Conf-720292--1

QUANTUM MONTE CARLO SIMULATIONS FOR DISORDERED BOSE SYSTEMS*

N. Trivedi
Materials Science Division
Argonne National Laboratory
Argonne, IL 60439

ANL/CP--75721

DE92 010343

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

MARCH 1992

CONFIDENTIAL

MAR 25 1992

/rlp

Distribution:

- 1-3. D. R. Hamrin
4. B. D. Dunlap
5. M. B. Brodsky
6. A. A. Abrikosov
7. Authors
8. Editorial Office

Submitted to Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics, University of Georgia, Athens, GA, February 17-21, 1992.

*Work Supported by the U.S. Department of Energy, BES-Materials Sciences, under Contract #W-31-109-ENG-38.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

102

QUANTUM MONTE CARLO SIMULATIONS FOR DISORDERED BOSE SYSTEMS*

N. Trivedi
Materials Science Division
Argonne National Laboratory
Argonne, IL 60439

The submitted manuscript has been authored
by a contractor of the U. S. Government
under contract No. W-31-109-ENG-38.
Accordingly, the U.S. Government retains a
nonexclusive, royalty-free license to publish
or reproduce the published form of this
contribution, or allow others to do so, for
U.S. Government purposes.

MARCH 1992

Submitted to Workshop on Recent Developments in Computer Simulation Studies in
Condensed Matter Physics, University of Georgia, Athens, GA, February 17-21, 1992.

*Work Supported by the U.S. Department of Energy, BES-Materials Sciences, under
Contract #W-31-109-ENG-38.

Quantum Monte Carlo Simulations For Disordered Bose Systems

Nandini Trivedi

Materials Science Division, Bldg. 223
Argonne National Laboratory
9700 S. Cass Avenue, Argonne, IL 60439

Abstract. Interacting bosons in a random potential can be used to model ^4He adsorbed in porous media, universal aspects of the superconductor-insulator transition in disordered films, and vortices in disordered type II superconductors. We study a model of bosons on a 2D square lattice with a random potential of strength V and on-site repulsion U . We first describe the path integral Monte Carlo algorithm used to simulate this system. The 2D quantum problem (at $T=0$) gets mapped onto a classical problem of strings or directed polymers moving in 3D with each string representing the world line of a boson. We discuss efficient ways of sampling the polymer configurations as well as the permutations between the bosons. We calculate the superfluid density and the excitation spectrum. Using these results we distinguish between a superfluid, a localized or 'Bose glass' insulator with gapless excitations and a Mott insulator with a finite gap to excitations (found only at commensurate densities). We discover novel effects arising from the interplay between V and U and present preliminary results for the phase diagram at incommensurate and commensurate densities.

1 Introduction

Some of the most important problems in condensed matter physics today deal with $T=0$ phase transitions driven by *quantum fluctuations*, e.g., metal-insulator[1] and superfluid-insulator[2] transitions. In this context I will describe some recent work on the localization problem for interacting bosons in 2D.

Besides the theoretical interest, we are motivated to explore disordered boson systems because of their relevance to a number of experiments. Some of the puzzles that can be addressed are the following:

- (i) The superfluid density ρ_s has been measured for ^4He adsorbed on a porous medium such as carbon black[3] for various coverages. It is found that ρ_s , extrapolated to $T=0$, is zero until a critical concentration ρ_c is reached and thereafter it increases as $\rho_s(T=0) \sim |\rho - \rho_c|^\zeta$, with $\zeta = 2.16$. This behavior is not completely understood; in particular, mean field theory[4]

predicts that $\zeta = 1$, whereas scaling theory[2] suggests $\zeta > 8/3$, both in disagreement with experiments.

- (ii) Thin disordered films of bismuth, for example, are found to undergo an insulator-superconductor transition with increasing film thickness[5]. This phase transition is expected to be in the same universality class as a boson model [6], since as the correlation length becomes much larger than the Cooper pair size it is possible to treat the Cooper pair as a bose field. Using scaling ideas it has been argued that at the transition the resistance is finite: $R^* = \alpha \hbar/e^2$ and α is universal. While this scenario is in qualitative agreement with experiment, α has so far not been reliably computed.
- (iii) A third question of current interest for which boson simulations are pertinent is the phase diagram of a disordered type II superconductor[7, 8]. This problem has assumed more importance recently in the context of the cuprate superconductors whose phase diagrams are likely to be significantly different from that obtained from mean field theory, given their short coherence lengths, high T_c 's and large anisotropy. The primary question is whether the transport behavior in a magnetic field is activated, in which case the resistivity is strictly zero only at $T=0$ (neglecting quantum fluctuations), or if there is a vortex glass phase[9, 10], in which the resistivity vanishes for a range of temperatures. Although experimental evidence[11, 12] is not yet conclusive, the universality of the exponents for different magnetic fields and even different materials, lend strong support to the vortex glass.

We use the path integral representation of bosons evolving in "imaginary" time. As will be described in detail below, the 2D quantum problem (at $T=0$) of bosons gets mapped onto a classical problem of 1D strings or directed polymers moving in 3D space, with each string representing the world line of a boson. The indistinguishability of the bosons requires that we sum over all permutations of the particles. For the third problem discussed above, the polymers are used to represent vortices in a type II superconductor. In this particular case the permutations are not relevant.

We build upon previous work by Ceperley and Pollock[13, 14] who used the path integral Monte Carlo scheme to study a continuum model of bosons with realistic ^4He interatomic potentials. We study an interacting lattice model with disorder, with an aim to exploring the interplay between randomness and interactions. There are two main difficulties that we face. The polymeric nature of the objects that we simulate limits considerably the sizes of systems and the number of Monte Carlo sweeps that can be studied compared with 3D classical simulations of particles or spin systems. In addition, disorder comes with its own bag of complications. To reduce sample-to-sample fluctuations it becomes necessary to average over disorder[15]. Disorder can also lead to problems with

equilibration or convergence, in which case the results may depend on the initial conditions[16]. Though considerable progress has been made in simulations of quantum phase transitions, their ability to confront experiments is still in its infancy. Nevertheless, we expect numerical simulations to play a major role in this area, just as they did in the study of spin glasses[17].

The boson model has proved difficult to treat analytically, primarily because the non-interacting limit is singular and there is no suitable limit to perturb around. In 1D, Giamarchi and Schulz[18] have used the renormalization group method. Some universal features of the boson model have been studied using scaling techniques by Ma et. al. [19] and Fisher et. al. [2]. Numerically this model has been explored by various techniques: We[20, 16] have done simulations of this model in 2D using path integral Monte Carlo techniques. The same model has been studied in 1D by Scalettar et. al. [21]. Real space renormalization group techniques have been used in the hard core or nearly hard core limit[22, 23] at commensurate densities. Hard core bosons is particularly amenable because of the reduced Hilbert space. Exact diagonalization studies[24] on 4×4 systems have also been performed. Variational methods have not been applied to this problem because of the lack of suitable wave functions in the presence of disorder and furthermore, to address the question of phase transitions would require constructing wave functions for each of the phases and then comparing their energies. However, in spite of the work discussed above, at present there are several questions regarding the nature of the phases and their characterization that remain open. In addition, the puzzles outlined above are as yet unresolved.

For completeness, I should mention that the problem of metal-insulator transition for fermions[1] in systems like Si:P is more complicated than the boson model discussed above because both charge and spin degrees of freedom must be included. Theoretical approaches (mostly by diagrammatic perturbation theory) have met with limited success[25]. Numerically, also this problem has proved rather intractable because of the so-called fermion sign problem[26].

The outline is as follows—The model is given in section 2, followed by a detailed discussion of the algorithm in section 3 which uses Monte Carlo methods to calculate the density matrix within a path integral formulation for bosons. In particular, we give an account of the techniques used to sample the configuration space of boson world lines efficiently. In section 4, we discuss how the different phases are characterized. Section 5 and 6 contain our results on the interplay between disorder and interactions. We conclude with a suggestive phase diagram for incommensurate and commensurate densities.

2 Boson Model

We consider a simple model of bosons on a 2D square lattice $N = L \times L$, described by the Hamiltonian H given by

$$H = \frac{-t}{2} \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c.) + \sum_i V_i n_i + \frac{U}{2} \sum_i n_i(n_i - 1) \quad (1)$$

where a_i ($a_i^\dagger$) is a boson annihilation (creation) operator at a site i and $n_i = a_i^\dagger a_i$. The first term describes the hopping of bosons between nearest neighbor sites with strength t . The second term is the interaction of the bosons with a random potential, with site energies V_i chosen from a uniform distribution $[-V, V]$ and the last term describes the on-site repulsive interaction between bosons with strength U . Our aim is to explore the competition between disorder and interaction; to see how different phases emerge and how they can be characterized.

This model can easily be augmented, depending on the physical situation, by including short range interaction (nearest and next-nearest neighbor) between bosons, and/or long range interaction, different types of disorder, e.g., unbounded disorder or uncorrelated disorder in the time direction (important for pinning studies in the vortex problem). Long range interactions are pertinent for modeling the vortex-vortex interaction and may also be important for a study of the novel phenomenon of quantum melting.

3 Path Integral Monte Carlo

The quantity containing all the information about a system is obviously the density matrix at an inverse temperature $\beta = 1/T$. The density matrix in the canonical ensemble is $\rho(R, R'; \beta) = \langle R | \exp(-\beta H) | R' \rangle$, where R and R' describe particular configurations of the N_b -particle system. The density matrix is the amplitude for the system starting in configuration R at (imaginary) time $t = 0$ to be in a configuration R' at $t = \beta$. Most of the discussion here will focus on the diagonal density matrix with $R' = R$ (i.e. paths that close on themselves after $t = \beta$). It is also possible to evaluate the off-diagonal matrix in order to obtain the condensate fraction.

For indistinguishable particles, we also include the possibility of exchanges between the particles. The diagonal density matrix for a bose system is symmetrized by summing over permutations P of the particles and is given by $\rho(R, R; \beta) = 1/N_b! \sum_P \langle R | \exp(-\beta H) | P[R] \rangle$. The partition function can be obtained from $Z = \text{Tr}[\rho]$. At high temperatures only the identity permutation contributes significantly to the sum but as the temperature is lowered, the thermal de Broglie wavelength $\lambda_T = \sqrt{\beta t / \pi}$ becomes of the order of the

interparticle spacing $r_0 = 1/\sqrt{\pi\rho}$ and exchanges between the particles become possible.

The first step in computing the density matrix is to break the total time β into tiny steps of size $\tau = \beta/N_\tau$. Upon inserting complete sets of states we obtain

$$\rho(R, R; \beta) = \frac{1}{N_b!} \sum_P \sum_{R_1} \dots \sum_{R_{(N_\tau-1)}} \rho(R, R_1; \tau) \rho(R_1, R_2; \tau) \dots \rho(R_{(N_\tau-1)}, P[R]; \tau) \quad (2)$$

In Eq. (2), R_m represents the ensemble of N_b particle coordinates on the m^{th} time slice, $R_m = (r_1(m), r_2(m), \dots, r_{N_b}(m))$, where $r_\ell = (x_\ell, y_\ell)$ is the position of the ℓ^{th} particle. We apply periodic boundary conditions along x , y and β directions. We have done simulations on lattice sizes up to 10×10 and densities $\rho = 1/2, 3/4$ and 1 . We have gone up to $\beta t = 4$ and used $N_\tau = 40 - 60$ time slices.

The importance of this break-up is that since the elemental density matrices $\rho(R_m, R_{m+1}; \tau)$ describe the propagation of the particles over a very short time τ (or equivalently, very high temperature), it may be possible to make some reasonable approximations for them. In the appendix, we describe one possible short time approximation for ρ . We shall use

$$\rho^A(R_m, R_{m+1}; \tau) = \prod_{\ell=1}^{N_b} \rho_1(r_\ell(m), r_\ell(m+1); \tau) \times \exp \left[-(\tau/2) \sum_j [\mathcal{U}_j(m) + \mathcal{U}_j(m+1)] \right] \quad (3)$$

In Eq. (3), ρ_1 is the single particle density matrix and

$$\mathcal{U}_j(m) = (U/2)n_j(m)(n_j(m) - 1) \quad (4)$$

where $n_j(m)$ is the number of particles at site j on timeslice m . Our algorithm differs from that of Ref.[21] in that we do not factor H into disjoint parts obtained by including only nearest neighbor hops at $t = \tau$; instead we use a more accurate short time approximation which allows the algorithm to converge with fewer time steps N_τ .

3.1 Monte Carlo: Basics

It is clear from Eq. (2) that an evaluation of the density matrix requires a sum (or in the continuous case, an integration) over a very large number of variables. For example, for the case of a 4 site chain and 3 bosons, there are 20 configurations and 3! permutations. If β is broken up into 10 time slices (which

is rather modest), a computation of ρ will require $6 \times 20^{10} \approx 10^{13}$ evaluations of the integrand. For a computer with a speed of 10 MFLOPS, this would take ~ 300 hrs. On the other hand, by Monte Carlo we can obtain the 1% accuracy level in about a minute!

In path integral Monte Carlo (PIMC), the power of Monte Carlo in performing the summations over the permutations and the co-ordinates of the N_b particles on the N_τ time slices in Eq. (2) is exploited. The PIMC algorithm discussed below is developed along the lines of the work of Ceperley and Pollock[14].

The path of a boson i.e. the position of a boson on all the N_τ time slices $\mathcal{P}_i = [r_i(0), r_i(1), r_i(2), \dots, r_i(N_\tau)]$ can be viewed as a polymer string. This allows the 2D quantum problem of bosons to be mapped onto a 3D classical problem of strings or directed polymers. One essential point is that because of the periodic boundary conditions along β and the permutations between the particles, the length of the polymers is not fixed, but can vary from N_τ to $N_b N_\tau$, the latter arising from a maximum permutation cycle of length N_b . Let $s = [P; R, R_1, \dots, R_{(N_\tau-1)}, R_{N_\tau}]$ denote a particular permutation of the bosons ($R_{N_\tau} = P[R]$) and the positions of the particles on the different time slices. In other words, s describes a particular snapshot of the spaghetti of the N_b polymer strings; an example is shown in Fig. 1(a). Our aim is to sample the probability function

$$\Pi_s = \rho(R, R_1; \tau) \rho(R_1, R_2; \tau) \dots \rho(R_{(N_\tau-1)}, P[R]; \tau) \quad (5)$$

This involves generating a sequence of M spaghetti snapshots, $s_1, s_2, \dots, s_M$, such that in the limit $M \rightarrow \infty$, the probability of finding a spaghetti configuration s_α in the sequence is $\propto \Pi_{s_\alpha}$.

We use a generalization of the Metropolis importance sampling method to generate the M points in configuration space. Let $W_{s,s'}$ be the probability that a system currently in state s makes a transition to a state s' in one Monte Carlo time step. (1 MC step involves choosing a permutation and attempting to move, on average, the N_b bosons on all the N_τ time slices). W satisfies the conditions, $W_{s,s'} \geq 0$ and $\sum_{s'} W_{s,s'} = 1$. In a two step process, via an intermediate state s_1 , $W_{s,s'}^{(2)} = \sum_{s_1} W_{s,s_1} W_{s_1,s'}$. It can be shown that if W satisfies the detailed balance condition, i.e., the rate of transition from s to s' is equal to the reverse process, then in an n -step process $\lim_{n \rightarrow \infty} W_{s,s'}^{(n)} = \Pi_{s'}$, where Π is unique and independent of the initial configuration.

The detailed balance condition is $W_{s,s'}/W_{s',s} = \Pi_{s'}/\Pi_s$ or equivalently, $W_{s,s'} = \min(1, \Pi_{s'}/\Pi_s)$. The above equation is not very useful yet, because we do not know Π in order to construct the transition probability. However, this is where we use the short time approximation of the elemental density matrices ρ^A mentioned above. For purposes of obtaining the transition probability, we approximate Π_s as follows:

$$\Pi_s \approx \rho^A(R, R_1; \tau) \rho^A(R_1, R_2; \tau) \dots \rho^A(R_{(N_\tau-1)}, P[R]; \tau) \quad (6)$$

where ρ^A is given in Eq. (3). We are now in a position, at least in principle, to use Monte Carlo to sample Π_s . The simulation is started with a particular snap-shot of the spaghetti. An attempt is made to (a) move a boson on a particular time slice to a new randomly chosen position, and (b) to permute two bosons without changing their co-ordinates. The move is accepted with probability given in Eq. (6). This procedure is repeated until an attempt to move all the bosons on all the time slices has been made, constituting one Monte Carlo step and data is accumulated over a large number of Monte Carlo steps. This procedure, though correct in principle, will not be successful in sampling the configuration space, primarily because the elastic forces between the different portions of a string (generated by the hopping term that connects adjacent time slices) hinder the movement of the polymer over short time scales. Thus more judicious techniques to sample the probability function are required. These technical aspects are discussed below.

3.2 Spaghetti Monte Carlo

Let us consider a specific example of $N_\tau = 4$. Our aim is to generate a sequence of spaghetti configurations s distributed according to the probability given in Eq. (5);

$$\Pi_s = \rho(R, R_1; \tau) \rho(R_1, R_2; \tau) \rho(R_2, R_3; \tau) \rho(R_3, R_4; \tau) \quad (7)$$

where $R_4 = P[R]$. Thus given an initial configuration s we now wish to find the rules by which to generate a new configuration s' .

3.2.1 Levels-Bisection Method

Eq. (7) can be written in terms of conditional probabilities as follows:

$$\begin{aligned} \Pi_s = \rho(R, R_4; 4\tau) & \left[\frac{\rho(R, R_2; 2\tau) \rho(R_2, R_4; 2\tau)}{\rho(R, R_4; 4\tau)} \right] \left[\frac{\rho(R, R_1; \tau) \rho(R_1, R_2; \tau)}{\rho(R, R_2; 2\tau)} \right] \\ & \times \left[\frac{\rho(R_2, R_3; \tau) \rho(R_3, R_4; \tau)}{\rho(R_2, R_4; 2\tau)} \right] \end{aligned} \quad (8)$$

This allows us to partition Π into levels

$$\Pi_s = \Pi_0 \Pi_1 \Pi_2 \dots \quad (9)$$

where at level 0, a permutation is chosen with probability $\Pi_0 = \rho(R, P[R]; 4\tau)$; at level 1, $\Pi_1 = \rho(R, R_2; 2\tau) \rho(R_2, R_4; 2\tau) / \rho(R, R_4; 4\tau)$, which is the conditional probability of finding a configuration of bosons R_2 midway, given that the boson path starts at R and ends at R_4 in time 4τ . Similarly, Π_2 is the probability of finding boson position 1/4-way at R_1 given the endpoints at R and R_2 and the probability of finding position 3/4-way at R_3 given endpoints at R_2 and R_4 .

By factorizing Π into levels, the problem gets relegated to sampling the individual Π_ℓ , $\ell = 0, 1, \dots$. Since in general, Π_ℓ involves density matrices at $t = n\tau$, we need to make an *ansatz* for ρ at longer times. This is done in analogy with the expression for ρ^A from Eq. (3) at time τ . We take

$$\rho^A(R_m, R_{m+n\tau}; n\tau) = \prod_{\ell=1}^{N_b} \rho_1(r_\ell(m), r_\ell(m+n); n\tau) \times \exp \left[-\frac{n\tau}{2} \sum_j [\mathcal{U}_j(m) + \mathcal{U}_j(m+n)] \right] \quad (10)$$

3.2.2 Choosing Moves Intelligently- A priori Sampling

Instead of choosing sites at random, we include information about the disorder potential in picking a site. The idea here is to factor the transition probability into an a priori sampling distribution T and an acceptance probability A , given by $W_{s,s'} = T_{s,s'} A_{s,s'}$. The detailed balance condition is then changed to

$$A_{s,s'} = \min \left(1, \frac{\Pi_{s'} T_{s,s'}}{\Pi_s T_{s,s'}} \right). \quad (11)$$

For simplicity it is often assumed that $T_{s,s'} = T_{s'}$, i.e. it depends only on the final state.

A reasonable choice for the sampling distribution for boson ℓ is

$$T = \frac{\rho_1(r_\ell(m), r_\ell(m+n/2); n\tau/2) \rho_1(r_\ell(m+n/2), r_\ell(m+n); n\tau/2)}{\rho_1(r_\ell(m), r_\ell(m+n); n\tau)} \quad (12)$$

which gives the probability of finding the boson at $r_\ell(m+n/2)$ at $t = (m+n/2)$ given that it is at $r_\ell(m)$ and $r_\ell(m+n)$ at $t = m$ and $t = (m+n)$ respectively.

The importance of this is evident- we are incorporating information about the disorder (contained in the single particle density matrices ρ_1) in the sampling distribution. The acceptance probability is now entirely governed by the interaction. To illustrate this, we consider once again 4 time slices.

3.2.3 Choosing Permutations

We include permutation cycles of length 2 only in our elementary move (the extension to larger cycle moves is straightforward). However, by the process of sweeping through the lattice several times, cycles of all lengths are generated. For the purposes of superfluidity, the long cycles are the important ones. Given a spaghetti snap-shot, the process of generating the next configuration proceeds by first picking two bosons, labeled 1 and 2 and attempting to permute them at $t = 4\tau$. The permutation is chosen with probability

$$\Pi_o = \rho_1(r_1(0), r_2(4); 4\tau) \rho_1(r_2(0), r_1(4); 4\tau) / \Sigma_P \quad (13)$$

where Σ_P is the sum of permutations for all pairs of particles.

3.2.4 Constructing New Paths

As depicted in Fig. 1(b), we have the old paths of the two bosons; polymer $\mathcal{P}_1 = [r_1(0), r_1(1) \dots P[r_1(4)]]$ and polymer $\mathcal{P}_2 = [r_2(0), r_2(1) \dots P[r_2(4)]]$ where $P[r_1(4)] = r_1(4)$ if the permutation in the previous step in Eq. (13) was not accepted, and $P[r_1(4)] = r_2(4)$ if the permutation was accepted; similarly for polymer $\mathcal{P}_2$.

The construction of the new polymer strings proceeds by first passing through level 1. This involves finding new positions $r'_1(t = 2\tau)$ and $r'_2(t = 2\tau)$ at the middle slice with a probability

$$T_1(s') = \prod_{i=1}^2 \frac{\rho_1(r_i(0), r'_i(2); 2\tau) \rho_1(r'_i(2), P[r_i(4)]; 2\tau)}{\rho_1(r_i(0), P[r_i(4)]; 4\tau)}. \quad (14)$$

These new moves are accepted with a probability given in Eq. (11). For the reverse process $T_1(s)$ is given by Eq. (14) with $r'_i(2) \rightarrow r_i(2)$. Furthermore,

$$\begin{aligned} \Pi_1(s) = \prod_{i=1}^2 & \frac{\rho_1(r_i(0), r_i(2); 2\tau) \rho_1(r_i(2), P[r_i(4)]; 2\tau)}{\rho_1(r_i(0), P[r_i(4)]; 4\tau)} \\ & \times \exp[-\tau\{\mathcal{U}_0 + 2\mathcal{U}_2 + \mathcal{U}_4\}] \end{aligned} \quad (15)$$

and $\Pi_2(s')$ is the above equation with $r_i(2) \rightarrow r'_i(2)$ and $\mathcal{U}_2 \rightarrow \mathcal{U}'_2$. Thus the acceptance probability obtained by substituting Eqs. (14,15) in Eq. (11) is

$$A_1(s, s') = \min(1, \exp[-2\tau(\mathcal{U}'_2 - \mathcal{U}_2)]) \quad (16)$$

and depends only on the interaction. If the new positions are accepted, we then continue on to the next level finding new positions at $t = \tau$ and $t = 3\tau$; if not, we go back to the initial step and attempt a new permutation. If positions on all the levels are accepted there is a final step related to the normalization of the permutation. Note that in Eq.(13), the normalization was set by Σ_P . For the reverse process, the normalization will be changed to Σ'_P . The move is thus finally accepted with probability Σ'_P/Σ_P .

This clearly illustrates the importance of the bisection method. The formation or acceptance of a new polymer string implies that it must be possible to generate new positions for each node on the polymer. If any node was unsuccessful the entire new polymer configuration must be rejected. By bisecting, then quartering and so on we are first ascertaining that the string exists over the larger sections and then zeroing in on the small parts. The algorithm is completely rigorous, and the fact that detailed balance is satisfied, implies that the probability distribution will eventually converge to Π , regardless of the approximations for Π_t and ρ^A .

4 Characterization of Phases

We find evidence for at least three phases: a superfluid (SF) phase with the superfluid density $\rho_s \neq 0$ and two insulating phases with $\rho_s = 0$. To further characterize the insulating phases, we calculate the excitation spectrum and find the localized (L) or the so-called Bose glass phase with gapless excitations and a Mott (M) phase with a finite gap to excitations. The Mott phase is found to occur only at a commensurate density of bosons (i.e. when the number of bosons is an integral multiple of the number of sites). The localized phase can arise in regions dominated by disorder as well as in regions dominated by interactions. As discussed below, we calculate the superfluid density, cycle distribution and the excitation spectrum to gain information about the phases.

4.1 Winding Number

The winding number $\mathbf{W} = (W_x, W_y)$ gives information about the response of a system to a twist in the boundary conditions. In the ground state, $\langle W_x^2 \rangle = \partial^2 \epsilon / \partial \theta^2$, where $\epsilon(\theta)$ is the dependence of the lowest eigenvalue on a twist θ along the x-direction; and similarly for $\langle W_y^2 \rangle$. If the ground state wave function is localized, it does not “see” the boundaries, provided the system is bigger than the localization length, and therefore $\langle W^2 \rangle = 0$. On the other hand, if the system is conducting, either metallic or superfluid, the twist tends to increase the energy and $\langle W^2 \rangle$ is finite. In the metallic case, this is an $\mathcal{O}(1)$ effect whereas in the superfluid it is an $\mathcal{O}(N_b)$ effect.

Another method of calculating $\langle W^2 \rangle$ is to count the number of times the path of a particle winds around a box with periodic boundary conditions [13]. It is given by $W_\mu = 1/N \sum_{i=1}^{N_r} j_\mu(t)$, with the current

$$j_\mu(t) = \sum_{\ell=1}^{N_b} [r_{\ell\mu}(t+1) - r_{\ell\mu}(t)] , \quad (17)$$

where $r_{\ell\mu}$ is the position of the ℓ th boson along $\mu = x$ or y . The net winding is zero in this system, however, the r.m.s fluctuations in W are non-zero and are related to the superfluid density ρ_s by

$$\frac{\rho_s}{\rho} = \frac{\langle W^2 \rangle}{2\rho\beta t} . \quad (18)$$

In Fig. (2) we compare the Monte Carlo results for ρ_s (obtained by counting the winding paths) with exact diagonalization (obtained by calculating the change of the free energy with the twist) for a small system. The agreement of the two methods provides a test of the equivalence of the two methods of obtaining ρ_s , as well as a stringent test of our code.

4.2 Excitation Spectrum

In our simulations, the two insulating phases— localized and Mott are indicated by the vanishing of ρ_s . In order to further characterize the insulating phases we calculate the spectrum of low lying *density* excitations in the Feynman-Bijl approximation, i.e. under the assumption that there is only one low-lying mode accessible to the system at each wavelength. Consider the trial state created by the density operator $\rho_k = \sum_j \exp(ikr_j)$ and orthogonal to the normalized ground state $|\Psi_0\rangle$:

$$|\Psi_k\rangle = \rho_k |\Psi_0\rangle - \langle \Psi_0 | \rho_k | \Psi_0 \rangle |\Psi_0\rangle. \quad (19)$$

The variational energy of this trial state is given by a generalization of the lattice f-sum rule [27] to disordered systems by

$$\omega_k \equiv E_k - E_0 = \epsilon_k |K| / S(k) \geq E_{gap} \quad (20)$$

where ϵ_k is the single particle (band) energy, K is the total kinetic energy, and $S(k) = (1/N)[\langle \rho_k \rho_{-k} \rangle - |\langle \rho_k \rangle|^2]$ is the structure factor. The insulating phases are distinguished by the long wave length behavior of the structure factor as discussed in section 5.

4.3 Cycle Distribution

A given permutation of bosons can be broken up into cycles of various lengths with the sum rule $N_c \mathcal{L}_c = N_b$, where N_c is the number of cycles of length $\mathcal{L}_c$. In Fig. (3) we show the cycle distribution for increasing amounts of disorder. In a system of 8 bosons, there are about 0.1 cycles of length 8 in the clean system, whereas for $V = 12$, it gets reduced to 0.006. On the other hand, weight in the short cycles increases from 1.3 to 2.8 as V is increased. Thus the weight of the cycle distribution shifts to smaller cycles as a tendency to localize is encountered, either due to interactions and/or disorder, and the number of long cycles that are indicative of conducting behavior are reduced.

5 Interplay between Disorder and Interaction

The behavior of ρ_s as a function of U is shown in Fig. (4). In the clean system, ρ_s/ρ is unity for $U = 0$ and decreases monotonically with increasing U , finally saturating at a finite value. For a finite V , in the non-interacting limit ρ_s vanishes for the infinite system, and is close to zero on our finite system. We have some preliminary results that indicate that the localized phase persists up to a critical value of U_{c1} that depends on the amount of disorder. Beyond U_{c1} , Fig. (4) clearly shows that an increase in U leads to an *enhancement* of ρ_s for small U , since the interaction term prohibits an extensive number of bosons from

occupying the one-particle localized ground state. Therefore in this region the interaction term screens the randomness and effectively delocalises the system.

The superfluid density ρ_s peaks when $U \approx V$ and then decreases for larger U . In the disordered system, even though ρ_s is non-monotonic as a function of U , it is always less than that in the clean system, as might be expected. It appears from Fig. (4), that for small disorder $V < V_c$ the system remains superfluid at large values of U . We believe this behavior should persist at arbitrarily large U . This persistence of a superfluid phase is in marked contrast to the results of ref.[2] where a localized phase appeared for any value of the disorder (even if bounded) in the hard core limit. However, for $V > V_c$ the system undergoes a transition from a superfluid to a localized phase at a critical value of U .

In Fig. (5) we show typical configurations in the SF phase, in which the polymers are seen to wander all over the box, and in the L phase where the polymers are essentially rigid.

We next calculate the density-density correlation function and find that in the superfluid phase $S(k) \sim k$. Since $\epsilon_k \sim k^2$, this confirms, from Eq. (20), the existence of phonon modes with a dispersion $\omega_k = ck$, where the sound velocity c decreases with disorder.

5.1 Competition between Bose Glass and Mott Insulator

The non-monotonic dependence of ρ_s on U arises for both incommensurate and commensurate densities. However, at commensuration there are some additional surprises. The behavior of ρ_s as a function of U for different disorder strengths is shown in Fig. (6). In particular, we find that in the range $6t \lesssim U \lesssim 8.5t$, ρ_s in the disordered system $V = 4t$ is *higher* than in the clean system. By studying the behavior of the structure factor, we find that disorder *enhances* the density fluctuations at large interaction at a commensurate density. For $8.5t \lesssim U \lesssim 11t$, the disordered system continues to be superfluid, while the clean system is already in a Mott phase.

Beyond $U \gtrsim 11t$, the disordered system also enters a Mott phase as indicated by the following observations:

- (a) The average single particle density at each point in the lattice is closely pinned to 1.
- (b) The correlation of the density with the underlying random disorder $\langle n_i V_i \rangle$ is vanishingly small.
- (c) The structure factor $S(k) \sim k^2$ and from Eq. (20) this implies that a Mott gap opens up in the excitation spectrum as shown in Fig. (7).

At $U = 14t$ for example, both the disordered system with $V = 4t$ and the clean one with $V = 0$ show the opening of a Mott gap that is *smaller* in the disordered

case. For comparison at $U/t = 6$, on the other hand, the spectrum is gapless in both cases and ρ_s is finite. Our numerical simulations indicate that at least for small disorder, there is a direct transition from the superfluid to the insulator at a critical value of the interaction which *increases* with the disorder. This puts into question the conjecture by Fisher et. al. [2] that the transition from the superfluid to the Mott phase would always be via an intermediate localized phase. We believe that at higher values of the disorder this is indeed the case as discussed in the next section.

6 Phase Diagram

It is clear that more detailed simulations are required on large systems, along with careful finite size scaling[15] in order to obtain the phase diagram and the different exponents that characterize the transitions. Here, we venture an educated guess about the phase diagram based on our simulations and physical arguments.

For the incommensurate density, we expect the phases in Fig. (8a), as argued in section (5). For $V = V_1 < V^-$, there is a L-SF transition. On the other hand, for $V = V_2 > V^-$, there is a reentrant behavior, where the system goes from L-SF-L. It was argued previously by Giamarchi and Schulz[18] that at incommensurate densities, there would be two insulating phases with a phase transition between them—one driven by disorder and the other driven by interactions. This was also claimed to be the case in the 1D simulations of Scalettar et. al. [21]. We, on the other hand believe that for finite U and V there is only one fixed point describing the SF-L transition.

In the commensurate case, the phase diagram is given in Fig. (8b). The three phases compete to give different types of transitions. Along $V = V_1$, we find a L-SF-M transition; for larger values of $V = V_2$, we find a L-SF-L-M transition and for yet higher disorder a direct L-M transition with increasing values of U .

7 Conclusions

We have performed path integral Monte Carlo simulations of a model of interacting bosons in a random potential in 2D at $T=0$. The problem was mapped onto a classical 3D problem of strings or directed polymers with one difference—the length of the polymers was not fixed but could vary because of the permutations between the bosons in the quantum problem. We discussed efficient ways to sample the configuration space of these polymeric objects. It is possible to extend the algorithm in order to improve its convergence. For example, the small time approximation for the density matrix can be made more accurate by including pair correlations[14]. It is also possible to include 3 and 4 particle

exchanges in the elementary moves. Another modification can be to include permutations in the intermediate states. Even without these modifications, the algorithm is completely rigorous since detailed balance is satisfied; however the above changes will certainly improve the convergence. Other extensions can be to calculate the off-diagonal density matrix by cutting one polymer and allowing it to wander. This will give information about the condensate fraction. The simulations have currently been done in the canonical ensemble, but it is possible to allow particle number fluctuations, which will give information about response functions from a single simulation.

Based on our simulations we have obtained the schematic phase diagrams for bosons at an incommensurate and commensurate density and have tracked the different phases— the superfluid, localized and Mott phases as functions of disorder and interactions. Some of the unexpected features that emerge are that in certain regions of parameter space it is indeed possible for both repulsive interactions and disorder to *enhance* the superfluidity. More careful finite size scaling analysis are in progress to obtain the exponents that characterize these transitions. We feel that quantum Monte Carlo simulations have proved to be a very useful tool in addressing a rather difficult class of problems. Further progress in answering some of the open experimental questions in adsorbed helium superconductor-insulator transitions and vortex glass transitions would be an important step forward.

Acknowledgments

I would like to especially thank Werner Krauth for his collaboration on developing the code, without which, needless to say, none of this would be possible. A large part of the work presented here was done in collaboration with him. I would also like to thank Salman Ullah for an on-going collaboration on the superconductor-insulator transition in films and the vortex glass simulations. And finally, I would like to thank David Ceperley for introducing me to Monte Carlo techniques and for many fruitful discussions. This work was supported by the U.S. Department of Energy, BES- Materials Sciences, under contract W-31-109-ENG-38.

Appendix: Approximate Density Matrix

Our aim here is to construct an approximation for the elemental density matrix $\rho(R_m, R_{m+1}; \tau)$ at short time $\tau \ll \beta$.

To begin, let us use the knowledge of the non-interacting problem. If U is zero in the Hamiltonian in Eq. (1), it reduces to a single particle problem with

$$H_1 = \frac{-t}{2} \sum_{\langle i,j \rangle} (a_i^\dagger a_j + h.c.) + \sum_i V_i n_i \quad (21)$$

The total density matrix ρ factorizes into a product of single particle density matrices ρ_1

$$\rho_{(U=0)}(R_m, R_{m+1}; \tau) = \prod_{\ell=1}^{N_b} \rho_1(r_\ell(m), r_\ell(m+1); \tau) \quad (22)$$

where

$$\rho_1(r_\ell(m), r_\ell(m+1); \tau) = \langle r_\ell(m) | \exp(-\tau H_1) | r_\ell(m+1) \rangle \quad (23)$$

For $U \neq 0$, we can now construct an approximate density matrix by taking the average of the interaction energy on the two slices

$$\begin{aligned} \rho(R_m, R_{m+1}; \tau) &= \prod_{\ell=1}^{N_b} \rho_1(r_\ell(m), r_\ell(m+1); \tau) \\ &\quad \times \exp \left(-\frac{\tau}{2} \sum_j [U_\ell(m) + U_\ell(m+1)] \right) \end{aligned} \quad (24)$$

Here we have also assumed that τ is small and have essentially neglected terms of order τ^2 arising from the commutation of the interaction term and H_1 .

A.1 Construction of ρ_1 : Matrix Squaring Method

We wish to construct $\rho_1(i, j; \tau)$ at short time $\tau \ll \beta$. We proceed by dividing up the short time τ into even tinier steps of size $\epsilon = (2^{-L})\tau$. We now have $\rho_1(\epsilon) = \exp(-\epsilon H_1) \approx 1 - \epsilon(T + V)$, where the first term in Eq. (21) is denoted by T , the kinetic energy operator, and the second term is denoted by V , the disorder. $\rho_1(\epsilon)$ is finite only along the diagonal, $\rho_1(i, i; \epsilon) = 1 - \epsilon V_i$, and for nearest neighbor sites, $\rho_1(i, j; \epsilon) = \epsilon/2$.

We can now easily construct $\rho_1(2\epsilon) = \rho_1(\epsilon)\rho_1(\epsilon)$ by matrix squaring. If this procedure is repeated L times, we will have $\rho_1(\tau = 2^L \epsilon)$. This allows the amplitude to spread out in a gaussian profile at time τ rather than being restricted to just the nearest neighbor sites.

References

- [1] P. A. Lee and T. V. Ramakrishnan, *Rev. Mod. Phys.* **57**, 287 (1985).
- [2] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, *Phys. Rev. B* **40**, 546 (1989).
- [3] K. Blum, *Thesis, Cornell University*, 1989.
- [4] P. B. Weichman, M. Rasolt, M. E. Fisher, and M. J. Stephen, *Phys. Rev. B* **33**, 4632 (1986).
- [5] D. B. Haviland, Y. Liu and, A. M. Goldman, *Phys. Rev. Lett.* **62**, 2180 (1989).
- [6] M. P. A. Fisher, G. Grinstein, and S. M. Girvin, *Phys. Rev. Lett.* **64**, 587 (1990).
- [7] D. R. Nelson and H. S. Seung, *Phys. Rev. B* **39**, 9153 (1989).
- [8] M. P. A. Fisher and D. H. Lee, *Phys. Rev. B* **39**, 2756 (1989).
- [9] M. P. A. Fisher, *Phys. Rev. Lett.* **62**, 1415 (1989).
- [10] D. S. Fisher, M. P. A. Fisher, and D. A. Huse, *Phys. Rev. B* **43**, 130 (1991).
- [11] R. H. Koch, V. Foglietti, W. J. Gallagher, G. Koren, A. Gupta, and M. P. A. Fisher, *Phys. Rev. Lett.* **63**, 1511 (1989).
- [12] P. L. Gammel, L. F. Schneemeyer, and D. J. Bishop, *Phys. Rev. Lett.* **66**, 953 (1991).
- [13] E. L. Pollock and D. M. Ceperley, *Phys. Rev. B* **36**, 8343 (1987); D. M. Ceperley and E. L. Pollock, *Phys. Rev. B* **39**, 2084 (1989).
- [14] D. M. Ceperley and E. L. Pollock, *Proc. of Elba Conference on Monte Carlo Methods for Physics*, eds. Fantoni, 1991.
- [15] S. Ullah and N. Trivedi, *Bull. Am. Phys. Soc.* **37**, 64 (1992).
- [16] W. Krauth, N. Trivedi, and D. M. Ceperley, *Phys. Rev. Lett.* **67**, 2307 (1991).
- [17] R. N. Bhatt and A. P. Young, *Phys. Rev. Lett.* **54**, 924 (1985).
- [18] T. Giamarchi and H. J. Schulz, *Europhys. Lett.* **3**, 1287 (1987); *Phys. Rev. B* **37**, 325 (1988).
- [19] M. Ma, B. I. Halperin, and P. A. Lee, *Phys. Rev. B* **34**, 3136 (1986).

- [20] W. Krauth and N. Trivedi, *Europhys. Lett.* **14**, 627 (1991).
- [21] G. G. Batrouni, R. T. Scalettar, and G. T. Zimanyi, *Phys. Rev. Lett.* **65**, 1765 (1990); R. T. Scalettar, G. G. Batrouni, and G. T. Zimanyi, *Phys. Rev. Lett.* **66**, 3144 (1991);
- [22] L. Zhang and M. Ma, to appear in *Phys. Rev. B* **45** 1992.
- [23] K. G. Singh and D. S. Rokhsar, preprint (1992).
- [24] K. Runge, preprint (1992).
- [25] D. Belitz and T. R. Kirkpatrick, *Phys. Rev. Lett.* **63**, 1296 (1989); M. Milovanovic, S. Sachdev and R. N. Bhatt, *Phys. Rev. Lett.* **63**, 82 (1989).
- [26] E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, *Phys. Rev. B* **41**, 9301 (1990).
- [27] N. Trivedi and D. M. Ceperley, *Phys. Rev. B* **40**, 2737 (1989); *Phys. Rev. B* **41**, 4552 (1990).

Figure Captions

Fig. 1(a) Configuration of 6 bosons in (1+1) dimension. The β direction is broken up into $N_\tau = 4$ time slices in this example. The boson world lines can be viewed as strings or directed polymers forming a spaghetti.

Fig. 1(b) Bisection method of constructing new paths. For $N_\tau = 4$, the old paths of two bosons are $\mathcal{P}_1 = [r_1(0), r_1(1), r_1(2), r_1(3), r_1(4)]$ and $\mathcal{P}_2 = [r_2(0), r_2(1), r_2(2), r_2(3), r_2(4)]$. We assume here that the bosons are not permuted. At the first level new positions $r'_1(2)$ and $r'_2(2)$ on $t = N_\tau/2$ are picked. If the moves are accepted, one proceeds to the next level where new positions $\{r'_1(1), r'_1(3)\}$ and $\{r'_2(1), r'_2(3)\}$ are picked. If accepted, we now have new paths $\mathcal{P}'_1 = [r_1(0), r'_1(1), r'_1(2), r'_1(3), r_1(4)]$ and $\mathcal{P}'_2 = [r_2(0), r'_2(1), r'_2(2), r'_2(3), r_2(4)]$.

Fig. 2 Comparison of path integral Monte Carlo and exact diagonalization results. The behavior of the superfluid density ρ_s/ρ is shown as a function of the repulsive on-site interaction between the particles U for disorder $V = 0$ and $V = 2t$ for a 4 site chain with 3 bosons. In the Monte Carlo code, ρ_s is obtained by counting the number of paths that wind around the box (with periodic boundary conditions), whereas in the exact diagonalization method, ρ_s is obtained from the dependence of the free energy on a twist at the boundary.

Fig. 3 The number of cycles N_c as a function of the cycle length $\mathcal{L}_c$. Data is shown for $V = 0$ and $V = 12t$ in a 4×4 system with $N_b = 8$, $U = 2t$ and $\beta t = 3$. The area under both curves is conserved and equals N_b . Note that the weight shifts to smaller cycles as disorder is increased.

Fig. 4 Interplay of disorder and interaction for incommensurate densities. The superfluid density ρ_s/ρ vs. interaction strength U/t is shown in a 6×6 system of density $\rho = 0.75$ and $\beta t = 4$. The values of the disorder parameter are $V/t = 0$ (triangles), 2 (squares) and 6 (circles). In the clean system, the effect of U is always to decrease ρ_s . In the presence of disorder, U initially enhances ρ_s until $U \approx V$ and then causes ρ_s to decrease beyond that.

Fig. 5 Two typical configurations are shown for a 4×4 system with 8 bosons at $\beta t = 3$ and $U = 2t$. (a) $V = 0$ with cycle distributions $\{2 \rightarrow 3 \rightarrow 8\}$, $\{1 \rightarrow 7\}$, $\{4 \rightarrow 5\}$ and $\{6\}$; and (b) $V = 12t$ with $\{3 \rightarrow 5 \rightarrow 7\}$, $\{1 \rightarrow 4\}$, $\{2 \rightarrow 6\}$ and $\{8\}$. We apply periodic boundary conditions along x , y , and β . Note that while the cycle distributions in these specific examples are not very different, the role of disorder is to localize the particles producing rigid world lines.

Fig. 6 Competition between Bose glass and Mott phases. Superfluid density ρ_s/ρ vs. interaction strength U/t in a 10×10 system of density $\rho = 1$ and $\beta t = 4$.

The values of the disorder parameter are $V/t = 0$ (triangles) and 2 (squares). Note that for $8.5 \lesssim U/t \lesssim 11$, the clean system is in a Mott phase, but in the presence of disorder the system becomes superfluid.

Fig. 7 Excitation spectrum along $[0,1]$ at $\rho = 1$. In a 10×10 system, in the superfluid phase the effect of disorder is shown by $U = 6t$, $V = 0$ (open triangles) and $U = 6t$, $V = 4t$ (open squares). In this case there is a linear mode with $E_k = ck$ with a sound velocity c that decreases with disorder. In the Mott phase the corresponding curves are $U = 14t$, $V = 0$ (filled triangles) and $U = 14t$, $V = 4t$ (filled squares). Here there is a finite gap to excitations which gets reduced by disorder.

Fig. 8(a) Phase Diagram at incommensurate density. For $V = 0$, the system is always superfluid (SF). At a finite $V = V_1 < V^-$, the system goes from a localized (L) to SF phase at $U = U_{c1}$. For $V^- < V = V_2 < V^+$, we see a L-SF-L at $U = U_{c1}$ and $U = U_{c2}$ respectively. For $V = V_3 > V^+$, the system is always localized.

Fig. 8(b) Phase Diagram at commensurate density. In this case there are 3 phases that compete, SF, L and Mott (M). For $V = 0$, there is a SF-M transition at $U_{c2} \sim 8t$. At a finite $V = V_1 < V^-$, (where V^- is the value of the disorder at the multicritical point), there is a L-SF-M transition where the surprise is that U_{c2} increases with V . For V above the multicritical point $V^- < V = V_2 < V^+$, we see a L-SF-L-M transition and above $V = V_3 > V^+$, there is a L-M transition.

TRIVED1
FIG. 1(a)

TRIVEDI
FIG. 3

TRIVEDI
FIG. 4

TRIVEDI
FIG. 5(a)

EF

TRIVED1
FIG. 5(b)

TRIVEDI
FIG. 6

TRIVED!
FIG. 7

TRIVED I
FIG. 8(a)

TRIVEDI
FIG. 8(b)

END

**DATE
FILMED**

5 / 18 / 92