n_x n_y)$ matrix $I + A^{\pm}$ given in (9), using the eigenvalues of $A_{\mu=0}^{-}$.

It follows from the structure of $A_{\mu=0}^{-}$ that its eigenvalues have a $Z_{n_\tau}$ symmetry: if $\Lambda_i$ is an eigenvalue so is $\Lambda_i e^{\frac{2\pi i n}{n_\tau}}$ ($n = 1, ..., n_\tau - 1$). The coefficients of the $\tilde{z}$ expansion in the fugacity powers are actually functions of the $\Lambda_i^{n_\tau}$.

The variation in these eigenvalues is significantly smaller, but the matrix to be diagonalized is $n_\tau^2$ times bigger, leading to a more time consuming diagonalization procedure.

The method used in our calculations consists of representing the determinant of (9) as

$$det(I + A)$$

(18)
with

\[
A = \begin{pmatrix}
0 & 0 & \ldots & B_1 B_2 \ldots B_{n_t} \\
-B_{n_t+1} B_{n_t+2} \ldots & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & -B_{n_{r_{\tau}}-1} B_{n_{r_{\tau}}} \\
\end{pmatrix}
\]  \ 
(19)

where the matrix \( A \) is of the size \( (n_x n_y n_{\tau_{n}}) \times (n_x n_y n_{\tau_{n}}) \). (In the last equation the \( B \) matrices are taken at \( \mu = 0 \).) The eigenvalues of this matrix have a reduced symmetry \( Z_{n_{r_{\tau}}} \rightarrow Z_{n_{r_{\tau}}/n_{t}} \) and thus variations of a larger magnitude than those of \( A \), but the diagonalization procedure is more efficient. On the other hand its eigenvalues are varying in a smaller range than the eigenvalues of the total time ordered product \( \prod_{l=1}^{n_{r_{\tau}}} B_l \). By finding the most appropriate ratio \( n_{r_{\tau}}/n_{t} \) we succeed to obtain the eigenvalues of \( A \) with the required precision and then taking the \( n_{r_{\tau}}/n_{t} \) power of them we obtain the \( \{\lambda_i\} \) and evaluate the expansions \((18)\) and \((17)\). Note that since the coefficients of the characteristic polynomials for \((18)\) and \((17)\) depend only on \( \lambda_i + \lambda_i^{-1} \), the above procedure, although introducing large variations in the \( \lambda_i \)'s themselves, does not lead to significant errors in the coefficients around half-filling. It is these coefficients which determine the behaviour of the smallest zeros of the GCPF and thus the phase structure of the model.

The physical observables are derived using eq.\((11)\). For a given configuration of Ising fields \( \{s_{i,l}\} \), the value of an operator \( O \) can be calculated
as a polynomial in the fugacity variable. Knowing the coefficient of each power of the fugacity in the $\tilde{z}$ expansion, one can then easily construct the corresponding coefficients for the contribution of this term to the observable by averaging each coefficient over the equilibrated ensemble. In this paper we measure only the expansion of the GCPF and hence we can predict the critical value of the chemical potential for which the relative weight of the the state with a finite doping fraction will be of the same order as the half-filled state. We expect that this prediction will be reflected in the behaviour of the hole occupation number and consistent with the critical values of $\mu$ obtained from an analysis of the complex zeros of the GCPF. Moreover, following the suggestion of Dagotto et al.\cite{dagotto1991} we evaluate the energy gap between the one pair state and the half-filled state.

3. Simulations and measurements

The simulation procedure is based on the algorithm described by White et al.\cite{white1992}. We use Metropolis algorithm for updating the configurations of Ising variables. Here we describe the procedure for the half-filling updating. (For clarity, we omit the spin labels in the following.) The generalization for the finite $\mu_0$ updating is straightforward.

The simulation starts from an arbitrary configuration for which we cal-
culate the equal-time Green’s function on a time slice $l$

$$G(l) = (I + P(l))^{-1} \tag{20}$$

where $P(l)$ is a time ordered product of the form

$$B_l...B_1B_{n_r}...B_{l+1} \tag{21}$$

To reduce the numerical errors in the evaluation of these products we apply the modified Gram-Schmidt (MGS) decomposition as proposed by White et al. [4]. Decomposing the products of each four matrices in (21) into a product of an orthogonal matrix, a diagonal one and an upper-triangular matrix whose diagonal elements equal to one enables us to deal with large variations in the matrix elements. The inversion of the $(I + P(l))$ appearing in the r.h.s. of (20) is also simplified by the MGS procedure. Once the equal-time propagator is evaluated on a time-slice $l$ we flip one of the spins $s_{i,l}$ and and accept the new configuration with respect to the ratio of the new and old statistical weights, defined as:

$$\frac{\text{det}M'^2}{\text{det}M^2} \times e^{\lambda \delta(s_{i,l})} \tag{22}$$

where $\delta(s_{i,l})$ is the difference in the potential term due to the flipped spin.

This ratio is determined by the value of the equal-time Green’s function (by its diagonal term corresponding to the flipped spin) and by a matrix $\Delta$
with only one nonzero element:

$$\Delta(i, l)_{j,k} = e^{-2dt\lambda s_i} \delta_{i,j} \delta_{j,k}$$  \hspace{1cm} (23)

If the new configuration is accepted we calculate the new Green’s function $G(l)'$ corresponding to this configuration using:

$$G(l)' = G(l) - \frac{1}{R} \times G(l) \Delta(i, l)(I - G(l))$$  \hspace{1cm} (24)

with

$$R = \frac{\text{det} M'}{\text{det} M} = 1 + (1 - G_{ii}) \Delta(i, l)_{ii}$$  \hspace{1cm} (25)

The nonlocal impact of the updated configuration is represented in the new Green’s function by eq. (24).

When the updating of the Ising fields on the $l$-th time-slice is completed we move to the next time slice using the relation:

$$G(l + 1) = B_{l+1} G(l) B_{l+1}^{-1}.$$  \hspace{1cm} (26)

Following the suggestion of [4], we evaluated the Green’s function from scratch every four time steps. This procedure is very time consuming, but is required in order that the numerical errors accumulated using eq. (26) are kept under control. Since the hopping term in the Hamiltonian is constant, the construction of the Green’s function from scratch reduces to a redefinition of the interaction matrix $e^{dtV}$ on each time-slice due to the updated Ising
fields. The computational effort involved in this procedure is minor as $V$ is a diagonal matrix and its exponentiation is fast. The hopping part is exponentiated only once at the start of the simulation procedure. Instead of using the checkerboard decomposition suggested by White et al., we expanded $e^{-dtK}$ taking advantage of its sparseness. Since this expansion is performed only once it can be done up to an arbitrary high order. We checked that taking a 10-th order expansion provided us with sufficiently high precision for the parameters used in the simulations described below.

4. Results and conclusions

The expansion coefficients of the GCPF as a polynomial in the fugacity variable were calculated at several values of the inverse temperature $\beta$ with the Coulomb repulsion fixed at $U = 4t$ (see eq.(1)). We present results obtained from simulations performed at half-filling and at chemical potential $\mu_0 = 0.9$. The spatial size of the lattice is $4^2$ throughout apart from one simulation at half-filling on a $10^2$ lattice at $\beta = 10.0$.

**Half-filling results:** The half-filling simulation was performed at $\beta = 0.3, 1.2, 2.5, 5.0$ and $10.0$ with $n_\tau = 4, 16, 20, 40$ and $80$ respectively. The euclidean time-spacing $dt$ was varied to check the numerical stability of the simulations and to allow comparison with the results of other groups [14].
The number of configurations required to get sufficiently low errors in the expansion coefficients is, in general, greater than 2000 and increases with \( \beta \).

The particle-hole symmetry is manifested via the equality between the coefficients of \( e^{\mu n \beta} \) and \( e^{-\mu n \beta} \). This symmetry follows directly from eqs. (16,17).

The \( z_n = < b_n > \) coefficient corresponds to the contribution of the \( n \)-hole state to the GCPF (canonical partition functions)\(^3\) and \( z_0 \) is the canonical partition function for the half-filled state. The latter is obtained with low error after a small number of measurements. The higher order coefficients require averaging over a larger number of configurations. For \( \beta \leq 5 \) all the \( 2(n_x n_y)^2 + 1 \) averaged coefficients were found to be positive.

As we extend our treatment to larger values of \( \beta \), negative coefficients appear in the expansion of the GCPF, but with large errors. Note that the coefficients arising from a single configuration do not have to be positive, as only the ensemble averages are identified as the canonical partition function at a given particle number. However, the low temperature simulation at half-filling does lead to a high variation of the coefficients in different field configurations and thus to the high errors. This is because updating at \( \mu = 0 \) minimizes the fluctuations in only \( z_0 \) (half-filling) which dominates the statistical weight at high \( \beta \). The large variations in these coefficients
indicates that this statistical weight, namely the determinant at $\mu_0 = 0$, becomes inefficient as $\beta$ gets large. A more appropriate choice is to update at $\mu_0 \neq 0$.

**Simulations at $\mu_0 \neq 0$:** We performed our simulations at $\mu_0 = 0.9$ and updated with respect to the absolute value of the weight function as described in the previous section at $\beta = 2.5, 3.5, 5.0, 5.4, 6.0$ and $7.5$ with $n_\tau = 20, 40, 40, 72, 48$ and $60$ respectively. In this simulation the value of the GCPF at $\mu_0$ is the average sign of $\det(M^+ \cdot \det(M^-)$. This requirement provides a useful check as to our numerical accuracy in extracting the coefficients of the characteristic polynomial. At $\beta = 2.5$ and $\beta = 5.0$, we compared the results of these simulations with those performed at half-filling updating and found that the normalized coefficients are equal within the statistical error.

In Table 1 and Fig.1 we present the expansion coefficients based on eq. (17) obtained from simulations performed either at half-filling or at updating chemical potential $\mu_0 = 0.9$. The normalization of the GCPF is chosen such that $Z(\mu = 0) = 1$. Our results are consistent with those obtained by Moreo et al. [14].

Fig.1 shows the coefficients $z_n$ ($n = 0, 1, 2, 3$) as a function of $\beta$, with normalization such that the GCPF $Z(\mu = 0) = 1$. The general tendency is
a sharp decrease of the coefficients with higher occupation number.

Figs. 2 and 3 show the hole density and the susceptibility respectively, as a function of the chemical potential. In these exploratory simulations, the coefficients corresponding to high occupation number are determined with large errors. However, the peak in the susceptibility at $\mu \approx 1.0$ is due to the low occupation levels which are determined with small errors. The structures at $\mu > 1.2$ do depend on the levels with large errors and require further investigation. As the temperature decreases the peak in the susceptibility sharpens significantly in the region $0.75 < \mu < 1.25$, especially for $\beta > 5.0$. At that $\beta$ the susceptibility does seem to signal some change in behaviour. This could be associated with the onset of a phase transition related to the occupation of holes. We explore this possibility further by analyzing the zeros of the GCPF in the complex fugacity plane.

We do this by finding the zeros of the averaged polynomial eq.(16). Since the large $n$ coefficients are evaluated with relatively low precision we checked the stability of the small zeros under truncation of the polynomial to $n = 4$. Table 2 gives the two smallest zeros for various values of the inverse temperature. In Fig.4 we plot these zeros of the partition function in the first quadrant of the complex $\mu$ plane. The zeros have the symmetries that
if $\mu$ is a zero, so also is $-\mu$ and their complex conjugates.

To a very good approximation, the imaginary part of these zeros of the partition function scales as $\frac{\pi}{\beta}$. For any finite value of $\beta$ the fugacity would remain negative yielding no phase transition in the physical region. However, at zero temperature ($\beta = \infty$) the $\text{Im}(\mu_c)$ vanishes and a phase transition may be possible. To extrapolate to the low temperature behaviour of the zeros we note an almost linear dependence between the imaginary part of the lowest zero and its real part, for values of $\beta \geq 5$. The linear fit of these zeros is shown in Fig.5. To clarify this point we show in Fig.6 the linear fit of $\text{Re}(\mu) \times \beta$ vs. $\beta$ in the same region of $\beta$. The lowest zero at $\beta = 2.5$ and 3 does not exhibit this scaling behaviour. Measuring the lowest zero of the partition function at high temperatures ($\beta = 0.3$ and $\beta = 1.2$) we find that the real parts of the zero to be 3.0 and 0.721 respectively with imaginary part $\frac{\pi}{\beta}$. The above is consistent with the lowest zero, $\mu_c$, scaling such that $\text{Re}(\mu_c) \times \beta$ is constant in the high temperature regime. At lower temperatures, $\beta = 2.5 - 3$, there is a crossover region into the low temperature regime where

$$\text{Re} \mu_c = -2.5/\beta + 1.1.$$  \hspace{1cm} (27)

This qualitative distinction between the high and low temperature regimes arises from a clear difference in the relative contributions of the finite particle
number states to the grand canonical partition function (see Table 1). In the high temperature regime the first two canonical partition functions are of the same order as the half-filled level and hence the corresponding states are excited even at zero chemical potential. On the other hand, these states in the low temperature GCPF are only excited by non-zero chemical potential. Based on the above observations, we conclude that there is the possibility of a phase transition at zero temperature and $\mu_c \approx 1.1$ but that no signal has been found for a phase transition at $T > 0$. Of course, the above simulations have been performed on a small system. There may well be large finite volume effects.

The above conclusion - that there may be a phase transition at zero temperature - will not alter if the lowest zero in the fugacity plane remains real (and hence necessarily negative). If there is a phase transition at nonzero temperature, then some complex zeros must be in the complex fugacity plane with $\text{Re}(e^{\mu_\beta}) > 0$ and pinch the positive real axis in the infinite spatial volume limit. No signal of the possible onset of this mechanism was observed on the $4^2$ lattice, i.e. no zeros were found in the first or fourth quadrants of the complex $e^{\mu_\beta}$ plane.

As we increase the spatial lattice size we should therefore observe either an
increase in the density of zeros adjacent to, or on, the negative real fugacity axis or, if the alternative mechanism is masked by finite size effects on the $4^2$ lattice, a migration of zeros to the $\text{Re}(e^{i\beta}) > 0$ complex half-plane. It is also important to confirm the scaling behaviour of eq. (27) for the lowest zero. Zeros adjacent to this one should also scale in an analogous manner with the temperature so that there is a well defined locus of zeros in the zero temperature limit. We intend to extend our simulations to $6^2$ and $8^2$ spatial lattices.

The absence of a critical positive fugacity above zero temperature can be interpreted in part as a realization of the Mermin-Wagner theorem [15], which claims absence of magnetic ordering in two dimensional spin systems at non-zero temperature. This theorem is in particular relevant to HTSC models based on the Heisenberg antiferromagnetic Hamiltonian resulting in the strong coupling treatment of the Hubbard model. If the isotropy of Heisenberg antiferromagnet is violated, e.g. by an interlayer interaction, the conditions of the theorem do not hold, thus relating the vanishing critical temperature for the superconductivity to the isotropy of the effective nearest neighbours coupling[16]. The 2D Hubbard model with effective interlayer interaction was recently studied by M. Frick et al. using the Projector Monte
Carlo technique[17],[18]. Their results show some evidence for HTSC. We note that the analysis described in our work can also be applied to the extended Hubbard model including effective interlayer interactions.

Finally, following the suggestion of Dagotto et al. [3] we calculate the binding energy of holes. The energy gap between the two and one-hole ground states, $E_2 - E_1$, is given by the slope of the linear fit to the ratio $\log \frac{z_2}{z_1}$ vs. $\beta$ (see Figs.7,8). Fig.7 presents the fit for the data in the range $2.5 \leq \beta \leq 7.5$ while, in Fig.8, we fit only the results for $\beta \geq 5.0$ in the light of the discussion above. The first fit shows an energy gap of $0.87 \pm 0.02$ which is very close to the result of Dagotto et al. $(0.88 \pm 0.02)[20]$. The energy gap obtained from the second fit is $0.85 \pm 0.02$. Analogous fits, (Figs.9,10), for $\log \frac{z_1}{z_0}$ vs. $\beta$ give the energy gap between the ground state with one hole and the corresponding state at half-filling, $E_1 - E_0$. The fits give $E_1 - E_0 = 0.83 \pm 0.02$ and $0.95 \pm 0.02$ respectively. The binding energy of holes is given by the difference

$$(E_2 - E_1) - (E_1 - E_0).$$

Thus the first fit yields positive binding energy with no pair creation expected while the latter suggests a binding energy of $-0.1$. Since this derivation of the energy gaps is valid only in the low temperature regime, which is distinct from the high temperature one, the second fit seems to be more appropriate.
We note that we have not included the spin wave contribution to the ratio of the canonical partition functions $z_1$ and $z_0$, since at low temperature, the spin wave contribution should become small. The result of our low temperature fit is close to that obtained by Dagotto et al. ($E_1 - E_0 = 0.98 \pm 0.02$). However, their fit included lower $\beta$ data thus requiring a spin wave contribution. Inclusion of a spin wave contribution to our canonical partition function at half-filling would raise the estimate of the one-hole ground state energy even higher, thus increasing the binding energy.

We conclude with suggested extensions of the above method. The predicted zero temperature phase transition can be confirmed by a lower temperature study. With this in mind, simulations at $\beta = 12 \ (n_r = 160)$ are under current investigation. A study of the finite size effects, in particular, the scaling properties of $\text{Im}(\mu_c)$ as a function of the volume is also necessary. It is also important to perform longer simulations in order that the analysis can be extended to larger values of the chemical potential. One can also generalize the method described above to derive polynomial expansions in the fugacity variable for other physical observables and thus extend the study of the nature of the phase transition and of its possible relevance to high $T_c$ superconductivity. This study would involve examining the persistence of
the antiferromagnetic order into the finite doping region\textsuperscript{19}.

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20. All the energies are given in units of the hopping parameter $t$—see Eq. (1).
Table 1.

| $\beta$ | $z_0$ | coeff. | err. | $z_1$ | coeff. | err. | $z_2$ | coeff. | err. | $z_3$ | coeff. | err. |
|---------|-------|--------|------|-------|--------|------|-------|--------|------|-------|--------|------|
| 0.3     |       | 0.171  | 2.E-4| 0.156 | 1.5E-4|      | 0.119 | 3.E-4  | 0.074 | 6.E-5 |
| 1.2     |       | 0.297  | 0.001| 0.223 | 2.E-4  |      | 0.097 | 4.E-4  | 0.025 | 2.5E-4|
| 2.5     |       | 0.477  | 0.002| 0.220 | 0.001  |      | 0.039 | 5.E-4  | 0.003 | 8.E-5 |
| 3.0     |       | 0.575  | 0.016| 0.189 | 0.002  |      | 0.022 | 1.E-4  | 0.001 | 1.E-5 |
| 5.0     |       | 0.872  | 0.005| 0.063 | 0.002  |      | 0.001 | 2.E-4  | 5.E-6 | 3.E-6 |
| 5.4     |       | 0.901  | 0.061| 0.049 | 0.002  |      | 7.E-4 | 3.E-5  | 4.E-6 | 2.E-7 |
| 6.0     |       | 0.946  | 0.056| 0.027 | 0.001  |      | 2.E-3 | 1.E-5  | 6.E-7 | 4.E-8 |
| 7.5     |       | 0.986  | 0.063| 0.007 | 5.E-4  |      | 2.E-5 | 1.E-6  | 1.E-8 | 1.E-9 |
| $\beta$ | $Re\mu$ | $Im\mu$ | $(Im\mu) \times \beta$ |
|-------|---------|---------|------------------|
|       | Full    | Trunc.  | Full    | Trunc.  | Full    | Trunc.  |
| 2.5   | 0.526   | 0.464   | 1.257   | 1.257   | 3.141   | 3.141   |
|       | 0.821   | 0.731   | 1.257   | 0.952   | 3.141   | 2.380   |
| 3.0   | 0.582   | 0.538   | 1.047   | 1.047   | 3.141   | 3.141   |
|       | 0.764   | 0.749   | 1.047   | 0.819   | 3.141   | 2.457   |
| 5.0   | 0.609   | 0.607   | 0.628   | 0.628   | 3.140   | 3.140   |
|       | 0.775   | 0.818   | 0.628   | 0.628   | 3.140   | 3.140   |
| 5.4   | 0.627   | 0.625   | 0.582   | 0.582   | 3.143   | 3.143   |
|       | 0.884   | 0.820   | 0.572   | 0.477   | 3.089   | 2.576   |
| 6.0   | 0.685   | 0.680   | 0.524   | 0.524   | 3.144   | 3.144   |
|       | 0.801   | 0.848   | 0.524   | 0.453   | 3.144   | 2.718   |
| 7.5   | 0.768   | 0.785   | 0.380   | 0.397   | 2.850   | 2.978   |
|       | 0.990   | 0.872   | 0.310   | 0.419   | 2.325   | 3.142   |
Figure Captions

1. Fig.1 $z_0, z_1, z_2,$ and $z_3$ as a function of $\beta$. Their associated statistical errors are also shown if larger than the resolution.

2. Fig.2 Average hole density (doping fraction) as a function of $\mu$ for $\beta$ between 2.5 and 7.5:
   - $\beta = 2.5$ and 3 — solid lines
   - $\beta = 5.0$ — dashed line
   - $\beta = 5.4$ — dashed-dotted line
   - $\beta = 6.0$ — dotted line
   - $\beta = 7.5$ — solid line;

3. Fig.3 Susceptibility as a function of $\mu$ for $\beta$ between 2.5 and 7.5:
   - $\beta = 2.5$ and 3 — solid lines
   - $\beta = 5.0$ — dashed line
   - $\beta = 5.4$ — dashed-dotted line
   - $\beta = 6.0$ — dotted line
   - $\beta = 7.5$ — solid line;

4. Fig.4 Two smallest zeros of the GCPF in the first quadrant of the complex $\mu$ plane for $\beta$ between 2.5 and 7.5:
\[ \beta = 2.5 \text{ — white dotted squares} \]
\[ \beta = 3.0 \text{ — black crosses} \]
\[ \beta = 5.0 \text{ — white circles} \]
\[ \beta = 5.4 \text{ — black circles} \]
\[ \beta = 6.0 \text{ — black squares} \]
\[ \beta = 7.5 \text{ — white squares;} \]

5. Fig.5 \( \text{Im}(\mu_c) \) plotted against \( \text{Re}(\mu_c) \). The solid line is a linear fit for \( \beta \) between 5.0 and 7.5;

6. Fig.6 \( \text{Re}(\mu_c)\beta \) as a function of \( \beta \). The solid line is a linear fit for \( \beta \) between 5.0 and 7.5;

7. Fig.7 \( \log(z_2/z_1) \) as a function of \( \beta \). The solid line is a linear fit for \( 2.5 \leq \beta \leq 7.5 \);

8. Fig.8 \( \log(z_2/z_1) \) as a function of \( \beta \). The solid line is a linear fit for \( 5.0 \leq \beta \leq 7.5 \);

9. Fig.9 \( \log(z_1/z_0) \) as a function of \( \beta \). The solid line is a linear fit for \( 2.5 \leq \beta \leq 7.5 \);

10. Fig.10 \( \log(z_1/z_0) \) as a function of \( \beta \). The solid line is a linear fit for
$5.0 \leq \beta \leq 7.5;$
Table Captions

1. Table 1 Expansion coefficients of the GCPF for $\beta$ between 0.3 and 2.5. $z_0$ corresponds to the half-filling and $z_n$ to the $n$–hole coefficients.

2. Table 2 Smallest zeros of the GCPF in the complex $\mu$ plane for $\beta$ between 2.5 and 7.5. The zeros are obtained from the full polynomial and the truncated one (up to 4-hole coefficient), to check the numerical stability of the results.