An Investigation of Mean-field Effects for a Bose Condensate in an Optical Lattice

S. B. McKagan$^{1, *}$, D. L. Feder$^2$, and W. P. Reinhardt$^1$

$^1$ Departments of Chemistry and Physics, University of Washington, Seattle, WA 98195 and $^2$ Department of Physics and Astronomy and the Institute for Quantum Information Science, University of Calgary, Calgary, Alberta, Canada T2N 1N4

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This paper presents a mean-field numerical analysis, using the full three-dimensional timedependent Gross-Pitaevskii equation (GPE), of an experiment carried out by Orzel et al. [Science 291, 2386 (2001)] intended to show number squeezing in a gaseous Bose-Einstein condensate in an optical lattice. The motivation for the present work is to elucidate the role of mean-field effects in understanding the experimental results of this work and those of related experiments. We show that the non-adiabatic loading of atoms into optical lattices reproduces many of the main results of the Orzel et al. experiment, including both loss of interference patterns as laser intensity is increased and their regeneration when intensities are lowered. The non-adiabaticity found in the GPE simulations manifests itself primarily in a coupling between the transverse and longitudinal dynamics, indicating that one-dimensional approximations are inadequate to model the experiment.

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I. INTRODUCTION

The creation of dilute gaseous Bose-Einstein condensates (BECs) in the laboratory in 1995 [1, 2, 3] has spurred much development in both experiment and theory [4, 5, 6]. Mean-field theory was able to explain most early BEC experiments, using the well-known Gross-Pitaevskii equation (GPE) [4, 5] which is valid for weakly interacting BECs at zero temperature because it assumes all atoms occupy a single macroscopic wavefunction:

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left( -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) + g|\psi(\mathbf{r}, t)|^2 \right) \psi(\mathbf{r}, t)$$

(1)

where $\psi(\mathbf{r}, t)$ is the single particle wave function for any atom in the BEC, $V(\mathbf{r}, t)$ is an external trapping potential, and $g = 4\pi a_s \hbar^2 / m$, where $a_s$ is the s-wave scattering length and $m$ is the atomic mass. These early successes included the anisotropic profile and momentum distribution of the ground state after ballistic expansion [1, 2, 3], the spectrum of collective excitations [4, 5], the dynamics of spinor condensates [10, 11], and the wave interference of interacting condensates [12, 13]. Perhaps unexpectedly, the time dependent GPE also accurately described strongly nonlinear excitations such as vortices [12, 13] and solitons [12, 13].

Given the overwhelming success of the GPE, there has been much interest in finding situations in which it breaks down and a more detailed theoretical description is needed. Indeed, the theoretical interpretation of the earliest experiments on collective excitations at finite temperature [4, 13, 20] has required a dynamical theory that includes the motion of the noncondensate [21, 22]. More recent experiments are geared toward inducing strong correlations among atoms, which are not captured by the GPE; these include molecules in Bose [23, 24] and Fermi [25, 26, 27] gases and exploring the BCS-BEC crossover [28, 29, 30], low-dimensional systems through tight confinement [31, 32, 33], quantum Hall-like states in rapidly rotating traps [34, 35] or using external lasers [36], and novel many-body states of atoms in optical lattices [37, 38, 39, 40, 41, 42].

In the experiments with optical lattices, the extent of correlations in the atomic gas has generally been measured by dropping all confining potentials and imaging the cloud after a period of ballistic expansion. When condensates are suddenly released from their confinement in shallow optical lattices formed from weak lasers, they form well-defined interference patterns corresponding to momentum-space Bragg peaks. This has been interpreted as an unequivocal signature of phase coherence over multiple lattice sites. As the laser intensity increases, however, the interference patterns partially or fully wash out [37, 38, 39]. The theoretical interpretation is that as tunneling is quenched, the initial macroscopic condensate splits into many separate subcondensates which may then lose some or all of their relative coherence; the resulting state has been described as ‘number squeezed,’ or ‘fragmented.’ Under various conditions one obtains full fragmentation, which leads to a quantum phase transition from a superfluid state to a Mott insulator [43].

In fact, the loss of fringe contrast after ballistic expansion is not as clear a signature of condensate fragmentation as is often assumed. Jean Dalibard and collaborators [44] recently demonstrated that high-visibility interference patterns resulted even under conditions where the phases from site to site of a one-dimensional (1D) optical lattice were random. A simple theoretical model that generalizes the interference pattern from two uncorrelated sources reproduces the experimental data. Under conditions similar to those of Orzel et al. [38] where num-
ber squeezing is expected to be present (though using a blue-detuned rather than a red-detuned lattice where the transverse confinement is much weaker), they observed an unattributed heating effect. A similar heating was observed by Morsch et al. [39], where radial modes excited by the non-adiabatic ramp-up of the 1D optical lattice rapidly damped and transferred energy to high-lying axial modes. Zakrzewski [40], using a time-dependent Gutzwiller mean-field approach to solving the Bose-Hubbard model, has found that non-adiabatic mean-field effects reproduce some of the results seen in the experiments of Greiner et al. [41].

The recent experiments indicate that fundamental questions need to be answered before fringe contrast can be used as a quantitative measure of the breakdown of mean-field theory in these systems. The effects of non-adiabaticity on the phase variations across the lattice have been addressed previously [42, 43, 44, 45]. 1D calculations based on the GPE found that the harmonically trapped condensate develops a pronounced ‘phase sag’ after slowly ramping up the lattice [46, 47]; the phase was found to increase approximately quadratically around the trap center. A flat phase profile at the end of the ramp, and a high-contrast interference pattern, can be restored if the harmonic trap parameters are simultaneously varied [48]. More recent effective 3D calculations demonstrate that collective modes are excited by slow ramps [49, 50], but the influence of these excitations on the resulting interference patterns was not addressed.

In order to clarify the various mean-field effects that can degrade the interference pattern when a condensate is released from an optical lattice, we have performed fully 3D numerical simulations based on the GPE of one of the above experiments, namely that of Orzel, Tuchman, Fenselau, Yasuda, and Kasevich [38] (referred to as OTFYK in what follows). See also [52]. If number squeezing were the main reason for the observed loss of fringe contrast as has been suggested [38], the GPE simulations should not be able to mimic the experimental data. We find, however, that we can reproduce the degradation of the interference patterns as the lattice depth approaches the regime where squeezing would be expected, and the subsequent restoration of contrast as the laser intensity is lowered, even in cases where ‘random’ phases have been applied to the individual wells at the largest lattice depths. At the level of the mean-field approximation, the behavior is due to the non-adiabatic response of the trapped condensate as the optical lattice is slowly turned on: the ramp induces axial currents and the excitation of strongly coupled transverse and longitudinal excitations. These in turn yield variations in the phase from site to site that cause the interference patterns to disappear. We expect that in the presence of damping (not included in the present analysis), the mean-field results would be close to, if not indistinguishable from, the experimental data.

The paper is organized as follows: In Section II, the ground states are obtained for a condensate in harmonic oscillator, gravitational, and optical lattice potentials as a function of laser intensity. The OTFYK experiment is described in Section III, and the observations are compared to results of a GPE model that assumes perfect adiabaticity of the optical lattice loading. Section IV, which is the heart of the paper, contains discussion of a GPE simulation of the full experimental protocol, including the turning on and turning off of the lattice, and the use of gravity to induce a relative phase shift of π between adjacent lattice sites. It is found that the experimental timescales for the lattice ramp are not generally sufficient to ensure adiabaticity. The resulting phase shifts mimic loss of coherence between adjacent lattice sites. In Sections V and VI it is demonstrated that interference patterns recover as the laser intensities are reduced, even if the site-to-site phases are artificially randomized at lattice maximum. In addition to the accumulation of axial phase variations, a second source of non-adiabaticity is found and discussed in Sections VII and VIII: a strong coupling between longitudinal and transverse oscillations. The results are compared to more recent experiments by the Kasevich group [52]. A brief summary and conclusions end the paper, in Section IX.

II. THE POTENTIAL AND GROUND STATE DENSITIES

In the OTFYK experiment, a BEC is first created in a cylindrically symmetric magnetic trap with the longitudinal axis oriented vertically, parallel to the ambient gravitational field. Counter-propagating laser beams are then slowly turned on, oriented vertically and aligned with the long axis of the magnetic trap. The lasers are red detuned, and thus the condensate is pulled into the anti-nodes, with spacing \(\lambda/2\), and also experiences strong transverse confinement. The full potential used to describe in the present numerical studies of this system is given by [57]:

\[
V(\rho, z, t) = U(t) \left(1 - e^{-\rho^2/r_0^2} \cos^2(kz)\right) + \frac{1}{2} m(\omega_\perp^2 \rho^2 + \omega_z^2 z^2) + mgz
\]  

where the first term is due to the laser, the second term to the magnetic trap, and the third term to gravity. The longitudinal coordinate \(z\) is in the vertical direction and the transverse coordinate \(\rho = \sqrt{x^2 + y^2}\). Table I gives the values of the experimental parameters as reported in the OTFYK paper.

Various parts of the trap are turned on and off at various points in the experiment, as described in Section III, so not all the terms in Eq. (2) are present at all times. The laser is generally ramped up slowly, so \(U\) varies as a function of time. As long as the magnetic trap is on, the gravitational term has no effect other than to give a linear shift the quadratic trapping potential, but it plays an important role when the magnetic trap is turned off.
TABLE I: Values of parameters used in the experiment and modeling.

| \( N \) | \( a_s \) | \( m \) | \( \omega_\perp \) | \( \omega_\parallel \) | \( k \) | \( r_b \) | \( U \) |
|--------|--------|------|------------|-------------|------|-----|-----|
| 30000  | 5.24nm | 1.44 \( \times 10^{-24} \)kg | 2\( \pi \) \( \times \) 19Hz | 2\( \sqrt{2} \)\( \omega_\perp \) | 2\( \pi \)/840nm | 50\( \mu \)m | 0 to 44\( E_R \) |

In our calculations, we neglect this term except when it is required for phase manipulation. Note that the laser creates not only a periodic trapping potential in the longitudinal direction, but also a Gaussian trapping potential in the transverse direction. This Gaussian term (which is not present for a blue-detuned laser) implies that as the laser strength increases, so does the transverse confinement of the BEC, and therefore the density increases. This turns out to be a very important effect.

Although the actual OTFYK experiments, as seen in Section III, consist of a sequence of well defined time dependent steps, it is useful to examine the density profiles of the stationary GPE ground states in the potential of Eq. (2). Ground states were obtained using numerical methods described in the Appendix, by evolution of the GPE in complex time \( (t \rightarrow it) \) with propagation converging to the lowest energy stationary states for each fixed value of \( U \). The results for three representative values of \( U \) are shown in Fig. 1. Figure 1(a) illustrates the density profile in the absence of the optical lattice. All experiments and theoretical simulations described herein start with this ground state of the condensate in the magnetic trap in the presence of gravity. Figures 1(b) and (c) illustrate the two dominant effects of the laser fields: first the condensate morphs from a single ellipsoidal and coherent structure into a vertical stack of disk like subcondensates. Also clearly seen is the very large effect of the transverse confinement: the condensate density envelope changes from oblate to prolate at the highest field densities.

III. AN INITIAL “ADIABATIC” SIMULATION OF THE EXPERIMENT

We have simulated each step of the OTFYK experiment using the full 3D GPE with the potential discussed in the previous section. To avoid repetition, we will describe the steps of the experiment and our simulation in parallel. The first step of the experiment is to create a BEC in a magnetic trap. This step can be simulated by using complex time evolution as described in the previous section. The results of the simulation for the harmonic trap only are shown in Fig. 1(a).

The next step in the experiment involved turning on the laser fields so that the intensity increases linearly from zero to some final intensity \( U_f \) (ranging from 7.2\( E_R \) to 44\( E_R \)) in a ramp time \( \tau_R = 200 \) ms. This ramp-up time was assumed by OTFYK to be slow enough to allow the condensate to follow the ramping adiabatically, so that the BEC stays in the appropriate ground state as the laser is turned up [55]; in the next section we will test this assumption of adiabaticity. If the final state of the BEC in the combined magnetic trap and lattice is the ground state of this system, then the sequence of states generated are just those which may be found by complex time evolution, as discussed in Section II. Then the ground states as a function of \( U \) shown in Figs. 1(b,c) can be used in a preliminary simulation of the OTFYK experiment.

The OTFYK paper described two regimes that exhibited markedly different interference patterns after the external potentials were dropped and the atomic cloud was allowed to ballistically expand. For low \( U_f \), the final state was expected to be fully phase coherent yielding a clean interference pattern [53]. The computed three-peak pattern for the \( U_f = 7.2E_R \) case is shown in Fig. 2(a). For high \( U_f \sim 40E_R \), the condensate was anticipated to be strongly number squeezed, leading to a random relative phase from site to site. Ballistic expansion would then yield no detectable interference pattern. Of course, the GPE cannot produce a number squeezed state, but if the random phases are put in ‘by hand’ it can mimic the experimental situation, as was done previously for the MIT interference experiment [12] by Röhr et al. [13] within the framework of the GPE. The numerical results for this case are shown in Fig. 2(b).

The three peak interference pattern of Fig. 2(a) is inconvenient for quantitative estimation of the extent of decay of coherence, so a third protocol was invoked by OTFYK. The experimenters used the presence of gravity, via an appropriate time delay, as discussed in the following section, to imprint a \( \pi \) phase difference between the condensate in each pair of neighboring wells. This produces a two-peak interference pattern, as illustrated in the simulated ballistic interference pattern of Fig. 2(c).
FIG. 2: Numerical simulations of three peak, washed out, and two peak interference patterns produced by imprinting phases on ground state of GP wave function in harmonic trap and $7.2E_R$ laser. The first row shows the phase along the longitudinal axis before expansion. The second row shows the density along the longitudinal axis after releasing the BEC and allowing it to expand for 8 ms. The third row shows a cross section of the density after expansion (indicated by the gray scale). Note the difference in the scale before and after expansions.

The three situations of Fig. 2 were simulated by painting phase patterns ‘by hand’ onto the ground state GP wave function in a $7.2E_R$ lattice and then allowing it to spatially expand by turning off all external potentials. The next section will show the condensate phase patterns obtained by a full time-dependent simulation of the actual experiment.

IV. FULL TIME-DEPENDENT GPE SIMULATION OF THE OTFYK EXPERIMENT

We have tested the assumption of adiabaticity by simulating a 200 ms laser turn-on in real time. In all cases the optical lattice was turned on starting with a numerically exact ground state condensate in the magnetic trap. The results of these tests, summarized in Fig. 3, are that a 200 ms switching time is nearly adiabatic for $U_f = 7.2E_R$, but not for $U_f = 40E_R$. Much longer times are needed for higher laser intensities not only because the laser is turned to higher intensity, but because the higher laser fields push more of the condensate into the outer wells; the required times for the condensate to tunnel through higher barriers to reach these outer wells are also longer.

As the lattice is raised, the value of the chemical potential varies from site to site, and atoms must flow from the trap center to the periphery in order to remain in equilibrium. For sufficiently deep lattices, the time needed to tunnel from site to site eventually exceeds the timescale of the ramp. The resulting non-adiabaticity for the $U_f = 40E_R$ case leads to significant deviations of both the density and phase profiles, compared with the true ground state. First, the density envelope is truncated, reflecting the inability of atoms to fully tunnel out to the cloud surface. Second, there is considerable ‘phase sag,’ illustrated in the second column of Fig. 3. This phase profile, which results from the axial velocities acquired by the atoms as they propagate ($v \propto \nabla \phi$), eventually becomes locked in for very deep lattices.

A simple estimate of the timescale required for adiabaticity is that it should at least exceed the inverse of the smallest collective mode frequency in the presence of the lattice. In deep lattices where the atomic profile in a given well is not much different from that of an ideal gas, the effective axial frequency shifts as $\tilde{\omega}_z = \omega_z \sqrt{m/m^*}$, where $m^*$ is the effective mass of the atom [60]. For a $40E_R$ lattice, $m^*/m \approx 900$ [60], which yields $2\pi/\tilde{\omega}_z \approx 600$ ms. It is reasonable to expect the full adiabatic ramp to require several times this, $t_R \sim 2$ s,
as is fully confirmed by the numerical results shown in Fig. 3. This value is an order of magnitude larger than that used in the experiment; since it is comparable to the lifetime of the BEC, such a long ramp is probably not experimentally feasible. An alternative protocol would have been to grow a coherent condensate ground state in the presence of the magnetic trap and optical lattice.

After turning the laser up to $U_f$ in 200 ms, the experimenters turn off the magnetic trap in 40 $\mu$s and hold the BEC in the vertically oriented laser for approximately $2.5 \text{ ms}$ in order to produce a $\pi$ offset between adjacent wells. The confinement of the laser is sufficient to prevent significant movement of the condensate during this time. However, the gradient of the gravitational potential between neighboring wells of the lattice causes dramatic Schrödinger phase evolution, since the condensate phase is given by $\theta = Vt/\hbar$, where $\Delta z = \lambda/2$ is the distance between the wells, after the condensate is held in the laser for a time $t_h$, there will be a phase difference between the condensates in two neighboring wells equal to $\Delta \theta = mg\Delta z/\hbar$. To achieve $\Delta \theta = \pi$, the hold time must be an odd multiple of $2\pi\hbar/mg\lambda = 0.557\text{ ms}$ for the parameters used in this experiment.

In our calculations, we follow this experimental procedure, using the exact hold time for $\Delta \theta = 5\pi$, $t_h = 2.785 \text{ ms}$, rather than the 2.5 ms quoted in OTFYK [61]. Simulations with $t_h = 2.5 \text{ ms}$ give an asymmetric density distribution after expansion, in which one peak is about twice as large as the other. This asymmetry is due to the asymmetry of the Fourier components of the wave function when the phase difference between the wells is not exactly $\pi$ [37].

A. Real Time Evolution for a Weak Laser

For a weak laser, the 200 ms turn-on is nearly adiabatic, but it is still important to check the results of the phase evolution and expansion of the actual state after the laser is turned on. The results of this calculation are shown in Fig. 4. These results are as expected in that there is approximately a $\pi$ phase difference between each neighboring well, and a clear two-peak interference pattern after expansion. Thus, although the simulated dynamics of the BEC in the weak laser are not as clean as the predictions of Fig. 2, the simulations confirm that the basic ideas of the discussion of Section III are correct in this case, and in agreement with the OTFYK observations.

B. Real Time Evolution for a Strong Laser

Fig. 5 illustrates the effect of ramping the lattice up to $40E_R$ in 200 ms. The resulting phase sag shown in the second column of Fig. 3 is repeated in Fig. 5(d). After holding the atoms in the laser for 2.785 ms, as shown in Fig. 4(d), the phase is so distorted that it begins to resemble the random pattern used in Fig. 2. In this context it is not surprising that the density profile after expansion, depicted in Fig. 4(e), is completely washed out. The loss of interference is driven entirely by non-adiabatic effect captured within a mean-field model. It is important to underline that these non-adiabatic effects are intrinsic to the ramp time, and are not affected by how the ramp is applied. We have performed simulations using a ramp with a smooth onset (based on a sine function) rather than the linear ramp discussed above, but the observed loss of interference was unchanged. We are thus able to qualitatively reproduce the loss of interference without invoking number squeezing.
We then calculate the absorption probability from the following equation (62):

\[ A(x, z) = 1 - \exp \left( -\sigma_0 \bar{n}(x, z) \right) \] (4)

where the absorption cross section \( \sigma_0 \) is given by:

\[ \sigma_0 = 6\pi \lambda^2 \] (5)

with \( \lambda = 780\text{nm}/2\pi \). We then smooth the data by taking a Gaussian convolution:

\[ \bar{A}(x, z) = \int dx' dz' A(x', z') e^{-((x-x')^2 + (z-z')^2)/w^2} \] (6)

where the \( 1/e \) width \( w = 17\mu\text{m} \) is chosen so that at very low laser strength \( (U_f = 5 - 8E_R) \) the ratio of the width of the interference peaks to their separation is \( \zeta = 0.22 \). This value of \( \zeta \) corresponds to the best experimental contrast reported in Ref. [38] (the parameter \( \zeta \) will be discussed further in Sec. VIII). The same method was used by OTFYK to analyze their experimental results, but they found that they needed a \( 1/e \) width of 25\( \mu\text{m} \), rather than 17\( \mu\text{m} \), to match their data [63].

Fig. 4 shows how the results of time-dependent numerical simulations compare with the experimental results. The three columns depict the raw numerical results for integrated density, the smoothed absorption probabilities, and the experimental results (copied with permission from the authors), respectively.

The numerical simulations can reproduce qualitatively the observed interference patterns for both weak and strong lasers. The flat phase profile after loading the atoms into a 7.2\( E_R \) lattice guarantees a clean interference pattern [53]. For a strong laser, the underlying mechanism for the loss of interference in our simulations (phase distortion due to non-adiabatic mean field effects) is entirely different from the mechanism proposed by the experimenters (number squeezing). A more quantitative analysis, given in Section VIII, reveals that the correspondence between simulation and experiment is not perfect, so it may be that number squeezing is in fact occurring in the experiment. However, the results of these simulations show that loss of interference is not in itself sufficient evidence of the presence of number squeezing.

### V. Restoring Interference

In the next phase of the experiment, instead of releasing the BEC after turning the laser up to 40\( E_R \), OTFYK first turn the laser down to 10\( E_R \) in 150 ms and then release the condensate after the short hold time. In the experiments the interference pattern, and by implication the coherence of the BEC, is restored by the adiabatic ramp-down. The results were originally explained in terms of the time-dependent two-mode model as the loss and return of coherence of the BEC. However, Fig. 6 illustrates that they can also be reproduced with numerical simulations of the GPE, and can therefore be explained in terms of mean-field effects. Indeed, the original interpretation of these experiments in terms of number squeezing has since been revised [52]. The dynamics are illustrated in Fig. 8 which shows the density and phase profiles after turning down the laser, before and after releasing the BEC. This figure shows that after turning the laser up and then down, the phase sag.
unwinds, so that at the end of the process, the site-to-site phase is relatively constant. There are variations in phase, but their size is on the order of \( \pi \), rather than 7\( \pi \). There is considerably more noise in the system after this process than there would have been if the laser were simply turned up to 10\( E_R \) without first going through the high barrier state, but this noise does not obscure the basic pattern.

### VI. RANDOM PHASE IMPRINTING

A further step, which was not done in the experiment, but which in principle could be done, is to imprint a random phase shift on each well when the laser strength is 40\( E_R \) and then turn the barrier back down. The two-mode model predicts that applying a random phase shift will destroy the ability of a mean-field state to heal back to a stationary (flat-phase) BEC state, but will have no effect on a strongly number-squeezed state. Since we have shown that the loss of interference is not sufficient to demonstrate number squeezing, it appears that random phase shifts could be used as an alternative test. If this is to be an effective test, applying a random phase shift should completely destroy the ability of the resulting BEC to produce a clean interference pattern.

We tested this idea numerically by running simulations similar to those described in the previous section, where we turned the laser up to 40\( E_R \) and then down to 10\( E_R \), but in this case we applied a random phase shift to each well before turning the laser down. The surprising result, illustrated in Fig. 9, is that the non-linear mean field dynamics ‘self-heals’ a truly random phase pattern just as it unwinds a mean-field induced phase sag: the interference...
FIG. 8: Real time evolution after turning laser up and then down. (a) Density profile along the longitudinal axis after turning laser up to $40E_R$ in 200 ms and then down to $10E_R$ in 150 ms. (b) Density profile along the longitudinal axis after turning off the magnetic trap holding the BEC in the laser (with gravity) for 2.785 ms. (c) Phase profile along the longitudinal axis after turning laser up to $40E_R$ in 200 ms and then down to $10E_R$ in 150 ms. (d) Phase profile along the longitudinal axis after turning off the magnetic trap holding the BEC in the laser (with gravity) for 2.785 ms. (e) Density profile along the longitudinal axis after releasing the BEC and allowing it to expand for 8 ms.

FIG. 9: Real time evolution after turning laser up, applying a random phase shift to each well, and then turning laser down. (a) Density profile along the longitudinal axis after laser is turned down. (b) Density profile along the longitudinal axis after turning off the magnetic trap holding the BEC in the laser (with gravity) for 2.785 ms. (c) Phase profile along the longitudinal axis after turning laser up to $40E_R$ in 200 ms and then down to $10E_R$ in 150 ms. (d) Phase profile along the longitudinal axis after turning off the magnetic trap holding the BEC in the laser (with gravity) for 2.785 ms. (e) Density profile along the longitudinal axis after releasing the BEC and allowing it to expand for 8 ms.

VII. PHASE OSCILLATIONS

An unexpected effect observed in the numerical simulations during the turn-on of the laser is a slow oscillation of the phase. The phase sag does not continue to grow, as has been seen in previous simulations using effective 1D models [47, 48], and which one might expect if the phase dynamics were due only to the mean field potential differences between the wells. Instead, as shown in Fig. 11, the phase oscillates, with the sag growing, then shrinking, then reversing.

These phase oscillations are the result of two non-adiabatic effects. First, if the lattice is ramped up too quickly, the local chemical potentials $\mu_{\text{loc}}$ in each well, defined by the expectation of the GPE operator, will not be identical. At the end of the ramp, the phase in each well will vary in time as $\phi_{\text{loc}} \sim \mu_{\text{loc}} t / \hbar$, causing
FIG. 10: Integrated density and absorption probability of expanded BEC after turning laser up, applying a random phase shift to each well, and then turning laser down.

FIG. 11: Phase accumulation, defined as phase difference along the longitudinal axis between $z = 6 \mu m$ and $z = 0 \mu m$ (after unwrapping), plotted as a function of time, as the laser is turned up to $U_f = 40E_R$ in 200 ms.

the overall phase profile to vary in time. The second, more important, source of the oscillations is the induction of transverse and longitudinal collective modes of the condensate. As the laser is turned up, the transverse confinement increases (see Fig. 1), and the BEC is pulled inward in the transverse direction and pushed outward in the longitudinal direction. This flow of superfluid gives rise to density oscillations along the longitudinal and radial axes, as illustrated in Fig. 12. As the lattice deepens, the frequency of the axial oscillations decreases because of the increasing effective mass \cite{52} and the time between classical turning points (where the phase is most flat) lengthens.

For a sufficiently deep lattice, the axial dipole mode period exceeds experimental timescales and the accumulated phases become effectively locked in. If the radial modes in each well all have the same frequency and are in phase, then the axial phase profile would be unaffected by their presence. In fact, for non-adiabatic ramps each disconnected well has a slightly different radial confinement frequency, so one would expect the longitudinal phase profile to change with time even for deep lattices. As discussed in the next section, these phase oscillations give rise to ‘collapses and revivals’ of the interference pattern which were not observed in the OTFYK experiments.

VIII. ZETA AND VISIBILITY

For more quantitative comparisons with experiment, it is useful to calculate the quantities used by OTFYK to compare their number squeezing model, their effective one dimensional GP model, and their data, namely \(\zeta\) and visibility \cite{53,54}. \(\zeta\) is defined as the ratio of the width of a single peak to the distance between the peaks and \(\zeta_0 = 0.22\) is the value of \(\zeta\) for \(U_f = 6E_R\). To determine \(\zeta\), we fit the cross section of the smoothed absorption probability through the longitudinal axis \(z\), \(A(0, z)\), to a double Gaussian:

\[
Be^{-(z-z_1)^2/2\sigma^2} + Ce^{-(z-z_2)^2/2\sigma^2}
\]

(7)
Small Gaussian fits (solid lines) for a range of laser strengths. The fit shown for 40\(E_R\) is the worst fit in the data set.

and then \(\zeta\) is the ratio of the width of the Gaussians to the distance between their centers:

\[
\zeta = \frac{\sigma}{(z_1 - z_2)}
\]

and \(\zeta_0\) is the value of \(\zeta\) for \(U_f = 6E_R\). Fig. 13 shows a sample of smoothed absorption cross sections and double Gaussian fits for a range of laser strengths. Visibility is defined as the difference between the average of the maxima of the two peaks and the minimum between the peaks, divided by their sum.

In a further analysis of the OTFYK experiment, Tuchman plots \(\zeta\) and visibility as a function of \(Ng\beta/\gamma\), where \(N\) is the number of particles in two wells, \(g\) is defined as in Eq. 1, and \(\beta\) and \(\gamma\) are defined by the following integrals over localized wave functions:

\[
\beta \equiv \int d^3r \psi_1^2(r)
\]

\[
\gamma \equiv \int d^3r \psi_1(r)\{ -\frac{\hbar^2}{2m} \nabla^2 + V^{ext}(r) \} \psi_2(r)
\]

Unlike \(\zeta\) and visibility, which are determined by fits to experimental data, the parameter \(Ng\beta/\gamma\) is derived from a two-mode model in which there are two fixed wave functions, \(\psi_1\) and \(\psi_2\), in each of two potential wells in the optical lattice. This parameter is essentially a measure of laser strength and density, and it is approximately exponential in laser strength. Our own calculations show that this factor varies somewhat depending on the details of the theoretical model used to determine it. Therefore, we prefer to plot \(\zeta\) and visibility versus laser strength \(U_f\), an experimentally determined parameter, rather than versus \(Ng\beta/\gamma\), which is based on particular theoretical model.

According to the numbers given in Ref. [38], a range of laser strengths from 6\(E_R\) to 50\(E_R\) corresponds approximately to a range of \(Ng\beta/\gamma\) from \(10^{1/2}\) to \(10^5\).

Fig. 14 shows \(\zeta\) and visibility for our simulations as a function of \(U_f\) (laser strength upon release). Each point corresponds to a simulation in which the laser strength is raised to \(U_f\) in 200 ms, the magnetic trap is turned off in 40 \(\mu\)s, the BEC is held in the laser for 2.785 ms, the laser is turned off and the BEC is allowed to expand for 8 ms. For each point, \(\zeta\) and visibility are calculated from a cross section of the smoothed absorption probability discussed in Sec. IV.C.

Perhaps the most striking aspect of the numerical results is that the values of both \(\zeta\) and visibility do not merely increase or decrease as a function of \(U_f\), but oscillate. These oscillations are due to the excitation of collective modes as discussed in the previous section, and do not appear in the experimental data or in the models employed in Refs. [38, 54]. It is possible that the oscillations present in the GPE simulations would be strongly damped in actual experiments, with the high radial energies being transferred to high-lying axial modes. When atoms are loaded into blue-detuned lattices, where the transverse confinement due to the external magnetic trap is weak compared to that of red-detuned lattices, considerable radial heating has been observed [40], leading to loss of interference contrast [41].

The observation of phase oscillations in numerical simulations leads to predictions that would be interesting to test experimentally. If the BEC were released when there was a peak in the amplitude of the phase oscillations, the interference pattern could be lost for a relatively low barrier height. If one waited a little longer to release the BEC until the phase flattened out again, the interference pattern would return for a few oscillations until disappearing due to damping. Note that these ‘collapses and revivals’ are completely driven by mean-field effects, and are unrelated to similar phenomena found.
FIG. 14: $(\zeta^2 - \zeta_0^2)^{1/2}$ and visibility versus $Ng\beta/\gamma$ and laser strength.

IX. CONCLUSIONS

We have shown that mean-field effects, as modeled by the three-dimensional time-dependent GPE, can explain both the loss and return of interference for a BEC in a one-dimensional optical lattice. The simulations yield behavior that is qualitatively similar to that observed of the OTFYK experiments [38] without the need to invoke physics beyond mean-field theory, such as number squeezing or condensate fragmentation. The central result of the present work is that ensuring adiabaticity during the loading of a BEC into a deep optical lattice is experimentally difficult to achieve, and that neglecting the rather large effects of mean-field excitations will lead to an incomplete description of future experiments.

The results of GPE simulations differ from the experimental data in a few small respects, however. The loss of contrast in the interference patterns, after dropping a deep optical lattice and allowing the cloud to expand, is not quite as pronounced as in the experiments. One explanation for the small difference is likely to be the presence of number squeezing, which is not captured by the GPE. Another possibility is that the radial excitations that are induced by the lattice ramp will rapidly damp into high-lying axial excitations in real experiments (the GPE has no damping mechanism), leading to heating and its attendant loss of contrast. These collective modes lead to phase oscillations that in turn yield periodic variations in the fringe contrast; though these ‘collapses and revivals’ were not seen in the original OTFYK experiments, similar oscillations attributed to quantum fluctuations have been observed more recently by the members of the same group [54]. Because the creation and destruction of interference patterns are widely used techniques to measure the presence of coherence and its loss, it is important to understand all the mechanisms that can affect this important experimental measure.

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APPENDIX A: NUMERICAL METHODS

The numerical simulation of the full three-dimensional time-dependent Gross-Pitaevskii Equation (GPE) is performed in Cartesian coordinates using a C code adapted from earlier work in the Reinhardt group. The time integration uses the variable step fourth-fifth order Runge-Kutta integrator odeint from Numerical Recipes in C. The spatial integration uses a pseudospectral method with fast Fourier transforms from the fftw library. The basic idea behind the pseudospectral method is that the wave function is expanded in terms of coordinate discretized trigonometric functions, reducing a partial differential equation into a set of coupled ordinary differential equations via fast Fourier transforms to coefficient basis. We have adapted the code using Type II Fourier transforms, which are appropriate to the boundary conditions of half of a symmetric box, to take advantage of the symmetry of the problem and reduce the analysis to one quadrant of the system. This adaptation increases the speed of the calculations by a factor of 8. In theory, since the system of interest is cylindrically symmetric, further improvement in speed could be achieved by using cylindrical coordinates and thus effectively reducing the problem two dimensions. In practice, the speed of the fast Fourier transforms appropriate to Cartesian coordinates eliminate the disadvantage of working in 3D and the 3D Cartesian code runs significantly faster than a 2D cylindrical coordinate code using the discrete variable representation method rather than the pseudospectral method.

For the results shown in this paper, we use 24.86 grid points per micron in the longitudinal direction (10.44 grid points per site) and 1.09 grid points per micron in the transverse directions. During the expansion of the BEC, we reduce the number of grid points per unit length in the longitudinal direction by a factor of 2 during the first 4 ms, and then by an additional factor of 2 during the next 4 ms. We have done sample runs with up to twice as many longitudinal grid points and four times as many grid points in each transverse direction and checked that this does not change the results. Many more grid points are needed in the longitudinal direction than in the transverse direction because of there is much more variation due to the laser, which has a wavelength of 0.84μm.

The simulations were done on a computer with four 3 GHz Xeon processors and 2 Gb of memory running Red Hat Linux. On this machine, using the Intel C compiler, the computations of the BEC expansion take about 4 hours using the minimum necessary number of grid points and the 200 ms laser turn-on computations take about 40-60 hours. (The code runs about 1.5 times faster when compiled with the Intel C compiler than when compiled with gcc.)

[1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science 269, 198 (1995).
[2] C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, Phys. Rev. Lett. 75, 1687 (1995), ibid. 79, 1170 (1997).
[3] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. 75, 3969 (1995).
[4] P. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 71, 463 (1999).
[5] A. J. Leggett, Rev. Mod. Phys. 73, 307 (2001).
[6] C. J. Pethick and H. Smith, Bose-Einstein Condensation in Dilute Gases (Cambridge University Press, 2002).
[7] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, C. G. Townsend, and W. Ketterle, Phys. Rev. Lett. 77, 988 (1996).
[8] D. S. Jin, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 77, 420 (1996).
[9] D. M. Stamper-Kurn, H.-J. Miesner, S. Inouye, M. R. Andrews, and W. Ketterle, Phys. Rev. Lett. 81, 500 (1998).
[10] H.-J. Miesner, D. M. Stamper-Kurn, J. Stenger, S. Inouye, A. P. Chikkatur, and W. Ketterle, Phys. Rev. Lett. 82, 2228 (1999).
[11] M. R. Matthews, B. P. Anderson, P. C. Haljan, D. S. Hall, M. J. Holland, J. E. Williams, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 83, 3358 (1999).
[12] M. R. Andrews, C. G. Townsend, H.-J. Miesner, D. S. Durfee, D. M. Kurn, and W. Ketterle, Science 275, 637 (1997).
[13] A. Röhr, M. Naraschewski, A. Schenzle, and H. Wallis, Phys. Rev. Lett. 78, 4143 (1997).
[14] M. R. Matthews, B. P. Anderson, P. C. Haljan, D. S. Hall, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 83, 2498 (1999).
[15] K. W. Madison, F. Chevy, W. Wohlleben, and J. Dalibard, Phys. Rev. Lett. 84, 806 (2000).
[16] J. R. Abo-Shaeer, C. Raman, J. M. Vogels, and W. Ketterle, Science 292, 476 (2001).
[17] S. Burger, K. Bongs, S. Dettmer, W. Ertmer, K. Sengstock, A. Sanpera, G. V. Shlyapnikov, and M. Lewenstein, Phys. Rev. Lett. 83, 5198 (1999).
[18] J. Denschlag, J. E. Simsarian, D. L. Feder, C. W. Clark, L. A. Collins, J. Cubizolles, L. Deng, E. W. Hagley, K. Helmerson, W. P. Reinhardt, et al., Science 287, 97 (2000).
[19] D. S. Jin, M. R. Matthews, J. R. Ensher, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. 78, 764 (1997).
[20] O. Maragò, G. Hechenblaikner, E. Hodby, and C. Foot, Phys. Rev. Lett. 86, 3938 (2001).
[21] S. A. Morgan, M. Rusch, D. A. W. Hutchinson, and K. Burnett, Phys. Rev. Lett. 91, 250403 (2003).
[22] B. Jackson and E. Zaremba, Phys. Rev. Lett. 88, 180402 (2002).
[23] R. Wynar, R. S. Freeland, D. J. Han, C. Ryu, and D. J. Heinzen, Science 287, 1016 (2000).
[24] C. McKenzie, J. H. Denschlag, H. Haffner, A. Browaeys, L. E. de Araujo, F. K. Fatemi, K. M. Jones, J. E. Simsarian, D. Cho, A. Simoni, et al., Phys. Rev. Lett. 88, 120403 (2002).
[25] M. Greiner, C. A. Regal, and D. S. Jin, Nature 426, 537 (2003).
[26] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, S. Riedl, C. Chin, J. H. Denschlag, and R. Grimm, Science 302, 2101 (2003).
[27] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, S. Gupta, Z. Hadzibabic, and W. Ketterle, Phys. Rev. Lett. 91, 250401 (2003).
[28] C. A. Regal, M. Greiner, and D. S. Jin, Phys. Rev. Lett. 92, 040403 (2004).
[29] M. Bartenstein, A. Altmeyer, S. Riedl, S. Jochim, C. Chin, J. H. Denschlag, and R. Grimm, Phys. Rev. Lett. 92, 120401 (2004).
[30] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, A. J. Kerman, and W. Ketterle, Phys. Rev. Lett. 92, 120403 (2004).
[31] H. Moritz, T. Stöferle, M. Köhl, and T. Esslinger, Phys. Rev. Lett. 91, 250402 (2003).
[32] B. L. Tolra, K. M. O'Hara, J. H. Huckans, W. D. Phillips, S. L. Rolston, and J. V. Porto, Phys. Rev. Lett. 92, 190401 (2004).
[33] T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger, Phys. Rev. Lett. 92, 130403 (2004).
[34] N. K. Wilkin and J. M. F. Gunn, Phys. Rev. Lett. 84, 6 (2000).
[35] B. Paredes, P. Fedichev, J. I. Cirac, and P. Zoller, Phys. Rev. Lett. 87, 010402 (2001).
[36] D. Jaksch and P. Zoller, New J. Phys. 5, 56 (2003).
[37] B. P. Anderson and M. A. Kasevich, Science 282, 1686 (1998).
[38] C. Orzel, A. K. Tuchman, M. L. Fenselau, M. Yasuda, and M. A. Kasevich, Science 291, 2386 (2001).
[39] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, Nature 415, 39 (2002).
[40] B. Paredes, A. Widera, V. Murg, O. Mandel, S. Fölling, J. I. Cirac, G. V. Shlyapnikov, T. W. Hänsch, and I. Bloch, Nature 429, 277 (2004).
[41] C. D. Fertig, K. M. O’Hara, J. H. Huckans, S. L. Rolston, W. D. Phillips, and J. V. Porto, Phys. Rev. Lett. 94, 120403 (2005).
[42] K. Xu, Y. Liu, J. Abo-Shaeer, T. Mukaiyama, J. Chin, D. Miller, W. Ketterle, K. M. Jones, and E. Tiesinga, e-print:cond-mat/0507288 (2005).
[43] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B 40, 546 (1989).
[44] Z. Hadzibabic, S. Stock, B. Battelier, V. Bretin, and J. Dalibard, Phys. Rev. Lett. 93, 180403 (2004).
[45] O. Morsch, J. H. Müller, D. Ciampini, M. Cristiani, P. B. Blakie, C. J. Williams, P. S. Julienne, and E. Arimondo, Phys. Rev. A 67, 031603(R) (2003).
[46] J. Zakrewski, Phys. Rev. A 71, 043601 (2005).
[47] S. E. Sklarz, I. Friedler, D. J. Tannor, Y. B. Band, and C. J. Williams, Phys. Rev. A 66, 053620 (2002).
[48] Y. B. Band and M. Trippenbach, Phys. Rev. A 65, 053602 (2002).
[49] J. Plata, Phys. Rev. A 69, 033604 (2004).
[50] L. Isella and J. Ruostekoski, Phys. Rev. A 72, 011601(R) (2005).
[51] Y. B. Band, I. Towers, and B. A. Malomed, Phys. Rev. A 67, 023602 (2003).
[52] S. McKinney (now McKagan), Ph.D. thesis, University of Washington (2004).
[53] A. K. Tuchman, Ph.D. thesis, Yale University (2004).
[54] A. K. Tuchman, C. Orzel, A. Polkovnikov, and M. A. Kasevich, e-print:cond-mat/0504762 (2005).
[55] M. L. Chiofalo and M. P. Tosi, Phys. Lett. A 268, 406 (2000).
[56] E. G. M. van Kempen, S. J. J. M. F. Kokkelmans, D. J. Heinzen, and B. J. Verhaar, Phys. Rev. Lett. 88, 093201 (2002).
[57] M. P. Bradley, J. V. Porto, S. Rainville, J. K. Thompson, and D. E. Fritsch, Phys. Rev. Lett. 83, 4510 (1999).
[58] The experiment also involved some runs in which the laser was turned up quickly, but these will not be discussed.
[59] P. Pedri, L. Pitaevskii, S. Stringari, C. Fort, S. Burger, F. S. Cataliotti, P. Maddaloni, F. Minardi, and M. Inguscio, Phys. Rev. Lett. 87, 220401 (2001).
[60] M. Krämer, L. Pitaevskii, and S. Stringari, Phys. Rev. Lett. 88, 180402 (2004).
[61] M. Kasevich, private communication, has confirmed that the 2.5 ms hold time quoted in the OTFYK paper was only an approximate value; the actual time was chosen to yield the most symmetric two-peak density distribution.
[62] W. Ketterle, D. S. Durfee, and D. M. Stamper-Kurn, in Proceedings of the International School of Physics - Enrico Fermi, edited by M. Inguscio, S. Stringari, and C. E. Wieman (IOS Press, 1999), p. 67.
[63] A. K. Tuchman, Private Communication.
[64] M. Greiner, O. Mandel, T. W. Hänsch, and I. Bloch, Nature 419, 51 (2002).
[65] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, Numerical Recipes in C (Cambridge University Press, 1992).
[66] B. Forseberg, A Practical Guide to Pseudospectral Methods (Cambridge University Press, 1996).
[67] The fftw library is available for free download from www.fftw.org. The specific transform routines we use are FFTW_RODFT00, FFTW_RODFT01, and FFTW_RODFT10.