Singularity of the density of states in the two-dimensional Hubbard model from finite size scaling of Yang-Lee zeros

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A finite size scaling is applied to the Yang-Lee zeros of the grand canonical partition function for the 2-D Hubbard model in the complex chemical potential plane. The logarithmic scaling of the imaginary part of the zeros with the system size indicates a singular dependence of the carrier density on the chemical potential. Our analysis points to a second-order phase transition with critical exponent $\frac{1}{2} = \frac{1}{2} \pm \frac{1}{4}$ which leads to a divergence of the electronic susceptibility. We interpret these results as reflecting singular behaviour of the density of states in the quasiparticle spectrum.

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I. INTRODUCTION

Quantum Monte Carlo techniques are widely applied in the investigation of the phase structure of the Hubbard model in an attempt to explore its relationship to high temperature superconductivity (HTSC). The pioneering works of Blankenbecler, Scalapino and Sugar [1] and Hirsch [2] outlined the finite-temperature Quantum Monte Carlo algorithms for treating systems of interacting fermions, thus allowing efficient numerical simulations of the model. These simulations showed remarkable stability for the half-filled model with on-site Coulomb repulsion, and could be extended to the doped case in the relatively high temperature regime. However, in the low-temperature and finite-doping regime, which is more relevant to HTSC, the simulations become less reliable due to the frequent appearance of field configurations with negative statistical weight, the so-called sign problem. This problem severely obscures numerical evaluation of thermodynamical averages of correlation functions and local condensates with subsequent difficulties in establishing the phase structure of the Hubbard model.

Barbour and Klepfish [3] explored an alternative method of detecting a phase transition in the Hubbard model. This method is based on the application of the general ideas of the Yang-Lee theorem [4] regarding the distribution of zeros of the grand canonical partition function in the complex fugacity plane. The theorem was originally proved for the Ising model and lattice gas[4]. Later extensions of this theorem include the case of higher-order Ising spins[5], Ising models with multiple spin interactions, the quantum Heisenberg model[6], the classical XY and Heisenberg models[6], and some continuous spin systems[8]. Recently, a generalization of the Yang-Lee theorem to the asymmetric first-order transition was made[9].

Following the Yang and Lee treatment, one identifies a phase transition by the appearance of zeros of the partition function in the complex chemical potential (μ) plane near the real axis, namely the physical region. For any finite system simulated on a lattice, these zeros will never be real. However, one may identify a group of zeros in the vicinity of the real axis which, if there is a phase transition, converge towards it as the system volume grows. The critical value of the chemical potential is thus the thermodynamic limit of the zero with the smallest imaginary part.

The 4² lattice simulations presented in Ref.[3] suggested that, from the scaling of the smallest zeros in the complex μ plane with the inverse temperature β, the two-dimensional single-band Hubbard model undergoes a phase transition only at zero temperature. This conclusion is in principle supported by the Mermin-Wagner theorem which states the absence of the off-diagonal long range order in two-dimensional systems at temperatures above zero [10]. However, it is not clear whether this theorem excludes any kind of phase transition in a doped two-dimensional Hubbard model. Therefore a thorough finite size analysis is required to validate or reject the above conclusion, as was pointed out in [11].

The distribution of zeros in the vicinity of the real axis, namely the angle of the zeros’ locus and the scaling of the location of these zeros in the complex plane, allows one to derive the critical exponents for the studied system [11], [12], [13]. This derivation is based upon the scaling hypothesis which is fundamental to the renormalization-group approach. In this work we apply the ideas developed in statistical mechanics models to investigate the criticalities in the Hubbard model of strongly correlated electrons.

One such criticality manifests itself through the macroscopic density of carriers. When the latter is derived by differentiating the free energy with respect to the chemical potential, it can serve as an indicator of a phase
transition controlled by the chemical potential. As in order-disorder transitions, one would expect a symmetry breaking signalled by an order parameter. In this model, the particle-hole symmetry is broken by introducing an “external field” which causes the particle density to become non-zero. Furthermore, the possibility of the free energy having a singularity at some finite value of the chemical potential is not excluded: in fact it can be a transition indicated by a divergence of the correlation length. A singularity of the free energy at finite “external field” was found in finite-temperature lattice QCD by using the Yang-Lee analysis for the chiral phase transition. A possible scenario for such a transition at finite chemical potential, is one in which the particle density consists of two components derived from the regular and singular parts of the free energy.

Since we are dealing with a grand canonical ensemble, the particle number can be calculated for a given chemical potential as opposed to constraining the chemical potential by a fixed particle number. Hence the chemical potential can be thought of as an external field for exploring the behaviour of the free energy. From the microscopic point of view, the critical values of the chemical potential are associated with singularities of the density of states. Transitions related to the singularity of the density of states are known as Lifshitz transitions. In metals these transitions only take place at zero temperature, while at finite temperatures the singularities are rounded. However, for a small ratio of temperature to the deviation from the critical values of the chemical potential, the singularity can be traced even at finite temperature. Lifshitz transitions may result from topological changes of the Fermi surface, and may occur inside the Brillouin zone as well as on its boundaries. In the case of strongly correlated electron systems the shape of the Fermi surface is indeed affected, which in turn may lead to an extension of the Lifshitz-type singularities into the finite-temperature regime.

In relating the macroscopic quantity of the carrier density to the density of quasiparticle states, we assumed the validity of a single particle excitation picture. Whether strong correlations completely distort this description is beyond the scope of the current study. However, the identification of the criticality using the Yang-Lee analysis, remains valid even if collective excitations prevail.

The paper is organised as follows. In Section 2 we outline the essentials of the computational technique used to simulate the grand canonical partition function and present its expansion as a polynomial in the fugacity variable. In Section 3 we present the Yang-Lee zeros of the partition function calculated on $6^2$ to $10^2$ lattices and highlight their qualitative differences from the $4^2$ lattice. In Section 4 we analyse the finite size scaling of the Yang-Lee zeros and compare it to the real-space renormalization group prediction for a second-order phase transition. Finally, in Section 5 we present a summary of our results and an outlook for future work.

II. SIMULATION ALGORITHM AND FUGACITY EXPANSION OF THE GRAND CANONICAL PARTITION FUNCTION

The model we are studying in this work is a two-dimensional single-band Hubbard Hamiltonian

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

(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, i.e. the actual chemical potential is shifted from $\mu$ to $\mu - \frac{U}{2}$.

The finite-temperature grand canonical partition function is given by

$$
Z = \text{Tr} \left( e^{-\beta \hat{H}} \right).
$$

(2)

Following Hirsch and White et al. we rewrite $Z$ as

$$
Z = \text{Tr} \prod_{l=1}^{n_{\tau}} \left( e^{-dt\hat{V}} e^{-dt\hat{K}} e^{dt\hat{N}} \right)
$$

(3)

where $\hat{K}$ corresponds to the nearest neighbour hopping term in the Hubbard hamiltonian and $\hat{V}$ to the on-site interaction including quartic products of fermion fields, and $\hat{N}$ to the particle number operator. This decomposition, based on the Trotter formula, introduces a systematic error proportional to $dt^2$. Thus $Z$ can be represented as a path integral of a 2+1-dimensional system where the range of the additional dimension (imaginary time) corresponds to the inverse temperature via $\beta = dt \times n_{\tau}$. The quartic interaction can be re-written in terms of Ising fields $s_{i,l}$ using the discrete HS transformation

$$
e^{-dt\hat{V}} = e^{-\frac{dtU}{2}} \sum_{s_{i,l}=\pm 1} e^{-dt s_{i,l} \gamma (n_{i+} - n_{i-})}
$$

(4)

where $i,l$ is the space-time index of a lattice site and the coupling $\gamma$ is related to the original on-site repulsion constant by

$$
cosh (dt\gamma) = \exp \left( \frac{dtU}{2} \right).
$$

(5)
This transformation 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

\[ Z = \sum_{\{s_i\} = \pm 1} \tilde{z} = \sum_{\{s_i\} = \pm 1} \text{det}(M^+) \text{det}(M^-) \]  

(6)
such that

\[ M^\pm = (I + P^\pm) = \left( I + \prod_{i=1}^{n_x} B^\pm_i \right) \]  

(7)
where the matrices \( B^\pm_i \) are defined as

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

(8)
with \( V_{ij} = \delta_{ij} s_i \) and \( K_{ij} = 1 \) if \( i, j \) are nearest neighbours and \( K_{ij} = 0 \) otherwise. The matrices in (7) and (8) are of size \((n_x n_y) \times (n_x n_y)\), corresponding to the spatial size of the lattice.

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

\[ < O >_{\mu} = \frac{\int O \tilde{z}(\mu) \, d\mu}{\int \tilde{z}(\mu) \, d\mu} = \frac{\sum_{\{s_i\}} O(\{s_i\}) \tilde{z}(\mu, \{s_i\})}{\sum_{\{s_i\}} \tilde{z}(\mu, \{s_i\})} \]  

(9)
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

\[ < O >_{\mu_0} = \frac{\int O \tilde{z}(\mu_0) \, d\mu_0}{\int \tilde{z}(\mu_0) \, d\mu_0} = \frac{\langle O \tilde{z}(\mu_0) \rangle_{\mu_0}}{\langle \tilde{z}(\mu_0) \rangle_{\mu_0}} = \langle \tilde{z}(\mu_0) \rangle_{\mu_0} \]  

(10)
The partition function \( Z(\mu) \) is given by

\[ Z(\mu) \propto \left\langle \frac{\tilde{z}(\mu)}{\tilde{z}(\mu_0)} \right\rangle_{\mu_0} . \]  

(11)
The angular brackets notation \( (<>_{\mu_0}) \) is to be understood here and in what follows as Monte Carlo integration with importance sampling based on the absolute value of the \( \tilde{z} \) calculated at an update chemical potential \( \mu_0 \). The normalization of \( Z \) is irrelevant as can be seen from eqn. (11).

It was shown in [3] that a unitary transformation equivalent to the particle-hole transformation allows the partition function to be represented as a power series in \( e^{\mu \beta} \) or \( e^{\mu \beta} + e^{-\mu \beta} \) whose powers are ranging between \([-n_x n_y, n_x n_y]\) or \([0, n_x n_y]\) respectively, where the coefficients of the first expansion are the canonical partition functions for a number of particles corresponding to the index \( n \), with \( n = 0 \) being the half-filling partition function. These coefficients are obtained by ensemble averaging of the following expansion of the statistical weight for each configuration

\[ \tilde{z}(\mu) = e^{\mu n_x n_y \beta} \sum_{n=-n_x n_y}^{n_x n_y} b_n e^{\mu \beta n} . \]  

(12)

or alternatively

\[ \tilde{z}(\mu) = e^{\mu n_x n_y \beta} \sum_{n=0}^{n_x n_y} a_n \left( e^{\mu \beta} + e^{-\mu \beta} \right)^n \]  

(13)
where the expansion coefficients in both these equations are obtained from the eigenvalues of the matrix \( P_{\mu=0} [3] \). Alternatively, each of these expansions can be done around the updating fugacity point, thus yielding for eqn. (13)

\[ \tilde{z}(\mu) = e^{\mu n_x n_y \beta} \sum_{n=0}^{n_x n_y} \bar{a}_n \left( e^{\mu \beta} + e^{-\mu \beta} - e^{\mu_0 \beta} - e^{-\mu_0 \beta} \right)^n \]  

(14)
with \( \mu_0 \) being the updating value of the chemical potential. A similar expression can be obtained for eqn. (12). The coefficient of the zeroth power in (14), normalised and averaged over the ensemble of the HS field configurations, is the average sign of the statistical weight calculated as

\[ < \text{sign} > = \frac{1}{N_c} \sum_{\{s_i\}} \tilde{z}(\mu_0) \]  

(15)
where \( N_c \) is the number of the HS field configurations accepted in the Monte Carlo integration. The statistical fluctuation in this coefficient reflects the sign fluctuations. The expansion for the partition function is then given by:

\[ Z(\mu) = e^{\mu n_x n_y \beta} \sum_{n=0}^{n_x n_y} \left\langle \tilde{a}_n \right\rangle_{\mu_0} \left( e^{\mu \beta} + e^{-\mu \beta} - e^{\mu_0 \beta} - e^{-\mu_0 \beta} \right)^n \]  

(16)

When the average sign is near unity, it is safe to assume that the lattice configurations reflect accurately the quantum degrees of freedom. Following Blankenbecler et al. [4] the diagonal matrix elements of the equal-time Green’s operator \( G^\pm = (I + P^\pm)^{-1} \) accurately describe the fermion density on a given configuration. In this regime the adiabatic approximation, which is the basis of the finite-temperature algorithm, is valid. The situation differs strongly when the average sign becomes small. We are in this case sampling positive and negative \( \tilde{z}(\mu_0) \) configurations with almost equal probability since the acceptance criterion depends only on the absolute value of \( \tilde{z}(\mu_0) \).
In the simulations of the HS fields the situation is different from the case of fermions interacting with dynamical boson fields presented in Ref. 1. The auxiliary HS fields do not have a kinetic energy term in the bosonic action which would suppress their rapid fluctuations and hence recover the adiabaticity. From the previous simulations on a $4^2$ lattice we know that avoiding the sign problem, by updating at half-filling, results in high uncontrolled fluctuations of the expansion coefficients for the statistical weight, thus severely limiting the range of validity of the expansion. It is therefore important to obtain the partition function for the widest range of $\mu_0$ and observe the persistence of the hierarchy of the expansion coefficients of $Z$. An error analysis is required to establish the Gaussian distribution of the simulated observables. We present in the following section results of the bootstrap analysis performed on our data for several values of $\mu_0$.

III. TEMPERATURE AND LATTICE-SIZE DEPENDENCE OF THE YANG-LEE ZEROS

The simulations were performed in the intermediate on-site repulsion regime $U = 4t$ for $\beta = 5, 6, 7.5$ on lattices $4^2, 6^2, 8^2$ and for $\beta = 5, 6$ on a $10^2$ lattice. The expansion coefficients given by eqn. (14) are obtained with relatively small errors and exhibit clear Gaussian distribution over the ensemble. This behaviour was recorded for a wide range of $\mu_0$ which makes our simulations reliable in spite of the sign problem. In Fig.1 (a-c) we present typical distributions of the first coefficients corresponding to $n = 1 - 7$ in eqn. (14) (normalized with respect to the zeroth power coefficient) for $\beta = 5 - 7.5$ for different $\mu_0$. The coefficients are obtained using the bootstrap method on over 10000 configurations for $\beta = 5$ increasing to over 30000 for $\beta = 7.5$. In spite of different values of the average sign in these simulations, the coefficients of the expansion (14) indicate good correspondence between coefficients obtained with different values of the update chemical potential $\mu_0$; the normalized coefficients taken from different $\mu_0$ values and equal power of the expansion variable correspond within the statistical error estimated using the bootstrap analysis. (To compare these coefficients we had to shift the expansion by $2 \cosh \mu_0 \beta$.)

We also performed a bootstrap analysis of the zeros in the $\mu$ plane which shows clear Gaussian distribution of their real and imaginary parts (see Fig.2). In addition, we observe overlapping results (i.e. same zeros) obtained with different values of $\mu_0$. The distribution of Yang-Lee zeros in the complex $\mu$-plane is presented in Fig.3(a-c) for the zeros nearest to the real axis. We observe a gradual decrease of the imaginary part as the lattice size increases. The quantitative analysis of this behaviour is discussed in the next section.

The critical domain can be identified by the behaviour of the density of Yang-Lee zeros’ in the positive half-plane of the fugacity. We expect to find that this density is temperature and volume dependent as the system approaches the phase transition. If the temperature is much higher than the critical temperature, the zeros stay far from the positive real axis as it happens in the high-temperature limit of the one-dimensional Ising model ($T_\epsilon = 0$) in which, for $\beta = 0$, the points of singularity of the free energy lie at fugacity value $-1$. As the temperature decreases we expect the zeros to migrate to the positive half-plane with their density, in this region, increasing with the system’s volume.

Figures 4(a-c) show the number $N(\theta)$ of zeros in the sector $(0, \theta)$ as a function of the angle $\theta$. The zeros shown in these figures are those presented in Fig.3(a-c) in the chemical potential plane with other zeros lying further from the positive real half-axis added in . We included only the zeros having absolute value less than one which we are able to do because if $y_i$ is a zero in the fugacity plane, so is $1/y_i$. The errors are shown where they were estimated using the bootstrap analysis (see Fig.2).

For $\beta = 5$, even for the largest simulated lattice $10^2$, all the zeros are in the negative half-plane. We notice a gradual movement of the pattern of the zeros towards the smaller $\theta$ values with an increasing density of the zeros near $\theta = \frac{\pi}{2}$ which is due to the increase of the lattice size. However, since no zeros are detected beyond this value of $\theta$ we can assume that $\beta = 5$ is too high a temperature for a phase transition.

At $\beta = 6$ we observe a qualitatively distinct behaviour for the two biggest lattice sizes ($8^2$ and $10^2$). The low-lying zeros are in the positive half-plane with angular density estimated as the slope of the linear interpolation between the points on the graphs of $N(\theta)$ for a given lattice size. These slopes increase with lattice size. Yet even the $10^2$ result extrapolated towards $\theta = 0$ yields a vanishing density of fugacity zeros on the positive real half-axis.

The $\beta = 7.5$ results show the density of zeros increasing with the simulation volume at small values of $\theta$. For the $8^2$ lattice the extrapolation of $N(\theta)$ gives a non-vanishing slope at zero angle. We interpret these results as signalling the existence of a criticality for this temperature. To obtain the scaling of the density of zeros near the positive half-axis we would have to extend the simulation to larger lattices (work which is currently in progress). On the basis of the existing results, we conclude that the system described in our simulations approaches criticality for the temperature corresponding to the lowest of our simulations, namely $\beta = 7.5$. We do not exclude the possibility that larger lattice simulations may show a phase transition for an even slightly higher temperature, as the $\beta = 6$ results indicate.
IV. FINITE SIZE SCALING AND THE SINGULARITY OF THE DENSITY OF STATES

As a starting point for the finite size analysis of the Yang-Lee singularities we recall the scaling hypothesis for the partition function singularities in the critical domain [11]. Following this hypothesis, for a change of scale of the linear dimension $L$

$$L \rightarrow \frac{L}{\lambda}$$

we obtain a transformation of the partition function

$$Z_L(\theta, \tilde{\mu}) = Z_{L/\lambda}(\theta_\lambda, \tilde{\mu}_\lambda)$$

(17)

where $\theta = (\tilde{T} - 1), \tilde{\mu} = (1 - \frac{\mu}{\mu_c})$ and $\theta_\lambda$ and $\tilde{\mu}_\lambda$ are the values of $\theta$ and $\tilde{\mu}$ under the rescaling transformation. This equation is correct up to a multiplication by an exponential stemming from the regular part of the free energy. In the scaling regime the following relationships hold

$$\theta_\lambda = \lambda^{\alpha_\theta} \theta$$

$$\tilde{\mu}_\lambda = \lambda^{\alpha_\mu} \tilde{\mu}$$

(18)

where $\alpha_\theta$ and $\alpha_\mu$ are the scaling exponents of the reduced temperature and reduced chemical potential respectively. While the $\lambda$ dependence of $\theta_\lambda$ and $\tilde{\mu}_\lambda$ expressed in the first two equations of the set (18) are correct for $\lambda \approx 1$, the third equation (in which $F_{\text{sing}}$ is the singular part of the free energy density), follows in general from the conservation of the partition function under the scaling transformation. Here and in what follows we assume that this transformation does not generate new couplings in the model. Hence, the zeros of $Z_L$ will be the same as the zeros of $Z_{L/\lambda}$.

Assume that the simulation temperature is sufficiently low to allow for a phase transition with respect to the chemical potential. In this case, the zeros of the grand canonical partition function will correspond to the zeros of a scaling function $Z$

$$Z_{L/\lambda}(\theta_\lambda^{\alpha_\theta}, \tilde{\mu}_\lambda^{\alpha_\mu}) = Z(\theta L^{\alpha_\theta}, \tilde{\mu}_L^{\alpha_\mu}) = 0.$$  

(19)

Solution of this equation determines the relationship between the reduced chemical potential and the temperature through a function $f_i$

$$\tilde{\mu}_i L^{\alpha_\mu} = f_i(\theta L^{\alpha_\theta})$$

(20)

where $i$ is the index of the root of the partition function. $\mu_c$ may vary with the temperature, and in particular we can regard $\mu_c(T_{\text{simulation}})$ as the critical chemical potential at the temperature of simulation. Thus, for $\theta = 0$ the previous equation becomes:

$$\tilde{\mu}_i L^{\alpha_\mu} = f_i(0)$$

(21)

which leads immediately to a determination of the exponent $\alpha_\mu$ from the logarithmic scaling of the zeros in the complex $\mu$ plane as

$$\log |\mu_L - \mu_c|_i = -\alpha_\mu \log L + \log f_i(0).$$

(22)

The notation of the last equation emphasizes the $L$-dependence of the chemical potential $\mu$.

The above derivation of the finite size scaling for the Yang-Lee zeros is a generalization of the ideas developed for a two-dimensional Ising model. In the present context, the essential difference between the Hubbard and Ising models, is in the phase boundary $T_c(\mu)$. We do not expect this difference to significantly alter the scaling relations with respect to the reduced chemical potential. For the Ising model the phase boundary in the $T - \mu$ plane is a straight line $\mu = \mu_c = 0$ (with the identification of $\mu$ as the external magnetic field). This line extends from $T = 0$ to $T = T_c$, with the latter being the critical temperature of a second-order phase transition. Below $T_c$ the phase transition with respect to the external field is first-order accompanied by the characteristic two-phase coexistence. We expect that for the Hubbard model the boundary will be given by a line parametrised as $T_c(\mu)$. As this line is not necessarily parallel to the $T$-axis, as one moves along either the $T$ or $\mu$ directions, the phase boundary will be crossed. Since the free energy is an analytic function on both sides of the boundary, the limits of its derivatives are independent of the path along which these limits are taken (as long as the boundary is not crossed). Therefore, we would expect the same order of singularity and phase transition with respect to either temperature or chemical potential.

In what follows we assume a transition weaker than a first-order one (an assumption supported by simulation results of Refs. [21], [22] for the 2D Hubbard model) although even for a first-order phase transition the finite-size scaling of the zeros is expected to be correct.

The critical exponent $\alpha_\mu$ is related to the average particle number via $\tilde{\mu}$ in the critical domain. We have to determine the relationship between $\alpha_\mu$ and $\delta$, where the latter is defined by

$$< n > \sim \tilde{\mu}^{\frac{1}{\nu}}$$

(23)

Following the real-space renormalization group treatment of Ref. [11] and assuming that the change of scale $\lambda$ is a continuous parameter, the exponent $\alpha_\theta$ is related to the critical exponent $\nu$ of the correlation length as $\alpha_\theta = \frac{1}{\nu}$. This result follows from the scaling of the correlation length $\xi$ as
\[
\xi(\theta \lambda) = \frac{\xi(\theta)}{\lambda}.
\]

(24)

Thus, iterating the scaling of \(\theta\) (Eq. 18) and reaching the point \(\lambda \approx \theta^{-\frac{1}{d}}\) we obtain

\[
\xi \sim |\theta|^{-\frac{1}{d\nu}} = |\theta|^{-\nu}.
\]

(25)

(The absolute value in the last equation corresponds to the points above and below \(T_c\).) Now recalling Eq. (18) and using the hyperscaling hypothesis (\(F_{\text{sing}} \sim \theta^{\nu d}\)) we find:

\[
F_{\text{sing}}(\theta, \tilde{\mu}) = |\theta|^{\nu d} F_{\text{sing}}(\pm 1, \frac{\tilde{\mu}}{|\theta|^{\nu \alpha}})
\]

(26)

where \(\theta \lambda\) has been scaled to \(\pm 1\) and \(\tilde{\mu}\lambda\) expressed in terms of \(\tilde{\mu}\) and \(\theta\). Differentiating this equation with respect to \(\tilde{\mu}\) yields:

\[
<n>_{\text{sing}} = (-\theta)^{\nu(d - \alpha\mu)} \frac{\partial F_{\text{sing}}(X, Y)}{\partial Y} \bigg|_{X = \pm 1}
\]

(27)

which determines the critical exponent of the particle density with respect to the reduced temperature as \(\nu(d - \alpha\mu)\). Substituting \(\theta \sim <n>_{\text{sing}}^{\frac{d - \alpha\mu}{\nu}(\mu - \mu_c)}\) into the argument \(Y = \frac{\tilde{\mu}}{|\theta|^{\nu \alpha \mu}}\) and demanding the hyperscaling \(\theta\)-dependence to be preserved in eqn. (26) we obtain:

\[
<n> \sim \frac{\tilde{\mu}}{|\theta|^{\nu \alpha \mu}}
\]

(28)

which defines the critical exponent \(\frac{1}{\beta} = \frac{d - \alpha\mu}{\nu\alpha\mu}\) in terms of the scaling exponent \(\alpha\mu\) of the Yang-Lee zeros.

Fig. 5 presents the scaling of the imaginary part of the \(\mu\) zeros for different values of the temperature. The linear regression slope of the logarithm of the imaginary part of the zeros plotted against the logarithm of the inverse linear dimension of the simulation volume, increases when the temperature decreases from \(\beta = 5\) to \(\beta = 6\). The results of \(\beta = 7.5\) correspond to \(\alpha\mu = 1.3\) within the errors of the zeros as the simulation volume increases from \(6^2\) to \(8^2\). As it is seen from Fig. 3, we can trace zeros with similar real part \((Re(\mu_1)) \approx 0.7\) which is also consistent with the critical value of the chemical potential given in Ref. [22] as the lattice size increases, which allows us to examine only the scaling of the imaginary part. Table 1 presents the values of \(\alpha\mu\) and \(\frac{1}{\beta}\) obtained from this figure.

| \(\beta\) | \(\alpha\mu\) | \(\frac{1}{\beta}\) |
|---------|---------|---------|
| 5       | 0.5 ± 0.05 | 3.0 ± 0.4 |
| 6       | 1.3 ± 0.2 | 0.5 ± 0.2 |
| 7.5     | 1.3 ± 0.3 | 0.5 ± 0.4 |

Table 1: The finite size scaling exponents and the critical exponent of particle-number singularity near criticality versus inverse temperature.

We also note that the location of the zeros corresponds to the singularity of the electronic susceptibility \(\chi\). In Fig. 6 we show \(\chi\), given by \(\chi = \frac{\partial \rho_{\text{reg}}}{\partial \mu}\), as a function of the chemical potential on an \(8^2\) lattice. The location of the peaks of the susceptibility, rounded by the finite size effects, is in good agreement with the distribution of the real part of the Yang-Lee zeros in the complex \(\mu\)-plane (see Fig. 3) which is particularly evident in the \(\beta = 7.5\) simulations (Fig. 4(c)). The contribution of each zero to the susceptibility can be singled out by expressing the free energy as:

\[
F = \sum_{i=1}^{2n_x n_y} (y - y_i)
\]

(29)

where \(y\) is the fugacity variable and \(y_i\) is the corresponding zero of the partition function. The dotted lines on these plots correspond to the contribution of the nearby zeros while the full polynomial contribution is given by the solid lines. We see that the developing singularities are indeed governed by the zeros closest to the real axis. The sharpening of the singularity as the temperature decreases is also in accordance with the dependence of the distribution of the zeros on the temperature.

The singularities of the free energy and its derivative with respect to the chemical potential, can be related to the quasiparticle density of states. To do this we assume that single particle excitations accurately represent the spectrum of the system. The relationship between the average particle density and the density of states \(\rho(\omega)\) is given by

\[
<n> = \int_0^\infty d\omega \frac{1}{1 + \frac{\omega - \mu - \mu_c}{\lambda}} \rho(\omega)
\]

(30)

which in the low-temperature regime \(\beta \to \infty\) becomes

\[
<n>_{\text{reg}} + <n>_{\text{sing}} = \int_0^\mu d\omega \rho(\omega)
\]

(31)

Assuming \(<n>_{\text{sing}}\) dependence upon the chemical potential as \(<n>_{\text{sing}} = (\mu - \mu_c)^{1/\delta}\) one obtains the zero-temperature approximation for the density of states as the particle susceptibility \(\chi\), namely

\[
\chi_{\text{sing}} = \frac{d <n>_{\text{sing}}}{d\mu} = \rho_{\text{sing}}(\mu) \propto \frac{1}{\delta(\mu - \mu_c)^{\frac{1}{\delta}-1}}
\]

(32)

and hence the rate of divergence of the density of states.

As in the case of Lifshitz transitions the singularity of the particle number is rounded at finite temperature. However, for sufficiently low temperatures, the singularity of the density of states remains manifest in the free energy, the average particle density, and particle susceptibility [15]. The regular part of the density of states does not contribute to the criticality, so we can concentrate on the singular part only. Consider a behaviour of the type
\( \rho_{\text{sing}}(\omega) \propto (\omega - \mu_c)^{\beta - 1} \) for \( \omega > \mu_c \) and \( \rho_{\text{sing}}(\omega) = 0 \) for \( \omega < \mu_c \). The integral (31) will give in the region \( T << (\mu - \mu_c) \) the low-temperature leading order behaviour for the particle density:

\[
<n>_{\text{sing}} (\mu) \propto (\mu - \mu_c)^{\beta}.
\]

with the value \( \delta \) for the particle number governed by the divergence of the density of states (at low temperatures) in spite of the finite-temperature rounding of the singularity itself. This rounding of the singularity is indeed reflected in the difference between the values of \( \alpha_\mu \) at \( \beta = 5 \) and \( \beta = 6 \).

\[ \text{V. DISCUSSION AND OUTLOOK} \]

We note that in our finite size scaling analysis we do not include logarithmic corrections. In particular, these corrections may prove significant when taking into account the fact that we are dealing with a two-dimensional system in which the pattern of the phase transition is likely to be of Kosterlitz-Thouless type [23]. The logarithmic corrections to the scaling laws have been proven essential in a recent work of Kenna and Irving [24]. Inclusion of these corrections would allow us to obtain the critical exponents with higher accuracy. However, such analysis would require simulations on even larger lattices.

The linear fits for the logarithmic scaling and the critical exponents obtained, are to be viewed as approximate values reflecting the general behaviour of the Yang-Lee zeros as the temperature and lattice size are varied. Although the bootstrap analysis provided us with accurate estimates of the statistical error on the values of the expansion coefficients and the Yang-Lee zeros, the small number of zeros obtained with sufficient accuracy does not allow us to claim higher precision for the critical exponents on the basis of more elaborate fittings of the scaling behaviour. The finite-size effects may still be significant, especially as the simulation temperature decreases, thus affecting the scaling of the Yang-Lee zeros with the system size. Larger lattice simulations will therefore be required for an accurate evaluation of the critical exponent for the particle density and the density of states. Nevertheless, the onset of a singularity at finite temperature, and its persistence as the lattice size increases, are evident.

The estimate of the critical exponent for the divergence rate of the density of states of the quasiparticle excitation spectrum is particularly relevant to the high \( T_c \) superconductivity scenario based on the van Hove singularities [23, 25, 27]. It is emphasized in Ref. [25] that the logarithmic singularity of a two-dimensional electron gas can, due to electronic correlations, turn into a power-law divergence resulting in an extended saddle point at the lattice momenta \((\pi,0)\) and \((0,\pi)\). In the case of the density of states diverging as the \( -\frac{1}{2} \) power, this singularity leads to a weak-BCS mechanism for superconductivity with \( T_c \) set at \( \approx 100K \) [28]. The extended saddle point behaviour has been confirmed by experimental results and numerical calculations [25, 26, 27, 28]. In numerical simulations the extended saddle point can be traced by a reconstruction of the quasiparticle spectral weight function from the simulation data on the Matsubara Green’s functions. This procedure requires solving an ill-posed inverse problem [23, 25] and is highly sensitive to the finite-doping simulation difficulties. The results obtained so far, cannot provide a quantitative description of the singularity. The Yang-Lee analysis, however, provides a scheme for a direct evaluation of the critical exponents.

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**Figure Captions**

**Figure 1**
Bootstrap distribution of normalized coefficients for expansion (14) at different update chemical potential $\mu_0$ for an $8^2$ lattice. The corresponding power of expansion is indicated in the top figure. (a) $\beta = 5$, (b) $\beta = 6$, (c) $\beta = 7.5$.

**Figure 2**
Bootstrap distributions for the Yang-Lee zeros in the complex $\mu$ plane closest to the real axis. (a) $10^2$ lattice at $\beta = 5$, (b) $10^2$ lattice at $\beta = 6$, (c) $8^2$ lattice at $\beta = 7.5$.

**Figure 3**
Yang-Lee zeros in the complex $\mu$ plane closest to the real axis. (a) $\beta = 5$, (b) $\beta = 6$, (c) $\beta = 7.5$. The corresponding lattice size is shown in the top right-hand corner.

**Figure 4**
Angular distribution of the Yang-Lee zeros in the complex fugacity plane. Error bars are drawn where estimated. (a) $\beta = 5$, (b) $\beta = 6$, (c) $\beta = 7.5$.

**Figure 5**
Scaling of the imaginary part of $\mu_1$ ($Re(\mu_1) \approx 0.7$) as a function of lattice size. $\alpha_{mn}u$ indicates the the fit of the logarithmic scaling.

**Figure 6**
Electronic susceptibility as a function of chemical potential for an $8^2$ lattice. The solid line represents the contribution of all the $2n_xn_y$ zeros and the dotted line the contribution of the six zeros nearest to the real-$\mu$ axis. (a) $\beta = 5$, (b) $\beta = 6$, (c) $\beta = 7.5$. 

