Extracting the Mott gap from energy measurements in trapped atomic gases

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(Dated: February 14, 2022)

We show that the measure of the so-called release energy, which is an experimentally accessible quantity, makes it possible to assess the value of the Mott gap in the presence of the confinement potential that is unavoidable in the actual experimental setup. Indeed, the curve of the release energy as a function of the total number of particles shows kinks that are directly related to the existence of excitation gaps. Calculations are presented within the Gutzwiller approach, but the final results go beyond this simple approximation and represent a genuine feature of the real system. In the case of harmonic confinement, the Mott gaps may be renormalized with respect to the uniform case. On the other hand, in the case of the recently proposed off-diagonal confinement, our results show good agreement with the homogeneous case.

PACS numbers: 03.75.Hh, 05.30.Jp, 71.30.+h

I. INTRODUCTION

It has been established that ultra-cold Bose and Fermi gases trapped in optical lattices provide experimental realizations of long-standing lattice models widely considered in condensed matter physics and statistical mechanics, such as the Bose and Fermi Hubbard models \[1,2\]. One of the most spectacular achievements was the observation of the superfluid to Mott-insulator transition as the optical lattice depth is varied \[3\]. This transition has been explained in light of the Bose-Hubbard model with on-site repulsive interactions and hopping between nearest-neighbouring sites. In the superfluid phase, each atom is spread out over the entire lattice, with long-range phase coherence, whereas in the insulating phase, exact numbers of atoms are localized at individual lattice sites, without phase coherence across the lattice: this phase is characterized by a gap in the excitation spectrum and a vanishing compressibility. Similarly, recent experiments have provided evidence on the formation of a Mott insulator of fermionic atoms in an optical lattice \[3\].

Several challenges arise when quantitatively comparing experimental data and theoretical results obtained from the analysis of infinite systems. One of the most important problems is due to inevitable spatial inhomogeneities induced by the optical trap, which is necessary to confine particles \[3,5\]. Further complications are connected to determine temperature effects present in experiments \[5\], and also to the limited available tools for the experimental characterization of the phases.

Here, we would like to focus our attention on the possibility to make quantitative estimations of the Mott gap $E_g$ from relatively simple quantities that can be experimentally addressed. In the presence of the optical trap, it is usually not possible to have a Mott insulating phase throughout the whole lattice and compressible regions intrude the system. This fact has been widely discussed both experimentally and theoretically and shows up through the typical “wedding-cake” profile of density \[3,5,7,9,10\]. Therefore, the system always possesses regions that are locally compressible and a precise determination of the Mott gap is subtler than in the homogeneous case. Some preliminary attempts to measure the excitation spectrum of interacting bosons have been performed by using Bragg spectroscopy \[11\]. Other approaches to characterize the appearance of Mott-insulating regions from experimentally accessible quantities have been also proposed \[12,13\]. Here, we would like to propose an alternative approach that is based upon energy measurements only and could give important insights about the appearance of Mott-insulating regions, as well as the actual value of the gap.

For an infinite and homogeneous system, the excitation gap $E_g$ can be calculated from the knowledge of the total energy for different particle numbers, namely $E_g = \mu^+ - \mu^-$, where $\mu^\pm = \pm (E_{N\pm 1} - E_N)$, $E_N$ being the ground-state energy with $N$ particles. The Mott gap $E_g$ is finite whenever $\mu^+ \neq \mu^-$ and, therefore, introduces a discontinuity in the first derivative of the energy with respect to the density.

In this paper, we will show that the existence of incompressible Mott regions and the values of the corresponding gaps can be obtained from so-called release energy $E^{rel}$, which may be measured experimentally \[14\]. Indeed, $E^{rel}$ is obtained by integrating the momentum distribution of the atoms after having switched off the confinement and let the atoms expand freely. The release energy is given by the sum of the kinetic and interaction energies just before switching off the trap \[14\]

\[ E^{rel} = E^{\text{kin}} + E^{\text{int}}. \]  

We notice that it would be much more difficult to extract the total energy, $E^{\text{tot}} = E^{\text{kin}} + E^{\text{int}} + E^{\text{pot}}$ that also includes the potential term due to the trap, since this would require the knowledge of the density profile in the presence of the trap, which is hard to reconstruct.

Specifically, we address two types of confinement \(i\) the usual harmonic confinement and \(ii\) a recently proposed off-diagonal confinement \[15\]. In such a confinement, the strength of the hopping parameter is varied across the
lattice, being maximum at the center of the lattice and vanishing at its edges, which naturally induces a trapping of the particles.

We consider bosons loaded in one- and two-dimensional optical lattices and use an insightful variational approach based upon the Gutzwiller wave function [10, 17]. Similar results must hold also in fermionic systems. Moreover, although approximated, this variational method is expected to correctly capture the behavior of the exact ground state. We find that the presence of Mott regions in the system is signaled by discontinuities in the derivative of the release-energy curve with respect to the total number of bosons, reminiscent of the presence of a gap in infinite homogeneous system. In the case of harmonic confinement, the measured gap may be substantially smaller than the one of the uniform system, whereas a much closer agreement is achieved by considering the off-diagonal confinement.

The emergence of strong signatures due to the formation of Mott domains in the energy measurements has been explored in Ref. [13], where it has been shown that the appearance of Mott domains is accompanied by minima in the release-energy curve as function of the on-site interaction parameter. Here, we make a further step in this direction and provide a direct and quantitative connection between energy calculations and Mott gaps, in presence of an external trap.

The paper is organized as follows: in section II we introduce the Bose-Hubbard model and describe the variational method, in section III we present our results, and finally, in section IV we draw our conclusions.

II. MODEL AND METHOD

Our starting point is the Bose-Hubbard model which describes interacting bosons on a lattice [6]:
\[
\hat{H} = -\frac{1}{2} \sum_{\langle i,j \rangle} t_{i,j} \hat{b}_i^\dagger \hat{b}_j + \text{h.c.} + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \sum_i \epsilon_i \hat{n}_i,
\]
(2)
where \(\langle \ldots \rangle\) indicates nearest-neighbor sites, \(\hat{b}_i^\dagger \) (\(\hat{b}_i\)) creates (destroys) a boson on site \(i\), and \(\hat{n}_i\) is the local density operator. \(U\) is the on-site interaction, \(t_{i,j}\) is the hopping amplitude, and \(\epsilon_i\) is a local energy offset due to an external trapping potential.

To study this model and describe its ground-state properties we use a mean-field approximation based on the Gutzwiller ansatz [10, 17]. This simple approach is able to capture important features of the true ground state and provides a qualitatively correct description of quantities such as the local density or the total energy, even in presence of spatial inhomogeneities [6, 10, 11, 17]. More involved wave functions with a long-range Jastrow factor [18], or numerically exact calculations [10] may be considered, but a much larger computational effort would be required. Instead, here we are just interested in showing that Mott gaps can be extracted from the behavior of the release energy as a function of the total number of particles, and we do not expect qualitative differences when considering more accurate approaches.

Within the Gutzwiller ansatz the ground-state wave function is approximated as
\[
|\Psi_G \rangle = \prod_i \left( \sum_{m=0}^{\infty} f_m^i |m\rangle_i \right),
\]
(3)
where \(|m\rangle_i\) is the Fock state with \(m\) particles at site \(i\) and \(f_m^i\) are variational parameters which have to be determined by minimizing the expectation value of the Gutzwiller ansatz on the Hamiltonian in Eq. (2). The sum in Eq. (3) runs from states with zero particles up to infinity; however, from a numerical point of view, we have to consider a cutoff and take only states up to a maximum number of particles (per site) \(M_{\text{max}} \gg \langle \Psi_G | \hat{n}_i | \Psi_G \rangle\) such
that the contribution of those states with higher density are negligible and observables are converged to a certain desired precision.

Equivalently, the Gutzwiller wave function can be introduced as the ground state of the following mean-field Hamiltonian \([20, 21]\):

\[
\hat{H}_{mf} = \frac{1}{2} \sum_{\langle i,j \rangle} t_{i,j} \left( \hat{b}_i^\dagger \Psi_j + \Psi_i^\dagger \hat{b}_j - \Psi_i^\dagger \Psi_j \right) + h.c. + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \sum_i (\epsilon_i - \mu) \hat{n}_i,
\]

where \(\Psi_i\) is the mean-field potential which is self-consistently defined as \(\Psi_i = \langle \Psi_G | \hat{b}_i | \Psi_G \rangle\); it can be shown that \(f_{mf}^a\) is related to the ground-state eigenvector components of the converged solution of the local Hamiltonian \([1, 20]\). The parameter \(\mu\) is the chemical potential that fixes the number of bosons. In the recent past, the Gutzwiller approach has been successfully used to study a wide range of bosonic systems, like for instance disordered potentials \([22]\), boson-boson mixtures \([23]\), and even time-dependent problems \([24, 26]\).

For the sake of simplicity and to simplify the presentation of the results, we first consider the one-dimensional (1D) case, which is the limiting case where a collection of non-interacting tubes is created. An almost 1D model may be easily generated by using different lasers in the three different spatial directions and has been experimentally considered \([11, 27]\). We mention that in 1D, within the Gutzwiller approach, the compressible phase has inevitably a finite condensate fraction. However, this approach correctly reproduces the opening of the excitation gap at the Mott transition; therefore, the presence of a condensate does not imply relevant quantitative differences on the estimation of the gap with respect to an unbiased calculation. Furthermore, we also report some results for two dimensions (2D) for which we obtain similar conclusions. We emphasize that all the results remain valid in higher spatial dimensions because the superfluid to Mott-insulator transition occurs in any dimension accompanied by the opening of a gap in the spectrum.

We consider a lattice with a harmonic potential of the form \(\epsilon_i = V_0 r_i^2\), where \(r_i\) is the distance of site \(i\) from the center of the lattice. In this case, the hopping amplitude is kept constant for all lattice sites \(t_{i,j} = t\). In addition, we also analyze the case of off-diagonal confinement in which \(\epsilon_i = 0\) and \(t_{i,i+1} = 4t \times i \times (L - i)/L^2\), where \(L\) is the total number of sites. In both cases, we evaluate local quantities which allow us to determine whether a certain region across the lattice is in a compressible or incompressible state, as well as the release energy of the system. In particular, we will show, besides the release energy, the local density \(n_i = \langle \Psi_G | \hat{n}_i | \Psi_G \rangle\) and its fluctuations \(\Delta_i = \langle \Psi_G | n_i^2 | \Psi_G \rangle - n_i^2\).

**FIG. 3:** (Color on-line) The same as in Fig. 2 for \(U/t = 15\).

**FIG. 4:** (Color on-line) Upper panels: first Mott gap obtained from the release energy as function of \(U/t\) for \(V_0/t = 0.01\), for comparison the homogeneous case is also reported (left); release-energy curves for different \(U/t\) and \(V_0/t = 0.01\). Lower Panel: first Mott gap as function of \(V_0/t\) for \(U/t = 15\). Calculations are shown for the 1D model.

**III. RESULTS**

Before showing the results for the confined system, which is relevant for experiments, let us briefly discuss the homogeneous case, with \(\epsilon_i = 0\) and \(t_{i,j} = t\). In this case, a superfluid-Mott transition takes place at integer fillings whenever the on-site interaction \(U\) is large enough. On the other hand, for any non-integer fillings the ground state is always superfluid and, therefore, compressible. In Fig. 11 we report the energy curve as a function of the density \(n\). Within the Gutzwiller approximation the values of the critical interaction may be determined analytically, i.e., \(U_c/t = D(\sqrt{n} + \sqrt{n+1})^2\), where \(n\) is an integer \([12]\). Whenever \(U < U_c\), the energy curve is smooth with a positive curvature, implying a finite compressibility and a vanishing gap. On the con-
trary, for $U > U_c$, there is a discontinuity in the curve at integer fillings, (the behavior in the vicinity of $n = 1$ is reported in Fig. 1), signaling the presence of the Mott gap. The latter one can be estimated by considering the change of the slope close to the discontinuity.

Let us now switch on the harmonic confinement by setting $V_0/t = 0.01$. In Figs. 2 and 3 we present the results for the release energy as function of the total number of bosons $N$, as well as the local quantities $n_i$ and $\Delta_i$ across the lattice sites. For the case with $U/t = 4$ (see Fig. 2) there are no insulating phases, no matter what the number of bosons is. The density profile is smooth, with a broad maximum at the center of the trap. In this case, all regions of the lattice are (locally) compressible and, therefore, the ground state is gapless. This is not the case for $U/t = 15$ (see Fig. 3), where insulating regions are expected. Indeed, what is found is the usual "wedding-cake" structure in the local density: the Mott regions with integer $n_i$ and vanishing $\Delta_i$ are surrounded by compressible regions which are locally gapless. We emphasize that the vanishing of $\Delta_i$ is consequence of the Gutzwiller approach; in a more accurate description of a Mott insulator, this quantity is indeed finite, though it is strongly reduced with respect to its value in the super-fluid regions. Here, the derivative of the release-energy curve clearly exhibits discontinuities that are reminiscent of the presence of a Mott gap. This discontinuity takes place whenever a new compressible region appears at the center of the trap, on top of the underlying Mott phase, see Fig. 4. In this way, we can define an energy gap for the confined system exactly as in the homogeneous system, namely $E_g^{\text{rel}} = \mu^{\text{rel}} - \mu^{\text{rel}}_{\text{rel}}$, where $\mu^{\text{rel}}_{\text{rel}} = \pm (E^{\text{rel}}_{N \pm 1} - E^{\text{rel}}_N)$ ($E^{\text{rel}}_N$ being the release-energy with $N$ particles). We would like to stress that similar results may be obtained taking $\mu^{\text{rel}}_{\text{rel}} = \pm (E^{\text{rel}}_{N \pm M} - E^{\text{rel}}_N)$, with $M \ll N$, which can be considered in experiments. For the case shown in Fig. 4 (i.e., for $V_0/t = 0.01$ and $U/t = 15$), we obtain that the first Mott gap is $E_g^{\text{rel}}/t \simeq 7.2$, to be compared with the Mott gap with $n = 1$ of the homogeneous case that gives $E_g/t \simeq 11.8$. The reduction of the measured gap comes from the fact that the release energy in the presence of the trap contains not only the information about the local creation of the new compressible region at the center of the trap, but also about all other sites of the lattice, which do not undergo the Mott transition. Therefore, the effect is spatially averaged over regions that are locally compressible and incompressible. Nevertheless, the effect that originates from the central sites is visible and allows us to provide an estimate of the gap associated with such a transition.

A summary of the results is reported in Fig. 6 where we show $E_g^{\text{rel}}$ (for the first Mott gap) as a function of $U/t$ for $V_0/t = 0.01$ and as a function of $V_0/t$ for $U/t = 15$. We find that, when the harmonic trap is increased, the Mott gap saturates to $E_g^{\text{rel}}/t \simeq 10.6$, which is close to the value of the homogeneous system. The initial depletion of the Mott gap as a function of $V_0$ is due to the presence of (large) regions of compressible sites close to the borders of the system; by further increasing $V_0$, these regions shrink and the gap eventually tends to approach the value of the uniform case.

We now briefly consider the two-dimensional case, see Fig. 5. Exactly as in 1D, in the appearance of a new compressible region at the center of the trap is accompanied by a discontinuity in the derivative of the release-energy curve. Similar conclusions to those in 1D are obtained, confirming the appearance of kinks in the release-energy curve in 2D where the Gutzwiller mean-field approach is more reliable.

We stress that in presence of a diagonal confinement is such that compressible and incompressible regions coexist. Indeed, the true gap of the overall confined system will be zero, as the global compressibility is always finite [5, 12]. Indeed, the total energy, as opposed to
the release energy, is a completely smooth curve with positive curvature (hence a vanishing real gap and finite compressibility). The total-energy curve as function of the total number of particles is shown in Fig. 6 for a 2D system. This curve is completely smooth, even when Mott insulating domains are present in the trap. In the experimental setup, the release-energy measurement corresponds to the actual total energy of the system, since in this case there is no potential energy. In Fig. 7, we present the results for a trapped system, since in this case there is no potential energy. In Fig. 7, we present the results for the trapped system, since in this case there is no potential energy. In Fig. 7, we present the results for the trapped system, since in this case there is no potential energy. In Fig. 7, we present the results for the trapped system, since in this case there is no potential energy.

Let us analyze the case of off-diagonal confinement. The number of sites is \( L = 200 \) and \( n = N/L \) is the density.

![Fig. 7](Color on-line) The same as in Fig. 3 but for an off-diagonal confinement. The number of sites is \( L = 200 \) and \( n = N/L \) is the density.

### IV. Conclusions

We have shown that relatively simple energy measurements may give important insights into the actual value of the Mott gap. In particular, it has been shown that the presence of the harmonic potential may renormalize the value of the gap with respect to the uniform case. On the other hand, much closer results may be achieved when the off-diagonal confinement will be experimentally realized. Although the experimental determination of the Mott gap from release-energy curves may be difficult, since small error bar on both energies and particle numbers are required, we hope that in the near future this method will be successfully applied.

We acknowledge useful discussions with M. Fabrizio, L. Fallani, C. Fort, S. Giorgini, V. Rousseau, and A. Trombettoni.

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