A Quantum Phase Transition in Hard-Core Bosons on an Optical Lattice in Three Dimensions

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Previous work [1] on the hard-core three-dimensional Bose-Hubbard model with period potential has demonstrated the existence of a superfluid-insulator phase transition and established bounds on temperature and lattice potential within which these phase transitions may occur. However, a quantitative phase diagram for this transition was heretofore unestablished. Using a QMC simulation in tandem with finite-size scaling methods, we locate precise values for the critical transition points.

I. Introduction

When bosonic particles like ^{4}He are lowered to very cold temperatures they exhibit the remarkable property of flowing without resistance. Superfluidity was discovered in 1937 by Peter Kapitsa, but has since been recognized to occur in a diverse set of systems, from excitons in semiconductors to neutron stars.

Over the last several years, ultracold atomic gases have provided a new experimental realization of superfluid and Mott insulator phase transitions. Some initial work has been done on creating an experimental superlattice on some small systems. In addition to experiment, mathematical analysis has shown that such a phase transition occurs for the hard-core Bose-Hubbard model at half-filling with a periodic lattice potential. Our work helps determine the precise critical transition points as these experiments are performed in the thermodynamic limit.

This paper is organized as follows: Section II describes the computational approach, Monte Carlo. Section III reviews the key general features of phase transitions such as the superfluid transition that is the focus of this work, and shows some results for the well-known Ising model of magnetism that was used as a preliminary project to develop an understanding of how to use Monte Carlo to study phase transitions. The finite size scaling method, which allows a more sophisticated analysis of data on small lattices to be used to understand the thermodynamic limit,

is discussed in Section IV, again with some data generated for the Ising model. Finally, sections V and VI contain new results obtained for the superfluid transition in the Bose-Hubbard model.

II. Background – Monte Carlo Method

The method we use to study bosonic gases on an optical lattice is Quantum Monte Carlo (QMC), in particular an algorithm called Stochastic Greens Function (SGF). The term Monte Carlo is attached to many algorithms and methods that differ substantially, but the essence of the method is to solve problems which are computationally infeasible when using deterministic methods and instead take a statistical mechanics approach interested in finding the probability of being in a certain state. The basic algorithm is the following:

(i) Generate a starting configuration

(ii) Propose a random change to the configuration

(iii) Accept or reject change based on relative probabilities of old and new configuration

(iv) Record some property of the resulting configuration

(v) Go back to (ii)

Once enough ('enough' depends on the algorithm used) configurations have been generated, the ensemble of configurations that has been generated converge on the sample generated by the correct probability distribution. In this way, Monte Carlo imitates a physical experiment. Crucially, Monte Carlo does this without knowledge of all possible states (enumeration) or, equivalently, knowing the partiton function. In statistical mechanics for instance, one needs to know the partition function to calculate how probable a particular state p_i is (and thereby to calculate the expectation value of an observable), but to calculate the ratio of probabilities, $\frac{p_{new}}{p_{old}} = e^{-\beta(E_{new}-E_{old})}$, knowing the partition function isn't necessary.

The Metropolis-Hastings algorithm is perhaps the simplest Monte-Carlo algorithm, and concerns only step (iii) of the above. It tells you how to accept or reject proposed changes: if $\frac{p_{new}}{p_{old}} > 1$, accept. Else, accept the change with probability $\frac{p_{new}}{p_{old}}$. It is easy to see how this approach is computationally simpler than deterministically evolving the system.

Many people regard Monte Carlo, especially because it involves random numbers, as a not very precise method. Monte Carlo and the Metropolis algorithm can in fact be put on a mathematical footing. The essence of how Monte Carlo can be used to generate configurations with a desired probability distribution is the following: the Metropolis algorithm (and in fact other methods like the heat-bath algorithm) define a probability $T(C, C')$ to go from one configuration C to another

C'. The rule $T(C, C')$ can be viewed as a matrix of probabilities which satisfies several specific conditions. First, T is a "stochastic matrix". It obeys $\sum_{C'} T(C, C') = 1$, because of any C the sum of the probabilities to go to all the different destinations C' is unity. Second, the Metropolis algorithm obeys "detailed balance" $p(C)T(C, C') = p(C')T(C'C)$. It can be shown from these two facts that the repeated action of T on any starting $C_(0)$ ultimately leads to a sequence of configuration in which C appears with probability $p(C)$

Quantum Monte Carlo, in this case, is a straightforward extension of this idea to a quantum system. The configuration the algorithm works on is a quantum world-line living in three spatial dimensions plus an additional β (inverse temperature) dimension that extends from zero to β – the program takes β as a fixed parameter – then suggests changes to this worldline and accepts or rejects the changes based on relative probabilities. For this reason it is sometimes said that QMC is merely classical Monte Carlo in one higher dimension.

III. Phase Transitions

A phase transition is a transformation of a thermodynamic system from one qualitative order to another, such as the familiar transition from solid to liquid. The transitions between the three familiar states of matter are examples of first-order phase transitions, in that at the critical point (e.g., a boiling point specified in temperature and pressure) there is a latent heat, a fixed amount of energy that must be absorbed or released by the system while it completes the phase transition. While latent heat is being transferred, the system stays at a constant temperature and in a mixed-phase regime wherein part of the system has undergone the phase transition and part has not; freezing or boiling water exemplifies this. A second class of phase transition that we are more interested in is the second-order or continuous phase transition, which is characterized by long-range correlations – the state of one component of the system gives you information about components of the system very far away – and power-law decay of correlations approaching the critical transition (from the side of the ordered phase). Phase transitions can be viewed in terms of an order-parameter which is exactly zero in the disordered phase – in systems where the parameter being varied is temperature, this (normally) means temperatures higher than T_c, the critical temperature – and non-zero in the ordered phase. In the Ising model, a simple model of magnetism that is one of the simplest models to show a phase transition, net magnetization is the order parameter. See Figure 1, showing net magnetization in the 2D Ising model, which I generated with code using the Metropolis-Hastings algorithm.

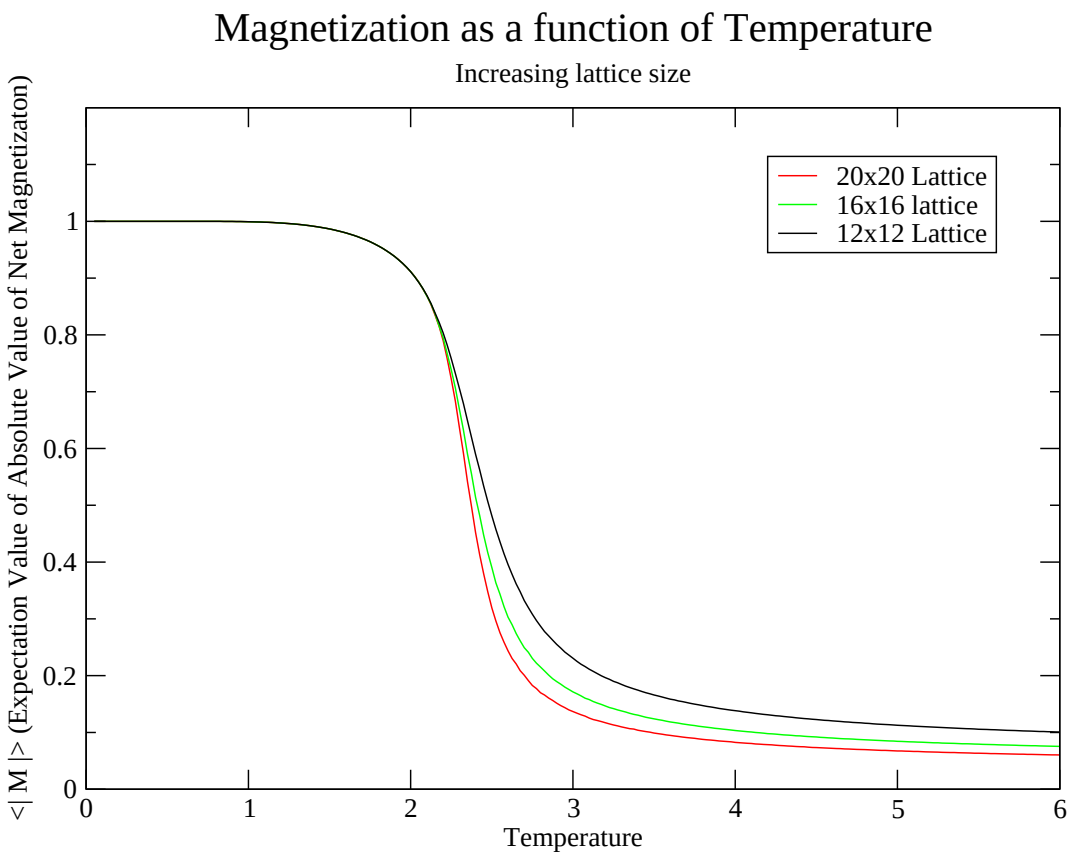

FIG. 1. My results for the expectation value of the absolute value of the magnetization of the 2D Ising model on three different lattice sizes are shown as a function of temperature. The exact critical temperature, in the limit of infinite lattice size, is $T_c = 2.269$. Already this raw data in lattices of just a few hundred sites suggests the order parameter does indeed start to build up at roughly this T_c.

$|M|$ was computed because true phase transitions cannot occur on finite lattice, so the order parameter M always vanishes. Put another way, an Ising model is equally likely to have spin $S = +1$ as spin $S = -1$. This symmetry ensures the average value of the spin must be zero on a finite lattice. The amazing thing about phase transitions is that this symmetry argument breaks down when the system is infinitely large, and symmetries can be "broken". We return to this point in the next Section.

Quantum phase transitions, on the other hand, can only be achieved by scaling some parameter (such as electric field) at $T = 0$, by definition. They are driven by quantum, rather than thermal fluctuations. However, they can be observed indirectly at small but finite temperatures where the

quantum fluctuations are on the same order as thermal fluctuations and the two compete. The energy scale characteristic of the quantum fluctuations is $\hbar\omega$ and that of thermal fluctuations is $k_B T$, so for $\hbar\omega > k_B T$, quantum fluctuations dominate. In this way, the critical value of the scaling parameter can be observed even at finite temperatures.

IV. Finite Size Scaling

We use computer simulations of bosons on a lattice to probe the behavior of physical systems, but computation time for simulations increases very rapidly as lattice-size grows. Of course, we are interested in describing the properties of a number of particles on the order of Avogadro's number (the thermodynamic limit), much larger than is feasible with current algorithms and processing powers. As such, we would like to be confident that the results of our simulation go to the thermodynamic limit for a relatively small lattice. Finite-size scaling offers such a guarantee. As mentioned previously, in second-order phase transitions the decay of correlations near T_c follows a power law. In particular, defining a reduced temperature $\tau \equiv \frac{(T-T_c)}{T_c}$, and some order parameter which depends on temperature and lattice size (such as magnetization in the Ising model), it can be shown that for temperatures near T_c the function describing this order parameter will take a rather constrained form of (1) for $\tau \approx 0$, where L is the size of the lattice, f is some unknown (well-behaved) function and

$$(1) \quad M^2(L,\tau) = L^{\frac{-2\beta}{\nu}} f(L^{\frac{1}{\nu}}\tau)$$

β and ν are critical exponents which describe the decay of correlations near criticality. This is a wonderful result, because it indicates that as $\tau \to 0$, $f(L^{\frac{1}{\nu}}\tau) \to f(0)$, and the equation can be rearranged to (2)

$$(2) \quad L^{\frac{2\beta}{\nu}} M^2(L,0) = f(0)$$

Armed with this, we can measure magnetization while tuning temperature for several different sizes of lattice, compute the quantity $L^{\frac{2\beta}{\nu}} M^2(L,\tau)$ for different values of the critical exponents β and ν, and look for a crossing. When we find one, we should have the both the correct critical exponents (which describe the long-range order of the system near criticality) and the correct critical transition value T_c, without having to build larger and larger lattices to be confident in our answers. This is called finite-size scaling.

V. The Bose-Hubbard Hamiltonian

The Bose-Hubbard model is the standard choice for studying bosons on an optical lattice. The

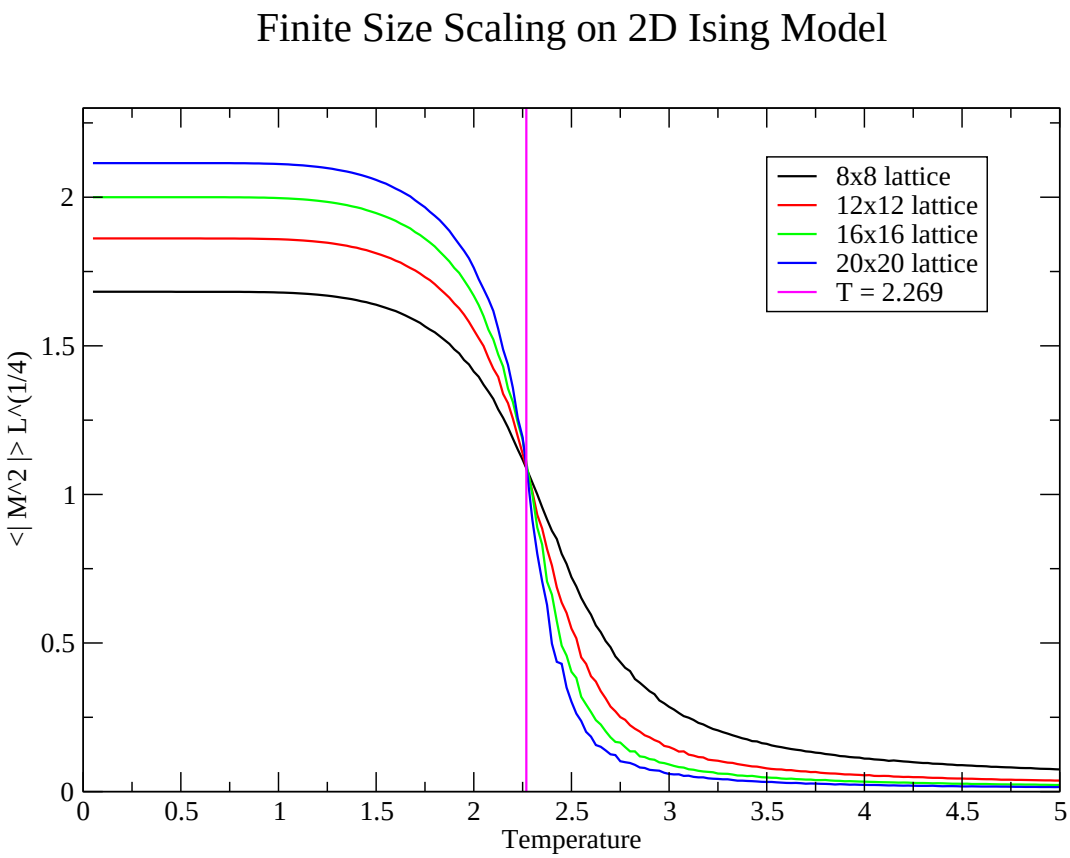

FIG. 2. This nice proof of concept graph shows finite size-scaling on the 2D Ising model. This simulation ran for a little over 25 minutes, and still managed to land within one percent or so of the correct critical temperature, on relatively modest lattices.

Bose-Hubbard Hamiltonian (3) includes a kinetic term contributing t energy for bosons (in this context ^{87}Rb atoms) hopping from one site to another, an on-site potential U for the repulsion between bosons sharing a lattice site, and a chemical potential μ which depends only on the total number of bosons. The superlattice is modeled by a periodic, one-body potential $\lambda(-1)^x$, where one sublattice has sites with potential $-\lambda$ and the other has potential $+\lambda$. The arrangement of the two sub-lattices resembles the arrangement of different colors on a checkerboard.

$$(3) \quad H = -t \sum_{<i\sim j>} (b_i^\dagger b_j + b_j^\dagger b_i) + \lambda \sum_i (-1)^x b_i^\dagger b_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i (\hat{n}_i)$$

We are interested in studying a particular variation of this model, a hard-core bosonic gas on a cubic lattice, and so we follow Aizenmen and Seirenger [1] (whose work we are expanding), by restricting the model to half filling ($N_{boson} = \frac{1}{2} N_{sites}$, i.e., we work in the canonical ensemble) and

modeling the bosons as a hard-core gas by letting $U = \infty$, making it impossible for the bosons to share a site. This reduces the Hamiltonian to the significantly simpler form (4).

$$(4) \quad H = -t \sum_{<i \sim j>} (b_i^\dagger b_j + b_j^\dagger b_i) + \lambda \sum_i (-1)^x b_i^\dagger b_i$$

This leaves only three parameters, t, λ, and temperature. We take t to be fixed at one, and are interested in varying λ and temperature to establish quantitative phase diagram for the predicted transition between a superfluid and a mott insulator. In particular, I chose superlattice potentials at evenly spaced intervals ($\lambda = 0, 0.2, 0.4$,etc) while sweeping up in temperature to find

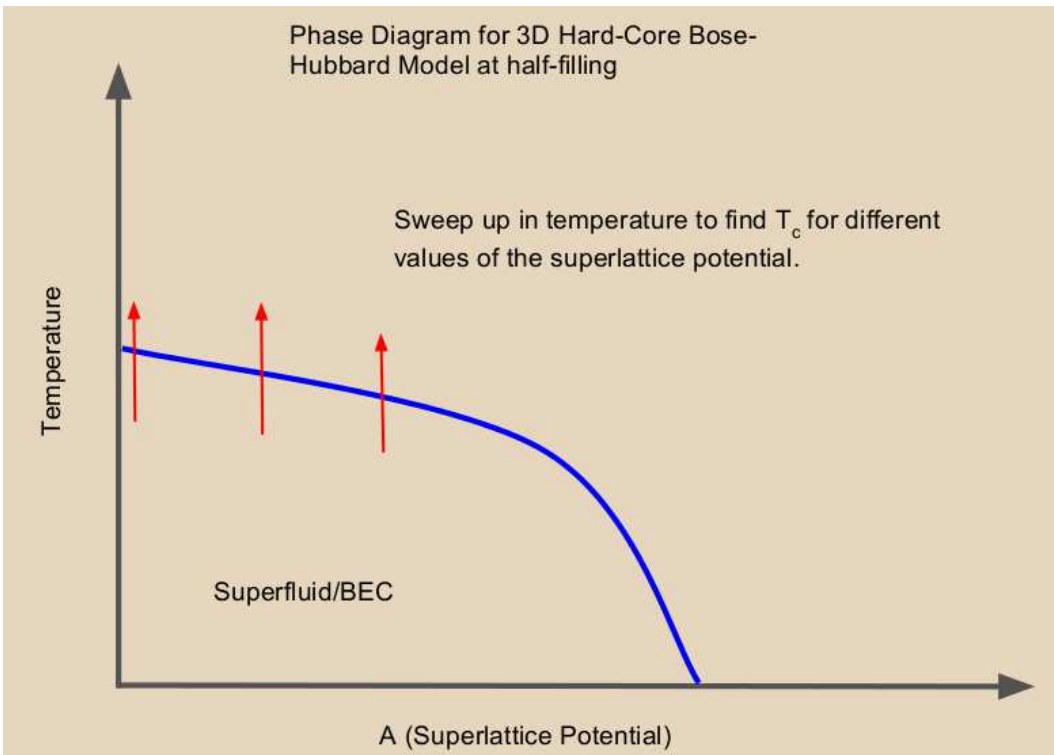

FIG. 3. Qualitative Phase diagram for Superfluid Transition. Red Arrows indicate where I actually run simulations to find the phase transition (where the red crosses the blue line).

T_c. We actually locate T_c through the use of two measures, superfluid fraction ρ_s, which is derived from the winding of the world-lines of the bosons, and the One-Body Green's Function, $b^\dagger(0,0,0)b(far)$, where far indicates the lattice site furthest from the zeroeth site on our finite lattices.

The "winding" of the bosons refers to counting the number of times a boson world-line exits one side of the lattice and reappears (as a result of periodic boundary conditions) on the other.

Roughly speaking, the reason "winding" measures superfluidity is that it is impossible for a single boson to travel so far (all the way across the simulation box) by itself. The only way winding can occur is through a coherent organization of the boson world lines in which one boson's world-line connects to another and then another and then another (recall bosons are indistinguishable), thereby forming a chain which can circumnavigate the entire simulation box. This linkage of world-lines is in fact the essence of superfluidity. It is made possible by the growth of the de Broglie thermal wavelength $\lambda_T = \frac{\hbar}{\sqrt{2\pi m k_B T}}$ as T is lowered, because λ_T measures how far an individual boson's world-line travels, and since λ_T grows as $T \to 0$ it becomes increasingly likely for many world-lines to entangle, forming the superfluid.

The Green's Function measures the likelihood of a boson being created at the zeroeth site (the corner of a cubic lattice) and then destroyed in the center of the lattice, which is as far as it can go when the lattice has periodic boundary conditions. Put somewhat more technically, $G(x,y) = \langle b_{(x,y)} b^\dagger_{(0,0)} \rangle$. The Fourier transform $G(k_x,k_y) = \sum_{x,y} e^{i(k_x x + k_y y)}\, G(x,y)$ measures the number of bosons with momentum (k_x,k_y). In particular, the number of bosons with zero momentum is just the sum of the real space Green's function over all sites $G(k_x=0,k_y=0) = \sum_{x,y} G(x,y)$. If $G(x,y)$ is nonzero even when $(x,y) = \text{far}$, then $G(k_x=0,k_y=0)$ will be enormous. In other words, one has Bose-Einstein condensation due to a large fraction of particles with zero momentum.

Thus the winding and the Green's function measure superfluidity and BEC respectively, and, to the extent that these are the same, provide a complementary way to locate the phase transition. Another way to check this critical temperature is to find some quantity that can be exploited using finite-size scaling. According to [2], this quantity is $L^1 \rho_s$.

The superfluid phase can be destroyed in two ways. First, one can increase temperature. This decreases the de Broglie thermal wavelength so that the bosons' world-lines can no longer cross, eliminating winding. A second way to destroy the superfluid is to increase the superlattice potential λ, as indicated in the schematic phase diagram (Figure 3), where it is obvious that increasing λ at fixed T moves out of the superfluid region. A way to understand this physically is that increasing λ makes it more difficult to hop. Indeed, to second-order in peturbation theory the effective hopping is given by $t_{\text{eff}} = \frac{t^2}{2\lambda}$, which reflects that moving between two low-energy sites on a checkerboard lattice is by hopping twice (hence the numerator t^2), inevitably passing through a high-energy site (hence 2λ). If the superfluid transition occurs at $\frac{T}{t_{\text{eff}}} = \frac{t^2}{2\lambda} \approx 2$, as indicated in Figure 3, we see that the transition temperature decreases with λ as $\frac{T}{t} \approx \frac{t}{\lambda}$.

This result, that the transition temperature $\frac{T}{t} \approx \frac{t}{\lambda}$, suggests that the superfluid phase should exist along the entire $T = 0$ axis, out to arbitrarily large λ. The interesting thing about the

Seiringer result is that there is a critical λ above which the superfluid vanishes even at $T = 0$ – that is, there is a quantum phase transition.

The physical origin of this quantum phase transition is suggested to be the appearance of a Mott insulator – a phase in which the number of strongly repulsive particles matches the number of sites so that motion is energetically very unfavorable. In this superlattice case, the number of particles is only half the total number of sites, but is equal to the number of low energy sites.

One signal of a Mott insulator is that energy cost to add particles take an abrupt jump after all low-energy sites have been filled: In a standard Mott insulator (no superlattice) the energy to add particles (chemical potential) jumps by the repulsion energy U when the number of particles exceeds the number of sites, as some double occupancy becomes unavoidable. In this problem, site-sharing is forbidden, so energy jumps by $2A$ once the number of particles exceeds half-filling.

VI. Results and Conclusions

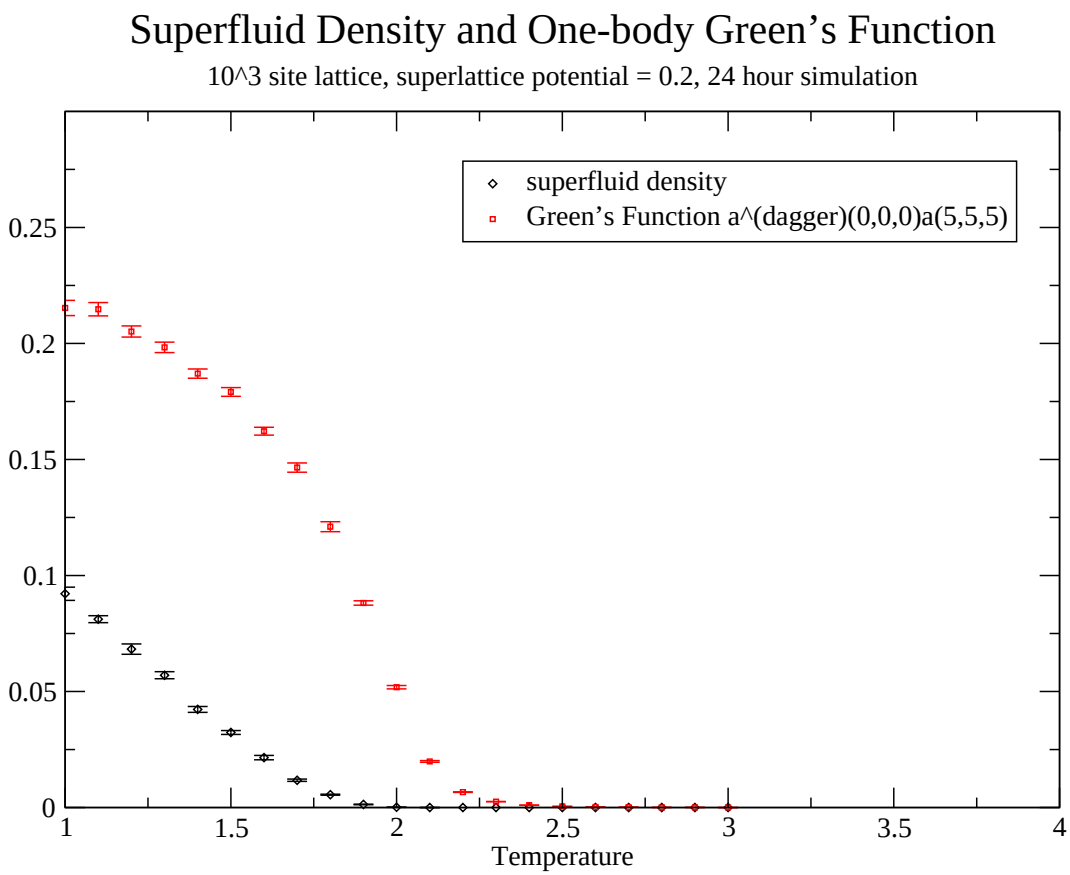

FIG. 4. Power law decay of correlations near criticality

Though we by no means have the comprehensive picture of the phase diagram that we want, we expect more results soon, and to date we have shown strong evidence (see Figure 4) of a phase transition on a 10^3 lattice in measures of both superfluidity and BEC.

In Figure 4 the superfluid fraction and the one-body Green's function disagree on the value of the phase transition by about 10%, a problem we hope will be resolved by going to larger lattices sizes. No matter the case, this data shows T_c occuring before or near the bound predicted by Aizenman *et al.*, $T_c \leq \frac{3}{2ln2} \approx 2.16$.

Tentatively, we have shown that the phase-transition from a superfluid/BEC to an insulator occurs where predicted for the hard-core model at half filling. Forthcoming future results should considerably improve our precision and confidence in the phase diagram. For future work, already underway, we will get results at the same superlattice potential for multiple lattice sizes (e.g. 8^3, 12^3, and 16^3) to exploit finite-size scaling, and perform parallel investigations at multiple values of the superlattice potential ($\lambda = 0, 0.2, 0.4$, etc.). These investigations we expect to yield a firm understanding of the phase diagram of this system at half-filling.

VII. Acknowledgements

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