Discerning Incompressible and Compressible Phases of Cold Atoms in Optical Lattices

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(Dated: November 4, 2009)

Experiments with cold atoms trapped in optical lattices offer the potential to realize a variety of novel phases but suffer from severe spatial inhomogeneity that can obscure signatures of new phases of matter and phase boundaries. We use a high temperature series expansion to show that compressibility in the core of a trapped Fermi-Hubbard system is related to measurements of changes in double occupancy. This core compressibility filters out edge effects, offering a direct probe of compressibility independent of inhomogeneity. A comparison with experiments is made.

PACS numbers: 03.75.Ss, 71.10.Fd

The search for stable quantum many-body phases forms the basis of quantum condensed matter, quantum chemistry and elementary particle physics. Stable states often arise as a consequence of energy gaps that set an energy scale for resilience. Examples of gapped condensed matter phases include superconductors and Mott insulators. In these phases gaps arise in the presence of (or as a result of) interactions to form many-body states that resist small perturbations from the environment. Gaps play a role in spectacular quantum effects in the solid state including zero resistance in superconductors or a dramatic rise in resistance in Mott insulators. Gaps set an energy scale for resilience. Examples of gapped states often arise as a consequence of energy gaps that play a role in spectacular quantum effects. Stable phases of matter and phase boundaries. We use a high temperature series expansion to show that compressibility in the core of a trapped Fermi-Hubbard model is related to measurements of changes in double occupancy. This core compressibility filters out edge effects, offering a direct probe of compressibility independent of inhomogeneity. A comparison with experiments is made.

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Compute the exact second order contribution to the grand potential for the high temperature regime studied here we also estimate in Ref. [3] find that the largest unknown, lattice temperature, can be kept below $U$ with values as low as $T \approx 0.8$ kHz and possibly lower.

To theoretically analyze observable signatures of incompressibility in a trapped Hubbard model we use a high temperature series expansion of the grand partition function $Z = \text{Tr} \exp(-\beta H)$ about the atomic, $t = 0$, limit. Such high temperature series expansions have a long history [23] and yield exact results for thermodynamic quantities of the Hubbard model in the limit $\beta t \ll 1$. Note that all experiments done with fermions in optical lattices currently lie in this high temperature regime when parameters are tuned to $U \gg t$. The high temperature series therefore offers a quantitatively reliable tool to compare to experiments. Our approach complements recent dynamical mean field studies that can be applied to lower temperatures [24]. We use up to 10th order in the expansion of the grand potential [21], $\Omega = -\ln (Z)/\beta$, to extract thermodynamic quantities for a uniform system ($\gamma = 0$). In terms of the series coefficients, $X^{(m)}$, the expansion reads:

$$-\beta \Omega = \ln z_0 + \sum_{m=2}^{\infty} (\beta t/z_0)^m X^{(m)}(w, \zeta), \quad (2)$$

where $\zeta = \exp(\beta \mu)$ is the fugacity of the uniform system, $\Omega \equiv \Omega/N$, $w = \exp(-\beta U)$ and $z_0 = 1 + 2 \zeta + \zeta^2 w$ is the partition function of a single site in the atomic limit. In a local density approximation (LDA) we assume the LDA is an excellent approximation for the high temperature regime and we can approximate with parameters for a uniform system. With the replacement $\zeta \rightarrow x_i = \exp(\beta \mu_i)$ the LDA becomes $\Omega^{\text{LDA}} = \sum_i \Omega_i$.

To show that the LDA is an excellent approximation for the high temperature regime studied here we also compute the exact second order contribution to the grand potential in a trapped system:

$$-\beta \Omega = \sum_i \ln z_{0,i} + (t/\beta)^2 \sum_{i,j \in n.n.} \frac{X^{(2)}_{ij}}{z_{0,i}^2 z_{0,j}^2} + \mathcal{O}((\beta t)^4), \quad (3)$$

where the second sum double counts nearest neighbors and

$$X^{(2)}_{ij} = I_{\delta,-\delta}[x_i + x_j^2 x_j w] + I_{-\delta,\delta}[x_j + x_j^2 x_i w] + x_i x_j [I_{-\delta-U,\delta+U} + I_{\delta-U,-\delta+U}] + x_i^2 w I_{\delta+U,-\delta-U} + x_j^2 w I_{-\delta+U,\delta-U}. \quad (4)$$

In the above expression the quantities $\delta \equiv \mu_i - \mu_j$ and $I_{\Delta,-\Delta} \equiv (\exp(\beta \Delta) - 1 - \beta \Delta)/((\beta \Delta)^2$ simplify to the uniform limit for $\Delta = 0$ and $I_{0,0} = 1/2$. The LDA is recovered in the limit $X_{ij} \rightarrow X^{\text{LDA}}_i \equiv (1-w)x_j^2/\beta U + x_i(1+x_j^2 w)$ yielding a simple expression for the grand potential of a trapped system in the continuum approximation (valid for large particle numbers): $-\beta \Omega^{\text{LDA}} \approx \int d^d r [\ln z_{0,r} + z(t/\beta Z_{0,r})^2 X^{\text{LDA}}_r]$, where $z$ is the coordination number. This second order high temperature expansion holds for any bipartite lattice in any dimension. As we show below there are no discernible differences between the LDA and the exact second order results for the parameters studied here.

We first focus on the compressibility which can distinguish the incompressible ground state of a gapped phase from a compressible metallic phase in a homogeneous system. The compressibility per particle is defined as $\kappa = N^{-1} \sum_i \partial n_i / \partial \mu$ where $N = \sum_i (n_i) = \sum_i x_i \partial_x [(-\beta \Omega)]$. We compute the compressibility with the 10th order series but find essentially no distinction from the second order results for $\beta t \lesssim 0.9$. The top panel of Fig. 1 plots the compressibility as a function of the chemical potential in the trap center for $t = 0.054$ kHz and $U = 5$ kHz. The arrows in the bottom panel indicate the Mott regime at $T = 0.2$ kHz.
We next study the system radius, \( R \), because the compressibility is not directly measurable in experiments. \( R \) is defined as the root mean square of the distance averaged with respect to the density. The central panel of Fig. 2 plots \( R \) in units of the Thomas-Fermi radius, \( R_{\text{TF}} = a(3N/4\pi)^{1/3} \), where \( a \) is the lattice spacing. The plateau in the middle panel of Fig. 4 results from a combination of edge effects and incompressibility at the trap center. As the chemical potential increases, we add more particles to the edge gas, and the size \( R \) scales as the size \( R_{\text{TF}} \), the relevant length scale for the edges. A similar plateau can be seen in the compressibility in units of the Thomas-Fermi compressibility at a value \( \kappa/R_{\text{TF}} = 1 \). Nonetheless, we have again found only weak, edge-dependent features that indicate the formation of a Mott insulator.

We are thus looking for a robust technique that probes the gapped phase without resorting to edge effects. We will show that the core compressibility per particle fulfills this requirement:

\[
\kappa^C \equiv N^{-1} \partial D / \partial \mu, \tag{5}
\]

where the double occupancy is conventionally defined as \( D = \partial (\Omega) / \partial U = \sum_{i} \langle n_i \rangle \langle n_i \rangle \). Our definition of \( D \) differs from the definition in Ref. \[6\]. In Ref. \[6\] a quantity related to its dimensionless derivative, \( \partial D / \partial N \), was measured, which directly relates to the ratio of core and total compressibility (without knowledge of \( \mu \)) via \( \partial D / \partial N = (\partial D / \partial \mu)(\partial \mu / \partial N) = \kappa^C / \kappa \).

Figure 2: Compressibility (dotted line) and core compressibility (solid line) versus chemical potential in a uniform system, \( \gamma = 0 \), with \( U = 7 \) kHz and \( t = 0.054 \) kHz. The top (bottom) panel sets \( T = 1 \) kHz (\( T = 0.5 \) kHz). The three incompressible regions correspond to a pinning of the density at 0, 1 and 2 for chemical potentials near \( \mu = -U/2, U/2 \) and \( 3U/2 \), respectively. For \( \mu \ll U/2 \), \( \kappa^C \) vanishes because the system shows very little double occupancy.

In Fig. 2 we plot \( \kappa^C \) and \( \kappa \) versus \( \mu \) for two different temperatures in a uniform system and find that \( \kappa^C \) is essentially identical to \( \kappa \) when the system has doubly occupied sites, but is zero otherwise. This is a key feature with useful implications for trapped systems: \( \kappa^C \), by taking the derivative of the double occupancy, measures the compressibility of the core region with density larger than one (see the insets of Fig. 3) and is therefore insensitive to the edges.

A comparison between the top and bottom panels of Fig. 2 shows that \( \kappa^C \) and \( \kappa \) agree at low temperatures and high chemical potentials. This can be understood by considering a single site in the atomic limit: \( (\kappa^C / \kappa)_{l=0} = (1 + \zeta)[2 + \zeta + w/\zeta]^{-1} \). At zero temperature we can see the implicit cutoff in the chemical potential (\( \kappa^C / \kappa \)) \( \rightarrow 0 \) for \( \theta(\mu - U/2) \). Measurements of \( \partial D / \partial N \) therefore exclude low chemical potentials (and thus edge effects) in trapped systems, yielding a measure of the core compressibility ratio (CCR), \( \kappa^C / \kappa \), at low temperatures, \( T \ll U \).

Figure 3: The core compressibility ratio versus on-site interaction strength for \( \mu = 4 \) kHz. The top panel fixes \( t = 0.054 \) kHz for several temperatures, \( T = 0.07 \) kHz (dot-dashed), 0.2 (dashed), 0.5 (solid) and 1.0 (dotted). The bottom panel fixes \( T = 0.2 \) kHz for \( t = 0.01 \) kHz (dashed) and 0.1 (dotted). The insets plot the density along a cross section in the cubic lattice for the same parameters as the bottom panel of Fig. 2 but in a trap and with \( \mu = 0.5 \) kHz (left) and \( \mu = 3.5 \) kHz (right). The circles are computed in a full second order expansion for the density while the solid line is computed in the second order LDA. The Mott gap pins the density near \( \langle n_i \rangle = 1 \) at the trap center (right panel). For \( \mu > U/2 \) (left panel) a central compressible region arises with \( n_i > 1 \) at the trap center.

The LDA is an excellent approximation for the parameters considered here. The circles in the insets of Fig. 3 plot the density computed without the LDA. Comparison with the LDA results (solid line) shows remarkable agreement for \( \beta t \ll 1 \). We have also compared the compressibility computed with and without the LDA and have found very little distinction (less than 4%) in the regime.
of validity of our high temperature series $\beta t \lesssim 1$. The LDA is thus a good approximation and the high temperature series expansion yields a highly accurate tool for quantitative comparison with ongoing experiments with strongly interacting ($t/U \ll 1$) fermions in optical lattices.

We now make contact with recent experiments of Ref. [6], reporting a measurement of the quantity $\delta d/\delta N$ where $\delta d$ stands for an approximate derivative taken by linear fitting to experimental data. This experiment measures the double occupancy fraction $d = 2D/N$ instead of the double occupancy $D$. Estimating $\delta d/\delta N \approx \partial d/\partial N = (2\kappa^C/\kappa N) - D/N^2$ we find that the difference is small near unity filling implying that Ref. [6] measures $\delta d/\delta N$.

Both the CCR and $\delta d/\delta N$ plotted in Fig. 4 show a distinct signature of the transition to the incompressible Mott phase. At low $U$ the core of the system lies in the compressible regime of the Fermi-Hubbard phase diagram, $n_1 > 1$. The peak structure in Fig. 4 originates from the choice of $\mu$ and the peaks in Fig. 2. Upon increasing $U$ we enter the Mott regime, $n_1 = 1$. (Note that compressibility alone cannot distinguish the Mott phase from a weakly compressible metallic phase.) Here the center of the trapped system opens a gap and the core compressibility drops exponentially to zero. The zeroing of the core compressibility (and the CCR) is therefore an indicator for the onset of a Mott insulating phase in the sample center. Recall that the total compressibility $\kappa$ shows very little structure as we enter the Mott phase of a trapped system, and the signal thus originates from the change in core compressibility (compare the top and bottom panels of Fig. 4).

The inset of Fig. 4 makes a more direct comparison with Ref. [8]. Here we match entropy in the dipole trap at a temperature fixed point appears for $U \approx \mu$ such that $\langle H \rangle \approx 0$. Here one finds a crossover from a high temperature Fermi-gas to a Mott phase. The bottom panel of Fig. 4 varies the hopping to demonstrate that there is only a small shift with different hoppings.

We have shown that observations of double occupancy of cold atoms in optical lattices reveal the core compressibility in a trapped Fermi-Hubbard model. This core compressibility clearly indicates the onset of incompressible states and describes recent measurements that show evidence for the Mott transition [6]. Ongoing work will generalize our proposed technique to bosonic systems. The core compressibility implicitly excludes edge effects to reveal compressibility near the trap center. Transitions to incompressible phases (e.g., metal-insulator transitions) nucleated at the sample center can be readily identified in experiments and compared with compressibility computed in uniform Hubbard models.

We thank T. Esslinger and his group, F. Hassler and S. Huber for valuable discussions. LP, MT and VS thank the Swiss National Science Foundation for support.

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