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Mott transition in anharmonic confinement

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Abstract. Two effects are identified that affect the visibility of the Mott transition in an atomic gas in an optical lattice confined in a power-law potential. The transition can be made more pronounced by increasing the power law, but at the same time, experimental uncertainty in the number of particles will induce corresponding fluctuations in the measured condensate fraction. Calculations in two dimensions indicate that a potential slightly more flat-bottomed than a quadratic one is to be preferred for a wide range of particle number fluctuation size.

PACS. 03.75.Lm Tunneling, Josephson effect, Bose-Einstein condensates in periodic potentials, solitons, vortices, and topological excitations

In a spectacular experiment a few years ago, the transition from a superfluid to a Mott insulator was realized in a gas of cold atoms in an optical lattice by Greiner et al. [1]. The experiment marked the birth of a new subfield of physics, where theoretical statistical-physics models, until then considered to be mostly of academic interest or crude approximations to real materials, can now be realized in experiment. With the help of atoms in optical lattices, it is hoped that fundamental questions regarding phase transitions can be addressed, as well as applications to e.g. quantum information. Nevertheless, a few practical issues remain to be sorted out. One such issue concerns the role of the confining potential.

A gas of spinless bosonic atoms in an optical lattice is known to be well described by the Hubbard model [2],

$$H = \frac{1}{2}\sum_r a_r^\dagger a_r^\dagger a_r a_r - \frac{t}{2}\sum_{<rr'>} a_r^\dagger a_{r'} + \sum_r [V(r)-\mu] a_r^\dagger a_r, \tag{1}$$

where t is the tunneling matrix element, μ is the chemical potential, $V(r)$ is the spatially dependent trapping potential, and r is a dimensionless site index. The operators a_r,$a_r^\dagger$ destroy and create a particle at the site r, respectively, and obey Bose commutation relations. The units are here chosen so that the on-site interaction strength, i.e., the prefactor of the first term in (1), is unity. The sum subscripted $\langle rr'\rangle$ runs over all pairs of nearest-neighbor sites. In the absence of an external potential $V(r)$, this Hamiltonian exhibits a quantum phase transition at zero temperature, separating two ground states [3]: when the tunneling matrix element t is strong enough, there is phase coherence over the entire sample which puts the system in its superfluid state, and there exists an accompanying Bose-Einstein condensed fraction of the gas that can be measured in time-of-flight experiments [4]. For weaker tunneling, phase coherence is lost, the number of atoms per site is locked to an integer, and number fluctuations are suppressed. This is the Mott insulating state.

In the experiment reported in reference [1], just as in nearly all experiments on optical lattices, the atoms were contained in a quadratic, i.e., harmonic-oscillator potential, in order for them not to escape. As a result, the transition between superfluid and Mott insulator is not simultaneous over the whole sample, but takes place via an intermediate state where part of the atomic cloud is superfluid and part is Mott insulating. Such a state is often called a "Mott plateau" state because of the characteristic density profile, in which the density is fixed to an integer in confined regions. This is well known and it is also well understood [5,6]. In effect, it is the local confining potential that contributes a (negative) addition to the chemical potential, resulting in a spatially dependent critical point for the phase transition.

In order to see a clear Mott transition one would need to get rid of the effects of the confining potential. It has therefore been proposed that the harmonic-oscillator potential could be replaced by a more flat-bottomed variety, e.g., a quartic or sixth-power potential, more similar to a square well [7]. In such a potential, the local chemical potential varies slowly in the center of the sample, where most atoms are residing, and the Mott transition would be sharper.

However, and this is the theme of the present paper, a pure Mott insulating state requires commensurate filling, i.e., the number of particles has to match the number of wells. In a quadratic potential this requirement is

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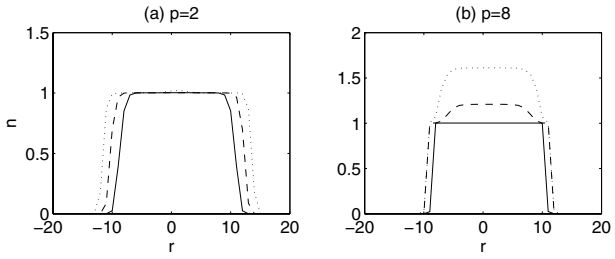

Fig. 1. Cross-section of the density profiles in a two-dimensional power-law potential with power law $p = 2$ (a), and $p = 8$ (b), respectively. The number of atoms is $N = 300$ (full lines), $N = 400$ (dashed), and $N = 500$ (dotted).

relaxed because excess atoms are absorbed into a superfluid region, where the filling is noninteger, at the surface of the sample. Using a flat-bottomed potential may put more severe constraints on the number of particles, which presents a problem, since in an actual experiment one does not have very precise control over this number. It is the purpose of the present study to explore the balance between on the one hand, the gradual character of the Mott transition, and on the other hand, the uncertainty in the particle number.

We consider two-dimensional systems in this study, since a power-law potential is more easily created in the plane than in three dimensions. The external potential is taken to be

$$V(r) = (|r|/r_0)^p, \tag{2}$$

where $|r|$ is the distance from the center in two dimensions measured in unit cells, r_0 is a constant length, and p is the power law. In experiments with trapped atoms, quadratic potentials are prevailing for natural reasons (the first term in the expansion around a minimum of a smooth function is in general quadratic). A fourth-order potential has been created by superimposing a Gaussian optical potential on a quadratic magnetic one in order to observe fast-rotating vortex configurations [8]. Other than that, realizations of high-order power-law potentials for atoms have been scarce. In two dimensions, an optical power-law potential could be realized using Gauss-Laguerre optical beams, Fourier optics, or masks. The confinement to two dimensions can be realized by applying an external field in that direction, or alternatively, by applying a strong optical-lattice potential in the third direction. The latter method, however, creates a number of two-dimensional systems with different numbers of particles, which will certainly affect the observability of the Mott transition considered here. A three-dimensional anharmonic trap would have to be created by combining several two-dimensional potentials. The technically easiest solution is probably to apply an anharmonic trap in a plane while the third dimension remains harmonically trapped. This will enhance the observability of the transition compared to the purely harmonic trapping, but not to the same extent as in the two-dimensional case.

Figure 1 shows a few examples of density profiles for a two-dimensional system in quadratic ($p = 2$) and $p = 8$ power-law potentials.

The most common way of detecting the state of an atomic gas in an optical lattice is by time of flight, that is, to release the sample from the trapping potential and image it after some time of expansion. From the resulting density profile one may deduce the fraction of coherent atoms, i.e., the condensate fraction [4]. Recently, experimental techniques have been developed for directly detecting Mott plateaus in situ [9,10]; nevertheless, that type of method addresses the occupation number and not the coherence, so the time-of-flight method remains the most straightforward. A harmonically trapped gas will in such an experiment exhibit a gradually increasing condensate fraction as the tunneling is increased.

In order to observe a sharper Mott transition, it was suggested in reference [7] that the potential can be made more similar to a square well. For a power-law potential of the form (2), the limit $p \to \infty$ corresponds to a square well of radius r_0. In a flat-bottomed potential, the typical situation will be that nearly all atoms will be in the same state (Mott insulating or superfluid), instead of having appreciable fractions of atoms in both states for a broad range of parameter values. However, now there appears a new problem: a flat-bottomed potential is much more sensitive to the exact number of particles. In a homogeneous Hubbard model, the Mott insulating state can only occur if the filling is commensurate, that is, if the number of particles is exactly an integer multiple of the number of wells: adding one particle to a Mott insulator results in a superfluid. In a power-law potential, there is no such restriction on the number of particles, but the region in phase space that can accommodate a partially Mott insulating system will be smaller for a flat-bottomed potential than for a more rounded one. This can be seen Figure 1, where the density profiles for a one-dimensional system with different particle numbers are compared. In the quadratic $p = 2$ trap, an increase of the number of particles does not have a dramatic effect on the profile or the number of Mott insulating atoms. In contrast, for a $p = 8$ potential illustrated in Figure 1b, it is seen how an increase in particle number from $N = 300$ to 400 takes most atoms out of the Mott phase.

In order to quantify this, we use the Gutzwiller mean-field method with a local-density approximation. The mean-field approximation is in two dimensions known to underestimate the size of the Mott insulating regions in phase space by about 40% [11], while the local-density approximation typically underestimates the superfluid fraction [5]. The fraction of Bose-Einstein condensed atoms is defined as

$$\frac{N_C}{N} = \frac{\sum_r |\langle a_r \rangle|^2}{\sum_r \langle a_r^\dagger a_r \rangle}. \tag{3}$$

This fraction can be inferred from experimental measurements [4] and is a direct quantitative measure of the state of the system. Inverting the definition of a local chemical potential,

$$\mu(r) = \mu - V(r) = \mu - \left(\frac{|r|}{r_0}\right)^p, \tag{4}$$

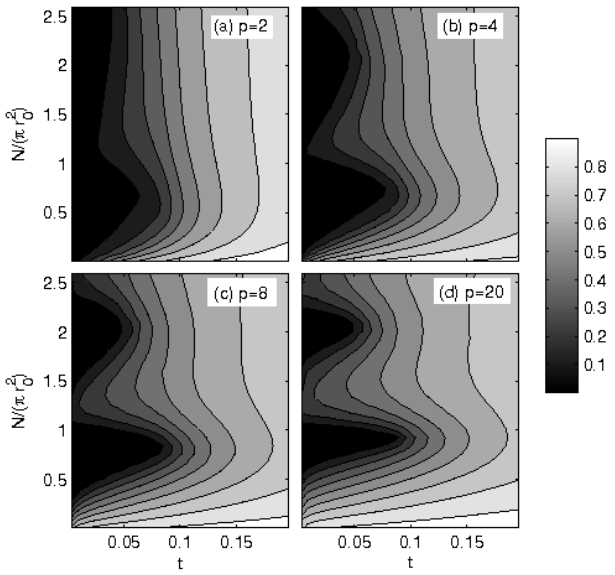

Fig. 2. Fraction of condensed atoms, N_C/N, for a Bose-Hubbard model in a power-law trapping potential as a function of the tunneling matrix element t and the number of atoms divided by the trap area, $N/\pi r_0^2$. The power law of the potential is (a) $p = 2$, (b) 4, (c) 8, and (d) 20.

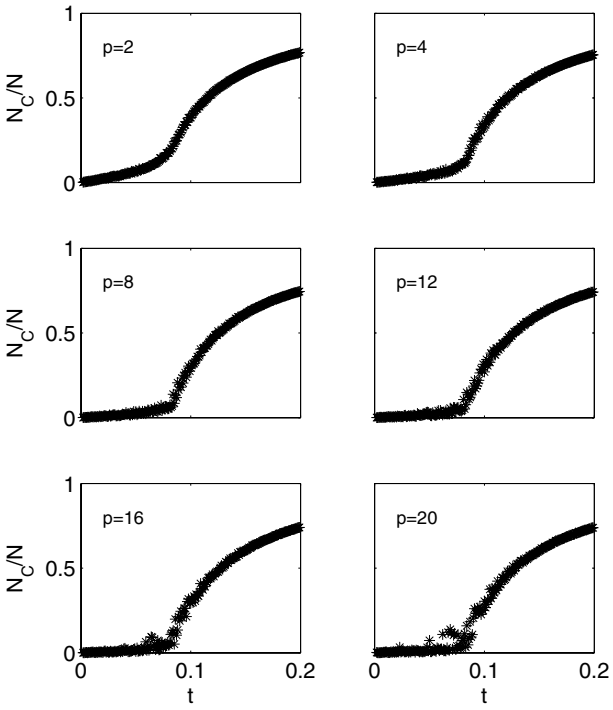

Fig. 3. Outcome of a simulated experiment measuring the fraction of condensed atoms N_C/N in a trap, traversing the Mott transition as the tunneling t is increased while the number of atoms is allowed to fluctuate within 10% according to a uniform random distribution. The different curves correspond to different power laws p of the two-dimensional trapping potential.

one can apply a local-density approximation to transform the spatial sum to a sum over $\mu' \equiv \mu(r)$, which in two dimensions reads

$$\frac{N_C}{N} = \frac{\int_{\mu_0}^{\mu} d\mu' \frac{dr}{d\mu'} 2\pi r(\mu') n_C(\mu')}{\int_{\mu_0}^{\mu} d\mu' \frac{dr}{d\mu'} 2\pi r(\mu') n(\mu')}, \tag{5}$$

where $n_C(\mu) = |\langle a \rangle|^2$ and $n(\mu) = \langle a^\dagger a \rangle$ are the condensate density and total density, respectively, for a homogeneous sample at chemical potential μ. The lower limit μ_0 is the chemical potential at which N vanishes; it obeys $\mu_0 \leq 0$ with the equality holding at vanishing tunneling matrix element t. These functions have been computed and tabulated, whereafter the integrals have been summed for a range of particle number N and tunneling matrix element t. The result is displayed in Figure 2. It is seen that for more flat-bottomed potentials, the transition between the Mott and superfluid states, i.e., from zero to non-negligible condensate fraction, is steeper. At the same time, the Mott state occupies a much smaller region in phase space for the flat-bottomed potentials. It is this tradeoff that has to be considered in experiment: in order to see a sharp Mott transition, one needs to have control over the number of particles.

Next, we simulate an experiment where the condensate fraction is measured for a series of increasing tunneling matrix element t (i.e., decreasing optical lattice irradiance), where N has been allowed to fluctuate. Experimentally, controlling the number of particles is very difficult [12], but the number can be measured afterwards to within certain bounds, so on performing a series of runs, one may apply post-selection, i.e., only the data from those runs that correspond to the desired number is included in the analysis. While the relative number between different shots is quite easy to measure, inferring the absolute number is more problematic and may produce a systematic error [13]. In the simulation, the average particle number $\langle N \rangle$ is chosen to lie in the most pronounced Mott insulating region seen in Figure 2. For definiteness, $\langle N \rangle$ was chosen to lie at the tip of the iso-condensate fraction curve for $N_C/N = 0.1$. Thus, for $p = 2$ we choose $\langle N \rangle = 0.73\pi r_0^2$, and so on; for $p = 20$ we choose $\langle N \rangle = 1.0\pi r_0^2$, corresponding to a filling of one particle per site. The fluctuations around the mean particle number are assumed to be uniform, as they would if the number was controlled by post-selection. Figure 3 shows the result for a fluctuation of 10 percent. As expected, for the quadratic $p = 2$ potential, the uncertainty in particle number has little effect, but the transition is gradual. In contrast, for the most flat-bottomed potential, $p = 20$, the transition would have been much sharper, but the uncertainty in the number of particles ruins the observability of this sharp transition. However, in the intermediate range of powers, both effects may apparently be working in favor: the transition is reasonably sharp as a function of t, yet the Mott insulating state covers a broad enough range of particle number N that the experimental uncertainty can be accommodated. Upon optical inspection, it seems that in this example, all power laws p between 2 and 20 yield about equally sensible results. As noted above, the use of the local-density approximation slightly underestimates the spatial size of

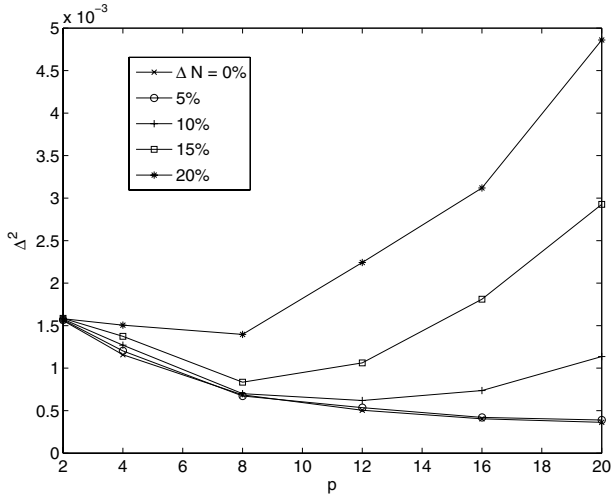

Fig. 4. Error in fitting the simulated data for the coherent fraction of atoms N_C/N, as a function of the power law of the trapping potential. The width ΔN of the simulated random distribution of particle number is indicated in the legend.

the superfluid regions in the trapped sample, and as a result, an exact calculation may have showed a slightly more rounded transition.

As an example calculation in order to quantify these considerations, we try to locate the transition by fitting the simulated data N_C/N to a function of the form

$$f(t) = \begin{cases} 0, & t < t_c, \\ \beta(t - t_c)^\alpha, & t \geq t_c, \end{cases} \tag{6}$$

where α, β, and t_c are fitting parameters; the resulting value for t_c is the critical point of the Mott transition. In Figure 4, the squared residual error of the fit,

$$\Delta^2 = \langle |N_C/N - f(t)|^2 \rangle, \tag{7}$$

is displayed for different power laws p and uncertainties in particle number ΔN. Clearly, the error in the fit is not dramatically different for different power laws, but for very small uncertainty, the minimum is of course obtained for the most flat-bottomed trap, $p = 20$. For the largest uncertainties of 15% and 20%, the best fit is obtained for the $p = 8$ trap, where the scatter in the data is smaller. Further numerical experimentation, not shown here, indicates that the $p = 2$ trap is best when the uncertainty exceeds about 30%. For the middle-ground case, with uncertainty 10%, it is an intermediate power law, $p = 12$, that produces the best fit. So indeed, for a modest uncertainty in particle number there seems to exist a range of power law where neither of the two competing processes is very strong, and the clearest Mott transition occurs for an intermediate power-law potential.

Summing up, in power-law potentials one faces a trade-off between two effects that affect the detectability of a Mott insulator. On the one hand, a flat-bottomed potential (i.e., a high power law) is preferred in order to make the Mott transition sharper. On the other hand, such a potential will increase the precision with which the number of particles has to be controlled. It was seen in an example simulation that for an uncertainty in number between ten and twenty percent, a power law of about 8 yields the most accurate determination of the Mott transition; if the uncertainty can be made smaller, then a very flat-bottomed potential with a power law above 10 yields the best result.

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