We have studied the t-J model using the Green Function Monte Carlo technique. We have obtained accurate energies well converged in the thermodynamic limit, by performing simulations up to 242 lattice sites. By studying the energy as a function of hole doping we conclude that there is no phase separation in the physical region, relevant for HTc superconductors. This finding is further supported by the hole-hole correlation function calculation. Remarkably, by approaching the phase separation instability, for \( J_c/t \sim 0.5 \), this function displays enhanced fluctuations at incommensurate wavevectors, scaling linearly with the doping, in agreement with experimental findings.

The simplest model taking into account spin interactions and hole kinematics is the \( t-J \) model \[1\]

\[
H = J \sum_{\langle i,j \rangle} (S_i \cdot S_j - \frac{1}{4} n_i n_j) - t \sum_{\langle i,j \rangle,\sigma} (c_i^\dagger c_j + h.c.),
\]

where \( c_{i\sigma} \) creates an electron of spin \( \sigma \) on the site \( i \), \( n_i \) and \( S_i \) being the electron number and spin operators respectively. Double occupations are not allowed and summations are extended to nearest neighbors.

Following \[4\], whenever the ground state energy per hole \( e_h(\delta) \) as a function of the doping \( \delta \)

\[
e_h(\delta) = (e(\delta) - e_0)/\delta
\]

has a minimum for a non zero value of \( \delta = x_c \) phase separation (PS) is energetically stabilized. In fact, by using the Maxwell construction, a macroscopic gain in energy can be obtained by phase separating the holes at all doping \( \delta < x_c \) in a hole rich phase with \( \delta = x_c \) and a fully AF region without holes with energy \( e_0 = -1.16944(4)J \) \[4\].

Many authors \[4,7–10\] have tried to clarify the important issue of PS by using numerical techniques. Calculations of exact ground state energies on small lattice sizes \[8\] do confirm the existence of PS at physical \( J/t \) and doping, but the sizes considered are far to be representative of the thermodynamic limit, where the question is meaningful. By contrast, using the high temperature expansion (HTE), PS was found only for large \( J/t \) \[1\].

Much more information, not only on PS, can be obtained by studying the behavior of the hole - hole correlation function:

\[
N(q) = \frac{1}{L} \sum_{i,j} e^{i q (R_i - R_j)} (1 - n_i)(1 - n_j)
\]

where \( L \) is the number of lattice sites. The onset of PS is characterized by the divergence of \( N(q) \) for small momenta \( q \). According to the HTE \[12\], \( N(q) \) displays some interesting feature at twice the spinless fermion Fermi vector but no PS in the physical region. These results are not affected by small size effects but are obviously limited by the difficulty of extrapolating an high temperature series to zero temperature.

In this letter we tackle the PS problem by the lattice Green Function Monte Carlo (GFMC) technique. This method allows to filter out from a given trial wavefunction \( |\psi_T\rangle \) the ground state \( |\psi_0\rangle \) of \( H \) by statistical application of the power method:

\[
|\psi_0\rangle \propto (\Lambda - H)^n |\psi_T\rangle,
\]

where \( \Lambda \) is a suitably large constant required to allow convergence to the ground state for large \( n \). In this scheme a Markov process is defined, acting on electron configurations \( \{ x \} \) with definite positions and spins, which are changed according to the Green Function \( G_{x'x} = \Delta \delta_{x',x} - H_{x'x} \) \[3\]. The algorithm is efficient even for large system size, provided all the \( G_{x'x} \) are non negative, otherwise one is facing the well known ”sign problem”. For the diagonal elements the above condition can be easily fulfilled by increasing \( \Lambda \). However an exceedingly large value of \( \Lambda \) -which is often the case especially for fermions- determines a slowing down of the algorithm, since there is a very small probability \( \sim 1/\Lambda \) to accept a new configuration \( x' \) and the algorithm remains almost always stacked in the old one \( x \). Thus one needs much more power iterations \( \langle 4 \rangle \) to generate statistically independent configurations. In order to overcome this difficulty, following \[4\], it is better to determine \textit{a priori} the number of diagonal moves before an off diagonal is accepted. Thus one can generate each time a new configuration without caring of a very large value of \( \Lambda \). A further improvement is to let \( \Lambda \rightarrow \infty \) with \( n = \Lambda \tau \), so that Eq. \[4\] becomes a more conventional imaginary time evolution by the operator \( e^{-H\tau} \). Further details of this technique will be given elsewhere.

The negative off-diagonal elements of the Green Function can be handled approximately by a recent achieve-
ment in GFMC: the fixed node technique (FN) for lattice Hamiltonians \[13\]. In order to control and improve the accuracy of the FN approximation in a systematic way, we have used a recent development, the GFMC with stochastic reconfiguration (GFMCSR) \[13\]. The GFMCSR results presented here have been obtained by keeping unchanged before and after each stochastic reconfiguration the energy, the kinetic energy and the nearest neighbor hole-hole correlation function. GFMCSR has to be implemented with a very large number $M$ of walkers in order to stabilize the simulation ($M \sim 2000 \div 4000$), whereas in the FN calculations $M = 800$ is by far sufficient to control the bias due to the finite walker population with the technique described in Ref. \[5\].

![FIG. 1. $e_h(\delta)$ computed with VMC (long dashed lines), FN (short dashed lines), GFMCSR (dotted lines) compared with the exact results \[20\] (full lines) for a 26 lattice size. Error bars are much smaller than the size of the symbols. Lines (guides to the eye) connect the two and four hole results.](image1)

A fundamental ingredient in GFMC is the choice of the guiding function in order to perform importance sampling, as described in \[5\]. At finite doping we have used a pure d-wave BCS guiding wave function \[16\] plus a long range density-density Jastrow factor \[19\]. At half filling instead we use the guiding function described in \[5\] that allows to obtain the exact answer for $e_0$, as there is no sign problem at zero doping for this particular guiding function. In the following we use the exact $e_0$ at the given size $L$ for all variational (VMC), FN and GFMCSR calculations of $e_h(\delta)$. Further we employ periodic boundary conditions tilted by 45 (\~{}11) degrees on square lattices with $L = 2l^2$ and odd integer $l \geq 5$ ($L = 26$).

We have compared our Monte Carlo calculations with the exact Lanczos results for the largest size $L = 26$ available in the literature \[20\]. We have found that the FN approximation improves the ground state energy of the best starting variational (and guiding) wavefunction by a factor of three (Fig. 1) and the GFMCSR by another similar factor, yielding finally an accuracy of less than 100K on the energy per hole, which is physically acceptable if compared with the low energy coupling of the model $J \sim 1500K$.

![FIG. 2. $e_h(\delta)$ computed with FN (dashed lines) and with GFMCSR (continuous lines) for $L = 50$ (triangles) and $L = 98$ (circles) at $J = 0.4t$. Lines are guides to the eye.](image2)

As shown in Fig. 1 this kind of accuracy depends weekly on the number of holes. However, for small lattices, the main difficulty to detect PS is the resolution in doping. By increasing the system size (see Fig. 2), the difference between FN calculation and the GFMCSR one remains of the same order, and much below the VMC energies. Thus we expect that the accuracy of the calculation is not very much size dependent, even for large systems where no exact solution is available. We remark that, as the accuracy of the calculation is improved from FN to GFMCSR, the minimum in the hole energy disappears for the largest size in Fig. 2. This suggests that the occurrence of PS at $J/t = 0.4$ and at this system size is an artifact of the FN. This approximation naturally enhances the tendency of PS because the FN acts only on the kinetic part of the Hamiltonian, thus implying a tendency to localize the holes. Nonetheless, as shown in Fig. 2, we have obtained, even within the FN, the stability of the uniform phase in the thermodynamic limit at $J/t = 0.4$. Thus we conclude that PS at this $J/t$ value is only a finite size effect.

![FIG. 3. $e_h(\delta)$ computed with FN for several lattice sizes.](image3)

Several authors \[7,8\] have used the infinite $L$ limit for $e_0$ even for the finite $L$ evaluation of $e_h(\delta)$. We have instead used the exact $e_0$ for each lattice size, and checked that for the largest size calculations both choices of $e_0$
lead to the same \( e_h(\delta) \). Indeed the small lattice size results are very sensitive at low doping to the particular choice of \( e_0 \), and this may explain the contradictory results presented in the literature so far. Moreover in Ref. 8 the most important and delicate low doping region is studied only with fairly small lattice sizes.

The absence of PS is also confirmed by the low momenta behavior of \( N(q) \), which will be discussed in the remaining part of this letter. In order to compute the ground state correlation functions \( N(q) \) we have used two different methods: the “forward walking technique” (FW) which allows the direct evaluation of the ground state expectation value, at the expense of very large error bars when the convergence to the ground state is particularly slow, as shown in 3; the second technique is based on Hellmann-Feynman theorem, and amounts to compute the ground state energy \( E(\lambda) \) of the Hamiltonian in presence of a small perturbation \( \lambda N(q) \), \( N(q) = \frac{d^2}{dq^2} E(\lambda) |_{\lambda=0} \), the derivative being estimated numerically by a few runs for different \( \lambda \)'s. The latter technique is much more stable, especially for large size, but each \( q \) value requires several simulations, whereas a single one is sufficient for the FW technique for all \( q \)'s. Thus we have used the more expensive method for the small \( q \) values where the FW convergence is more difficult, and we have checked the consistency of both methods in the remaining momentum region. Moreover the FW technique is limited to the FN approximation and has not been extended within the GFMCSR scheme yet. For the 26 site cluster the FN results for \( N(q) \) are accurate within 3%, as compared with the exact diagonalization data. Since this accuracy is already very good for determining the qualitative features of \( N(q) \), we have chosen to work within FN, avoiding to implement the much more expensive GFMCSR on large clusters.

In Fig. 3 the \( N(q) \) is plotted for several dopings and lattice sizes. Inside the PS region, at \( J = t \) (Fig. 3b), \( N(q) \) shows a divergent peak at small \( q \), as can be expected from general arguments. Instead for \( J = 0.4t \) (Fig. 3a) the charge correlations approach zero as \( q \to 0 \), confirming the absence of PS even at the lowest doping. Nevertheless enhanced fluctuations are clearly evident along the \((1, 1)\) and \((1, 0)\) directions. We believe that these incommensurate peaks are a genuine feature of the ground state of the model, because they do not appear for instance at the VMC level, and it is extremely important to use many power iterations 4 to eliminate the bias due to the VMC guiding wavefunction. The \( N(q) \) at this \( J/t \) value is very weakly size dependent, so that the overall shape of this function in the thermodynamic limit should not differ too much from the one shown in Fig. 3 (a). Thus \( N(q) \) should be always finite even for small \( q \), ruling out PS and charge density wave instability. Even though we found some peaks at incommensurate wavevectors, that maybe reminiscent of some dynamical stripe order, they are not consistent with a static stripe structure (the peaks should diverge).

In fact we tried to stabilize some static stripe order similarly to what was done within Density Matrix Renormalization Group (DMRG) 21, but in our approach the uniform phase remains always the most stable one at \( J/t = 0.4 \). The stabilization of the stripe phase with DMRG is probably due to the use of open boundary condition in one direction. We have not attempted to use open boundary condition as, i) the momentum is not defined on finite lattices, ii) it is more difficult to reach the thermodynamic limit, iii) the gap to the first excited state is much reduced, especially close to a PS instability, yielding a much slower convergence of the power method 4.

Remarkably, as \( \delta \) is increased the peak at finite momentum moves far from the \( \Gamma \) point at a distance that scales linearly with the doping with a coefficient which is surprisingly close to 4\( \pi \). This is exactly the coefficient obtained experimentally in \( La_{2-x}Nd_xSr_2CuO_4 \) 22. We have also found that this peak position does not depend on \( J/t \), implying that the 4\( \pi \delta \) slope could be a general feature of the \( t-J \) model in the region without PS. It
is reasonable to expect that the interaction of electrons with the ions could further enhance the intensity of this incommensurate peaks, leading not only to a qualitative but also to a quantitative agreement with experiments.

In conclusion we have performed accurate calculations of the ground state energy of the 2D $t-J$ model with three methods: VMC, FN and GFMC.$^\mathrm{CSR}$.

![Graph showing the low doping PS phase diagram of the $t-J$ model](image)

As summarized in the phase diagram picture (Fig. 5) we find no evidence of PS for $J \leq 0.4t$, at least for $\delta \geq 2.5\%$, which represents the smallest doping considered here (6 holes in a $L = 242$ sites), and a transition to the phase separated regime at a critical $J_c \sim 0.5t$. The small doping difference between FN and GFMC.$^\mathrm{CSR}$ for the occurrence of PS at $J = t$ strengthens the validity of the FN phase separation diagram. These results are in acceptable quantitative agreement with Ref. $^4$ but we believe that our calculation represents a much better attempt to control the finite size effects, which are very important, especially at small doping. Instead, in the large doping region, the best agreement is found with the exact diagonalization data $^4$ on small clusters. Close to PS we have computed the equal time charge correlations and enhanced fluctuations at incommensurate momenta have been found. The fact that the position of these peaks approach the $\Gamma$ point linearly with the doping cannot be explained within a simple model for the holes, like e.g. the spinless fermion one, as was proposed by $^2$ to explain the shape of $N(q)$ using HTE. In this case in fact the characteristic incommensurate wavevector $2k_F$ approaches the $\Gamma$ point in a much more singular fashion $2k_F \sim \sqrt{\delta}$. On the other hand the hard-core boson model is unable to produce any feature at momenta different from $\Gamma$. Further study is probably necessary to clarify this point. We emphasize however that, within the $t-J$ model, it is possible to reproduce the qualitative features of the experimental findings of incommensurate charge fluctuations, without i) electron-phonon coupling and ii) long range forces to push the $q = 0$ PS instability to finite $q$ value $^8$.

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