Signature of Quantum Criticality in the Density Profiles of Cold Atom Systems

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In recent years, there is considerable experimental effort using cold atoms to study strongly correlated many-body systems. One class of phenomena of particularly interests is quantum critical (QC) phenomena. While prevalent in many materials, these phenomena are notoriously difficult theoretical problems due to the vanishing of energy scales in QC region. So far, there are no systematic ways to deduce QC behavior of bulk systems from the data of trapped atomic gases. Here, we present a simple algorithm to use the experimental density profile to determine the T=0 phase boundary of bulk systems, as well as the scaling functions in QC regime. We also present another scheme for removing finite size effects of the trap. We demonstrate the validity of our schemes using exactly soluble models.

In a recent paper, we gave a general scheme to derive thermodynamic functions of bulk systems at finite temperature from the density profile of trapped gases within local density approximation (LDA)\[7\]. This scheme has recently been implemented by Salomon’s group at ENS to map out the global phase diagram and equation of state of unitary Fermi gas\[8, 9\]. The study of quantum phase transitions, however, involves other challenges. First of all, these are phase transitions at T = 0 caused by changes of the parameters of the system. In addition, there are systems with phase transitions only at T = 0 but not at finite temperatures. How to access the phase boundary of bulk systems, as well as the scaling functions in QC regime. We also present another scheme for removing finite size effects of the trap. We demonstrate the validity of our schemes using exactly soluble models.

The fully spin polarized fermi gas, n_r can be calculated analytically. In such cases, if we plot the “scaled density” A(μ, T) ≡ T^{−1−d/z+1/νz}(n(μ, T) − n_r), or the scaled compressibility C(μ, T) ≡ T^{−1−d/z+2/νz}[κ(μ, T) − κ_r(μ, T)] versus μ for different temperatures, then all curves will intersect at the same point μ = μ_c. Once μ_c is determined, one can then plot A(μ, T) or C(μ, T) versus 1/(μ − μ_c)/T^{1/νz}. The scaled density curves for all temperatures will collapse into a single curve, which is the scaling function G(u) (or G’(u)).

This scheme can easily be implemented in cold atom experiments within LDA, which takes the measured density n^{ex}(x) at point x at temperature T as its bulk value n(μ, T) with μ replaced by μ(x) = μ − V(x), where V(x) is the confining trap; i.e. n^{ex}(x) = n(μ(x), T). With T and μ determined from the measured density profile, n = n(μ, T) of the bulk system is readily obtained from the non-uniform density profile n^{ex}(x) of the trapped gas. To locate the critical point μ_c, one simply plots A^{ex}(r) = T^{−1−d/z+1/νz}(n^{ex}(r) − n_r) versus μ(r) for different samples at different temperatures T and looks for their common intersection. Such intersection will only occurs if z and ν assume their correct values. Recalling that z is typically either 1 or 2, and ν can be estimated from our knowledge of various universality classes, the number of trials needed in practice to produce the common intersection is very small.

Even if n_r is unknown, its regularity allows one to expand it around (μ = μ_c, T = 0), n_r(T, μ) = n_r(0, μ_c) + \sum_{(n,m)\neq(0,0)}\alpha_{n,m} T^n (μ − μ_c)^m. One can then implement the previous scheme by retaining the first few terms in the series, treating their coefficients \alpha_{n,m} as parameters to be adjusted to obtain a crossing of the scaled densities or compressibilities at various temperatures.

(B) Quantum criticality of 1D hard core bosons: To demonstrate our scheme, we use 1D hard core bosons and 1D free Fermi gas as examples. Since both systems have exact solutions in confining traps and in free space, we can then characterize the accuracy of LDA by comparing
the density calculated from it with that calculated from the solution in a harmonic trap, (denoted as $n^{ex}(x)$), which now plays the role of experimental data. Our hamiltonian is $H = -J \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} (\hat{b}_\mathbf{R}^\dagger \hat{b}_{\mathbf{R}'} + \text{h.c.}) + V_R n_R$, where $\mathbf{R}$ labels the lattice sites, $(\mathbf{R}, \mathbf{R}')$ are nearest neighbors, $\hat{b}_{\mathbf{R}}^\dagger$ creates a boson at $\mathbf{R}$, $V_R = \frac{1}{2} M \omega^2 R^2$ is the harmonic potential, and $n_R = \frac{1}{2} (\hat{b}_{\mathbf{R}}^\dagger \hat{b}_{\mathbf{R}} + \text{h.c.})$. The hardcore constraint is implemented by restricting $n_R = 0$ or 1. It is well known that the wavefunction for 1D hardcore bosons, $\Psi_B(R_1, R_2, ..., R_N)$, is of the form $\Psi_B = A \Psi_F$. The density profile of hard core bosons is then given by that of the free Fermi gas, 
\begin{equation}
 n^{ex}(x) = \sum_{n=0,1,2,...} |u_n(x)|^2 f(E_n), \tag{2}
\end{equation}
where $u_n$ is the eigenfunction of $H$ with energy $E_n$, and $f(x) = 1/(e^{(x-\mu)/T} + 1)$ is the Fermi function. For homogeneous systems (where $V_R = 0$), the density is
\begin{equation}
 n(\mu, T) = \int_{-\pi/a}^{\pi/a} \frac{dk}{2\pi} f(\epsilon_k) = \int_{-2J}^{2J} dE N(E) f(E) \tag{3}
\end{equation}
where $\epsilon_k = -2J \cos ka$, $N(E) = (\pi a)^{-1} (4J^2 - E^2)^{-1/2}$ is the density of states, and $a$ is the lattice constant. Note that both Eq. (2) and (3) also apply to free fermions.

The $T = 0$ phase diagram of this system is shown in Figure 1. There are two QC points, $\mu_c = -2J$ and +2J in the $T - \mu$ plane, corresponding to the transition from vacuum ($n = 0$) to a Tomonaga-Luttinger Liquid (TLL) and from the TLL to Mott phase ($n = 1$); denoted as $I$ and $II$, respectively. The region $T > |2J + \mu|$ (QCII in Fig.1) is a quantum critical region, where thermal excitations dominate over the excitation energy of the system (measured from $\mu$). Similar region appears near QC point $I$ by particle-hole symme-

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Phase diagram of 1D hard core Bose gas. $I$ and $II$ are the quantum critical points of vacuum (V) to Tomonaga-Luttinger Liquid (TLL), and Mott (M) to TLL transitions. The quantum critical regions associated with quantum critical point $I$ and $II$ are denoted as QCII and QCIII, given by $|\mu + 2J| < T$ and $|\mu - 2J| < T$ respectively. The shaded region in the vacuum and the Mott phase represent the low fugacity regime of particle and holes.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{Scaled density (top) and scaled compressibility (bottom) vs. $\mu(x) - \mu_c / T 2$. All the data collapse onto a single curve. The parameters are the same as Fig. 2.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{Scaled density (top) and scaled compressibility (bottom) vs. $(\mu(x) - \mu_c) / T$. All the data collapse onto a single curve. The parameters are the same as Fig. 2.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig4.png}
\caption{Scaled density (top) and scaled compressibility (bottom) vs. $(\mu(x) - \mu_c) / T$. All the data collapse onto a single curve. The parameters are the same as Fig. 2.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.png}
\caption{Scaled density (top) and scaled compressibility (bottom) vs. $(\mu(x) - \mu_c) / T$. All the data collapse onto a single curve. The parameters are the same as Fig. 2.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig6.png}
\caption{Scaled density (top) and scaled compressibility (bottom) vs. $(\mu(x) - \mu_c) / T$. All the data collapse onto a single curve. The parameters are the same as Fig. 2.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig7.png}
\caption{Scaled density (top) and scaled compressibility (bottom) vs. $(\mu(x) - \mu_c) / T$. All the data collapse onto a single curve. The parameters are the same as Fig. 2.}
\end{figure}
the scaled quantities are \( A^{\mu}(x) = n^{\mu}(x)T^{-1/2} \) and \( C^{\mu}(x) = \kappa^{\mu}(x)T^{1/2} \). In Figure 2, we have plotted \( A^{\mu}(x) \) and \( C^{\mu}(x) \) versus \( \mu(x) \) for different temperatures. We find that for \( T \leq 0.3J \), all the curves at different temperatures intersect at \( \mu^{c}_I/J = -1.98 \) and \( \mu^{c}_{II}/J = 1.998 \), corresponding to the critical points \( I \) and \( II \) in Fig.1. Comparing with the exact value \( \mu^{c}/J = -2 \) and 2, one sees that LDA is accurate to 99% even for a system with \( 10^2 \) particles. At \( T > 0.3J \), the scaled compressibility at different temperatures fail to intersect at the same point, showing that QC properties appear only when \( T \leq 0.3J \). Similar intersections are found when we plot the scaled compressibility with local chemical potential (see Figure 2). To construct the scaling function, we plot the scaled density and scaled compressibility at different \( T \) against the scaled variable \( \mu(x)/T^{1/(2\nu)} \) around QCI and \( II \). We see from Figure 3 that all data collapse onto a single curve near \( \mu^{*} \), which is the scaling function for these QC points.

\( D \) Finite size scaling: Although the small error of the LDA scheme (about 1%) is hardly of concern to current experiments, it is a matter of principle whether it can be eliminated. This question is not academic, for it will also be of experimental relevance as the resolution of density measurements continue to improve. Moreover, it is also relevant for understanding the results of numerical calculations. Here, we show that this error can be corrected by a (more involved) algorithm that make use of finite size scaling rather than LDA. Using renormalization group arguments\[12\] \[13\], it has been shown that for a bulk system close to a QC point, if one switches on a harmonic potential, then the singular part of a thermodynamic quantity near \( x = 0 \) follows certain scaling relations. The validity of these scaling relations has been well tested for quantum spin systems\[12\] \[13\]. For example, under a scale change \( b \), the singular part of the density below \( d_c \) scales as

\[
n_s(\mu, T, \omega^2, x) = b^{(d+2)+1/\nu} g(\mu h^b, T h^b, \omega^2 h^b, x/b),
\]

where \( \mu = \mu - \mu_c, \ y = 2 + 1/\nu, \) and \( g \) is scaling function. Choosing \( T h^b = 1 \), the scaled density \( A(\mu, T; D, x) = T^{-1-d/2\nu} n_s(\mu, T, \omega^2, x) \) at point \( x \) satisfies

\[
A(\mu, T, \omega^2, x) = g \left( \frac{\mu}{T^{1/2}}, \omega^2/ T^{1/2}, x T^{1/2} \right).
\]

Defining \( D = \omega^2/ T^{1/2} \), Eq.5 becomes

\[
\overline{\mu}(\mu, T; D, x) = g \left( \frac{\mu}{T^{1/2}}, D, x T^{1/2} \right),
\]

where \( \overline{A}(\mu, T; D, x) \equiv A(\mu, T, D T^{1/2}, x) \). Then we have \( \overline{A}(\mu, T; D, 0) = g(0, D, 0) \). Hence, if we plot \( \overline{A} \) versus \( \mu \) at \( x = 0 \) for different \( T \) with \( D \) held fixed, then different curves with different \( T \) (but same \( D \)) will intersect at \( \mu_c \) since \( \overline{A}(\mu_c, T; D, 0) = g(0, D, 0) \). A similar analysis shows scaled compressibility \( T^{-1-d/\nu} x^{1/2} \) at constant \( D \) also intersect at \( \mu_c \).

For 1D hard core bosons, \( z = 2, \nu = 1/2, \ n_s = n \), we have \( \overline{A}(\mu, T; D, x) = n^{\mu}(\mu, \omega, T; x) T^{-1/2} \) near \( x = 0 \). Our scheme is to plot \( n^{\mu}(\mu, \omega, T; 0) T^{-1/2} \) versus \( \mu \) for a family of samples with different \( T \) and \( \omega \) but with identical values for the ratio \( D = \omega^2/ T^{1/2} \). These plots, together with similar plots for the compressibility, are given in Figure 4, with the ratio \( D \equiv (1/2 M \omega^2 a^2/J)/(T/J)^{1/2} = 0.25 \). We find that, to machine accuracy, different curves intersect exactly at \( \mu_c/J = 2.0 \). Moreover, if we plot \( n^{\mu}(\mu, \omega, 0) T^{-1/2} \) against the variable \( \tilde{\mu} = (\mu - \mu_c)/T^{1/2} \), we see in Fig. 5 that all curves

FIG. 4: Determining \( \mu_c \) of bulk systems using a finite-size scaling scheme: the scaled density and scaled compressibility are plotted against \( \mu \) for different \( T/J = 0.02, 0.03, 0.05, 0.07 \) (red, blue, purple, brown, and pink curves) for 1D hard core bosons in harmonic traps. The value \( D \) defined in the text is set equal to 0.25.

FIG. 5: Scaled density (top) and scaled compressibility (bottom) vs. \( (\mu - \mu_c)/T^{1/2} \) with \( \nu = 1 \). All curves in Figure 4 collapse onto a single curve. The parameters are the same as Fig. 4.
collapse to the same curve, which is the scaling function \( g(u, D, 0) \).

By holding \( D \) fixed, we need to know the densities \( \{ n^{ex}(\mu, T; \omega) \} \) for a range of \( T, \mu \) and \( \omega \) values. Thus, this scheme is clearly more laborious than the LDA scheme. Still, it is of conceptual importance to demonstrate that the \( \mu_c \) of bulk systems can be obtained exactly without errors. The recent work by Salomon’s group [9] mapping out the equation of state of a unitary gas indicates that the construction of the entire family \( \{ n^{ex}(\mu, T; \omega) \} \) is feasible. Our scheme will also be useful in numerical studies of trapped atoms, especially for unsolved problems where the existence of quantum criticality is in question.

\[ \text{(E) Finite temperature phase transition:} \quad \text{Previously, we have pointed out that within LDA, the phase boundary } \mu_c(T) \text{ of a finite temperature continuous phase transition will show up as a kink in the in the compressibility } \kappa^{ex}(x) = \partial n^{ex}(x)/\partial \mu(x) \text{ at position } \omega^* \text{ such that } \mu_c(T) = \mu(x^*). \quad \text{As with the quantum critical field discussed in main text, LDA will contain a systematic error due to finite size effects, even though it is very small. This error can also be corrected in a similar way. The analog of Eq. (4) for a finite temperature phase transition is} \]

\[ n_s(T, \mu, \omega^2, x) = b^{-d+1/\nu} n_s(\overline{\mu}(T)) b^{1/\nu} x^{d_\nu} x/b, \quad (7) \]

where \( \overline{\mu}(T) \equiv \mu - \mu_c(T) \) and \( \nu \) is the correlation length exponent for finite \( T \) transition. (For example, \( \nu = 0.67 \) for the 3D xy universality class.) Setting \( \omega^2 b^\nu = 1 \), Eq. (7) implies the scaling form

\[ n_s(T, \mu, \omega^2, x) = \omega^x \mathcal{F}(\omega^{-2/y}\overline{\mu}(T), \omega^{2/y} x), \quad (8) \]

where \( x = (2/y)(d - 1/\nu) \) and \( \mathcal{F} \) is a scaling function. Similar analysis gives \( \kappa_s(T, \mu, \omega^2, x) = \omega^{(2/y)(d-2/\nu)} \mathcal{F}(\omega^{-2/y}\overline{\mu}(T), \omega^{2/y} x) \). The full density \( n \), however, contains both singular (\( n_s \)) and regular (\( n_r \)) contributions; i.e. \( n = n_s + n_r \). The unknown regular contribution \( n_r \) can be eliminated by measuring the difference in density profiles at different trap frequencies \( \omega \neq \omega_1 \) relative to some reference value \( \omega_1 \). Fixing \( \omega_1 \), the function

\[ B_\nu(\mu; \omega) = n(T, \mu, \omega_1^2, 0) - n(T, \mu, \omega^2, 0) / \omega_1^x - \omega^x \quad (9) \]

will assume the value \( \mathcal{F}(0, 0) \) at \( \mu = \mu_c(T) \) for all \( \omega \). This means that if we plot \( B_\nu(\mu; \omega) \) as a function of \( \mu \), different curves for different \( \omega \) will intersect at the exact phase boundary \( \mu_c(T) \).

The fact that the entire phenomenology of quantum criticality of bulk systems - its existence, its dynamical critical exponent, its scaling function, and the location of the quantum critical point - can all be deduced from the \( T 
eq 0 \) density profile of trapped gases as demonstrated here further adds to the list of valuable information deducible from density measurements [7]. At present, the field of quantum gases is moving rapidly in the direction of high precision measurements, a direction essential for realizing the full power of quantum simulation [7]. The extraordinarily high resolution for density imaging recently achieved by Greiner’s group [14, 15] shows that the accuracy needed for deducing bulk properties from trapped gases has been achieved. The recent success of Salomon’s group in deducing the phase diagram of a unitary gas [8, 9] demonstrates the feasibility of our algorithms. All these developments strongly suggest the power of quantum simulation is ready to be harvested.

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[1] Greiner, M., Mandel, O., Esslinger, T., Hänsch, T.W., and Bloch, I. Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms. Nature. 415, 39-44 (2002)
[2] Schneider, U., Hackermuller, L., Will, S., Best, Th., Bloch, I., Costi, T.A., Helmes, R.W., Rasch, D., and Rosch, A. Metallic and Insulating Phases of Repulsively Interacting Fermions in a 3D Optical Lattice Science. 322, 1520-1525 (2008)
[3] Jördens, R., Strohmaier, N., Günter, K., Moritz, H., and Esslinger, T. A Mott insulator of fermionic atoms in an optical lattice. Nature. 455, 204-207 (2008)
[4] Gemelke, N., Zhang X., Hung, C.L., and Chin, C. In-situ Observation of Incompressible Mott-Insulating Domains of Ultracold Atomic Gases. Nature. 460, 995-998 (2009)
[5] Spielman, I.B., Phillips, W.D., and Porto. J.V. Condensate fraction in a 2D Bose gas measured across the Mott-insulator transition. Phys. Rev. Lett. 100, 120402 (2008)
[6] Bloch, I. Ultracold Quantum Gases in optical lattices. Nature Phys. 1, 23 - 30 (2005).
[7] Ho, T.L., and Zhou, Q. Obtaining the phase diagram and thermodynamic quantities of bulk systems from the densities of trapped gases. Nature Physics. 6, 131 - 134 (2010)
[8] Nascimbène, S., Navon, N., Jiang, K.J., Chevy, F., and Salomon, C. Exploring the thermodynamics of a universal Fermi gas. Nature. 463, 1057-1060 (2010)
[9] Navon, N., Nascimbène, S., Chevy, F., and Salomon, C. The Equation of State of a Low-Temperature Fermi Gas with Tunable Interactions. Science. 328, 729 - 732 (2010)
[10] Fisher, M.P.A., Weichman, P.B., Grinstein, G. and Fisher, D.S. Boson localization and the superfluid-singlet transition. Phys. Rev. B. 40, 546-570 (1989)
[11] Zhou, Q and Ho, T.L. Universal Thermometry for Quantum Simulation. arXiv:0908.3015 (2009)
[12] Platini, T., Karevski, D., and Turban, L. Gradient critical phenomena in the Ising quantum chain. J. Phys. A: Math. Theor. 40, 1467-1479 (2007)
[13] Campoonerini, M., and Vicari, E. Trap-size scaling in confined particle systems at quantum transitions. Phys. Rev.
A 81, 023606 (2010)

[14] Gericke, T., Würtz, P., Reitz, D., Langen, T., and Ott, H. High-resolution scanning electron microscopy of an ultracold quantum gas. Nature Physics. 4, 949 (2008)

[15] Bakr, W.S., Gillen, J.I., Peng, A., Fölling, S., and Greiner, M., A quantum gas microscope for detecting single atoms in a Hubbard-regime optical lattice. Nature. 462, 74-77 (2009)

[16] Campostrini, M., and Vicari, E. Critical behavior and scaling in trapped systems. Phys. Rev. Lett. 102, 240601 (2009)