Quantum Criticality from in-situ Density Imaging

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We perform large-scale Quantum Monte Carlo (QMC) simulations for strongly interacting bosons in a 2D optical lattice trap, and confirm an excellent agreement with the benchmarking in-situ density measurements by the Chicago group [1]. We further present a general finite temperature phase diagram both for the uniform and the trapped systems, and demonstrate how the universal scaling properties near the superfluid(SF)-to-Mott insulator(MI) transition can be observed by analysing the in-situ density profile. The characteristic temperature to find such quantum criticality is estimated to be of the order of the single-particle bandwidth, which should be achievable in the present or near future experiments. Finally, we examine the validity regime of the local fluctuation-dissipation theorem (FDT), which can be used as a thermometry in the strongly interacting regime.

In this recent decade, systems of ultracold atoms have become the most promising candidate for the realization of quantum simulators, which are designed to explore various challenging and exotic many-body physics. One of the most well-understood ultracold systems is made of bosonic atoms loaded in an optical lattice, whereby the 3D SF-MI phase transition had been observed in time-of-flight (TOF) experiments [2] and then directly compared to theory with great accuracy [3]. However, the TOF images do not directly represent physical quantities of atoms inside the optical lattice and thus subject the quantitative study of critical phenomena to question, especially given the complexity of the expansion dynamics during the TOF imaging [4]. As a result, several schemes have been proposed to determine the critical properties based on density-related quantities [4, 5], which have been successfully measured via in-situ spatially resolved density imaging in a bosonic systems loaded into a 2D optical lattice [6]. Before these theoretical schemes could be trusted and applied, an essential step is to validate them from the first principle calculation in the parameter regime of realistic experiments.

In this paper, we perform an ab-initio QMC simulation [10] to have a direct comparison with the in-situ data of Chicago group [1] in a 2D optical lattice with a harmonic trap, and find an excellent agreement (see Figs. 1(a) and (b)). We then calculate the finite temperature phase diagram for a uniform system, and justify the validity of the local density approximation (LDA), except near the phase boundary. We further quantitatively confirm the universal scaling properties near the SF-MI quantum phase transition point through the finite temperature density profile in a trapped system. The characteristic temperature, $T^*$, to find such quantum criticality is comparable to the single particle bandwidth, and therefore is achievable in the present or near future experiments. Finally, we show the regime where the local fluctuation-dissipation theorem (FDT) is valid, providing a useful thermometry in the strongly interacting regime. Our work therefore paves the way for the future experimental realization of quantum simulators.

![Fig. 1](https://example.com/fig1.png)

**FIG. 1**: (Color online) Density profiles measured by Chicago group (blue squares) and by our QMC simulation (green lines) for (a) a shallow lattice and (b) a deep lattice. $\alpha(V_{\text{lat}})$ is the lattice constant(strength), and $E_R$ is the recoil energy. (c) is the finite temperature phase diagram of a uniform 2D system. Green thick line is the SF-MI phase boundary at $T = 0$. Red/blue lines are boundaries of SF(MI) at $T/U = 0.01$, 0.05, 0.1, and 0.15 from left to right (from right to left). The regime of MI phase is defined in the text. The vertical dashed lines are the chemical potential range in Figs. 3 and 4.

Our numerical simulation starts from the single-band Bose-Hubbard model: $\hat{H} = -J \sum_{\langle i,j \rangle} (\hat{a}_i^\dagger \hat{a}_j^\dagger + h.c.) + U \sum_i \hat{n}_i (\hat{n}_i - 1) - \sum_i \mu(\hat{r}_i) \hat{n}_i$, where $\hat{a}_i$ and $\hat{n}_i$ are the boson field operator and density operator at the $i$th lattice site. $\mu(\hat{r}_i) \equiv \mu - V(\hat{r}_i)$ with $\mu$ the global chemical potential and $V(\hat{r}_i) = V_{\text{lat}} \times (x_i^2 + y_i^2)$ being the isotropic trap-
potential at lattice position, $r_i = (x_i, y_i)$. Within a 5% uncertainty in the total particle number $N$, direct comparisons of the density images show excellent and quantitative agreements (see Fig. 1(a) and (b)) both in the weak and strong lattice strengths. A small deviation in the trap center of Fig. 1(b) is due to some experimental equilibration issues [11]. Hence, our results convincingly indicate that the bosonic atoms loaded into an optical lattice is an excellent quantum simulator. In Fig. 1(c), we show the finite temperature phase diagram in a uniform 2D system. The boundaries between SF and normal phases (red lines) are determined by vanishing SF density [12]. Strictly speaking, MI phase does not exist at $T > 0$, but we can still definite its regime (blue lines) empirically by a small compressibility, $\kappa \equiv \partial n / \partial \mu < 0.02 / U$. As a result, one can clearly see how both the SF and MI regimes shrink as $T$ increases, leading to the normal phase in the intermediate regime. Such finite temperature phase diagram of a uniform system can help in the determination of the phase boundaries in a trapped system within the LDA [13], as shown in Figs. 2(a) and (b). The density profile ($\rho(r)$) as well as local compressibility ($\kappa(r) \equiv \partial \rho(r) / \partial \mu$) are obtained within the QMC simulation, but both of them can be well-reproduced within the LDA, except for the narrow regime near the phase boundary [14]. Such rounding of $\kappa(r)$ originate from the finite size effect and the finite temperature Berezinskii-Kosterlitz-Thouless (BKT) transition. From our direct comparison, however, the phase boundary determined by the largest curvature points of $\kappa(r)$ is still very close to the position obtained within the LDA (within one or two lattice sites), and also agrees with the onset of the local SF density. Therefore, practically speaking, one can still apply LDA to estimate the phase boundary even in the 2D trapped system at finite temperature. In the following, we will use another scheme to investigate the phase boundary as well as the quantum criticality near the SF-MI quantum phase transition from the density profile.

It is well-known that near the second order phase transition, the correlation length diverges and universal scal-
value of \(\mu_c\). The obtained result is identical (<0.1%) to the result of a uniform system after finite size scaling [2], and also very close (<1%) to the one we obtain above in a trap system (Fig. 3(a)). Our results verify the proposal to map out the zero temperature phase diagram in a realistic trapped system.

After determination of \(\mu_c\) in Fig. 3(b) we show the rescaled singular density \(n_s/T\) as a function of rescaled chemical potential, \((\mu - \mu_c)/T\), in the DBG model, and find a very nice convergence for the universal scaling function \(G\) (see Eq. (1)) in a wider temperature regime. This is a clear evidence of the scaling theory near the critical point of SF-MI transition. Similarly, we also show the universal functions for \(H\) and \(H(G^{-1})\) in Figs. 3(c) and (d) respectively. The later results are also shown for both the particle side and hole side of the phase transition points (i.e. the \(C_1\) and \(C_2\) points in Fig. 1(c)).

In our calculation here, we find that the universal scaling function is very sensitive to the value of exponents, i.e. no intersection point for \(\mu_c\) and no convergence of the scaling function can be obtained if using exponents of other universal classes. This can be also observed when we calculate the universal scaling function near the Mott tip, as shown in Fig. 4(a) and (b). For these data at \(J/U = 0.054\) (i.e. \(C_3 - C_4\) line in Fig. 1(c)), exponents obtained from the \(O(2)\) rotor model works much better than the DBG model, consistent with the general understanding that the low energy effective model at the Mott tip is governed by the former. The crossover from the DBG model to the \(O(2)\) rotor model near the Mott tip is of great interest, but is beyond the scope of this paper.

From the experimental point of view, however, it is somehow more important to know the characteristic temperature, \(T^*\), below which the universal scaling behavior is observable. The effective model itself cannot provide this information, and therefore our \textit{ab-initio} QMC data becomes very crucial. In Fig. 4(c), we show how the universal scaling of the DBG model is affected by temperature at \(J/U = 0.03\). We can see that \(\kappa_c\) keeps almost a constant in the low temperature limit up to some higher temperature, \(T^*\), above which their universal value starts to deviate due to higher order effects. For compressibility near \(\kappa_c\) (i.e. \(\mu \sim \mu_c\)), such \(T^*\) becomes much larger. If we set the minimum range for observing the scaling law in real space (within LDA) is about 10 lattice sites, the corresponding \(T^* \sim 6J\) is about the order of the single particle band width. Although such low temperature measurement is challenging, but should be still experimentally accessible in the near future. When \(J/U\) is close to the MI tip, due to the crossover from the DBG model to the \(O(2)\) model, we find that \(T^*\) is reduced and the range to observe the universal scaling behavior becomes smaller (see Fig. 4(d)). Therefore, at least within the QMC simulation, our results confirm the possibility of observe the universal scaling theory near the critical point in the present experimental parameter regime.

Accurate thermometry is the essence in the observation of universal scaling behavior. Earlier scheme to fit the outskirt density profile with a noninteracting model hardly works in the strongly interacting regime we consider here. It has been proposed that the fluctuation-
dissipation theorem (FDT) can be a feasible thermometry scheme (independent of any theoretical model)\(^2\)\(^1\)\(^2\), but in realistic experiments, it is more practical to consider the local version of the FDT. We start from the identity, \(\frac{d\chi}{d\mu} = \frac{\langle \delta N^2 \rangle}{k_B T} \), where \(\delta N \equiv \sum_i \delta n_i\) is the total number operator. Therefore, the local compressibility can be related to the local density fluctuation by:

\[
\kappa(r_i) = \frac{\langle \delta n_i^2 \rangle}{k_B T} + \sum_j \langle \delta n_i \delta n_j \rangle/k_B T,
\]

where the last term is the non-local density correlations. In the normal phase regime away from the critical point, this term should be negligible due to the short correlation length, i.e. \(k_B T \kappa(r_i) = \langle \delta n_i^2 \rangle\). In order to investigate the regime when the local FDT is valid, we define \(\chi(r_i) \equiv k_B T \kappa(r_i)/\langle \delta n_i^2 \rangle\), and show the result of a typical parameter in Fig. 5(a), where there is a wide regime (not only in the outskirt regime) to find a constant plateau, which can estimate the system temperature with a reasonably high precision. More generally, in Fig. 5(b) and (c), we find the regime for \(\chi \approx 1\) is always in the normal phase regime of small \(J/U\) and \(\mu\) in a uniform 2D system at \(T/U = 0.05\) and 0.25 respectively. The solid and dashed lines in (a) indicate the SF and MI boundaries. The vertical line in (b) is the range of chemical potential in (a).

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\(1\) N. Gemelke et al., Nature 460, 995 (2009). The experimental data shown here are provided privately by Chicago’s group in their later experiment.

\(2\) M. Greiner et al., Nature 415, 39 (2002).

\(3\) S. Trotzky et al., arXiv:0905.4882 (2009).

\(4\) F. Gerbier et al., Phys. Rev. Lett. 101, 155303 (2008).

\(5\) S. Fang, R.-K. Lee, and D.-W. Wang, Phys. Rev. A 82, 031601 (2010).

\(6\) Qi Zhou and Tin-Lun Ho, arXiv 1006:1174. (2010)

\(7\) K. R. A. Hazzard, E. J. Mueller, arXiv:1006.0969 (2009).

\(8\) L. Pollet et al., Phys. Rev. Lett. 104, 245705 (2010).

\(9\) W. S. Bakr, et al., Nature 462, 74(2009); J. F. Sherson, et al., Nature 467, 68 (2010).

\(10\) L. Pollet, K. Van Houcke and S. M.A. Rombouts, J. Comp. Phys. 225, 2249-2266 (2007)

\(11\) C.-L. Hung et al., Phys. Rev. Lett. 104, 160403 (2010).

\(12\) E. L. Pollock and D. M. Ceperley, Phys. Rev. B 36, 8343 (1987).

\(13\) Q. Zhou et al., Phys. Rev. Lett. 103, 085701 (2009).

\(14\) L. Pollet, N.V. Prokof’ev, and B.V. Svistunov, arXiv:1009.4159 (unpublished); also the private communication with L. Pollet, Q. Zhou, and T.-L. Ho.

\(15\) T. Donner, et al., Science 315, 1556 (2007).

\(16\) C.-L. Hung, et al., arXiv:1009.0016 (unpublished).

\(17\) S. Sachdev, Quantum Phase Transitions (Cambridge University Press, 1999)

\(18\) M. P.A. Fisher et al., Phys. Rev. B 40, 546 (1989).

\(19\) M. Caprara, and E. Vicari, Phys. Rev. A 81, 023606 (2010).

\(20\) Considering the finite size (L) and finite temperature (T) effects, the superfluid density (\(\rho_s\)) in a uniform system should have the following scaling form: \(\rho_s (\delta T; L) \sim \delta^{d+(d+z-2)} R(L \delta^z; T/\delta^z)\), where \(\delta = \mu - \mu_c\). We then determine the phase boundary for various sizes at different temperature. The obtained \(\mu_c\) is almost the same (< 0.1%) as the result calculated from the trap scaling method [19].

\(21\) P.N. Ma, L. Pollet, and M. Troyer. arXiv:1007.3529 (2010).

\(22\) Qi Zhou and Tin-Lun Ho, arXiv:0908.3015