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Effective parameters for weakly coupled Bose–Einstein condensates

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Abstract. The dynamics of quantum fluctuations of weakly coupled Bose– Einstein condensates (BECs) can be described by an effective Bose–Josephson Hamiltonian. By requiring that the mean-field approximation on this effective Hamiltonian reproduces the low energy dynamics of the Gross–Pitaevskii equation, we obtain parameters for the effective Hamiltonian. This approach is particularly suitable when the BECs are in the Thomas–Fermi regime. Considering the problem of the splitting of a trapped BEC into two BEC fragments, our results for the dynamics of the depletion, collapses and revivals of the phase coherence are in good agreement with a recent numerical microscopic calculation from Streltsov *et al* (2007 *Phys. Rev. Lett.* **99** 030402). In addition, the excitation energy of the lowest symmetric mode, which is the first relevant mode for the symmetric splitting process, is reproduced with reasonable accuracy all the way from the mean-field Josephson regime to the Fock regime.

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1. Introduction

The system of two or many atomic Bose–Einstein condensates (BECs) weakly linked together has attracted considerable attention in the last decade. Different dynamical scenarios have been predicted and measured: these include the mean field predicted regimes of Josephson oscillations [2, 3], macroscopic quantum self trapping [4], the ac and dc Josephson analogous effect [5, 6] and their corresponding experimental observations [7]–[10]; the prediction of quantum regimes of collapses and revivals of the phase of two superfluids [11]–[14] and their experimental observation in a multi-well system [15], the characterization of quantum and thermal fluctuations [16] and the observation of thermal noise [17] and indications of number squeezing [18].

Whereas the majority of theoretical investigations (see for example [19] and references therein) have been made by assuming and studying an effective Bose–Hubbard or Bose–Josephson type of Hamiltonian, considerably less attention has been devoted to the problem of how to obtain accurate energy parameters for these effective Hamiltonians. Some analytical expressions have been given by Zapata *et al* [3], and in the work of one of us [5]. In particular, the validity of the Josephson Hamiltonian description for the mean field regimes has been numerically confirmed in this last work [5, 6].

The purpose of this paper is to show that the second quantized form of the effective Josephson Hamiltonian allows the quantitative understanding of the splitting dynamics recently numerically solved using advanced many-orbital mean-field theory by Streltsov *et al* [1]. The mapping between Josephson and exact many body Hamiltonians is well known in the tight binding regime. Here, we demonstrate how to extend the effective two mode Josephson model to describe the on-going physics, relaxing the tight binding condition, including the Thomas–Fermi limit. This is confirmed by good agreement of depletion dynamics and excitation spectra obtained by numerical methods in [1]. This shows that our approach is capable of capturing the physics of quantum fluctuations that play an important role in the splitting process of a BEC [14, 20] in typical experimental situations where the BEC is usually in the Thomas–Fermi regime.

2. Description of the model

In this paper, we focus on the problem of an initially trapped weakly interacting BEC with negligible depletion which is slowly separated into two parts by a barrier potential growing in the middle of the trapping potential [14, 20, 21]. As the barrier potential grows the degenerate Bose gas evolves from a mean-field Josephson regime to the Fock regime, where the Bose gas is fragmented into two BECs. In the Josephson regime the atoms are free to tunnel from the left to the right wells. In contrast, in the Fock regime the tunneling energy E_J is lower than the interaction energy cost of exchanging one atom, which we refer to as the charging energy E_C in analogy with the original Josephson effect in superconductors. As a consequence the tunneling process loses the typical collective character of the Josephson oscillations. The ground state has a strong overlap with the Fock state of half the atoms on the left and the other half of the atoms occupying a state on the right (see figure 3).

In addition to the above equilibrium considerations, the problem of the splitting of a BEC is a dynamical one [20, 21]. Depending on how slow the barrier is raised the atomic cloud may end up in the Fock ground state or in a superposition of excited states, which manifests itself in a time dependence of the phase fluctuations (see figure 2).

2.1. The effective Hamiltonian

In this paper, we are only interested in the dynamics and the fluctuations of macroscopic observables such as the atom number and the phase difference associated with the split BECs. To calculate these quantities a microscopic description is not needed and we assume an effective Hamiltonian which has the following second quantized form

$$H = (E_{\rm J}/N) \left(c_a^{\dagger} c_b + c_b^{\dagger} c_a \right) + (E_{\rm C}/8) \left(c_a^{\dagger} c_a - c_b^{\dagger} c_b \right)^2, \tag{1}$$

where c_a and c_b (c_a^{\dagger} , c_b^{\dagger}) are destruction (creation) operators of particles in the left and right wells. The same form for the Hamiltonian can be obtained by a variational approach starting from the full many body Hamiltonian [4]. In that case, the two modes associated with c_a and c_b are explicitly calculated and the parameters E_C and E_J are then deduced as matrix elements of the appropriate operators between these modes [4, 22]. Our approach does not assume any particular expression for the modes.

The parameters $E_{\rm C}$ and $E_{\rm J}$ are tuned to match the mean field solution of equation (1) to the mean field predictions for the macroscopic observables of the many particle problem, i.e. the Gross–Pitavskii equation (GPE). This phenomenological approach is in some sense very similar to the description of Josephson junction systems in condensed matter where the microscopic details are not known.

The above Hamiltonian (1) is not the most general form of a Josephson-type Hamiltonian. The chosen form implies a sinusoidal current–phase relationship which is a good approximation for the parameters considered here. The first term may contain different powers of $c_a^{\dagger}c_b$ which would give rise to different current–phase relationships, e.g. in the regime of hydrodynamic flow between the wells [23].

We do not discuss in this paper the possibility of having the chemical potential difference between the wells larger than the first intra-well excitation energy, which is a typical situation in condensed matter.

2.2. The Josephson energy $E_{\rm J}$

We estimate the Josephson energy E_J from solutions of the time-independent GPE. We calculate the ground state and the first asymmetric solution with a node at the barrier. The Josephson energy E_J is half the difference between the energies of the two states which follows from the assumed sinusoidal current–phase relationship. This method is straightforward to implement in the case of a symmetric double well potential. In the absence of such symmetry one can use inequality (8) of [3] which becomes an equality for one-dimensional (1D) flow.

2.3. The charging energy $E_{\rm C}$

The charging energy $E_{\rm C}$ is calculated as $E_{\rm C} = 4\partial \mu/\partial N$ where μ is the total chemical potential extracted from the GPE solution. When the two BECs have a negligible overlap this corresponds to $E_{\rm C} = 2\partial \mu_1/\partial N_1$ where μ_1 and N_1 are the chemical potential and the equilibrium atom number on the left well, respectively [3, 5].

In the Thomas–Fermi limit $\partial \mu / \partial N = g / V_{\text{TF}}$, where V_{TF} is the volume (area or segment in 2D and 1D, respectively) where the Thomas–Fermi wavefunction differs from zero. Note that in a variational approach with static wavefunctions $\partial \mu / \partial N$ is approximated by its variational counterpart $E_{\text{C}} = U = g \int |\Psi|^4$. This gives a systematic error as high as 43% in 3D, 33% in 2D and 20% in 1D in the Thomas–Fermi limit.

3. Dynamical splitting of a BEC

3.1. Trap parameters

We consider the Hamiltonian of a 1D symmetric double well trap with an even number of bosons as defined in [1]. A BEC of $N = 200^{87}$ Rb atoms is initially prepared in an elongated, quasi-1D harmonic trap of longitudinal $\omega_{\parallel} = 2\pi \times 44.7$ Hz and transverse $\omega_{\perp} = 2\pi \times 1.1$ kHz frequencies. We set the length unit as $L = 1 \mu m$, and the time and energy scale consistently as in [1]. With these units the 1D reduced atom–atom interaction is $U(x - x') = \lambda_0 \delta(x - x')$ with $\lambda_0 = 0.1$. At time t = 0 a barrier potential $V_{\text{laser}} = V_0 \exp(-x^2/2\sigma^2)$ of Gaussian shape with $\sigma = 2.6$ is ramped-up linearly in time, i.e. $V_0(t) = (t/T_{\text{ramp}})V_0^{\text{max}}$ to a height of $V_0^{\text{max}} = 30$ and with ramp-up time of T_{ramp} . The total time-dependent 1D trap potential is then $V(x, t) = (x^2/2\sigma^2) + V_{\text{laser}}$. In the present 1D calculation the value of the Thomas–Fermi parameter per well is $\eta_{1D} = a(N/2)l_{\parallel}/l_{\perp}^2 \approx 6$.

3.2. Energy parameters of the effective Hamiltonian

Our Hamiltonian (1) is time-dependent. The time dependence originates from the dependence of $E_{\rm C}$ and $E_{\rm J}$ on the barrier height, which evolves in time. Figure 1 shows the dependence of the calculated $E_{\rm C}$ and $E_{\rm J}$ on the barrier height. Note that whereas $E_{\rm C}$ is almost constant $E_{\rm J}$ goes to zero very quickly as the barrier grows. When the barrier height is approximatively at 0.23 of the final barrier height $E_{\rm J}$ crosses $E_{\rm C}$ and the ground state starts strongly overlapping the so called fragmented condensate.



Figure 1. $N = 200^{87}$ Rb atoms are trapped in a double well potential formed by a barrier of height V_0 in the middle of an harmonic trap (see text for the actual parameters and dimensionless units). (a) Overlap of the ground state with the fragmented (Fock) state versus barrier height. As the barrier height exceeds 0.223 of its final maximum barrier height, the Josephson energy E_J crosses the charging energy E_C and the ground state starts strongly overlapping a Fock state. (b) For each value of the barrier height V_0 we calculate the parameters E_J (solid line) and E_C (dashed line) as described in section 2 entering the effective Josephson Hamiltonian (1).

3.3. Evolution of the quantum fluctuations

We solve numerically the many-body Schrödinger equation corresponding to (1). We consider the symmetric c_g and antisymmetric c_e combination of the operators c_a and c_b , that is $c_g = (c_a + c_b)/\sqrt{2}$ and $c_e = (c_a - c_b)/\sqrt{2}$. We deduce the dynamic evolution of the expectation values $\langle c_g^{\dagger} c_g \rangle/N$ and $\langle c_e^{\dagger} c_e \rangle/N$ corresponding to the populations of a condensate wavefunction with even symmetry and of a condensate wavefunction with odd symmetry. Figure 2 shows the time evolution of these two quantities. Before the barrier starts to rise, almost all the atoms occupy the ground state with a very small depletion of order of $\langle c_e^{\dagger} c_e \rangle/N \sim 2 \times 10^{-3}$. As the barrier rises the depletion in the antisymmetric state grows.

We compare the depletion calculated from the dynamics with the one obtained using the adiabatic approximation, i.e. from the ground state of (1) considered as time-independent. For t < 200 the expectation values $\langle c_g^{\dagger} c_g \rangle / N$ and $\langle c_e^{\dagger} c_e \rangle / N$ are very close to the adiabatic solution, which is represented by the smooth dot-dashed line in figure 2.

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Figure 2. An initially coherent BEC of $N = 200^{87}$ Rb atoms evolves towards a twofold fragmented state during the ramping-up of a barrier in the middle of a trap. The figure shows the fractional populations of a symmetric (solid line) and antisymmetric (dashed line) wavefunction versus time (the ramping-up time is $T_{\text{ramp}} = 1000$). For t < 200 the population evolutions follow the adiabatic curves (thin solid and dashed lines). The further oscillations are characteristic of collapses and revivals. The revival period is related to the charging energy by $4\pi\hbar/E_{\text{C}}$ (see text). The results of this figure are in good agreement with the corresponding exact numerical results of figure 1 in [1].

For t > 200, we observe oscillations of the populations of the symmetric and antisymmetric states. The oscillatory behavior denotes the collapses and revivals of the phase coherence as explained in [11]–[14]. The amplitude and the period of the oscillations are in good agreement with the microscopic calculation reported in figure 1 of [1]. The revival time is governed by the charging energy $E_{\rm C}$. In most of the experimentally accessible situations for atomic BEC the timescale is of order of one second. Note that the corresponding revival times are about 10 μ s for a typical superconductor and as much as 10¹⁶ s for superfluid helium [12].

3.4. First excited state

We also compare the barrier height V_0 dependence of the excitation energy of the second excited state calculated from (1) with that reported in figure 1(b) of [1]. This excitation energy corresponds to the first excited state that can be partially populated by a nonadiabatic rise of the barrier. The result of the comparison is shown in figure 3 and represents the main result of this paper. The agreement is better than 12% for barrier height $V_0/V_0^{\text{max}} > 0.18$. For $V_0/V_0^{\text{max}} < 0.2$, i.e. the Josephson regime, the energy of the considered excited state is in good agreement with the energy of two Josephson excitations $2\sqrt{E_JE_C}$. For $V_0/V_0^{\text{max}} > 0.24$, i.e. the Fock regime, the considered excitation energy tends towards $E_C/2$. For $V_0 = V_0^{\text{max}}$ the revival time 327.9 obtained from the simulation in figure 2 corresponds to an energy of 0.01916, in perfect agreement with the value of excitation energy $E_C/2 = 0.01917$. These are also in reasonable agreement with the



Figure 3. Energy of the second excited state versus barrier height V_0 . This energy corresponds to the first excited state that can be partially populated by a nonperfectly adiabatic rise of the barrier. The solid line is obtained from the numerical diagonalization of the Hamiltonian (1). Crosses are the numerical results of [1]. The agreement is satisfactory for $V_0/V_0^{\text{max}} > 0.18$. For $V_0/V_0^{\text{max}} < 0.2$, the energy of the considered excited state is in good agreement with the energy of two Josephson excitations $2\sqrt{E_J E_C}$ (green dashed line). For $V_0/V_0^{\text{max}} > 0.24$, the spectrum is dominated by the charging term $E_C/2$ (magenta dashed line).

simulation of [1] for which the corresponding values are 0.0197 from the dynamics and 0.0188 from the calculated spectrum.

4. Conclusions

We have shown that an effective Josephson Hamiltonian approach is a reasonable description also in situations where the role of excited states is considered to be relevant (Thomas–Fermi regime), see the discussions in [1, 20]. The method discussed in this paper can be naturally extended to the case of a Bose gas loaded in an optical lattice. Since the atomic confinement in a typical optical potential can be quite high, the Thomas–Fermi parameter $\eta_{3D} = aN_i/l$ (with N_i being the atom number per site) can be of order of unity or even bigger, especially in 1D optical lattices. Therefore the corrections mentioned in this paper apply to the Bose– Hubbard Hamiltonian description [24]. Neglecting finite size effects due to finite number of atoms per well, the replacement of the variational energy integral $U = g \int |\Psi|^4$ with Ψ a Wannier wavefunction, by $\partial \mu_i / \partial N_i$ where μ_i is the chemical potential should give a better approximation for calculating the depletion of a BEC in an optical lattice. **IOP** Institute of Physics DEUTSCHE PHYSIKALISCHE GESELLSCHAFT

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