Mean-field treatment of the damping of the oscillations of a one-dimensional Bose gas in an optical lattice

Julio Gea-Banacloche,[1,*] Ana María Rey,[2,3] Guido Pupillo,[2,4] Carl J. Williams,[2] and Charles W. Clark[2]
[1]*Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA*
[2]*National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA*
[3]*ITAMP, Harvard-Smithsonian Center of Astrophysics, Cambridge, Massachusetts 02138, USA*
[4]*IQOQI of the Austrian Academy of Sciences, 6020 Innsbruck, Austria*
(Received 15 November 2004; published 9 January 2006)

We present a theoretical treatment of the surprisingly large damping observed recently in one-dimensional Bose-Einstein atomic condensates in optical lattices. We show that time-dependent Hartree-Fock-Bogoliubov (HFB) calculations can describe qualitatively the main features of the damping observed over a range of lattice depths. We also derive a formula of the fluctuation-dissipation type for the damping, based on a picture in which the coherent motion of the condensate atoms is disrupted as they try to flow through the random local potential created by the irregular motion of noncondensate atoms. When parameters for the characteristic strength and correlation times of the fluctuations, obtained from the HFB calculations, are substituted in the damping formula, we find very good agreement with the experimentally observed damping, as long as the lattice is shallow enough for the fraction of atoms in the Mott insulator phase to be negligible. We also include, for completeness, the results of other calculations based on the Gutzwiller ansatz, which appear to work better for the deeper lattices.

DOI: 10.1103/PhysRevA.73.013605 PACS number(s): 03.75.Kk, 03.75.Lm

I. INTRODUCTION

The transport properties of atomic Bose-Einstein condensates have recently been the subject of much interest. In a pure harmonic trap, the dipole mode of the motion—where the cloud of atoms oscillates back and forth without altering its shape—is known to be stable. On the other hand, if an optical lattice is used to create a one-dimensional array of potential wells and barriers, one may find, even in a single-particle picture, a damping of the oscillations due to the nonquadratic nature of the resulting dispersion relation [1–6]. When interactions between atoms are included, at the mean-field level, one finds dynamical instabilities [7] that may result in a very large damping [8,9]. All these effects are, however, only expected to be substantial when the quasimomentum of the cloud of atoms is sufficiently large (typically, of the order of $\pi\hbar/\lambda$, where $\lambda/2$ is the lattice spacing).

In recent experiments with ^{87}Rb atoms [10,11], confined to move in one-dimensional "tubes," a surprisingly large damping of the dipole mode was observed, for very weak optical lattices and very small cloud displacements. We note that no (or very little) damping was observed for the same system in the absence of the tight transverse confinement [12,13]. In the experiments [10], the oscillation frequency in the harmonic trap $\omega_0/2\pi$ was about 60 Hz, whereas the photon recoil energy $E_R=h^2/(2m\lambda^2)$ corresponded to a frequency $E_R/h=3.47$ kHz. Under these conditions, for a shallow lattice, the maximum displacement of the condensate in the experiment (7 to 8 lattice sites) should not result in a momentum larger than about $0.1(\pi\hbar/\lambda)$, which is well within the quadratic part of the lattice dispersion curve. Likewise, the quasimomentum spread arising from the finite size of the cloud itself was also quite small (of the order of $2\pi\hbar/13\lambda$, since the Thomas-Fermi radius of the cloud is about 13λ).

Since these results were first presented (and, in some cases, predating them), a number of theoretical treatments have been put forward that, directly or indirectly, address various relevant aspects of the underlying dynamics, from different perspectives. It has been shown, for instance [14–16], that the momentum cutoff for the dynamical instability may be substantially lowered for commensurate lattices, and, probably more relevant for the experimental situation, that the boundary between regular and irregular motion becomes "smeared out" due to quantum fluctuations. Numerical calculations based on a truncated Wigner representation [17] have also shown that the fraction of atoms with momenta in the unstable region can indeed cause damping of the center of mass motion of the whole system. As we shall show below, this fraction is, in fact, a non-negligible number, for the experimental parameters, even for relatively shallow lattices, because of the large depletion caused by the very tight transverse confinement.

In a recent series of papers [6,18], several of us have characterized the damping mechanisms that may dominate, for these systems, in different parameter ranges. Perhaps the most important conclusion of these papers is that the very deep lattices (lattice potential V larger than about $5E_R$) can be described very well by an extended fermionization model, in which most atoms localize in a Mott-insulator state with unit filling of the lattice, and the remaining atoms are free to move above the Mott state with a renormalized kinetic energy. Both the atoms in the Mott state and the remaining atoms are treated as effective noninteracting fermions whose

*Email address: jgeabana@uark.edu

dynamics are governed by a combination of the trap potential and appropriate kinetic energy terms. These references also show, however, that there is a region of values of the ratio of interaction energy to kinetic energy (referred to as the "intermediate region" in [6]) where the single-particle models, whether bosonic or fermonic, are inadequate to describe the dynamics of the Bose-Hubbard model, which is the main underlying theoretical tool for most of the studies described above. This intermediate region, in the experiments of [10], covers all the lattices studied with V smaller than about $5E_R$, although there is some concern that for the shallowest lattices the tight-binding approximation leading to the Bose-Hubbard model itself may not be entirely accurate.

The present paper is an attempt to fill in this gap by presenting mean-field-based calculations for the Bose-Hubbard dynamics in the "intermediate region" where the fraction of atoms having undergone the transition to the Mott insulator state is still negligible, and the system is mostly superfluid, yet the interaction energy cannot be neglected. Our main calculational tool is time-dependent Hartree-Fock-Bogoliubov (HFB) theory, and we show that this approach does indeed reproduce qualitatively many of the features of the damping observed in the experiments, although it generally underestimates its magnitude for any given lattice depth. We also report the results of calculations based on the Gutzwiller ansatz, which fail to show any damping for the shallower lattices but do so for depths greater than about $3E_R$.

An important feature common to both calculations is that they show fairly large, and seemingly random, fluctuations in the particle density difference for neighboring sites. Furthermore, in the Gutzwiller ansatz calculation, this randomness is clearly tied to the damping of the center of mass motion (see Fig. 5 below). Since the site-to-site distance is $\lambda/2$, spatial fluctuations on this scale are clearly associated with large quasimomentum components, and hence, at least initially, with the dynamics of the noncondensate fraction (since, as argued above, the momentum of the condensate in these experiments should always be much smaller than π/λ). This has motivated us to develop a phenomenological model for the damping in which these site-to-site density fluctuations are treated as providing, through the interaction term, an effective "external" random potential for the motion of the whole cloud. This approach yields a formula for the damping which exhibits good agreement with the experimental data when parameters for the characteristic strength and correlation times of the fluctuations, obtained from the HFB calculations, are substituted in it.

Our HFB calculations also show that the motion of the center of mass of the noncondensate fraction is typically more strongly damped than the condensate. This noncondensate damping is consistent with the results of single-particle models based on Fermi statistics [1,6]. The results of [6], in particular, show this damping to be related to the overlap of the displaced cloud with localized eigenstates of the combined quadratic and periodic potentials. (Such localized eigenstates, when expressed in terms of Bloch waves, naturally involve states of high momentum.) Note also that a damping of the center of mass motion of a system of noninteracting particles is also consistent with the notion that their individual dynamics are irregular (i.e., chaotic or quasichaotic), since in that case their contributions to the center of mass position get out of step over time, and eventually average to zero [19]. Although in our "intermediate" regime it is probably not warranted to treat the noncondensate atoms as noninteracting fermions, the results quoted above strongly suggest that irregular dynamics will be obtained generically for any atomic gas in a combination of periodic and quadratic potentials when sufficiently high-momentum states are involved, regardless of whether it is a condensate or not. What we envision, then, as characteristic of this regime is a situation in which a non-negligible fraction of the (noncondensate) atoms undergoes this randomlike motion, and eventually causes, through the interaction term, a breaking up of the regular motion of the entire cloud.

The layout of the paper is as follows. In Sec. II we present the results of quantum Monte-Carlo ground-state calculations that establish the existence, for the experimental parameters, of a large noncondensate fraction that arises as a direct consequence of the enhanced effective on-site interaction (due to the tight transverse confinement); we also show a non-negligible occupation of high-momentum states. In Sec. III the "effective external potential" treatment of the interaction term is developed, leading to our phenomenological damping formula. Section IV then presents the results of Hartree-Fock-Bogoliubov calculations, which we use to estimate the parameters appearing in the damping formula. Results from calculations based on the Gutzwiller ansatz are presented in Sec. V. Finally, Sec. VI is devoted to further discussions and conclusions.

II. HAMILTONIAN AND STATIC (GROUND-STATE) RESULTS

The starting point for our theoretical treatment is a Hamiltonian of the "tight binding" or Bose-Hubbard form [20],

$$\hat{H} = -J\sum_{\langle j,i\rangle} \hat{a}_j^\dagger \hat{a}_i + \Omega\sum_j j^2 \hat{n}_j + \frac{U}{2}\sum_j \hat{n}_j(\hat{n}_j - 1). \qquad (1)$$

In this expression, the sum $\langle i,j\rangle$ is taken over nearest neighbors, $\hat{a}_j$ ($\hat{a}_j^\dagger$) are bosonic field operators that annihilate (create) an atom at the lattice site j, $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$, and $\Omega = m\tilde{\omega}_0^2\lambda^2/(8E_R)$ characterizes the strength of the harmonic trap. The on-site interaction energy is

$$U = \frac{2a\hbar}{\sqrt{2\pi}E_R}\left(\frac{\tilde{\omega}_x\tilde{\omega}_y\tilde{\omega}_z}{a_x a_y a_z}\right)^{1/3}, \qquad (2)$$

where $\tilde{\omega}_{x,y,z}$ are the oscillation frequencies at individual lattice sites along the three axes, obtained with a harmonic approximation expanding around the minima of the potential wells, $a_{x,y,z} = \sqrt{\hbar/m\tilde{\omega}_{x,y,z}}$ are the effective harmonic oscillator lengths and $a = 5.31\times 10^{-9}$ m is the s-wave scattering length. For the experiment $\tilde{\omega}_x/2\pi = \tilde{\omega}_y/2\pi = 35$ kHz and $\tilde{\omega}_z = \sqrt{4E_R^2 s}/\hbar$, where s is the longitudinal periodic potential strength in units of the recoil energy, $s = V/E_R$. Recalling that the recoil energy is only of the order of 3.47 kHz$\times 2\pi\hbar$, and that, for the cases considered here, $s < 6$, it is easy to see that

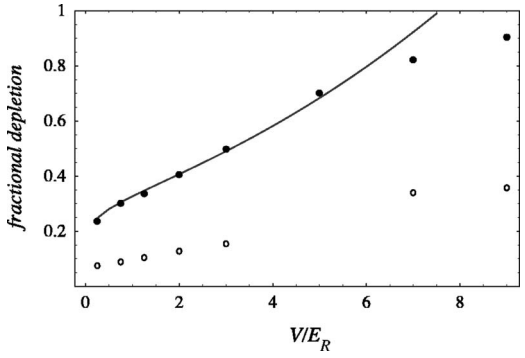

FIG. 1. Black dots: fractional quantum depletion ($\tilde{n}/n=1-n_c/n$) vs lattice depth V. Open circles: the fraction of $\tilde{n}$ with momenta $>\pi\hbar/\lambda$. Solid line: Eq. (4) with $n=2.2$ (approximate atom density in the experiment at the center of the trap) and $\alpha=0.37$ (best fit).

the transverse confinement is much stronger than the longitudinal one and the system is effectively one-dimensional. Alternatively, the "hopping" energy J, which is defined in the usual way as

$$J=-\int w_0^*(x)H_0w_0(x+\lambda/2)dx \tag{3}$$

(where w_0 are the first-band Wannier functions, H_0 is the lattice Hamiltonian, and $\lambda/2$ is the lattice constant) is extremely small in the transverse directions because of the exponentially small overlap of the corresponding Wannier functions.

The definition (2) above implies that the parameters U, J, and Ω in (1) are understood to be in units of E_R. The summation indices in Eq. (1) range from $-M/2$ to $M/2$, where $M+1$ is the total number of wells (100–200 in our numerical calculations), and $j=0$ at the center of the trap.

We have used a numerical quantum Monte-Carlo [21] method to derive the single-particle density matrix for the Hamiltonian (1) at very low temperature (0.01 J, in our calculations), for a total number of atoms $N=80$. The latter is the estimated number of atoms in the central tube of the experiment of Ref. [10]. We point out that the computation of average properties by this method for systems' sizes comparable to the experimental ones is typically unfeasible in dimensions larger than one. From the computed density matrix we obtain the quantum depletion shown in Fig. 1. The curve is a fit to the formula

$$1-\frac{n_c}{n}=\alpha\sqrt{\frac{U}{nJ}} \tag{4}$$

which gives the depletion in the homogeneous case (that is, in the absence of the harmonic trap, $\Omega=0$). n_c is the density of condensate atoms, n the total density, and α a parameter that can be calculated from the Bogoliubov spectrum of excitations [22,23]. To be precise, for a homogeneous condensate in a lattice, the usual Bogoliubov analysis yields, in D dimensions and with M lattice sites, a formula like (4) with a constant α given by

$$\alpha=\frac{1}{M}\frac{1}{4\sqrt{2}}\sum_{\mathbf{q}\neq 0}\left[\sum_{i=1}^{D}\sin^2\left(\frac{q_i\pi}{M}\right)\right]^{-1/2}. \tag{5}$$

Here, the numbers q_i give the quasimomentum of the excitations. In the continuous limit, the expression (5) diverges in one dimension, in accordance with the Mermin-Wagner-Hohenberg theorem that establishes that one cannot have a totally homogeneous (translationally invariant) condensate in one dimension; however, for a bounded system the sum (5) always yields a finite value for $D=1$, although, in general, a much larger one than in the two- or three-dimensional case. This is, qualitatively speaking, the main reason why one finds a much larger depletion in these one-dimensional "tubes" than in two- or three-dimensional geometries at comparable densities.

Since, in the harmonic trap potential, the spectrum of excitations is modified and n is not uniform, α in Fig. 1 has been treated as an adjustable parameter. We find that, even for very shallow lattices, some 20–40% of the atoms are not part of the condensate. The figure also shows (open circles) the fraction of these noncondensed atoms that have quasimomenta greater than $\hbar\pi/\lambda$ (also calculated from the numerical single-particle density matrix).

We note Eq. (4) was derived under the tight-binding approximation which assumes that atoms only populate at the lowest vibrational level of each lattice site and neglects tunneling to next-to-nearest-neighbors sites. These assumptions become invalid in the limit $s\to 0$ and therefore Eq. (4) becomes questionable for the very shallow lattices. Nevertheless, recent studies done in Ref. [17] for shallow lattices using parameters appropriate to the experiments of Ref. [10] have shown that for $s>0.25$ most of the atoms still remain in the first band. This observation together with the fact that tunneling to next-nearest neighbor sites only introduces corrections to the value of α, indicate that Eq. (4) can account for the correct physics for $s>0.25$. Moreover the model to be developed in Sec. III below can be generalized to include corrections due to next-nearest-neighbor couplings if necessary.

For the $s=0$ case (no lattice) the noncondensate population is no longer a relevant quantity for the dipole dynamics. In fact, according to the generalized Kohn theorem [24] the dipole oscillations of a harmonically confined gas are always undamped independently of the temperature, dimensionality, quantum statistics, and interaction effects.

In other studies, we have observed that the Mott insulator begins to form around $V=3E_R$ in this system, as characterized by a small decrease in the density fluctuations around the center of the trap that first becomes visible at this point. Nonetheless, Fig. 1 shows that the Bogoliubov result (4) for $\tilde{n}$ remains approximately valid until around $V=5E_R$, which inspires some confidence that the mean-field analysis that follows may be at least semiquantitatively valid even for those very highly depleted systems.

III. A DAMPING MODEL

In some recent work, one of us [25] has developed a formalism to describe the effect on matter waves of

coherence-breaking processes such as random "localizing" events, momentum kicks, or perturbation by (time-dependent) random external potentials. All these processes can be shown to lead to a damping of the center of mass motion of the system.

Given the relatively large fraction of atoms, calculated in the previous section, with quasimomenta large enough to cause local density fluctuations on a scale of one or two lattice sites, it seems natural to consider these density fluctuations (whose existence, in the relevant parameter regime, will be established by the numerical HFB and Gutzwiller calculations in the next couple of sections) as providing a sort of random potential for the atomic cloud to flow through, and to expect the damping to arise as a consequence of this. The goal of this section is to make this picture plausible and quantitative, first by rederiving the damping due to an external random potential, then by showing how the Heisenberg equations of motion derived from the Hamiltonian (1) can be cast into a similar form through a standard factorization ansatz, and, finally, deriving from all of this a damping formula.

In our tight-binding model, the center of mass position operator is

$$\hat{x}_{cm} = \frac{\lambda}{2N}\sum_j j\hat{n}_j. \tag{6}$$

The commutator of $\hat{x}_{cm}$ with the Hamiltonian (1) yields a center of mass velocity operator

$$\hat{v} = -\frac{iJ\lambda}{2N\hbar}\sum_j (\hat{a}_j^\dagger \hat{a}_{j+1} - \hat{a}_{j+1}^\dagger \hat{a}_j), \tag{7}$$

which is essentially the same as the current operator in [23]. A further commutation yields the time derivative of $\hat{a}_j^\dagger \hat{a}_{j+1}$:

$$i\hbar\frac{d}{dt}\hat{a}_j^\dagger \hat{a}_{j+1} = (2j+1)\Omega \hat{a}_j^\dagger \hat{a}_{j+1} + U\hat{a}_j^\dagger(\hat{n}_{j+1} - \hat{n}_j)\hat{a}_{j+1} + J(\hat{a}_{j-1}^\dagger \hat{a}_{j+1} - \hat{a}_j^\dagger \hat{a}_{j+2} + \hat{n}_{j+1} - \hat{n}_j) \tag{8}$$

with an analogous result for the derivative of $\hat{a}_{j+1}^\dagger \hat{a}_j$. In the "intermediate region" in which we are interested here, where the evolution of the system is not adequately described by single-particle models (bosonic or pseudofermionic), we expect the overall damping to arise from the interaction term (proportional to U) in (8).

Before we get to work on that term, however, consider what would happen if one were to replace it in (1) by a random external potential, proportional to $\Sigma V_j \hat{n}_j$. Equations (6) and (7) would be unchanged, whereas Eq. (8) would become

$$i\hbar\frac{d}{dt}\hat{a}_j^\dagger \hat{a}_{j+1} = (2j+1)\Omega \hat{a}_j^\dagger \hat{a}_{j+1} + (V_{j+1} - V_j)\hat{a}_j^\dagger \hat{a}_{j+1} + J(\hat{a}_{j-1}^\dagger \hat{a}_{j+1} - \hat{a}_j^\dagger \hat{a}_{j+2} + \hat{n}_{j+1} - \hat{n}_j). \tag{9}$$

Now consider formally taking the ordinary quantum-mechanical expectation value of Eq. (9) and integrating it over an interval $(t-\Delta t, t)$, to get

$$\langle \hat{a}_j^\dagger \hat{a}_{j+1}(t)\rangle = \langle \hat{a}_j^\dagger \hat{a}_{j+1}(t-\Delta t)\rangle - \frac{i}{\hbar}\int_{t-\Delta t}^{t} (V_{j+1} - V_j)(t') \times \langle \hat{a}_j^\dagger \hat{a}_{j+1}(t')\rangle dt' + \cdots, \tag{10}$$

where $\cdots$ represents terms that do not contain V_j's. Substituting (10) back into the (expectation value of the) second term on the right-hand side of (9), one obtains two kinds of terms: some linear in the V_j, and some quadratic in V_j. The linear ones involve products of a V_j at the time t and field operators at an earlier time, and we may assume that they vanish in an ensemble average over different realizations of the random process V_j, provided it has a sufficiently short correlation time. The ensemble average of the quadratic terms, on the other hand, yields

$$-\frac{i}{\hbar}\int_{t-\Delta t}^{t} \langle (V_{j+1} - V_j)(t)(V_{j+1} - V_j)(t')\rangle \langle \hat{a}_j^\dagger \hat{a}_{j+1}(t')\rangle dt' \simeq -\frac{i}{\hbar}\tau_c \langle (V_{j+1} - V_j)^2\rangle \langle \hat{a}_j^\dagger \hat{a}_{j+1}(t)\rangle, \tag{11}$$

where τ_c is the characteristic correlation time for the randomly fluctuating potential, $\langle (V_{j+1} - V_j)^2\rangle$ is the average (squared) strength of the fluctuations, and it has been assumed that $\langle \hat{a}_j^\dagger \hat{a}_{j+1}\rangle$ (essentially, the velocity of the system) does not change appreciably over the time scale of τ_c. (This is, basically, the Markov approximation.) The result, since the left-hand side of (9) is multiplied by $i\hbar$, is clearly a damping term for $\langle \hat{a}_j^\dagger \hat{a}_{j+1}\rangle$, or, by (7), for the on-site velocity $v_j \equiv i\langle \hat{a}_j^\dagger \hat{a}_{j+1} - \hat{a}_{j+1}^\dagger \hat{a}_j\rangle$:

$$\frac{dv_j}{dt} = -2\gamma_j v_j + \cdots \tag{12}$$

with

$$\gamma_j = \frac{1}{2\hbar^2}\tau_c \langle (V_{j+1} - V_j)^2\rangle. \tag{13}$$

The question now is whether it is possible to extract, from the interaction term in (8), something that looks like an "external" random potential, as in Eq. (9). That this is, in fact, possible follows if one replaces the bosonic field operators $\hat{a}_j$ by $\hat{a}_j = z_j + \hat{\delta}_j$, where z_j is a c number equal to $\langle \hat{a}_j\rangle$ (the local mean field), and $\hat{\delta}_j$ a zero-average operator. Substituting in the interaction term in (8), we get

$$\hat{a}_j^\dagger(\hat{n}_{j+1} - \hat{n}_j)\hat{a}_{j+1} = (|z_{j+1}|^2 - |z_j|^2)\hat{a}_j^\dagger \hat{a}_{j+1} + \hat{a}_j^\dagger(z_{j+1}^* \hat{\delta}_{j+1} + z_{j+1}\hat{\delta}_{j+1}^\dagger + \hat{\delta}_{j+1}^\dagger \hat{\delta}_{j+1} - z_j^* \hat{\delta}_j - z_j \hat{\delta}_j^\dagger - \hat{\delta}_j^\dagger \hat{\delta}_j)\hat{a}_{j+1}. \tag{14}$$

The first term on the right-hand side of (14) is a "deterministic" term which can be combined with the first term on the right-hand side of (9); indeed, it is the combination of these two terms that yields the Thomas-Fermi profile in the ground state when the kinetic energy term (the J term) in (9) is negligible. The second term in (14), on the other hand, is where we expect the main "noise" to arise. To determine its

contribution to the equation of motion for the expectation value $\langle \hat{a}_j^\dagger \hat{a}_{j+1} \rangle$, we express the remaining $\hat{a}_j$ operators in terms of $\hat{\delta}_j$, assume expectation values of the form $\langle (\hat{\delta}^\dagger)^p \hat{\delta}^q \rangle$ vanish unless $p=q$, and factor terms such as $\langle \hat{\delta}_j^\dagger \hat{\delta}_j^\dagger \hat{\delta}_j \hat{\delta}_{j+1} \rangle$ in a standard way, as $2\langle \hat{\delta}_j^\dagger \hat{\delta}_j \rangle \langle \hat{\delta}_j^\dagger \hat{\delta}_{j+1} \rangle$. The result is

$$\begin{aligned}\langle \hat{a}_j^\dagger (z_{j+1}^* \hat{\delta}_{j+1} + z_{j+1} \hat{\delta}_{j+1}^\dagger + \hat{\delta}_{j+1}^\dagger \hat{\delta}_{j+1} - z_j^* \hat{\delta}_j - z_j \hat{\delta}_j^\dagger - \hat{\delta}_j^\dagger \hat{\delta}_j) \hat{a}_{j+1} \rangle \\ = 2(\langle \hat{\delta}_{j+1}^\dagger \hat{\delta}_{j+1} \rangle - \langle \hat{\delta}_j^\dagger \hat{\delta}_j \rangle)(z_j^* z_{j+1} + \langle \hat{\delta}_j^\dagger \hat{\delta}_{j+1} \rangle) + (|z_{j+1}|^2 - |z_j|^2) \\ \times \langle \hat{\delta}_j^\dagger \hat{\delta}_{j+1} \rangle = 2(\tilde{n}_{j+1} - \tilde{n}_j) \langle \hat{a}_j^\dagger \hat{a}_{j+1} \rangle + (|z_{j+1}|^2 - |z_j|^2) \langle \hat{\delta}_j^\dagger \hat{\delta}_{j+1} \rangle, \end{aligned} \tag{15}$$

where the noncondensate density $\tilde{n}_j \equiv \langle \hat{n}_j \rangle - |z_j|^2$ has been introduced. The second term on the right-hand side of (15) appears to be a small noise-induced contribution to the deterministic part of (14). The first term has the desired form. We can then replace the expectation value of the interaction term in (8) by a deterministic term, which we shall not consider further, and a noiselike term

$$2U(\tilde{n}_{j+1} - \tilde{n}_j) \langle \hat{a}_j^\dagger \hat{a}_{j+1} \rangle. \tag{16}$$

If the evolution of the $\tilde{n}_j$ is sufficiently chaotic, one could imagine integrating the Heisenberg equations many times for very slightly different initial conditions and obtaining each time a different realization of the "random process" $\tilde{n}_j$. Then, if the Markovian condition holds, one can follow the same steps as for the external potential V_j in Eqs. (9)–(13) above and, by identifying V_j with $2U\tilde{n}_j$, conclude that, on average, a damping

$$\gamma_j = \frac{2U^2}{\hbar^2} \tau_c \langle (\tilde{n}_{j+1} - \tilde{n}_j)^2 \rangle \equiv \frac{2U^2}{\hbar^2} \tau_c \langle f_j^2 \rangle \tag{17}$$

will be observed in this system, for the on-site velocity v_j. (For conciseness, we have introduced the notation $f_j \equiv \tilde{n}_{j+1} - \tilde{n}_j$). The overall damping of the center of mass motion could be estimated by taking a weighted average of the γ_j (although, if the γ_j are very different from site to site, the assumption of a single damping constant for the center of mass motion may not be a very good approximation).

Our model is, therefore, that the condensate atoms are slowed down as they attempt to move through a randomly fluctuating effective potential created (through the interaction term) by the noncondensate atoms, as the latter are "shaken" out of equilibrium by the displacement of the trap. It may be worthwhile, at this point, to go over and attempt to justify the various assumptions that have been made.

The interpretation of $\tilde{n}_{j+1} - \tilde{n}_j$ as an essentially random variable appears justified from time-dependent HFB calculations (about which much more will be said in the next section) such as the one illustrated in Fig. 2 for a lattice of depth $V=1E_R$: the top part shows the time trace of $\tilde{n}_1 - \tilde{n}_0$, and the bottom figure the logarithm of the absolute value of its (time-)autocorrelation function, with a linear fit showing an approximately exponentially decaying envelope. It is, however, not quite as clear whether the Markov approximation is valid: after all, $\tilde{n}_j$ is not an external field, but one of the system's dynamical variables, and it certainly must develop

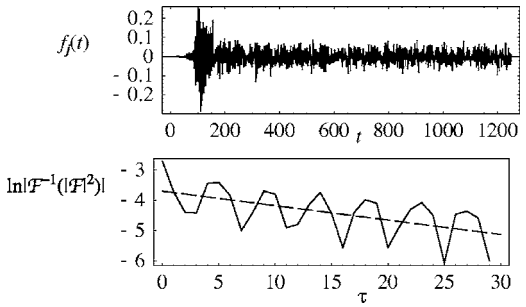

FIG. 2. (a) $\tilde{n}_{j+1} - \tilde{n}_j$ for $V=1E_R$ and $j=0$; (b) Fit (dashed line) to $\ln|\mathcal{F}^{-1}\{|\mathcal{F}[f_j(t)]|^2\}|$, for the first 30 time steps, for the f_j shown in (a). The slope of this line is taken to be $1/\tau_c$, for this particular value of j. Time is in units of $\hbar/E_R$ in both cases.

correlations and become entangled with other dynamical variables as the system evolves. Still, we take this as the simplest approximation, and note that, as will be seen in the next section, over the range considered, the time scale τ_c for the decay of correlations in $\tilde{n}_{j+1} - \tilde{n}_j$ (which is, essentially, $\hbar/J$) is indeed well-separated from the time scale of the damping of the center of mass oscillations.

Besides the above approximations, we have neglected "anomalous averages" such as, e.g., $\langle \hat{\delta}_j \hat{\delta}_j \rangle$, and we have used a standard "bosonic" ansatz to factor expectation values of products of four operators into expectation values of products of two operators. We do this in the spirit of all mean-field theories; namely, as something to try and see how it works. We certainly do not expect it to be a good approximation once (extended) fermionization becomes important.

Note that if, instead of using the bosonic ansatz, we had taken the simplest approach of factoring $\langle \hat{a}_j^\dagger (\hat{n}_{j+1} - \hat{n}_j) \hat{a}_{j+1} \rangle$ as $\simeq \langle \hat{a}_j^\dagger \hat{a}_{j+1} \rangle \langle \hat{n}_{j+1} - \hat{n}_j \rangle$ (and then separated out the condensate part from $\langle \hat{n}_{j+1} - \hat{n}_j \rangle$), the resulting "noise" term would have differed from (16) by a factor of 2, and hence the damping formula (17) would have been four times smaller. This may be a reasonable estimate of the possible error involved in our factorization assumptions.

Equation (17) does not, by itself, tell us what the actual damping is; for that, one needs to know the parameters characterizing the strength of the noise, $\langle f_j^2 \rangle$, and its characteristic correlation time τ_c. A possible way to obtain a very rough order-of-magnitude estimate for these quantities has been sketched in [25], by rewriting Eq. (17) in terms of the discrete Fourier transform (momentum components) of the $\tilde{n}_j$ (the order of magnitude of which can be estimated from Fig. 1), and assuming that τ_c should be of the order of magnitude of $\hbar/J$, since this is the "hopping rate," and that is the time scale over which one would expect local density fluctuations to decay. This simple approach does indeed yield the order of magnitude of the experimentally observed damping.

As we shall show below, using values for $\langle f_j^2 \rangle$ and τ_c derived from HFB calculations in the formula (17) does lead to very good agreement with the experimentally observed damping.

IV. HFB CALCULATIONS

In this section we report on the results of calculations using the time-dependent Hartree-Fock-Bogoliubov approxi-

mation [26,27]. The starting point of this approximation is the Heisenberg equation of motion for the field operator:

$$i\hbar\frac{d}{dt}\hat{a}_j = (\hat{K} + \Omega j^2 + U\hat{a}_j^\dagger\hat{a}_j)\hat{a}_j, \tag{18}$$

with $\hat{K}$ the tight binding kinetic energy operator: $\hat{K}A_j = -J(A_{j+1}+A_{j-1})$ (here A_j can be any function or operator defined at the point j), and Ωj^2 the external confining potential, which is quadratic in our system. By expressing the field operator, as before, as $\hat{a}_j = z_j + \hat{\delta}_j$, replacing this ansatz in Eq. (18), and treating the cubic term in a self-consistent mean-field approximation, coupled equations of motion for the condensate, z_j, and the fluctuating field $\hat{\delta}_j$ can be obtained:

$$i\hbar\frac{d}{dt}z_j = [\hat{K} + \Omega j^2 + U(|z_j|^2 + 2\tilde{n}_j)]z_j + U\tilde{m}_j z_j^*, \tag{19}$$

$$i\hbar\frac{d}{dt}\hat{\delta}_j = (\hat{K} + \Omega j^2 + 2Un_j)\hat{\delta}_j + Um_j\hat{\delta}_j^\dagger, \tag{20}$$

here $n_j = \langle\hat{a}_j^\dagger\hat{a}_j\rangle$, $\tilde{n}_j = \langle\hat{\delta}_j^\dagger\hat{\delta}_j\rangle$, $m_j = \langle\hat{a}_j\hat{a}_j\rangle$, and $\tilde{m}_j = \langle\hat{\delta}_j\hat{\delta}_j\rangle$. By using a Bogoliubov transformation that expresses the operators $\hat{\delta}_j$ in terms of quasiparticle creation and annihilation operators $\hat{\alpha}_k$, $\hat{\alpha}_k^\dagger$ and amplitudes $\{u_j^k(t)\}$, $\{v_j^k(t)\}$, as $\hat{\delta}_j = \Sigma_k[u_j^k(t)\hat{\alpha}_k - v_j^{k^*}(t)\hat{\alpha}_k^\dagger]$, one obtains equations of motion for the amplitudes $\{z_j\}$, $\{u_j^k(t)\}$, and $\{v_j^k(t)\}$ known as HFB equations. They describe the coupled dynamics of condensate and noncondensate atoms and conserve particle number and energy. As coupled, nonlinear equations, they have the potential to describe a wide range of dynamics, including deterministic chaos.

A difficulty with the time-independent HFB equations is that they violate the Hugenholtz-Pines theorem and yield an initial ground state with a depletion that is too small [22], when compared to the exact numerical results in Fig. 1. We have, therefore, used the Popov approximation [27] (which ignores the anomalous terms $\tilde{m}_j$) to calculate the ground state of the undisplaced trap, but then, after displacing the trap, we propagate in time using the full HFB equations (without the Popov approximation), because propagating in time with the Popov approximation does not conserve particle number or energy. Due to this mixing of approximations (in a sense, we are starting from the "wrong" initial state), as well as to the intrinsic limitations of the HFB approximation, our HFB results must be taken with some caution. Nonetheless, one may gain at least some qualitative insights from them, as illustrated, for instance, in Fig. 3, which shows how the noncondensate atoms relax rather rapidly (in agreement with the expectation of strongly inhibited transport for the high-momentum states), and with a substantial amount of noise.

Our HFB calculations do exhibit damped center of mass oscillations for all the values of V in the experiment, and for sufficiently deep lattices (about $V > 4E_R$ in our calculations) they even exhibit the overdamped relaxation seen in the experiments (i.e., the value of the damping exceeds the oscillation frequency), although in the experiments this transition to overdamped motion was seen already for shallower lattices, between $V = 2E_R$ and $V = 3E_R$. Quantitatively speaking, the HFB results do predict, in general, a smaller damping than is seen experimentally for any given lattice depth V, and also, even with the Popov approximation, a smaller ground-state depletion than the Monte-Carlo calculations in Fig. 1. This lack of precise quantitative agreement is not terribly surprising, given the fact that for all of these systems the depletion of the condensate is really not very small when compared to the mean-field density; hence neglecting higher powers of the $\hat{\delta}_j$ operators cannot be very accurate. The qualitative agreement, however, suggests that the HFB approximation does retain all the physical ingredients needed to predict the kind of damped oscillations seen in the experiments in this regime.

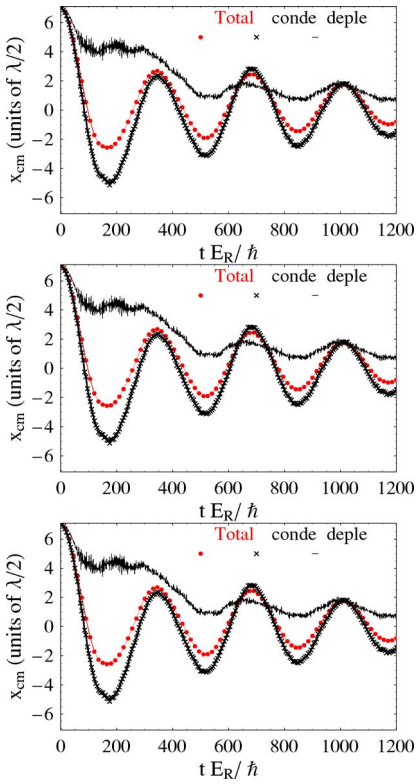

FIG. 3. (Color online) Result of the direct numerical integration of the HFB equations for, from top to bottom, $V = 3E_R$, $V = 4E_R$, and $V = 5E_R$. In all cases the position of the center of mass of the noncondensate atoms is given by the noisier top trace, that of the condensate by the lighter lower trace (small crosses), and the total is given by the line drawn with the circles. Time is in units of $\hbar/E_R$ and the position is in units of the lattice spacing.

With all of the above in mind, we have attempted to use the results of the HFB calculations to estimate the quantities $\langle f_j^2\rangle$ and τ_c in the damping formula (17), in the following manner. First, we generate a time series for $\tilde{n}_j(t)$ for all j and for a relatively large number of oscillation periods, and we simply average all these values to estimate $\langle f_j^2(t)\rangle$. We also calculate the Fourier transform $\tilde{f}_j(\omega) \equiv \mathcal{F}(f_j)$ of each time series, and then calculate the inverse Fourier transform, $\mathcal{F}^{-1}$, of the power spectrum $|\tilde{f}_j(\omega)|^2$; by the convolution theorem of Fourier transforms, this should equal the autocorrelation

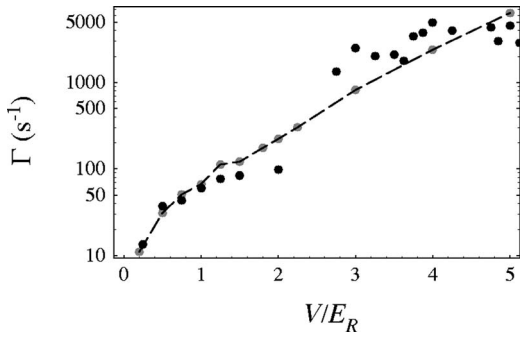

FIG. 4. Gray dots (connected by dashed lines): the value of Γ calculated from Eq. (3), using the time series that results from integrating the HFB equations. Black dots: experimental data.

of $f_j(t)$. We therefore estimate a correlation time by fitting an exponential to the decay of the absolute value of $\mathcal{F}^{-1}(|\tilde{f}_j|^2)$, for relatively short times (of the order of $30\hbar/E_R$). [Representative results are shown in Fig. 2(b).] We obtain in this way a (generally different) value of τ_c and $\langle f_j^2(t)\rangle$ for every lattice site j. The final estimate of the overall damping Γ is obtained by taking a weighted average of all the γ_j, using the equilibrium density as the weighting function. This results in the gray dots in Fig. 4, which are to be compared to the experimental data shown as the black dots in the same figure.

We are faced with the somewhat paradoxical result that, while the HFB calculations generally underestimate the damping, the formula (17), using HFB values, agrees quite well with the experiments and even appears to overestimate the damping in places (such as around $V=2E_R$).

We do not have, in principle, a reason to doubt the relative accuracy of the HFB estimate of the fluctuations' correlation time τ_c (which does turn out to be between $2\hbar/J$ and $3\hbar/J$ for the values of V considered). On the other hand, the fact, pointed out above, that the HFB calculations predict a noncondensate density lower than the true one, suggests that the HFB estimate of $\langle f_j^2(t)\rangle$ may be proportionately low as well. If this is the case, it would indicate that the formula (17) generally overestimates the damping, perhaps because of the assumption of totally uncorrelated condensate and noncondensate fluctuations that goes into its derivation. The agreement with the experiment shown in Fig. 4 would then appear to be more precise than it is actually supposed to be. Nonetheless, generally speaking, the physical picture invoked in the derivation of the damping formula appears to be correct, even if oversimplified in some details (e.g., validity of the Markov approximation).

V. RESULTS FROM GUTZWILLER-ANSATZ CALCULATIONS

It is well known that an alternative to the HFB calculations is provided by a mean-field theory based on the Gutzwiller ansatz. While in the HFB method the interaction term in (1) is treated approximately, and the kinetic energy term is treated exactly, yielding a theory best suited for weakly interacting superfluids, the Gutzwiller ansatz is equivalent to treating the interaction term in (1) exactly and

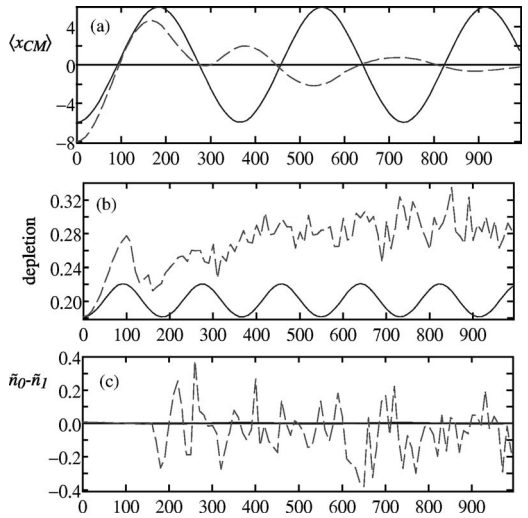

FIG. 5. Results of Gutzwiller calculations for $V=3E_R$ and initial displacements $d=6$ (solid line) and $d=8$ (dashed line). (See text for details.)

approximating the kinetic energy term as follows

$$\hat{a}_{j+1}^\dagger \hat{a}_j = [\langle \hat{a}_{j+1}^\dagger \rangle + (\hat{a}_{j+1}^\dagger - \langle \hat{a}_{j+1}^\dagger \rangle)][\langle \hat{a}_j \rangle + (\hat{a}_j - \langle \hat{a}_j \rangle)]$$
$$\simeq \langle \hat{a}_{j+1} \rangle^* \hat{a}_j + \hat{a}_{j+1}^\dagger \langle \hat{a}_j \rangle - \langle \hat{a}_{j+1} \rangle^* \langle \hat{a}_j \rangle. \quad (21)$$

As a result of this, the Gutzwiller ansatz works best for very strongly interacting systems, and it is, in fact, capable of describing qualitatively the Mott transition [28], which the HFB method cannot do.

In Eq. (21), the mean field $\langle \hat{a}_j \rangle$ is obtained self-consistently by diagonalization of the resultant effective Hamiltonian, to which a chemical potential term $-\mu \Sigma n_j$ is added in order to get the desired average number of particles. Once the initial state has been calculated, the relevant equations of motion are as given, for instance, in [15,28].

What we find from the Gutzwiller approach is that the predicted depletion for the ground state is substantially lower than the one calculated numerically in Fig. 1, for all except the deepest lattices, and accordingly no appreciable damping is seen, for the experimental parameters, until $V=4E_R$ or so. For $V=3E_R$ a displacement of the trap potential by six lattice sites fails to give any visible damping, but a displacement of eight lattice sites does give substantial damping, as shown in Fig. 5(a).

The other graphs in Fig. 5, also for $V=3E_R$, highlight other interesting features of this transition from undamped to damped motion, which are in rough agreement with our prior expectations. Figure 5(b) shows the fractional depletion as a function of time for the two displacements $d=6$ (solid) and $d=8$ (dashed). Although the initial depletion is the same (the ground-state value), the time evolution leads to a depletion that, in the case of regular motion, is largest at the times when the condensate is moving faster. In the case $d=8$ one can see the depletion initially growing as the speed [the slope of the corresponding curve in Fig. 5(a)] increases, and eventually becoming rather large, after which damped motion follows. Note, for reference, that the Monte-Carlo prediction

from Fig. 1 for this case would be a ground-state depletion of about 0.5. On the other hand, the smallest depletion calculated in Fig. 1, for $V=0.25E_R$, is 0.24, which here would appear to be just large enough to result in damped motion.

Figure 5(c) shows the time dependence of $\tilde{n}_0-\tilde{n}_1$ (the subscript "0" refers to the center of the trap). The regular case, for $d=6$, is a solid line invisible on the scale of the figure (<0.005 in magnitude). Again, the damping appears to be strongly correlated with the site-to-site density fluctuations.

As we did for the HFB calculation, we can extract values for $\langle f_j^2 \rangle$ and τ_c from the time series obtained by the Gutzwiller approach, and substitute them in Eq. (17). The results, for $V/E_R=4,5$, are actually quite close to those obtained from the HFB calculation. For smaller V, of course, the calculation would not make sense, since the time dependence of $\tilde{n}_j-\tilde{n}_{j+1}$ predicted by the Gutzwiller ansatz in this region is always regular, rather than noiselike.

It is perhaps worth noting that the strong dependence on the displacement d exhibited by the Gutzwiller calculations is not seen in the HFB calculations, which always yield damped motion, even for very small displacements, although the strength of the damping does decrease continuously with d, as does the size of the density fluctuations. The strong dependence on the displacement exhibited by the Gutzwiller calculations is a signature of its mean-field character: The factorization approximation used in the Gutzwiller ansatz completely neglects nonlocal correlations. In contrast, the HFB approximation goes beyond mean field and accounts for quantum fluctuations around the condensate and nonlocal correlations. In Ref. [16] the authors present a detailed analysis of the role of quantum fluctuations and nonlocal correlations in the dynamics. They show that in one-dimensional (1D) systems classical mean-field theories such as the Gutzwiller ansatz predict a very sharp transition from underdamped to overdamped dynamics. The mean-field transition depends on the interactions' strength and interpolates between the classical modulation instability at $p_c=\hbar\pi/\lambda$ deep in the superfluid regime to $p_c=0$ near the Mott insulator transition. Quantum fluctuations, included in an analysis beyond mean field such as the HFB approximation, lead to substantial broadening of the nonequilibrium transition and induce a decay of the center of mass oscillations before the classical equations of motion become unstable.

VI. DISCUSSION AND CONCLUSIONS

To recapitulate, then, we believe that the damping in this "intermediate" regime can be explained as arising from the large depletion due to the tight transverse confinement, which leads to the population of high-momentum states in the nonquadratic part of the lattice dispersion curve. The condensate atoms' motion is then damped through their interactions with the random field created by these noncondensate atoms when their equilibrium state is perturbed. The dramatic growth of Γ with V illustrated in Fig. 4 arises from several causes: first, the depletion increases with lattice depth, as shown by Fig. 1 and Eq. (4); second, the interaction U itself increases, albeit weakly (as $V^{1/4}$); third, the tunneling rate J decreases, and the correlation time $\tau_c \sim \hbar/J$ in (17) increases accordingly (the "damping medium" becomes more "sluggish").

The main limitations of the formula (17) have been pointed out when it was derived. Since it only accounts for the damping induced by the interactions, it vanishes in the $U \to 0$ limit, even though, as we mentioned in the Introduction, a noninteracting bosonic gas exhibits a sort of damping in a lattice, associated with the nonharmonic nature of the total potential (see, e.g., [6]). At the other limit point, $U \to \infty$, Eq. (17) predicts an infinite damping, which is clearly also not correct. The reason is that Eq. (17) is based on a self-consistent factorization approximation that, strictly speaking, is only valid in the weakly interacting limit.

We note that, in these regimes where Eq. (17) does not apply, previous studies [1,3,4,17,18] have shown that treatments based on single-particle solutions can provide a very accurate description of the damping. On the other hand, in the complex intermediate regime where it is not possible to use the simplicity of the single-particle solutions, we have shown that Eq. (17) does manage to describe the damping. Moreover, it connects in a simple way the damping rate to physical parameters and therefore allows a clearer understanding of the physics responsible for the dissipative dynamics exhibited by 1D lattice systems in this regime.

ACKNOWLEDGMENTS

J. Gea-Banacloche is grateful to NIST for their hospitality, and ARO for partial support. A.M.R. acknowledges additional support by a grant from the Institute of Theoretical, Atomic, Molecular and Optical Physics at Harvard University and Smithsonian Astrophysical observatory. All the authors acknowledge many helpful discussions with James (Trey) Porto and W. D. Phillips, and their team.

[1] V. Ruuska and P. Törmä, New J. Phys. **6**, 59 (2004).
[2] L. Pezzè, L. Pitaevskii, A. Smerzi, S. Stringari, G. Modungo, E. DeMirandes, F. Ferlaino, H. Ott, G. Roati, and M. Inguscio, Phys. Rev. Lett. **93**, 120407 (2004).
[3] H. Ott, E. de Mirandes, F. Ferlaino, G. Roati, V. Türck, G. Modugno, and M. Inguscio, Phys. Rev. Lett. **93**, 120407 (2004).
[4] M. Rigol and A. Muramatsu, Phys. Rev. A **70**, 043627 (2004).
[5] M. Rigol, V. Rousseau, R. T. Scalettar, and R. R. P. Singh, Phys. Rev. Lett. **95**, 110402 (2005).
[6] A. M. Rey, G. Pupillo, C. W. Clark, and C. J. Williams, Phys. Rev. A **72**, 033616 (2005).
[7] B. Wu, R. B. Diener, and Q. Niu, Phys. Rev. A **65**, 025601 (2002), and references therein.
[8] S. Burger, F. S. Cataliotti, C. Fort, F. Minardi, M. Inguscio, M. L. Chiofalo, and M. P. Tosi, Phys. Rev. Lett. **86**, 4447 (2001).

[9] A. Smerzi, A. Trombettoni, P. G. Kevrekidis, and A. R. Bishop, Phys. Rev. Lett. **89**, 170402 (2002).
[10] 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).
[11] T. Stöferle, H. Moritz, Ch. Schori, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **92**, 130403 (2004).
[12] O. Morsch, J. H. Müller, M. Cristiani, D. Ciampini, and E. Arimondo, Phys. Rev. Lett. **87**, 140402 (2001).
[13] F. S. Cataliotti, S. Burger, C. Fort, P. Maddaloni, F. Minardi, A. Trombettoni, A. Smerzi, and M. Inguscio, Science **293**, 843 (2001).
[14] A. Polkovnikov and D.-W. Wang, Phys. Rev. Lett. **93**, 070401 (2004).
[15] E. Altman, A. Polkovnikov, E. Demler, B. Halperin, and M. D. Lukin, Phys. Rev. Lett. **95**, 020402 (2005).
[16] A. Polkovnikov, E. Altman, E. Demler, B. I. Halperin, and M. D. Lukin, Phys. Rev. A **71**, 063613 (2005).
[17] J. Ruostekoski and L. Isella, Phys. Rev. Lett. **95**, 110403 (2005).
[18] G. Pupillo, A. M. Rey, C. J. Williams, and C. W. Clark, e-print cond-mat/0505325.
[19] For a semiclassical picture of this see T. A. B. Kennedy, Phys. Rev. A **70**, 023603 (2004).
[20] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998).
[21] N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsyn, Phys. Lett. A **238**, 253 (1998); JETP **87**, 310 (1998).
[22] A. M. Rey, D. Phil. thesis, University of Maryland at College Park, 2004 (unpublished).
[23] A. M. Rey, K. Burnett, R. Roth, M. Edwards, C. J. Williams, and C. W. Clark, J. Phys. B **36**, 825 (2003).
[24] W. Kohn, Phys. Rev. **123**, 1242 (1961); J. F. Dobson, Phys. Rev. Lett. **73**, 2244 (1994).
[25] J. Gea-Banacloche, J. Phys. B **39**, 69 (2006).
[26] A. M. Rey, B. L. Hu, E. Calzetta, A. Roura, and C. W. Clark, Phys. Rev. A **69**, 033610 (2004).
[27] A. Griffin, Phys. Rev. B **53**, 9341 (1995).
[28] D. Jaksch, V. Venturi, J. I. Cirac, C. J. Williams, and P. Zoller, Phys. Rev. Lett. **89**, 040402 (2002).