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# Analogy between a two-well Bose-Einstein condensate and atom diffraction

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We compare the dynamics of a Bose-Einstein condensate in two coupled potential wells with atoms diffracting from a standing light wave. The corresponding Hamiltonians have an identical appearance, but with a different set of commutation rules. Well-known diffraction phenomena as *Pendellösung* oscillations between opposite momenta in the case of Bragg diffraction, and adiabatic transitions between momentum states are shown to have analogies in the two-well case. They represent the collective exchange of a fixed number of atoms between the wells.

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## I. INTRODUCTION

The most common approach to the description of a trapped Bose-condensed gas is based on the mean-field approximation, which yields the Gross-Pitaevski equation for the macroscopic wave function. This wave function, which depends on the number of atoms, plays the role of the mode function for the Maxwell field. This approach is reliable when the condensate is trapped in a single quantum state in a potential well. However, when the condensate is separated into two or more parts, so that more than one quantum state is populated, the mean-field approach is not evidently justified. It has been shown by Javanainen and Yoo [1] that two originally separate parts of a condensate that are initially in a Fock state and that are brought to overlap will reveal an interference pattern that varies in position from one realization to another. This effect, which has also been observed experimentally [2], cannot be described by a single macroscopic wave function. A simple model for a condensate in a double potential well is defined by a field-theoretical Hamiltonian for a boson-Hubbard dimer [3,4], which can be expressed in terms of SU(2) angular-momentum-type operators with a quadratic term. This latter term represents the interaction between atoms in a well. The mean-field approximation is basically equivalent to classical equations of motion for the expectation values of the SU(2) operators [5,6]. The quantum regime has mainly been studied numerically, leading to collapse and revival [5], and to nonclassical dynamics arising from the periodic modulation of the coupling between the wells [7]. The formation of a two-well condensate by the raising of the barrier has been analyzed theoretically [8]. The situation of a Bose-Einstein condensate (BEC) in a two-well trap is also studied experimentally [9,10].

A very similar Hamiltonian describes the situation of an atom diffracting from a standing-wave optical potential. This problem has received attention already in the early days of laser cooling [11]. More recent work has developed the band structure of the energy spectrum [12], and a number of regimes have been distinguished that allow an analytical description [13]. In a simple version of the model, the Hamiltonian is identical in form as in the two-well problem mentioned above. Now the quadratic term represents the kinetic energy of the atom. The only difference between the two cases is that the commutation rules for the operators in

the diffraction case are slightly simplified compared to the case of SU(2) symmetry.

In this paper, we discuss the analogy and the differences between these two systems. We point that a number of analytical solutions known for the diffraction problem can be carried over to the two-well system. The physics of these cases is discussed.

## II. BEC IN A DOUBLE POTENTIAL WELL

We consider a potential consisting of two wells. When the barrier between the wells is not too low, the ground state and the first excited state  $|g\rangle$  and  $|e\rangle$  of a single atom are well approximated as the even and odd superposition of the lowest bound states in the two wells. Therefore, these states can be described as

$$|g\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle), \quad |e\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle), \quad (1)$$

with  $|1\rangle$  and  $|2\rangle$  the localized states in either well. When the energy separation between the excited and the ground state is indicated as  $\hbar\delta$ , the off-diagonal element of the one-particle Hamiltonian  $\hat{H}_1$  between the localized states is

$$\langle 1|\hat{H}_1|2\rangle = -\hbar\delta/2.$$

At the low energies that are of interest here, the two-particle interaction is well approximated by the standard contact potential  $U(\vec{r}, \vec{r}') = (4\pi\hbar^2 a/m)\delta(\vec{r} - \vec{r}')$ , with  $a$  the scattering length. The second-quantized field operator is now

$$\hat{\Psi}(\vec{r}) = \hat{a}_g\psi_g(\vec{r}) + \hat{a}_e\psi_e(\vec{r}) = \hat{a}_1\psi_1(\vec{r}) + \hat{a}_2\psi_2(\vec{r}), \quad (2)$$

in terms of the wave functions  $\psi_i$  and the annihilation operators  $\hat{a}_i$  of the single-particle states. The annihilation operators and the corresponding creation operators obey the standard bosonic commutation rules. The corresponding Hamiltonian is

$$\hat{H} = \int d\vec{r} \hat{\Psi}^\dagger(\vec{r}) H_1 \hat{\Psi}(\vec{r}) + \int d\vec{r} d\vec{r}' \hat{\Psi}^\dagger(\vec{r}) \hat{\Psi}^\dagger(\vec{r}') U(\vec{r}, \vec{r}') \hat{\Psi}(\vec{r}) \hat{\Psi}(\vec{r}'). \quad (3)$$

The wave functions  $\psi_1$  and  $\psi_2$  of the localized states have the same form, and we assume that they do not overlap. Then the interaction term can be expressed exclusively in the parameter  $\kappa$  defined by

$$\hbar \kappa = \frac{4\pi\hbar^2 a}{m} \int d\vec{r} |\psi_1(\vec{r})|^4, \quad (4)$$

which measures the strength of the interatomic interaction. Performing the integrations in Eq. (3) leads to the expression for the Hamiltonian

$$\hat{H} = -\frac{\hbar\delta}{2}(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + \frac{\hbar\kappa}{2}(\hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_1 \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_2), \quad (5)$$

where we took the zero of energy halfway the two energy levels of a single atom. This is also known as the boson-Hubbard dimer Hamiltonian [3].

Hamiltonian (5) can also be expressed in terms of SU(2) operators by applying the standard Schwinger representation of two modes. This leads to the definition

$$\hat{J}_0 = \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_1 - \hat{a}_2^\dagger \hat{a}_2), \quad \hat{J}_+ = \hat{a}_1^\dagger \hat{a}_2, \quad \hat{J}_- = \hat{a}_2^\dagger \hat{a}_1. \quad (6)$$

These operators are related to the Cartesian components of angular momentum by the standard relations  $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$  and  $\hat{J}_0 = \hat{J}_z$ . They obey the commutation rules for angular-momentum operators

$$[\hat{J}_0, \hat{J}_\pm] = \pm \hat{J}_\pm, \quad [\hat{J}_+, \hat{J}_-] = 2\hat{J}_0, \quad (7)$$

which generate the su(2) algebra. Hamiltonian (5) can be rewritten in the form

$$\hat{H} = -\frac{\hbar\delta}{2}(\hat{J}_+ + \hat{J}_-) + \hbar\kappa\hat{J}_0^2 + \frac{\hbar\kappa}{4}(\hat{N}^2 - 2\hat{N}), \quad (8)$$

with  $\hat{N} = \hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2$  the operator for the total number of particles. Obviously, Hamiltonian (8) commutes with  $\hat{N}$ , and it is block diagonal in the number of particles  $N$ . For each value of  $N$ , Hamiltonian (8) can be expressed as

$$\hat{H}_N + \frac{\hbar\kappa}{4}(N^2 - 2N),$$

with the  $N$ -particle Hamiltonian

$$\hat{H}_N = -\frac{\hbar\delta}{2}(\hat{J}_+ + \hat{J}_-) + \hbar\kappa\hat{J}_0^2, \quad (9)$$

where the operators are now restricted to the  $N+1$  Fock states  $|n, N-n\rangle$  with  $n=0, 1, \dots, N$ , with  $n$  particles in well

1 and  $N-n$  particles in well 2. In the language of angular momentum, this manifold of states corresponds to the angular-momentum quantum number  $J=N/2$ , and the  $2J+1$  Fock states are eigenstates of  $\hat{J}_0$  with eigenvalue  $\mu=n-N/2$  with  $\mu=-J, -J+1, \dots, J$ . Note that  $\mu$  is half the difference of the particle number in the two wells. For an even number of particles, the angular-momentum quantum number  $J$  as well as the “magnetic” quantum numbers are integer, whereas these number are half integer in case of an odd number of particles. The action of the operators  $\hat{J}_0$  and  $\hat{J}_\pm$  on the Fock states has the well-known behavior

$$\begin{aligned} \hat{J}_0|\mu\rangle &= \mu|\mu\rangle, & \hat{J}_+|\mu\rangle &= f_{\mu+1}|\mu+1\rangle, \\ \hat{J}_-|\mu\rangle &= f_\mu|\mu-1\rangle, \end{aligned} \quad (10)$$

with  $f_\mu = \sqrt{(J+\mu)(J-\mu+1)}$ . The  $\mu$  dependence of the strength of the hopping operators  $\hat{J}_\pm$  reflects the bosonic accumulation factor, which favors the arrival of an additional bosonic atom in an already occupied state.

When the quadratic term in Eq. (9) would be replaced by a linear term, the evolution would be a uniform rotation in the  $(2J+1)$ -dimensional state space with angular frequency  $\sqrt{\delta^2 + \kappa^2}$ . The presence of the quadratic term makes the dynamics considerably more complex. Therefore, we compare this dynamics with another well-known case in which a similar quadratic term appears.

### III. STANDING-WAVE DIFFRACTION OF ATOMS

The translational motion of a two-level atom in a far detuned standing-wave light field is described by the effective Hamiltonian

$$\hat{H}_d = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} - \frac{\hbar\omega_R^2}{\Delta} \cos^2 kz, \quad (11)$$

with  $\Delta = \omega_0 - \omega$  is the difference of the resonance frequency and the optical frequency, and  $\omega_R$  is the Rabi frequency of each of the traveling waves that make up the standing wave. The Hamiltonian takes a particularly simple form in momentum representation, since the kinetic-energy term is diagonal in momentum and the potential energy changes the momentum by  $\pm 2\hbar k$ . Therefore, we introduce momentum eigenstates  $|\mu\rangle$  which have the momentum  $2\mu\hbar k$ . Then apart from an irrelevant constant, Hamiltonian (11) can be represented in the algebraic form

$$\hat{H}_d = -\frac{\hbar\delta}{2}(\hat{B}_+ + \hat{B}_-) + \hbar\kappa\hat{B}_0^2, \quad (12)$$

where  $\kappa = 2\hbar k^2/m$  determines the kinetic-energy term and  $\delta = \omega_R^2/2\Delta$  the atom-field coupling. The operators occurring on the right-hand side (r.h.s.) are defined by the relations

$$\hat{B}_0|\mu\rangle = \mu|\mu\rangle, \quad \hat{B}_\pm|\mu\rangle = |\mu \pm 1\rangle. \quad (13)$$

They differ from the corresponding relations (10) in that now the strength of the hopping operators is uniform.

This Hamiltonian (12) has the same form as Eq. (9), even though they describe completely different physical situations. The difference is mathematically characterized by the commutation relations. The SU(2) relations (7) are replaced by the simpler set

$$[\hat{B}_0, \hat{B}_\pm] = \pm \hat{B}_\pm, \quad [\hat{B}_+, \hat{B}_-] = 0, \quad (14)$$

which is easily found from their explicit expressions (13). The two operators  $\hat{B}_\pm$  are found to commute. A result of this difference is that the state space in the two-well case has a finite dimension  $2J+1=N+1$ , whereas the momentum space has an infinite number of dimensions.

A mathematically identical set of operators occurs in the description of the dynamics of the Wannier-Stark system, consisting of a particle in a periodic potential with an additional uniform force [14]. In that case, the eigenstates of  $\hat{B}_0$  represent the spatially localized Wannier states, rather than the momentum states.

We recall three approximate solutions of the evolution governed by Hamiltonian (12), which are valid in different situations, and which allow analytical solutions.

The Raman-Nath regime is valid for interaction times that are so short that the atom has no time to propagate. Then the quadratic term in Eq. (12) can be neglected, and the evolution is determined by the atom-field coupling  $\delta(t)$ . The evolution operator is simply  $\hat{U} = \exp[i\phi(\hat{B}_+ + \hat{B}_-)/2]$ , where  $\phi = \int dt \delta(t)$  is the integral of the coupling constant over the evolution period. The matrix elements of the resulting evolution operator for the pulse can be found by operator algebra in the form [14]

$$\langle \mu' | \hat{U} | \mu \rangle = i^{\mu' - \mu} J_{\mu' - \mu}(\phi), \quad (15)$$

in terms of Bessel functions. For an initial state  $|\mu\rangle$  with a well-determined momentum, the time-dependent state following the pulse can be expressed as

$$|\Psi(t)\rangle \approx \sum_{\mu'} e^{-i\kappa t \mu'^2} |\mu'\rangle \langle \mu' | \hat{U} | \mu \rangle. \quad (16)$$

This leads to explicit analytical expressions for diffraction experiments [11]. The probability of transfer of  $n$  units of momentum is proportional to  $|J_n(\phi)|^2$ .

The Bragg regime is valid when the coupling  $\delta$  between neighboring momentum states is small compared to the kinetic-energy separation  $\approx 2\hbar\kappa\mu$  of the initial state  $|\mu\rangle$  from its neighboring states  $|\mu+1\rangle$ . This initial state leads to an oscillating time-dependent state between the two states  $|\mu\rangle$  and  $|\mu\rangle$  with the same kinetic energy

$$|\Psi(t)\rangle = \cos \frac{\Omega_\mu t}{2} |\mu\rangle + i \sin \frac{\Omega_\mu t}{2} |-\mu\rangle, \quad (17)$$

apart from an overall phase factor. This can only occur when the momentum transfer  $2\mu$  (in units of  $2\hbar k$ ) is an integer, which corresponds precisely to the Bragg condition.

The *Pendellösung* frequency is given by  $\Omega_\mu = \delta / (2\kappa)^{2\mu-1} / [(2\mu-1)!]^2$  [13]. This expression is fully analogous to the effective Rabi frequency for a resonant multiphoton transition, with nonresonant intermediate states [15,16].

The regime of adiabatic coupling arises for a time-dependent atom-field coupling  $\delta(t)$  that varies sufficiently slowly, so that an initial energy eigenstate remains an eigenstate. The adiabaticity condition in the present case reads

$$\frac{d\delta}{dt} \ll \kappa \delta. \quad (18)$$

When an atom passes a standing wave with a sufficiently smooth variation of the intensity, and the Bragg condition is fulfilled, the presence of two initially degenerate eigenstates  $|\pm\mu\rangle$  leads to interference after the passage, which produces two outgoing beams. Because of the similarity between the two Hamiltonians (9) and (12), these well-known diffraction cases can be expected to have analogies in the dynamics of the two-well problem.

#### IV. SYMMETRY CONSIDERATIONS OF GENERIC HAMILTONIAN

Hamiltonians (9) and (12) can be represented in the generic form

$$\hat{H} = -\hbar \delta \hat{L}_x + \hbar \kappa \hat{L}_z^2, \quad (19)$$

with  $\hat{L}_x = (\hat{L}_+ + \hat{L}_-)/2$ ,  $\hat{L}_z = \hat{L}_0$ , where the operators  $\hat{L}_i$  represent  $\hat{J}_i$  or  $\hat{B}_i$ , depending on the commutation rules and the corresponding algebra that they obey. In the two-well case, the eigenstates  $|\mu\rangle$  of the operator  $\hat{L}_z$  represent number states in the two-well case, with the eigenvalue  $\mu$  half the number difference between the wells. In the diffraction case, the states  $|\mu\rangle$  are momentum eigenstates. In this latter case, the coupling between neighboring momentum states is independent of  $\mu$  [Eq. (13)], whereas in the two-well case the  $\mu$  dependence of the hopping operator indicated in Eq. (10) reflects the bosonic accumulation effect. A consequence of this is also that the Hamiltonian in the diffraction case couples an infinite number of states  $|\mu\rangle$ , whereas in the two-well case the number of coupled states has the finite value  $N+1$ . In the diffraction case, we restrict ourselves to the situation that the Bragg condition is respected. Therefore, both in the diffraction case and in the two-well case  $\mu$  attains either integer or half-integer values. The action of  $\hat{L}_z$  is the same in both cases.

Hamiltonian (19) is invariant for inversion of  $\mu$ . In order to demonstrate this, we introduce the inversion operator  $\hat{P}$ , defined by the relation  $\hat{P}|\mu\rangle = |-\mu\rangle$ . In the diffraction case, the operator  $\hat{P}$  corresponds to inversion of momentum, which does not change the kinetic energy. In the two-well case, the operator  $\hat{P}$  represents interchanging the particle numbers in the two wells, which has no effect on the interparticle interaction. The commutation rules of the inversion operator with the operators  $\hat{L}_i$  are specified by  $\hat{P}\hat{L}_z\hat{P}$

$= -\hat{L}_z$ ,  $\hat{P}\hat{L}_\pm\hat{P}=\hat{L}_\mp$ , so that  $\hat{P}$  inverts  $\hat{L}_y$  and  $\hat{L}_z$ , and commutes with  $\hat{L}_x$ . It follows that Hamiltonian (19) commutes with  $\hat{P}$ , so that it is invariant for inversion of  $\mu$ . Therefore, the Hamiltonian has vanishing matrix elements between the even and the odd subspaces, which are the eigenspaces of  $\hat{P}$  with eigenvalue 1 and  $-1$ , respectively. For half-integer  $\mu$  values, these spaces are spanned by the states

$$|\mu\rangle_+ \equiv \frac{|\mu\rangle + |-\mu\rangle}{\sqrt{2}}, \quad |\mu\rangle_- \equiv \frac{|\mu\rangle - |-\mu\rangle}{\sqrt{2}}, \quad (20)$$

for positive values of  $\mu$ . In the case of integer  $\mu$  values, the state  $|\mu=0\rangle$  also belongs to the even subspace. The even and odd subspace evolve independently from one another. This symmetry property of  $H$  depends on the fact that it is quadratic in the operator  $\hat{L}_z$ .

The action of the quadratic term in Hamiltonian (19) on the new basis is simply given by the relation  $\hat{L}_z^2|\mu\rangle_\pm = \mu^2|\mu\rangle_\pm$ . The action of the coupling term in the Hamiltonian can be expressed in a general form by introducing coefficients  $F_\mu$  for non-negative values of  $\mu$ . In the case of the  $\text{su}(2)$  algebra, we define  $F_\mu = f_\mu$ , whereas in the diffraction case we simply have  $F_\mu = 1$ . The matrix elements of  $\hat{L}_x$  can be fully expressed in terms of the coefficients  $F_\mu$  for positive  $\mu$ . Within the even or the odd subspace, the operator  $\hat{L}_x$  has off-diagonal matrix elements only between two states for which the values of  $\mu$  differ by one, and we find

$$\pm\langle\mu+1|\hat{L}_x|\mu\rangle_\pm = \frac{1}{2}F_{\mu+1}, \quad (21)$$

provided that the value of  $\mu$  is positive. These matrix elements coincide with those on the basis of the states  $|\mu\rangle$ . For the state  $|\mu=0\rangle$ , which belongs to the even subspace of a manifold of states with integer  $\mu$  values, the matrix element is

$$+\langle 1|\hat{L}_x|0\rangle = F_1/\sqrt{2}. \quad (22)$$

On the other hand, in a manifold of states with half-integer  $\mu$  values,  $\hat{L}_x$  has a single nonzero diagonal element for  $\mu = 1/2$ , that is given by

$$\pm\langle 1/2|\hat{L}_x|1/2\rangle_\pm = \pm F_{1/2}. \quad (23)$$

Hence, in the case of half-integer  $\mu$  values, the Hamiltonian projected on the even and the odd subspace differ exclusively in the diagonal matrix element for  $\mu = \frac{1}{2}$ , for which we find

$$\pm\langle 1/2|\hat{H}|1/2\rangle_\pm = \frac{\hbar\kappa}{4} \mp \frac{1}{2}\hbar\delta F_{1/2}. \quad (24)$$

For integer values of  $\mu$ , the Hamiltonian for the odd subspace is identical to the Hamiltonian for the even subspace

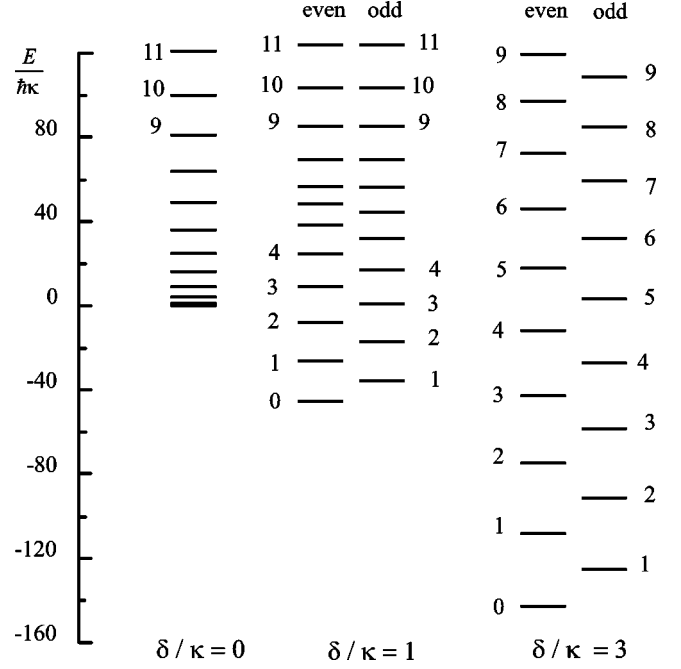


FIG. 1. Energy levels in units of  $\hbar\kappa$  for the double well with  $N=100$  particles, for various values of  $\delta/\kappa$ . The levels are labeled by the quantum number  $\mu$ .

with  $\mu \geq 1$ . The only difference is that the even subspace also contains the state  $|0\rangle$ , which is coupled to the other states by the matrix element

$$+\langle 1|\hat{H}|0\rangle = \langle 0|\hat{H}|1\rangle_+ = -\hbar\delta F_1/\sqrt{2}. \quad (25)$$

In both cases, the difference between the Hamiltonian parts on the even and odd subspaces are proportional to  $\delta$ . These differences are responsible for the energy splitting between the even and the odd energy eigenstates. Moreover, since these differences in the Hamiltonian parts occur for low values of  $\mu$ , we expect that for a fixed value of  $\delta/\kappa$ , the even-odd energy splittings decrease for increasing  $\mu$  values. This is confirmed by numerical calculations. In Figs. 1 and 2, we display the energy levels of the Hamiltonian, for a few values of  $\delta/\kappa$ , both for the double-well case (with  $N=100$ ), and for the diffraction case. The energy levels are found to be alternately even and odd, with increasing energy. In the two-well case, the energy shifts and splittings due to the coupling are larger for the same value of  $\delta/\kappa$  and the same value of  $\mu$ . This arises from the factor  $F_\mu$ , which is unity in the diffraction case, whereas in the two-well case it decreases from  $\sim J=N/2$  at  $\mu=0$  to zero at  $\mu=J$ . In fact, the condition for weak coupling is that matrix elements coupling the states  $|\mu\rangle$  and  $|\mu-1\rangle$  are small compared with their unperturbed energy separation. This condition can be expressed as

$$\lambda_\mu = \frac{\delta}{2\kappa} \frac{F_\mu}{2\mu-1} < 1. \quad (26)$$

This confirms that for a given value of  $\delta/\kappa$ , the region of weakest coupling occurs for the highest values of  $\mu$ . In the



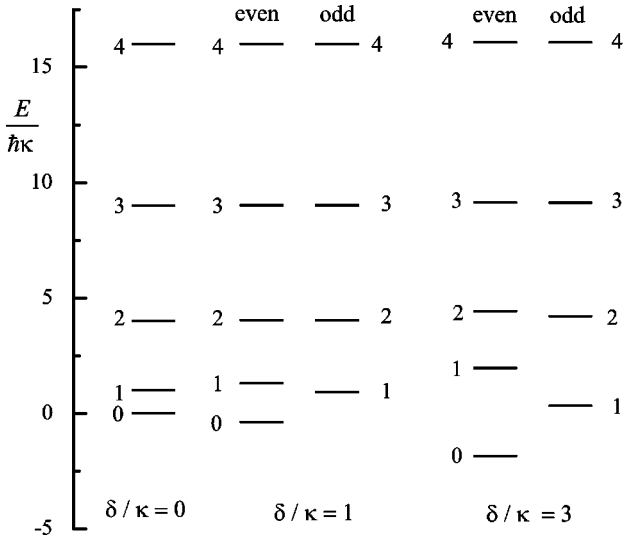


FIG. 2. Energy levels in units of  $\hbar\kappa$  for the diffraction case, for various values of  $\delta/\kappa$ .

two-well case, the lowest-energy states start out to be nearly equidistant for low- $\mu$  values as long as  $\lambda_\mu$  is large.

## V. PENDELLÖSUNG OSCILLATIONS

The energy splittings between the even and the odd eigenstates give rise to time-dependent states that oscillate between the states  $|\pm\mu\rangle$ . In the diffraction case, they correspond to the well-known Pendellösung oscillations in the Bragg regime. Here we show that similar oscillations can occur for the two-well problem, and we give an analytical estimation of the oscillation frequencies. For the generic Hamiltonian given by Eq. (19), the Bragg condition is fulfilled when inequality (26) holds.

The energy differences between the even and odd states to lowest order in  $\lambda_\mu$  can be found from the effective Hamiltonian for two degenerate states that are coupled via a number of nonresonant intermediate states. This situation occurs for the states  $|\pm\mu\rangle$ , with their  $2\mu-1$  intermediate states. In this case, the intermediate states can be eliminated adiabatically, as demonstrated in Sec. 18.7 of Ref. [15]. The resulting effective Hamiltonian for these two states  $|\pm\mu\rangle$  has an off-diagonal element that is the ratio between two products. The numerator contains the product of the successive  $2\mu$  matrix elements  $-\hbar\delta F_\mu/2$  of the Hamiltonian coupling neighboring states, and the denominator is the product of the  $2\mu-1$  unperturbed energy differences of the degenerate states  $|\pm\mu\rangle$  with the successive intermediate states. In the diffraction case, this result coincides with the calculation given in Ref. [12], which was obtained by diagonalizing a tridiagonal matrix and keeping only the lowest order in  $\delta/\kappa$ .

Generalizing this result to the present case of the two states  $|\pm\mu\rangle$ , we find that the effective Hamiltonian has the diagonal element

$$\langle \pm\mu | \hat{H}_{eff} | \pm\mu \rangle = \hbar\kappa\mu^2, \quad (27)$$

and the off-diagonal element

$$\langle \mp\mu | \hat{H}_{eff} | \pm\mu \rangle = -\hbar\Omega_\mu/2, \quad (28)$$

with  $\Omega_\mu$  an effective oscillation frequency given by

$$\Omega_\mu = (-1)^{2\mu+1} \frac{1}{2^{2\mu-1}} \frac{\delta^{2\mu}}{\kappa^{2\mu-1}} \frac{1}{[(2\mu-1)!]^2} F. \quad (29)$$

The factor  $F$  is just the product of the coefficients  $F_\mu$  successively coupling the states intermediate between  $|\mu\rangle$  and  $|\pm\mu\rangle$ . In the diffraction case, we simply have  $F=1$ , whereas in the case of SU(2) symmetry, applying to the double well, we find

$$F = \frac{(J+\mu)!}{(J-\mu)!}. \quad (30)$$

These expressions are valid both for integer and half-integer values of  $\mu$ . The eigenstates of the effective Hamiltonian are the even and odd states, and the eigenvalue equations are  $\hat{H}_{eff}|\mu\rangle_\pm = (\hbar\kappa\mu^2 \mp \hbar\Omega_\mu/2)|\mu\rangle_\pm$ . For integer values of  $\mu$ , the frequency  $\Omega_\mu$  is negative, so that the even states  $|\mu\rangle_+$  are shifted upwards and the odd states are shifted downwards in energy. The opposite is true for half-integer values of  $\mu$ . In both cases, the ground state is even, and the energy eigenstates for increasing energy are alternatingly even and odd. In view of the results of the numerical calculation mentioned above, one may expect that this alternating behavior of the even and odd eigenstates is valid for all finite values of the ratio  $\delta/\kappa$ . It is interesting to notice that in the special case that  $\mu = J \equiv N/2$ , Eq. (29) for the two-well case coincides with the ground-state energy splitting of two coupled quantum anharmonic oscillators, which model two coupled vibrational degrees of freedom in a molecule [17].

For an initial state  $|\mu\rangle$ , the effective Hamiltonian  $\hat{H}_{eff}$  leads to a time-dependent state that is given by Eq. (17), apart from an irrelevant overall phase factor. This shows that the oscillating solution (17) corresponding to the Bragg regime of diffraction can be generalized to the case of a condensate in a double well. The same expression (17) remains valid, while the oscillation frequency  $\Omega_\mu$  is determined by Eqs. (29) and (30). This describes a state of the condensate atoms in the double well in the weak-coupling limit. In this case, the state oscillates between the Fock states  $|n_1, n_2\rangle = |N/2 + \mu, N/2 - \mu\rangle$  and  $|n_1, n_2\rangle = |N/2 - \mu, N/2 + \mu\rangle$ .

Obviously, when the initial state is given by  $|\mu\rangle_\pm$ , the system is in a stationary state, and no oscillations occur. In this case, Pendellösung oscillations can still be induced by including in the Hamiltonian a term that is linear in  $\hat{L}_z$ . In the diffraction case, there is no obvious physical realization of such a term. For the Wannier-Stark system, where the quadratic term in  $\hat{L}_z^2$  is absent, the linear term can be realized by imposing a uniform force, which gives rise to Bloch oscillations [14,18]. In the case of the BEC in a double well, a term  $\hbar\xi\hat{L}_z$  in the Hamiltonian can be realized by imposing an energy difference  $\hbar\xi$  between the single-particle ground states in the two wells. When this term is periodically varying, it can be used for coherent control of the condensate [20]. The additional term couples the even and odd sub-

spaces, thereby breaking the symmetry of the Hamiltonian. On the basis of the states  $|\mu\rangle_{\pm}$ , the effective Hamiltonian attains the off-diagonal element

$${}_{\pm}\langle\mu|\hat{H}_{eff}|\mu\rangle_{\mp}=\hbar\xi\mu. \quad (31)$$

When we assume that both  $\delta$  and  $\xi$  are small compared with the splitting due to the interparticle interaction  $\kappa$ , so that we remain in the Bragg regime, the two states  $|\pm\mu\rangle$  remain decoupled from the other number states, and we have an effective two-state system. In practice, the parameter  $\xi$  can be easily controlled, so that many effects of two-state atoms [19] can also be realized for these two states. For example, in analogy to the excitation of ground-state by an adiabatic sweep across the resonance, one could create an effective transfer from the state  $|\mu\rangle$  to the state  $|\mu\rangle$  by varying the parameter  $\xi$  adiabatically from a positive to a negative value that is large compared to  $\Omega_{\mu}$ . This gives an effective collective transfer of  $n=2\mu$  atoms from one well to the other one.

## VI. TIME-DEPENDENT COUPLING

When the coupling  $\delta(t)$  varies with time, the time-dependent eigenstates of the Hamiltonian are coupled to each other. The eigenstate that correlates in the limit  $\delta \rightarrow 0$  to the state  $|\mu\rangle_{\pm}$  is denoted as  $|\varphi_{\mu}^{\pm}\rangle$ . Note that even eigenstates are only coupled to other even eigenstates, and odd eigenstates to odd eigenstates. The coupling results from the time dependence of the eigenstates. In fact, the term in the Schrödinger equation coupling  $|\varphi_{\mu}^{\pm}\rangle$  to  $|\varphi_{\nu}^{\pm}\rangle$  is proportional to

$$\left\langle \varphi_{\nu}^{\pm}(t) \left| \frac{d}{dt} \right| \varphi_{\mu}^{\pm}(t) \right\rangle = -\langle \varphi_{\nu}^{\pm}(t) | \hat{L}_x | \varphi_{\mu}^{\pm}(t) \rangle \frac{\hbar \dot{\delta}(t)}{E_{\nu}^{\pm} - E_{\mu}^{\pm}}, \quad (32)$$

$\mu \neq \nu.$

This coupling is ineffective in the case that the r.h.s. of Eq. (32) is small compared with  $(E_{\nu}^{\pm} - E_{\mu}^{\pm})/\hbar$ . In this case, an initial eigenstate remains an eigenstate at all times. This is the standard case of adiabatic following, which has been discussed in the diffraction case [13]. Since within the even or the odd subspace there are no degeneracies, the dynamics of adiabatic following is particularly simple. When the coupling coefficient  $\delta$  is smoothly switched on, with the system initially in the state  $|\mu\rangle = (|\mu\rangle_{+} + |\mu\rangle_{-})/\sqrt{2}$ , the time-dependent state is obviously

$$|\Psi(t)\rangle = e^{-i\vartheta(t)} (|\varphi_{\mu}^{+}\rangle e^{-i\eta(t)/2} + |\varphi_{\mu}^{-}\rangle e^{i\eta(t)/2})/\sqrt{2}, \quad (33)$$

with  $\vartheta(t) = \int^t dt' [E_{\mu}^{+}(t') + E_{\mu}^{-}(t')]/2\hbar$  the average phase and  $\eta(t) = \int^t dt' [E_{\mu}^{+}(t') - E_{\mu}^{-}(t')]/\hbar$  the accumulated phase difference of the two eigenstates. In a time interval that the coupling  $\delta$  is constant, the phase difference  $\eta(t)$  increases linearly with time, and state (33) gives rise to expectation values oscillating at the single frequency  $[E_{\mu}^{+}(t') - E_{\mu}^{-}(t')]/\hbar$ . When the coupling is switched off again, the phase difference approaches a constant limiting value  $\bar{\eta} = \eta(\infty)$ . State (33) at later times corresponds to a linear superposition of the states  $|\pm\mu\rangle$  proportional to

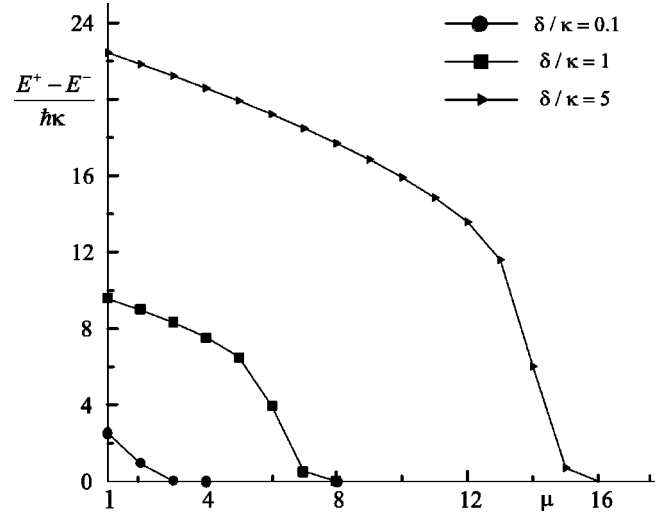


FIG. 3. Even-odd energy splittings for the double well as a function of the quantum number  $\mu$ , for various values of  $\delta/\kappa$  and for  $N=100$  particles.

$|\mu\rangle \cos(\bar{\eta}/2) + |\mu\rangle \sin(\bar{\eta}/2)$ . Again, as we see, this effect that is known in the diffraction case also has a counterpart for the double-well problem, where adiabatic switching of the coupling between the wells leads to a linear superposition of the Fock states  $|n_1, n_2\rangle = |N/2 + \mu, N/2 - \mu\rangle$  and  $|n_1, n_2\rangle = |N/2 - \mu, N/2 + \mu\rangle$ . By proper tailoring of the pulse, the final state can be made to coincide with either one of these Fock states, with the even state  $|\mu\rangle_{+}$  or with the odd state  $|\mu\rangle_{-}$ , depending on the precise value of the accumulated phase difference  $\bar{\eta}$ , which in turn is determined by the energy difference  $E_{\mu}^{+} - E_{\mu}^{-}$  between the even and the odd eigenstate. In Fig. 3, we plot this energy difference in the two-well case, for  $N=100$ , and for a few values of  $\delta/\kappa$ . This shows that these splittings decrease monotonously for increasing quantum number  $\mu$ . When  $\delta/\kappa$  is not small, the decrease starts out to be slow, and then falls rapidly to zero.

In contrast, when the coupling term  $\delta(t)$  has the form of a short pulse around time zero, such that the action of the quadratic term can be neglected during the pulse, the initial state  $|\mu\rangle$  couples to all other states  $|\mu'\rangle$ . The state vector has exactly the same form (16) as for diffraction in the Raman-Nath regime. For the two-well problem, the evolution operator takes the form  $\hat{U} = \exp(i\phi\hat{L}_x)$  with  $\phi = \int dt \delta(t)$ , which has matrix elements that can be expressed in the Wigner rotation matrices [21] by

$$\langle \mu' | \hat{U} | \mu \rangle = i^{\mu' - \mu} d_{\mu', \mu}^J(\phi), \quad (34)$$

with  $J=N/2$ . A comparison with Eq. (15) shows that for the two-well-problem, the Wigner functions play the same role as the Bessel functions in the diffraction case.

## VII. CONCLUSION

In this paper, we have analyzed both the similarity and the difference between the dynamical behavior of atom diffraction from a standing wave and a Bose-Einstein condensate in

a double-well potential. In both cases, the Hamiltonian is given by the generic form (19), the only difference being in the commutation rules for the operators  $\hat{L}_i$  with  $i=x,y,z$ . Well-known diffraction phenomena as Pendellösung oscillations between opposite momenta in the case of Bragg diffraction, and the result of adiabatic transitions between momentum states have counterparts in the behavior of the atom distribution over the two wells, in the case that the coupling between the wells is weak compared to the interatomic interaction or slowly varying with time. A common underlying reason for these effects is the symmetry of the Hamiltonian for inversion  $\mu \leftrightarrow -\mu$ , and the energy splitting between even and odd states arising from the coupling term. In these cases, effective coupling occurs between the states  $|n_1, n_2\rangle$  and  $|n_2, n_1\rangle$  with opposite imbalance between the particle numbers in the two wells. These states are coupled without population of the intermediate states, so that a number of  $n_1 - n_2$  particles oscillate collectively between the two wells. The interparticle interaction is essential for this effect to oc-

cur. A simple analytical expression is obtained for the Pendellösung frequency. An initial state  $|n_1, n_2\rangle$  with a well-determined number of atoms in each well can be transferred to a linear superposition of  $|n_1, n_2\rangle$  and  $|n_2, n_1\rangle$ , which is a highly entangled state of the two wells. A similar analogy is obtained to diffraction in the Raman-Nath regime. For the double-well problem this requires that the coupling is sufficiently short to ignore dynamical effect of the atomic interaction during the coupling. The well-known diffraction pattern in terms of the Bessel function is replaced by elements of the Wigner rotation matrix for the double well. These effects do not show up in the mean-field approximation, where the Gross-Pitaevski equation holds.

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