Finite-temperature phase transitions in a two-dimensional boson Hubbard model

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We study finite-temperature phase transitions in a two-dimensional boson Hubbard model with zero-point quantum fluctuations via Monte Carlo simulations of quantum rotor model, and construct the corresponding phase diagram. Compressibility shows a thermally activated gapped behavior in the insulating regime. Finite-size scaling of the superfluid stiffness clearly shows the nature of the Kosterlitz-Thouless transition. The transition temperature, \(T_c\), confirms a scaling relation \(T_c \propto \rho_0^x\) with \(x = 1.0\). Some evidences of anomalous quantum behavior at low temperatures are presented.

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Recently quantum phase transitions\(^1,2\) have drawn a lot of attention in systems of interacting particles. Typically strong interactions suppress the itineracy of particles to induce a strongly correlated insulating phase, whereas with weak interactions a conducting phase is stable. The criticality of these zero-temperature phase transitions can be investigated at low, but finite, temperatures. How quantum fluctuations associated with a quantum critical point (QCP) have influence on phases at finite temperatures\(^3,4,5\) is a theoretically interesting and an experimentally relevant question.

At finite temperatures, it is expected that a quantum phase transition turns into a classical one with the same order parameter or disappears. Remnant quantum fluctuations near a QCP may bring anomalous properties\(^6\), which can be captured by scaling relations, and lead to crossover behaviors as temperature rises. Some possibilities such as reentrant behaviors due to the interplay of quantum and thermal fluctuations have been proposed\(^7\).

These issues can be clarified by direct investigations of a generic quantum mechanical model. So far most of the theoretical investigations heavily rely on the exact solution of the quantum Ising model, available strictly in one dimension\(^4\). Interacting bosonic systems simulated via Monte Carlo methods, not suffering from negative sign problems, will be an ideal place to study these problems. In previous works, a quantum XY model, equivalent to hard-core bosons at half-filling, showed the Kosterlitz-Thouless (KT) transition\(^2\) at finite temperature in two dimensions\(^8,9\). In the model with nearest neighbor repulsion, destruction of the solid order as well as the superfluidity by thermal fluctuations was observed\(^10\). However, generic finite-temperature phase diagrams have not been constructed.

In this work, we investigate the thermally driven phase transitions of a two-dimensional quantum rotor model, which is believed to share the same critical properties of a soft-core generic boson Hubbard model\(^11\), via Monte Carlo simulations. The results are summarized in the phase diagram as shown in Fig. 1. Finite-size scaling properties of the superfluid stiffness confirm that the nature of the classical phase transition associated with the destruction of superfluidity is consistent with that of the KT transition, and clearly support the scenario of the universal jump at the critical point\(^12\). Finite temperature, \(T_c\), sets the size in the temporal direction, leading to a scaling behavior\(^4,11\) \(T_c \propto \rho_0^x\) with \(x = 1.0\), where \(T_c\) is the transition temperature and \(\rho_0\) is the superfluid stiffness at zero temperature. The compressibility diverges at the transition. In the insulating regime at low temperature, thermally activated behavior of the compressibility with a finite energy gap is observed. Some anomalous dependence of energy and specific heat on \(T\), possibly due to quantum fluctuations, are observed for \(T < 0.25U\).

The Hamiltonian of a boson Hubbard model reads

\[
H = \frac{U}{2} \sum_j n_j (n_j - 1) - \mu \sum_j n_j - w \sum_{<ij>} (b_j^\dagger b_i + b_i^\dagger b_j^\dagger),
\]

where \(b_j(b_j^\dagger)\) is the boson annihilation (creation) operator.

![FIG. 1: (Color online) Phase diagram on the space of hopping strength, \(t(=\sqrt{\mu_0(n_0 + 1)/w})\), and temperature, \(T\), in unit of \(U\). The solid line denotes the classical phase transitions, which terminates at a QCP at \(T = 0\). The dotted line represents crossover between gapped fluid and normal fluid.](image-url)
at the \(j\)-th site, and \(n_j\) is the number operator. \(U\) and \(w\) stand for the strengths of the on-site repulsion and of the nearest neighbor hopping, respectively, and \(\mu\) is the chemical potential.

It is convenient to put \(\mu/U + 1/2 = n_0 + \bar{n}\) with an integer \(n_0\) and \(-1/2 < \bar{n} \leq 1/2\) so that \(n_0\) represents the background number of bosons per site and \(\bar{n}\) is a charge offset. When \(\bar{n} = 0\), the density of bosons is fixed to a commensurate filling across the transition. For non-integer \(\bar{n}\), however, an integer filling in a Mott insulator shifts to a non-integer filling in a compressible fluid. We study the phase transition of the latter case in \((2+1)\)-dimensional \(L \times L \times L_\tau\) square lattices, where \(L\) denotes the size in a spatial dimension and \(L_\tau\) in the temporal dimension.

Since the phase transition of the model in Eq. (1) is characterized by the establishment of phase coherence, we may rewrite the Hamiltonian in terms of the phase angle \(\theta_j\) of bosons by replacing \(b_j(b_j^\dagger) = \sqrt{\rho_0} e^{-i\theta_j}(\sqrt{n_j + 1} e^{i\theta_j})\) with \(n_j = \frac{1}{\beta} \partial \theta_j\). Under the assumption that the nature of the transition is governed only by the fluctuations of \(\theta_j\), not those of the hopping strength, we replace \(n_j \rightarrow n_0\) so that \(b_j(b_j^\dagger) = \sqrt{n_0} e^{-i\theta_j}(\sqrt{n_0 + 1} e^{i\theta_j})\). Then, the Hamiltonian is reduced to a quantum rotor model

\[
H = \frac{U}{2} \sum_j n_j(n_j - 1) - \mu \sum_j n_j - 2t \sum_{<ij>} \cos(\theta_i - \theta_j),
\]

where \(t = \sqrt{n_0(n_0 + 1)} w\). Here we take the number of bosons \(n_j \geq 0\).

Through a path integral mapping, we can construct the corresponding classical action\[14\]

\[
S = \sum_r \frac{\epsilon U}{2} J_r^2 (J_r^2 - 1) - \epsilon \mu J_r - \ln I_{J_r}(2ct) - \ln I_{J_r}(2ct)
\]

with the partition function

\[
Z = \sum_{\{J_r\}} e^{-S[J]},
\]

where \(\epsilon = \beta/L_\tau\) is a lattice constant in the imaginary time axis for an inverse temperature \(\beta\), \(J_r\) is an integer current at site \(r = (j, \tau)\) with a spatial index \(j\) and a temporal index \(\tau\), which is conserved at each site as denoted by \(\nabla \cdot J_r = 0\), and \(I_m(x)\) is the modified Bessel function given by the relation \(e^{K \cos \theta} = \sum_{m=-\infty}^{\infty} I_m(K) e^{im\theta}\). In this work, we investigate the properties of the model in Eq. (3) via Monte Carlo simulations using a recently proposed worm algorithm \[13\]. In order to reduce the systematic errors in discretizing the imaginary time axis, we need to take \(\epsilon \sqrt{\epsilon U} \ll 1\). We take \(U/e = 0.5 - 2\) for \(t \ll U\) and set the energy unit \(U = 1\).

The superfluid stiffness in a finite system is given by\[14\]

\[
\rho_L = \beta^{-1} L^{2-d} \langle W_x^2 \rangle,
\]

where \(W_x = L^{-1} \sum_r J_r^x\) and \(\langle \ldots \rangle\) denotes the averages over the probabilities determined by the partition function of Eq. (4), and \(d\) is the spatial dimensionality. Similarly the compressibility is

\[
\kappa = \beta L^{-d} [\langle N^2 \rangle - \langle N \rangle^2],
\]

with \(N = L^{-1} \sum_r J_r^x\). The energy expectation is given by

\[
\langle H \rangle = L^{-1} \langle \partial S / \partial e \rangle,
\]

and the specific heat is \(C_V = L^{-d} (\partial \langle H \rangle / \partial T)\).

We consider the case for \(\mu = 0.9\) so that \(n_0 = 1\) and \(\bar{n} = 0.4\). Figure (b) shows the finite-size scaling behavior of the superfluid stiffness as a function of (a) \(t\) and
(b) $\beta$. Finite-size scaling properties of the transition can be obtained by plotting the curves in terms of a scaling variable $L/\xi$, where $\xi$ is the correlation length. Here we assume an essential singularity \[ \xi \approx \exp(b\delta^{-1/2}), \]
where $\delta = t - t_c$ (or $\beta - \beta_c$) is a tuning parameter and $b$ is a non-universal scaling factor. In terms of this scaling variable, we obtain high-quality data collapsing onto a single curve for different sizes, consistent with the nature of the KT transition. The scaling behavior also supports the scenario of the universal jump of the superfluid stiffness \[ (\pi/2)\beta_c \rho_\infty = 1, \]
at the critical point in the thermodynamic limit. By extrapolating the single curves to the critical point, we find that $(\pi/2)\beta_c \rho_\infty \approx (a)1.01$ and $(b)1.06$. These numbers are, however, sensitive to fitting parameters $b$ and $t_c(\beta_c)$.

Figure 3a shows the behavior of the compressibility. The finite-size scaling ansatz of the compressibility is written in the form
\[ \kappa = L^{z-d} \tilde{X}_\kappa(L(t - t_c)^{1/\nu}, \beta/L^z), \]
where $\tilde{X}_\kappa$ is a dimensionless scaling function and $z$ is the dynamical critical exponent. For the generic superfluid-insulator transition (GSIT), $z = 2$ is expected. The crossing behavior of the compressibility curves for different sizes at the critical point $t^0 = 0.023 \pm 0.001$, therefore, represents the scaling properties near the QCP, where $t^0$ is the critical hopping strength at zero temperature. For different values of $\mu$, we have similar results with $t^0$ just shifted.

We find that the compressibility diverges at the transition. In the superfluid side, $\kappa \sim 1/(t - t^0)$. This strongly supports that the long-range density fluctuations drive the transition. In the insulating side, the compressibility has an activated form $e^{-\Delta_{\text{gap}}/T}$ with a finite energy gap $\Delta_{\text{gap}}$. This dependence is shown in Fig. 3b for different $t$, from which we can calculate $\Delta_{\text{gap}}$ as shown in the inset. For small $t$, we need a large number of Monte Carlo steps to obtain equilibrium and have bigger error bars in determination of $\Delta_{\text{gap}}$. The gap vanishes around $t = t^0$ as expected.

Thus we have a so-called ‘V-shaped’ phase diagram (Fig. 1). In the insulating regime, the Mott insulator exists at $T = 0$, which turns into an activated gapped fluid with a finite energy gap at low temperature. It gradually disappears in a high-temperature normal fluid. This crossover line can be specified by the condition $\Delta_{\text{gap}}/T \approx 1$. The phase coherence in a superfluid at $T = 0$ is destroyed by quantum fluctuations to form a QCP or by thermal fluctuations at $T > 0$ to define classical phase transitions. The phase boundary in Fig. 1 is obtained by tuning $t$ for given $T$ (black circles) as well as by tuning $\beta$ for a given $t$ (red squares). Note that the phase boundary follows a scaling relation $T_c \propto |t - t^0|^\nu$, which implies that $\beta$ determines the correlation length in the temporal direction, where $\nu$ is the correlation length critical exponent. The boundary in Fig. 1 is consistent with the expectation $z\nu = 1$ for the GSIT.

It is interesting to check the predicted scaling relation \[ T_c \propto \rho_0^x \]
in this model. Figure 4 shows that the zero-temperature superfluid stiffness $\rho_0^x$, denoted by dotted line, which obtained via extrapolation of values at $T > 0$, follows $\rho_0^x \propto (t - t^0)$, implying that $x = 1.0$. It is consistent with the hyperscaling argument suggesting $x = z/(d + z - 2)$.

We expect that this quantum criticality disappears as temperature rises, which means quantum fluctuations possibly leave some tracks in bulk properties at low temperatures. Figure 5 shows the specific heat, $C_V$, and the energy expectation values, $\langle H \rangle$, as a function of $T$ for different $t$. Sharp rises of $C_V$ in the conducting regime or round up-rises in the insulating regime are followed by
indents, regions indicated by ▲, which apparently represent anomalous behavior due to quantum fluctuations and disappear at high temperatures for $T \gtrsim 0.25$. This feature strongly suggests a crossover in normal fluid from quantum mechanical to classical regime. Similarly the curves of $\langle H \rangle$ show bumps, indicated by ▼, only in the range where quantum critical fluctuations are expected to have effects.

In summary, we have investigated the phase transitions at finite temperature in a two-dimensional quantum rotor model in which intrinsic zero-point fluctuations are present. Finite-size scaling of the superfluid stiffness shows an essential singularity of the KT phase transition and the universal jump at the critical point. The compressibility diverges at the transition. In the insulating regime, the compressibility shows a thermally activated behavior, $\kappa \sim e^{-\Delta_{\text{exp}}/T}$, from which we can successfully evaluate the gap. This indicates that the insulating behavior at low temperature gradually crosses over to the behavior of normal fluid as temperature increases. The transition temperature $T_c$ shows a scaling behavior $T_c \propto |t - t_c^0|$, showing that finite $T$ limits the length of quantum fluctuations in the temporal direction, and a hyperscaling relation $T_c \propto p_0$. The behavior of the specific heat and the energy expectation values, $\langle H \rangle$, have bumps at low temperatures, which disappear in the high temperature region, $T \gtrsim 0.25$. Insets: The curves of the energy expectation values, $\langle H \rangle$, have bumps at low temperatures possibly due to the effects of quantum fluctuations.

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![FIG. 4: (Color online) Superfluid stiffness for different $\beta$. As $\beta$ increases, the size dependence becomes smaller. This allows us to extrapolate the curves to obtain zero-temperature superfluid stiffness, $\rho_0$, in the thermodynamic limit as denoted by dotted line. It shows that $\rho_0 \propto |t - t_c^0|$ with $t_c^0 \approx 0.22$.](image)

![FIG. 5: (Color online) Specific heat, $C_V$, as a function of $t$ for different $\beta$. Sharp rises in the conducting regime, signature of the superfluid transition, or round up-rise of $C_V$ in the insulating regime are followed by indents which disappear in high temperature region, $T \gtrsim 0.25$. Insets: The curves of the energy expectation values, $\langle H \rangle$, have bumps at low temperatures possibly due to the effects of quantum fluctuations.](image)

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