Hard Core Bosons on the Triangular Lattice at Zero Temperature: A Series Expansion Study

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We use high order series expansions to investigate the phase diagram of a system of hard-core bosons on the two-dimensional triangular lattice, with nearest neighbour repulsion. For commensurate filling $n=1/3,2/3$ we identify a quantum phase transition at $t/V\approx 0.208$ from a solid phase to a superfluid.

1. Introduction

The possibility of an exotic *supersolid* phase of matter, where long range crystalline order and superfluidity may co-exist, was conjectured over thirty years ago and has remained controversial and unobserved until, perhaps, very recently [1].

On the other hand the existence of supersolid phases in lattice models of interacting hard-core bosons is evident from mean-field studies [2] and more recently, from more reliable quantum Monte Carlo studies, particularly for the triangular lattice [3,4].

Our goal in this work is to study a model of hard-core bosons on the triangular lattice via long series expansions, an approach which complements the extant Monte Carlo work. The series approach also offers some advantages, allowing us to compute not only bulk ground state properties but also energies of elementary excitations.

The Hamiltonian of the model is

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

where the first term is a nearest neighbour hopping, the V-term is a nearest neighbour repulsion, and we also include a chemical potential term. The site occupancy is $n_i=0,1$. In figure 1 we show the 3-sublattice decomposition of the triangular lattice, and commensurate ground states for $n=1/3,\ 2/3$ (here $n=\langle n_i\rangle$ the average site occupancy). These two states are related by a particle-hole transformation, and it suffices to study the $n=1/3$ state. We write the Hamiltonian in the usual perturbative form $H=H_0+\lambda H_1$ where the hopping term is taken as the perturbation. Thus at $t=0$ the ground state is that shown in Figure 1(b), with all sites on sublattice α (say) occupied and sublattices β, γ empty. The perturbation will induce hopping of bosons to other sublattices and at some critical t_c we expect all sublattices to be equally filled. This will be a phase transition between a normal solid and superfluid.

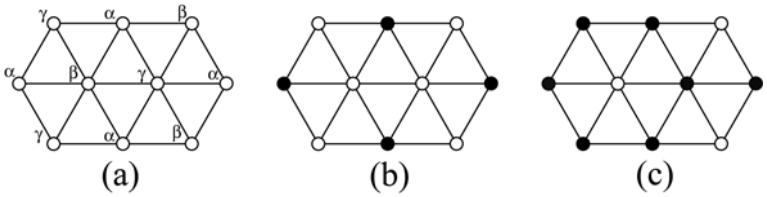


Fig. 1. The lattice and unperturbed $n=1/3,\ 2/3$ states.

2. Methodology

The series expansion method [5], which we employ in this work, is based on writing the Hamiltonian in the usual perturbative form $H=H_0+\lambda H_1$, with

$$H_0 = \sum_{\langle ij \rangle} n_i n_j$$
$$H_1 = -t \sum_{\langle ij \rangle} (a_i^\dagger a_j + a_j^\dagger a_i)$$

where we have set the repulsion parameter V to 1, and dropped the chemical potential term which is constant for fixed n. We compute power series in t, to order t^{10}, for various quantities of interest, and analyse the resulting series via standard Padé and differential approximant methods. To order t^{10} a total of 231955 distinct clusters need to be included.

For small t the system will retain crystalline long-range order of the $\sqrt{3} \times \sqrt{3}$ type, shown in Fig. 1(b), (c). As t increases to the critical point t_c the sublattice occupancies will become equal and the crystalline phase is replaced by a uniform superfluid. The transition can be identified and located via a divergence in the `specific heat' d^2E_0/dt^2, where E_0 is the ground state energy, through the vanishing of a suitably defined order parameter, through the structure factor or via the opening/closing of energy gaps for elementary excitations.

3. Results

The series themselves are presented in a fuller paper [6], and we confine ourselves here to some typical results. Figure 2(a) shows the ground state energy per site, versus t, obtained from differential approximants. The error is estimated to be no greater than the width of the line, except near $t \approx 0.21$ where different approximants begin to splay out. Also shown is the second derivative d^2E_0/dt^2, which is analogous to a specific heat, and is seen to diverge at around $t \approx 0.21$, signifying the phase transition.

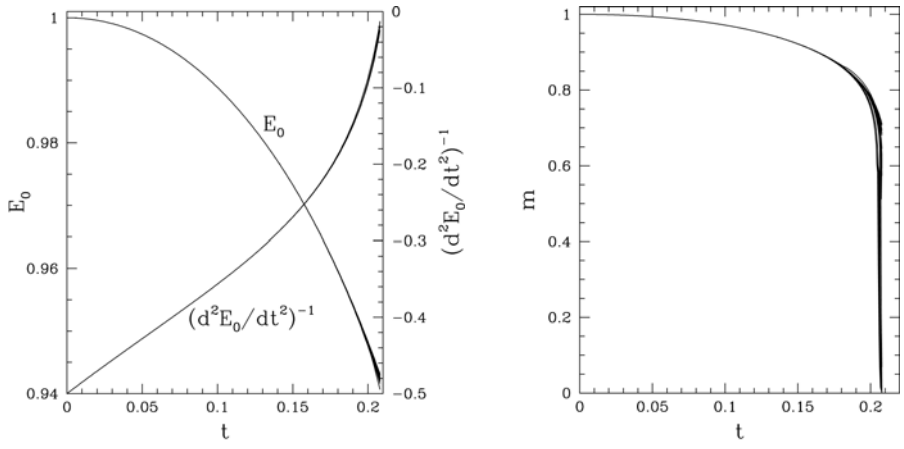
An order parameter for the solid $n=1/3$ phase can be defined as

$$m = \langle n_\alpha \rangle - \langle n_\gamma \rangle = (3\langle n_\alpha \rangle - 1)/2$$

which equals 1(0) in the fully order (disordered) phase. In Fig. 2(b) we show m versus t. As is evident, m drops rapidly to zero at around $t=0.208$. If we assume a normal second order phase transition with a power law

$$m \sim (1 - t/t_c)^\beta \qquad t \to t_c -$$

we obtain an estimate for the critical exponent $\beta \approx 0.09$.



(a) (b)

Fig. 2. (a) Ground state energy and `specific heat' versus t; (b) crystalline order parameter m versus t. The curves are the results of differential approximants to the exact series.

Another quantity of interest is the static structure factor

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

Note that this differs from the usual definition by the subtraction of the second term, which is necessary to implement the linked cluster method efficiently. The effect of this term is to remove the δ-function peak at $\mathbf{k}=0$ and to reduce it at the ordering wavevector $\mathbf{k}=\mathbf{k}^*=(4\pi/3, 0)$. At the transition point t_c, where $\langle n_i\rangle$ is independent of 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 Figure 3 where we show $S(\mathbf{k})$ along symmetry lines in the Brillouin zone for various t values.

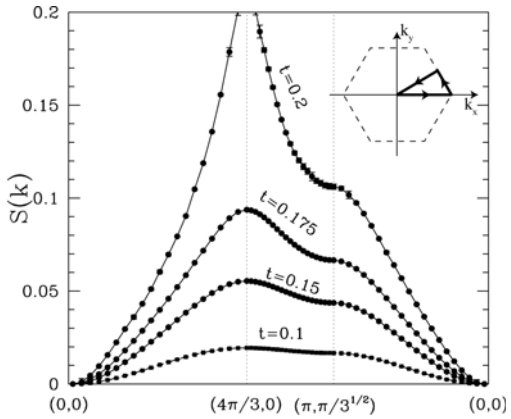


Fig. 3. The static structure factor $S(\mathbf{k})$ along high-symmetry cuts through the Brillouin zone for various t at $n=2/3$ filling. The inset shows the Brillouin zone, and path chosen.

The most precise estimate of the transition point t_c is obtained by analysis of the series $[S(\mathbf{k}^*)]^{-2.5}$, which vanishes approximately linearly at t_c, and yields $t_c=0.208(1)$.

4. Conclusions

We have shown that the series method can be successfully used to study a system of hard-core bosons on a lattice, at zero temperature. We have locate the quantum phase transition for commensurate $n=1/3, 2/3$ fillings at $t/V=0.208(1)$, in good agreement with the most recent Monte Carlo estimate of 0.195±0.025. Our results suggest a 2nd order transition but the possibility of a weak 1st order transition cannot be excluded.

The case of $n=1/2$, where the supersolid phase is expected, is more difficult, and is the subject of ongoing work.

Acknowledgments

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