Rotation of atoms in a two dimensional lattice with a harmonic trap

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Rotation of atoms in a lattice is studied using a Hubbard model. It is found that the atoms are still contained in the trap even when the rotation frequency is larger than the trapping frequency. This is very different from the behavior in continuum. Bragg scattering and coupling between angular and radial motion are believed to make this stability possible. In this regime, density depletion at the center of the trap can be developed for spin polarized fermions.

Recent spectacular progress in manipulating neutral atoms has opened the way to the simulations of complex quantum systems of condensed matter physics, such as high-Tc superconductors, by means of atomic systems with perfectly controllable physical parameters. The systems studied include Bose-Einstein condensations (BEC) for both atoms and molecules, paired states for fermions (BCS), the crossover between BEC and BCS \([1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]\).

So far, most of the experimental studies involving cold atoms were conducted in continuum. One of the major goals of studying ultracold gases in optical lattices is to understand the physics in condensed matter systems. In addition to topics already investigated in continuum systems there are many effects of interest lately: Superfluid to Mott insulator transition \([13]\), Bloch oscillation of particles in lattice due to Bragg scattering \([14]\), parametric atomic down conversion in BEC \([15]\), and so on.

In this letter, we will address the effect of a lattice on the rotation of atoms in a harmonic trap. Many phenomena of rotation atoms in a continuous trap have already been investigated, both experimentally and theoretically: the appearance of vortices \([16, 17]\) in BEC and BCS samples \([11]\), quantum Hall states for fast rotating fermions \([13]\), and vortex lattices in the lowest Landau level for BEC \([17, 19]\). On the other hand, lattices lead to many new effects under rotation, such as structural phase transitions of vortex matter \([20]\). Also, near the superfluid–Mott insulator transition, the vortex core has a tendency toward the Mott insulating phase \([21]\), and second-order quantum phase transitions between states of different symmetries were observed at discrete rotation frequencies \([22]\).

In particular, it is well known that in a continuum the centrifugal force prevents atoms from rotating beyond the harmonic trap frequency. That means that if the rotation is too fast the centrifugal force lets the atoms escape the trap. Therefore, a quadratic-plus-quartic potential was assumed to prevent the atoms from flying away from the trap at fast rotation frequencies \([23]\). In a lattice, however, as will be shown in this paper, it is possible for atoms to stay in the trap even if the rotation frequency is larger than the harmonic trapping frequency and density depletion at the center of the trap can then be developed for such a regime.

For completeness, we first review the rotation of a particle in a two dimensional (2D) continuum. In the rotating frame, the Hamiltonian for the particle is

\[
H_c = -\frac{\nabla^2}{2} + \frac{\omega^2 \rho^2}{2} - \Omega L_z
\]

with \(L_z = -i\partial/\partial \phi\), \(\omega\) is the trapping frequency and \(\Omega\) the rotation frequency. Throughout this paper, units \(\hbar = m = 1\) are used, where \(m\) is the mass of the particle. Eq. (1) is formally identical to the Hamiltonian of a particle of charge one placed in a uniform magnetic field \(2\Omega\hat{z}\) and confined in a potential with a spring constant \(\omega^2 - \Omega^2\). This equation can be solved by separation of variables \((r, \phi)\) in polar coordinates where the radial equation is given as

\[
\left(\frac{1}{2\rho} \frac{\partial}{\partial \rho} \frac{\partial}{\partial \rho} + \frac{(\omega^2 - \Omega^2) \rho^2}{2}\right) \psi_r = \epsilon \psi_r.
\]

This decoupling of radial and angular degrees of freedom is different from the motion in a lattice, which is to be discussed later. For \(\Omega \leq \omega\), Eq. (1) has eigenvalues \([17]\)

\[
E_{j,k} = \omega + (\omega - \Omega) j + (\omega + \Omega) k
\]

where \(j, k\) are non-negative integers. Note that the angular momentum states are eigenstates \([17]\) such that there are only level crossings when \(\Omega\) changes. At \(\Omega = \omega\), the ground states become infinitely degenerate lowest Landau levels.

When \(\Omega\) is bigger than \(\omega\) \((\omega'^2 = \Omega^2 - \omega^2 > 0)\), at \(r \rightarrow \infty\), the radial equation becomes \(\psi_r'' + r^2 \omega'^2 \psi_r = 0\), which gives the non-vanishing asymptotic solution \(\psi_r \propto \exp \left[\pm i \omega' r^2 / 2\right]\). However, because the harmonic trap potential at \(r \rightarrow \infty\) approaches infinity, the wavefunction at \(r \rightarrow \infty\) has to vanish. This contradiction indicates that at \(\Omega > \omega\), Eq. (1) has no solution. This means that the atoms would leave the trap because the centrifugal force \(\Omega^2 r\) exceeds the restoring force \(-\omega^2 r\) in the xy plane.

Numerically, a system is treated by necessity as having a finite size. Thus a procedure needs to be determined to distinguish a “non-existing” wave function (meaning that the particles have left the trap) from a wave function where the particles are held in the trap. To this end, we discretize the simple analytic problem of Eq. (1) using a
The results can be visualized like in Fig. 1 For well-contained particles the analytic (Eq. (3)) and numeric (Fig. 1) solutions agree in that the ground state energy $E_g$ does not depend on the rotation frequency $\Omega$. As soon as the particles are not contained anymore (since the centrifugal force is now stronger than the trap) the ground state energy plunges immediately. As can be seen in Fig. 1 this plunge happens slower for larger mesh sizes. What is important here is that $E_g$ depends in this (unphysical) case strongly on the mesh size. A similar case can be made by looking at the probability density $|\psi_r|^2$ of the particles in the trap, as shown in Fig. 2 For the case of a rotation frequency too large to contain the particles in the trap, it can be seen that only the fine-gridded solution (here with the mesh size $h=0.25$) approaches our physical understanding of the particles being driven outward by putting the probability density all to the boundary of the numerically available space. Therefore, the wavefunctions depend on the mesh size only if the atoms are not contained and thus is another good measure (along with a varying $E_g$) for this situation.

We now study the case of zero-temperature atoms in a lattice placed inside a harmonic trap. We will see that in this case, the particles stay contained even when the rotation frequency $\Omega$ is slightly larger than the trapping frequency $\omega$. In the rotating frame, the single band Hubbard Hamiltonian is

$$H = \sum_{\langle i,j \rangle} (-t - i\Omega K_{i,j}) c_i^+ c_j + H.c. + \sum_i V(\vec{r}_i)n_i \tag{4}$$

where $\langle i,j \rangle$ indicates a sum over nearest neighbors, $V(\vec{r}_i) = \Omega^2 r_i^2 / 2$ is the harmonic trap potential, $t$ is the hopping term that describes tunneling between neighboring sites, $n_i = c_i^+ c_i$ is the number operator with $c_i^+$ ($c_i$) the fermion creation (annihilation) operator at site $i$, and $H.c.$ means Hermitian conjugate. In this paper, $t$ is set to one and used as a reference unit for $\omega$ and $\Omega$. $\Omega K$ represents the centrifugal term with $K_{i,j} = r_i r_j \sin \alpha_{i,j}/d^2$, where $r_i$ denotes the distance from the axis of rotation to the $i$th site, $\alpha_{i,j}$ is the angle subtended by the $i$th and $j$th sites with respect to the axis of rotation, $d$ is the lattice constant, and $\beta = 0.493$ is the dimensionless constant characterizing the lattice geometry and depth $22, 24$. We note that, different from that in continuum, the effective mass in the lattice $\mu(k) = (2t d^2 \cos kd)^{-1}$ depends on momentum $k$ and may become negative. To avoid confusion here it should be noted that without a trap, the particles will immediately fly away independent of the magnitude of $\Omega$. This means that the lattice potential (in particular, the tunneling $t$ term) has absolutely no confining effect on the atoms. As a result, the addition of the lattice potential to the trap potential cannot explain the above-threshold rotation which will be explained here.

Figure 1 shows that in the presence of the lattice $E_g$ does not depend on the rotation frequency for $\Omega < \omega$ as it is the case for a continuum. For comparison, in Fig. 1 we choose the lattice constant such that $\mu(k = 0) = 1$ and find that the $\Omega$-dependence for $\Omega > \omega$ of $E_g$ is the same as for the case of the “discretized continuum” (with the same effective mass $\mu = 1$) by setting the mesh size $h = 1/\sqrt{2}$. The similarity in the energy dependence for the lattice and discretized continuum let us conclude that it is just a consequence of the discrete nature of the lattice. Besides, it is to be remembered that the infinite degeneracy of the ground state at $\Omega = \omega$ in the continuum is lifted in the lattice and thus the physics associated with the lowest Landau levels will be different from that in the continuum. A detailed study of this will follow in the future.

Figure 2 shows the density distribution at various $\Omega$ around $\omega = 0.1$. Two features deserve attention: First, the atoms still are contained at $\Omega = 0.11 >
FIG. 3: Ground state density distributions at $\Omega = 0.09$ (a), $0.105$ (b) and $0.11$ (c). As the rotation frequency $\Omega$ becomes larger than the trapping frequency $\omega = 0.1$, the ground state wave functions gradually change into the 4-lobe structure and the atoms are kept hold in the trap. For better visibility, the maximum density are normalized to one for each plot.

$\omega$ because if we increase the lattice size, both the ground state wave function $|\psi|^2$ and energies $E_g$ do not change. At larger rotation frequency $\Omega$, different lattice size/shape (SIZE/CONSTANTS) lead to different density distributions and ground state energies, which we interpret as particles escaping the trap. In addition, the density at the center of the trap becomes depleted, which is impossible for the ground state in the continuum as shown in Ref. [18]. When the lowest four states become degenerate, the ground state develops a 4-lobe structure (Fig. 3). Moreover, when $\Omega$ increases beyond $\omega$, the ground states continue to change smoothly and move away from the center as shown in Fig. 3, the particles in the ground states only move away from the center to a distance determined by the rotation frequency, but don’t leave the trap altogether. It is also found that with the same $\omega$, the particles in the ground state of a smaller lattice leave the trap at smaller values of $\Omega$, as opposed to the universal threshold $\omega$ that is present in continuum. This difference between the lattice and the continuum is one of the major results of this paper. Note that the symmetric 4-lobe structure is determined by the primitive cell geometry’s fourfold symmetry, not by the overall lattice shape, because, for example, 150X100 lattice gives the same diagonal density distribution as 150X150 at $\omega = 0.1$ and $\Omega = 0.11$. In other words, the fourfold degeneracy reflects the discrete rotational symmetry of the underlying square plaquette in the lattice [22]. Furthermore, when the 4-lobe structure is finally formed, both at $x = 0$ and $y = 0$ the densities approach zero.

The atoms rotating in the lattice are always in motion, so there are always currents between neighbor-

ing sites, which are calculated using $J_{ij} = i[n_i, H_{ij}] = i(t(a_i a_j^+ - H.c.) + \Omega(a_i a_j^+ + H.c.)$ [22]. One example of the current pattern is shown in Fig. 4. While the properties of the 4-lobe states will be for future publication, the important thing here is that the persistent motion allows Bragg scattering to explain the stabilization of atoms in the lattice.

FIG. 4: The current distribution at one of the lobe in Fig. 3. A center for the current pattern is clearly seen at site (-10,-10) by nearly disappearing current at that site. However, Fig. 4 shows that the density at this site is nonzero, different from a vortex core.

To appreciate the role of Bragg scattering, we recall the Bloch oscillations in the lattice [14]; the driving voltage across the lattice does not produce a net current for the electrons, instead it produces periodic current, as the Bragg scattering completely reflects the electrons. So it may not be so surprising to see that the Bragg scattering can hold the atoms in the trap even when $\Omega$ is slightly larger than $\omega$. Furthermore, as the continuous symmetry is broken in the lattice, the correlated motion in radial and angular direction allows Bragg scattering between these directions. This is believed to also be the reason for the containment of the particles for rotation frequencies beyond $\Omega = \omega$. Additionally, we note that Bragg scattering is not limited to the Hubbard Hamiltonian Eq. (4), because the discretized continuum Hamiltonian Eq. (1) with large mesh sizes gives similar results (the dashed line in Fig. 1) as that in lattice Eq. (4).

So far, we have shown that the quantum statistics of atoms does not play a role for the stabilization. Next, we point out that density depletion at the center of the trap for spin polarized fermions is possible. To this end, spin polarized fermions without interaction are considered in the lattice at zero temperature. The overall density of putting $N$ rotating fermions into a lattice, according to Pauli’s exclusion principle, is the summation of the density of the lowest $N$ states. Note that the very low lying states all have zero population at the center of the trap, which causes the non-interacting fermions not only to have a density plateau at $\Omega < \omega$ (the solid curve in Fig. 5) like in the continuum [18], but one also sees density depletion at $\Omega > \omega$ as shown by dashed line and dot-dashed line in Fig. 5. This is another major result of this paper. In comparison, the density depletion cannot
be realized in a continuum with a harmonic trap because the atoms fly away at $\Omega > \omega$.

![Graph](image_url)

**FIG. 5:** Density distribution of 50 noninteracting spinless fermions at the cross section with $y = 0$. When $\Omega$ is close to but smaller than $\omega = 0.1$, the plateaus are developed reflecting the underlying Landau-level wave functions [18]. On the other hand, when $\Omega$ is larger than $\omega$, density at the center is depleted.

In the above, coupling between the angular motion and radial motion as well as Bragg scattering were used to explain the stabilization. One may also think that the effective mass, which depends on $k$ and could be negative in the lattice, may also stabilize the atoms. However, the wave packets with $\mu(k) > 0$ will not be contained in the trap at $\Omega > \omega$ if only the effective mass contributes to the stabilization. Therefore, while it may play an important role, the effective mass alone cannot explain the stabilization.

In lattices, when $\omega$ is comparable to or greater than $\mu$, the coupling between the angular motion and radial motion is enhanced. As this enhancement makes the Bragg scattering between radial direction to angular direction larger, the atoms will stay in the lattice with larger rotation frequency. This means that to experimentally demonstrate the above threshold rotation, larger trapping frequency is desirable. However, deep harmonic trap makes the single band Hubbard model not be reasonable for describing an optical lattice system [23]. Therefore, some intermediate trapping frequency is preferred for demonstrating the above-threshold rotation experimentally.

To conclude, the rotation of atoms in an optical lattice is studied using a Hubbard model. It is found that the atoms are contained in the trap even when the rotation frequency exceeds the trapping frequency, which is very different from the continuum case. Bragg scattering and the coupling of angular and radial motion make the above stability possible. In this regime, density depletion at the center of the trap can be developed for spin polarized fermions.

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