Hard-core bosons on the triangular lattice at zero temperature: A series expansion study

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(Received 10 October 2005; revised manuscript received 23 January 2006; published 1 May 2006)

We use high order linked cluster series to investigate the hard-core boson model on the triangular lattice, at zero temperature. Our expansions, in powers of the hopping parameter t, probe the spatially ordered "solid" phase and the transition to a uniform superfluid phase. At the commensurate fillings $n=\frac{1}{3},\frac{2}{3}$ we locate a quantum phase transition point at $(t/V)_c \simeq 0.208(1)$, in good agreement with recent Monte Carlo studies.

DOI: 10.1103/PhysRevB.73.172401 PACS number(s): 73.43.Nq, 75.50.Ee, 75.40.Gb

There is considerable interest at present in the physics of a system of hard-core bosons on the two-dimensional triangular lattice, described by the Hamiltonian

$$H = -t\sum_{\langle ij\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + V\sum_{\langle ij\rangle} n_i n_j - \mu\sum_i n_i, \tag{1}$$

where each lattice site can be occupied by 0 or 1 bosons ($n_i=0,1$). The first term represents hopping between nearest neighbor sites, the V term is a nearest neighbor repulsion, $n_i=a_i^\dagger a_i$, and μ is the chemical potential. This Hamiltonian also arises as a limiting case ($U=\infty$) of the so-called "Bose-Hubbard" model, where multiple occupancy is allowed, albeit at a cost in energy.

Interest is this model has arisen, in the main, because of the possibility of an exotic "supersolid" phase where long-range crystalline order and superfluidity may co-exist. Such a phase was conjectured over thirty years ago and has remained controversial and unobserved until, perhaps, very recently.[1] On the other hand evidence for supersolid phases has been found in lattice models of interacting hard-core bosons, and the possibility of experimental realizations with atoms in optical potentials[2] provides an exciting prospect of direct verification of the theoretical predictions.

As is well known, a lattice model of hard-core bosons with nearest-neighbor repulsion can be mapped directly to a spin-$\frac{1}{2}$ antiferromagnet, in general in the presence of a magnetic field. Techniques developed and used for the magnetic system can then be used to study the boson problem. The early work of Liu and Fisher[3] studied the phase diagram of the model, on a bipartite lattice, using the usual mean-field approximation, and showed the existence of a supersolid phase under certain conditions. More recently Murty *et al.*[4] have used first-order spin-wave theory to study the model on the two-dimensional triangular and kagome lattices, and also find a stable supersolid phase. These lattices are attractive candidates for exotic quantum phases because of frustration and low dimensionality, and the consequent enhancement of quantum fluctuations. Both of these studies[3,4] involve, however, approximations whose validity is difficult to judge.

A series of recent studies,[5–9] using quantum Monte Carlo methods, have confirmed the presence of a supersolid phase, albeit within a smaller range of parameters than predicted at the mean-field level. Of particular interest is the existence of a supersolid phase at and near half-filling ($n=\frac{1}{2}$), contrary to early expectations.[5]

Our goal in this paper is to investigate the ground state properties of the triangular lattice hard-core boson model via the technique of high-order series expansions,[10,11] an approach complementary to the Monte Carlo work. A particular advantage of the series approach is the ability to locate critical points reliably and accurately. Another advantage is that the infinite bulk lattice is treated directly and there are no finite size corrections to the series coefficients. To the best of our knowledge the hard-core boson problem has not previously been studied using this approach, although there has been some work on the Bose-Hubbard model without the nearest neighbor repulsion.[12]

As already mentioned above, the hard-core boson Hamiltonian has a particle-hole symmetry. Under the transformation $\bar{a}_i=a_i^\dagger$, $\bar{n}_i=1-n_i$ the Hamiltonian (1) becomes

$$\bar{H} = N\left(\frac{1}{2}zV-\mu\right) - t\sum_{\langle ij\rangle}(\bar{a}_i^\dagger\bar{a}_j + \bar{a}_j^\dagger\bar{a}_i) + V\sum_{\langle ij\rangle}\bar{n}_i\bar{n}_j - (zV-\mu)\sum_i \bar{n}_i \tag{2}$$

which, apart from a constant, is identical in form to the original. Here $z(=6)$ is the coordination number of the lattice. Thus the phase diagram is symmetric about the half-filled case $n=\frac{1}{2}$. Consequently our series for the commensurate filling $n=\frac{1}{3}$ are unchanged for $n=\frac{2}{3}$, and we consider the two cases together.

It is also useful to display the equivalent spin Hamiltonian, obtained via the transformation

$$a_i \to S_i^-, \quad a_i^\dagger \to S_i^+, \quad n_i \to S_i^z + \frac{1}{2} \tag{3}$$

which yields, apart from a constant

$$H_{\rm spin} = V\sum_{\langle ij\rangle} S_i^z S_j^z - 2t\sum_{\langle ij\rangle}(S_i^x S_j^x + S_i^y S_j^y) - \left(\mu - \frac{zV}{2}\right)\sum_i S_i^z, \tag{4}$$

i.e., a Heisenberg model with an exchange anisotropy (XXZ model) in a magnetic field. A phase with $\langle S^z\rangle \neq 0$, $\langle S^x\rangle=0$ then corresponds to a solid phase or normal fluid, while a phase with nonzero magnetization in the x-y plane corre-

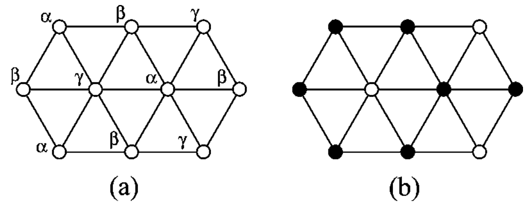

FIG. 1. (a) The three-sublattice decomposition of the triangular lattice; (b) Unperturbed configuration for $n=\frac{2}{3}$ (the filled circles represent occupied sites).

sponds to a superfluid (if $\langle S^z \rangle$ is uniform) or a supersolid (if $\langle S^z \rangle$ is spatially modulated).

The series expansion method is based on writing the Hamiltonian in the form

$$H = H_0 + \lambda H_1, \tag{5}$$

where H_0 is exactly solvable and H_1 is treated perturbatively. A linked-cluster approach[10,11] is the most efficient, permitting the series to be derived to quite high order. Here we take the nearest neighbor repulsion term as H_0, and the hopping term as the perturbation. The Hamiltonian (1) is particle conserving and hence the chemical potential term can be dropped in the calculations. For convenience we also set $V=1$ to fix the energy scale. The perturbation parameter is then $\lambda=-t$, and our series are obtained in powers of t. As the series are of finite length we are unable to effectively probe the large t region of the phase diagram. In magnetic language, our unperturbed state is a commensurate Néel type state, and x-y spin fluctuations are included perturbatively. We are unable to treat the superfluid/supersolid phases directly. Nevertheless, as we shall show, a great deal of useful information about the model can be obtained.

The triangular lattice can be decomposed into three equivalent sublattices, which we denote α, β, γ, as shown in Fig. 1(a). For filling $n=\frac{2}{3}$ the unperturbed ground state has two sublattices (say α and β) fully occupied and the third (γ) empty. This corresponds to a solid phase, with a density modulation with wave vector $\mathbf{k}=\left(\frac{4\pi}{3},0\right)$, and is shown in Fig. 1(b). It is also referred to as the $\sqrt{3}\times\sqrt{3}$ phase. Although the ground state is threefold degenerate, these do not mix in any finite order of perturbation theory and we can start from one of the partners. Turning on the hopping term allows particles to occupy the other sublattice, and at some critical value t_c the average sublattice occupancies will become equal. This represents the transition from solid to superfluid. An order parameter can be defined as follows:

$$m \equiv \langle n_\alpha \rangle - \langle n_\gamma \rangle = 3\langle n_\alpha \rangle - 2 \tag{6}$$

which equals 1(0) in the fully ordered (disordered) phase. The transition can also be located from the behavior of nearest neighbor correlators $C_{\alpha\beta} \equiv \langle n_\alpha n_\beta \rangle$, or from the static structure factor $S(\mathbf{k})$ at $\mathbf{k}=\mathbf{k}^*$, where $\mathbf{k}^*=\left(\frac{4\pi}{3},0\right)$ is the wave vector for the $\sqrt{3}\times\sqrt{3}$ phase. For $n=\frac{1}{3}$ a completely analogous treatment can be used, with the unperturbed ground state having one sublattice (say γ) fully occupied, and the other sublattices empty.

We turn now to our results, for the commensurate phase with $n=\frac{2}{3}$. The unperturbed ground state ($\sqrt{3}\times\sqrt{3}$) is shown in Fig. 1(b). The order parameter m [Eq. (6)] will decrease with increasing t, and, assuming a normal second order transition, will go to zero with a power law

$$m \sim (t_c - t)^\beta, \quad t \to t_c^-, \tag{7}$$

where β is a critical exponent.

We have computed a series expansion for m, up to order t^{12}. The series coefficients are given in Table I. Dlog Padé approximants and integrated differential approximants[13] have been used to analyze this series, with the resulting estimates

$$t_c = 0.21(1), \quad \beta = 0.09(1). \tag{8}$$

The estimate t_c=0.21 is consistent with the most recent Monte Carlo estimate[6] of 0.195±0.025. We are unaware of any previous estimate of the exponent β. The order and uni-

TABLE I. Series for ground state energy per site $E_0(t)$, order parameter m, difference of shortest correlator $C_{\alpha\beta}-C_{\alpha\gamma}$, and static structure factor S at $\mathbf{k}^*$ for the $n=2/3$ case. Nonzero coefficients t^n up to order $n=12$ are listed.

n	$E_0(t)$	m	$C_{\alpha\beta}-C_{\alpha\gamma}$	$S(\mathbf{k}^*)$
0	1.000000000	1.000000000	1.000000000	0.000000000
1	0.000000000	0.000000000	0.000000000	0.000000000
2	−1.000000000	−2.250000000	−2.750000000	1.500000000
3	−1.000000000	−4.500000000	−5.500000000	3.000000000
4	$-9.500000000\times10^{-1}$	-1.019750000×10^{1}	-1.052083333×10^{1}	8.168333333
5	−2.355555556	-3.750666667×10^{1}	-3.819305556×10^{1}	3.518166667×10^{1}
6	−7.937379630	-1.418886375×10^{2}	-1.498124375×10^{2}	1.428442162×10^{2}
7	-2.616389136×10^{1}	-5.619014174×10^{2}	-5.933175977×10^{2}	6.107654281×10^{2}
8	-9.005836612×10^{1}	-2.307990196×10^{3}	-2.428296319×10^{3}	2.667494106×10^{3}
9	-3.229654053×10^{2}	-9.596323715×10^{3}	-1.008214369×10^{4}	1.170747249×10^{4}
10	-1.201486606×10^{3}	-4.067064188×10^{4}	-4.264450526×10^{4}	5.234712003×10^{4}
11	-4.607510926×10^{3}	-1.750821492×10^{5}	-1.832564264×10^{5}	
12	-1.792870548×10^{4}	-7.572580451×10^{5}		

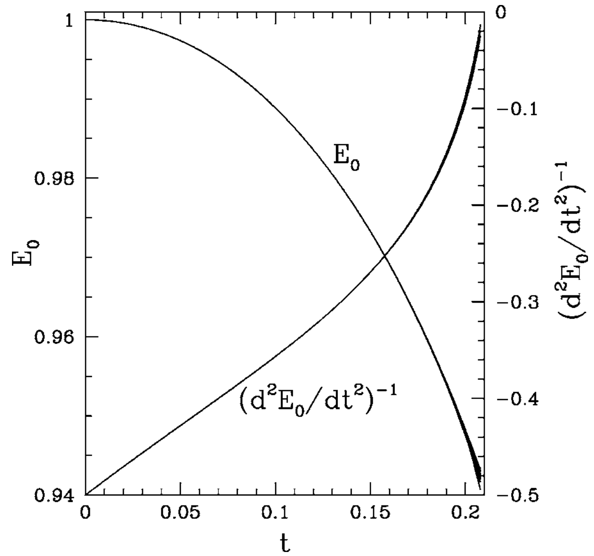

FIG. 2. The ground state energy per site E_0 and $(d^2E_0/dt^2)^{-1}$ versus t for $n=2/3$ filling. The results of several different integrated differential approximants to the series are shown.

versality class of this transition remains unclear. Our exponent estimate $\sim 0.09(1)$ is similar to that of the three-state Potts model in two dimensions ($\beta=1/9$). On the other hand the three-state Potts model in three dimensions is believed to have weak first-order transitions.

Another way of estimating the critical point is to compute the series for the ground state energy $E_0(t)$ and for the second derivative d^2E_0/dt^2 (analogous to a "specific heat"). This analysis is less precise, but the results are consistent with (8). In Fig. 2 we show E_0 and the inverse of the second derivative as functions of t, for $0<t\leq t_c$. The results of several different integrated differential approximants to the series are shown. The second derivative is seen to diverge at $t\sim 0.21$.

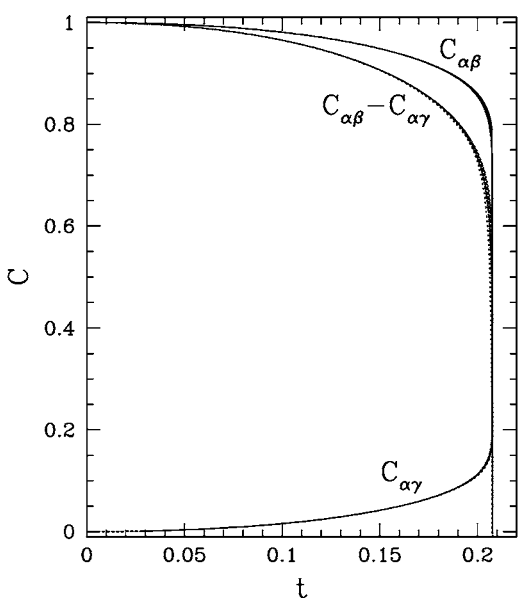

FIG. 3. The nearest neighbor correlators $C_{\alpha\beta}$ and $C_{\alpha\gamma}$ and their difference, versus t, for $n=2/3$ filling. Several different integrated differential approximants to the series are shown.

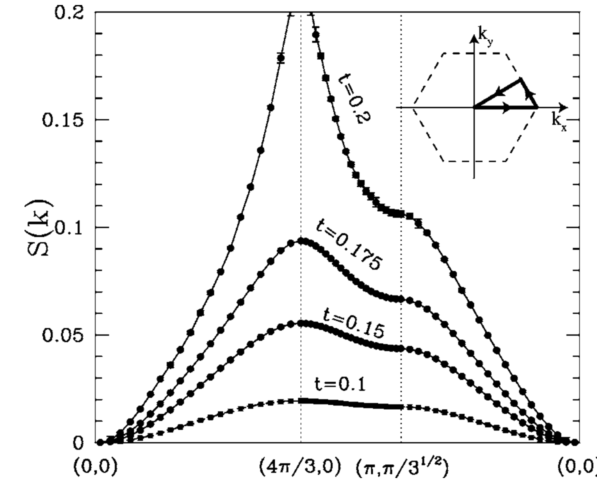

FIG. 4. The static structure factor $S(\mathbf{k})$ along high-symmetry cuts through the Brillouin zone for various t at $n=2/3$ filling. The inset shows the Brillouin zone, and path chosen.

We have also obtained series in t for the pair correlators $C_{ij}\equiv\langle n_in_j\rangle$. One such series is given in Table I)—we are happy to provide others on request. Figure 3 shows three curves, as functions of t: the nearest neighbor correlators $C_{\alpha\beta}$ and $C_{\alpha\gamma}$, and their difference. The difference $C_{\alpha\beta}-C_{\alpha\gamma}$ decreases from 1 as t increases, and vanishes at the critical point where all sublattices are equally occupied. This gives an independent estimate of t_c, consistent with (8).

Another quantity of interest is the static structure factor

$$S(\mathbf{k})=\frac{1}{N}\sum_{i,j}\left(\langle n_in_j\rangle-\langle n_i\rangle\langle n_j\rangle\right)e^{i\mathbf{k}\cdot(\mathbf{R}_j-\mathbf{R}_i)} \qquad (9)$$

This differs from the more usual definition (e.g., Ref. 5) by the subtraction of the second term, which is necessary to

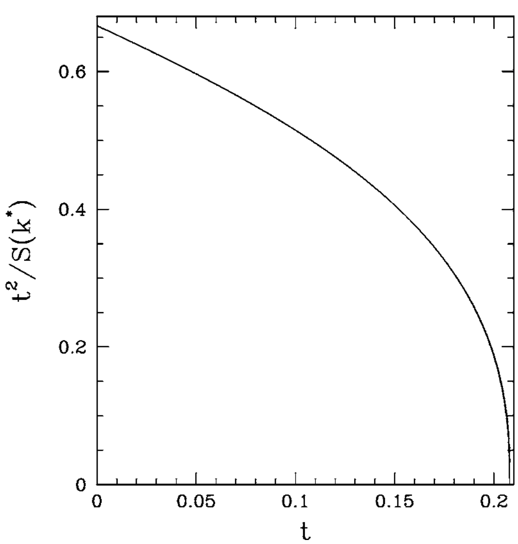

FIG. 5. The static structure factor $S(\mathbf{k}^*)$ versus t at $n=2/3$ filling. Several different integrated differential approximants to the series are shown. Since the series begins with a t^2 term we divide this out for convenience.

implement the linked cluster method efficiently. The effect of this term is to remove the δ-function peak at $\mathbf{k}=0$, and reduce it at the special wave vector $\mathbf{k}^*$. At the transition point t_c, where $\langle n_i \rangle$ is independent of the sublattice, the contribution of this second term vanishes, and our $S(\mathbf{k})$ is expected to show a δ-function peak at $\mathbf{k}^*$. This is confirmed in Fig. 4, where we show $S(\mathbf{k})$ curves along symmetry lines in the Brillouin zone for various t values.

At $\mathbf{k}=\mathbf{k}^*$, the Dlog Padé approximants to the series $S(\mathbf{k}^*)$ give a critical point estimate $t_c=0.208(3)$ with exponent $-0.40(3)$. To obtain a more accurate estimate of $S(\mathbf{k}^*)$ versus t, we use integrated differential approximants to the series $[S(\mathbf{k}^*)]^{-2.5}$ (which vanishes linearly at t_c). The result is shown in Fig. 5, from which we can locate the critical point more accurately, at $t_c=0.208(1)$.

In summary, we have successfully used series methods to investigate the commensurate $n=1/3,2/3$ phases of the hard-core boson model with nearest neighbor repulsion, on the triangular lattice. The ground state energy, order parameter, nearest neighbor correlators, and static structure factor all give consistent indications of a quantum phase transition at $(t/V)_c \simeq 0.208(1)$, in good agreement with the most recent Monte Carlo estimate of 0.195 ± 0.025. We are unable to exclude the possibility of a weakly first-order rather than second-order transition, but this is equally true of the Monte Carlo work. However, recent field theoretical work[14] argues that the transitions in this model are *deconfined quantum critical points*, i.e., second order.

The most recent work finds a stable supersolid phase in the model at half-filling $\left(n=\frac{1}{2}\right)$ with a transition to a uniform superfluid at $t/V \simeq 0.1$. To study this case with series is more difficult, and is left for future work.

ACKNOWLEDGMENTS

This work forms part of a research project supported by a grant from the Australian Research Council. We are grateful for the computing resources provided by the Australian Partnership for Advanced Computing (APAC) National Facility and by the Australian Centre for Advanced Computing and Communications (AC3).

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