The single-atom box: bosonic staircase and effects of parity

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We have developed a theory of a Josephson junction formed by two tunnel-coupled Bose-Einstein condensates in a double-well potential in the regime of strong atom-atom interaction for an arbitrary total number N of bosons in the condensates. The tunnel resonances in the junction are shown to be periodically spaced by the interaction energy, forming a single-atom staircase sensitive to the parity of N even for large N. One of the manifestations of the staircase structure is the periodic modulation with the bias energy of the visibility of the interference pattern in lattices of junctions.

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Bose-Einstein condensates (BECs) have a unique ability to give rise to individual quantum states occupied with a macroscopically large number of particles. The interference of the wavefunctions of such macroscopic states leads to a variety of macroscopic quantum phenomena, the most studied of which is the Josephson effect: the flow of current across a potential barrier due to the interference of the condensate states on the two sides of the barrier. For a long time since the original discovery [1], this effect has been studied in solid-state "Josephson junctions" [2]: two weakly-coupled superconductors, in which the condensates are formed by Cooper pairs [3]. At energies smaller than the binding energy of electrons in Cooper pairs, the characteristics of Josephson junctions can be discussed directly in terms of the properties of the Cooper-pair condensates [4]. In this case, the two dynamic variables of the Josephson junction (JJ) are the phase difference ϕ between the condensate wavefunctions on the two sides of the barrier and the half-difference n of the number of Cooper pairs in the two condensates. Since the phase ϕ and the "charge" n are conjugate quantum variables [5], the dominant qualitative feature of the JJ dynamics is the transition from the classical dynamics of ϕ in large junctions to the classical dynamics of n in small junctions. The classical charge regime is characterized by the correlated transfer of individual Cooper pairs [6], with the simplest "Cooper-pair box" system [7, 8] providing the most basic demonstration of this transfer in the "Cooper-pair staircase": the step-wise increase of n with the junction bias that corresponds to successive transfers of Cooper pairs one by one through the junction. The transition between the quasiclassical dynamics of ϕ and n is affected by the energy dissipation in the junction [9] (with the classical-n regime requiring small dissipation) but can generally be understood as competition between the tunnel amplitude and the interaction energy of Cooper pairs.

In the case of solid-state JJs, the bosonic junction model is partly a pedagogical simplification. With ultracold atoms in optical traps of double-well structure, this model, however, can [10, 11] and recently has been realized directly. It has been studied experimentally both in the regime of larger-scale BECs in the wells with relatively weak transverse confinement [12–14], when they exhibit the Josephson effect governed by the classical dynamics of the phase difference ϕ, and in the "Mott insulator" regime [15, 16], when the total number N of atoms in the double-well structure is small $N = 1, 2$ and the number difference n behaves quasiclassically. One of the main dynamic features of the regime of classical n is the existence of resonances, as a function of the energy bias ϵ, corresponding to the tunneling of individual atoms [17–19]. The goal of this work is to study these "single-atom" resonances for an arbitrary number of atoms N in the BEC Josephson junction, in both the interaction-dominated Mott-insulator regime and the case of large-scale BECs. We show that the main features of the single-atom effects in BEC junctions are quite similar to those in solid-state JJs [6–8], and in particular, include the periodic spacing of resonances in the "single-atom staircase". There are, however, several new effects produced by the fixed total number of bosons N in the BEC junction, as opposed to solid-state JJs where the total number of particles is not well-defined. One is the modulation of the strength of the resonances with the number difference n, which reflects the collective nature of the tunnel coupling of the BECs even in the regime of single-atom tunneling. Another is the dependence of the resonances on the parity (even or odd) of the total number of bosons N.

We consider N bosons in a double-well potential approximated by a two-site Bose-Hubbard model [20–23]:

$$H_0 = \frac{U}{2}\sum_{i=1,2} n_i(n_i-1) - \Delta(a_1^\dagger a_2 + a_2^\dagger a_1) - \epsilon(n_1 - n_2)\,. \quad (1)$$

Here $n_i = a_i^\dagger a_i$ and $a_i^\dagger$ (a_i) creates (annihilates) a boson in the lowest-energy state localized in the ith well, Δ is the tunnel coupling of these two states, 2ϵ is their difference in on-site energy, and U is the on-site interaction. The Hamiltonian (1) conserves the total number of bosons $N = n_1 + n_2$, and after separation of N, it takes the following form (up to a constant energy shift):

$$H_0 = Un^2 - 2\epsilon n - \Delta(a_1^\dagger a_2 + a_2^\dagger a_1)\,. \tag{2}$$

Here $n \equiv (n_1 - n_2)/2$ is the occupation number difference between the two wells. While N does not enter the Hamiltonian (2) explicitly, it influences the junction dynamics by limiting the range of the possible values of the number difference $n \in \{-N/2, -N/2+1, ..., N/2\}$, i.e., to integer or half-integer n for even or odd N, respectively. In general, the kinematics of the model defined by Eq. (1) or (2) gives Schwinger's representation of the angular momentum $\vec{J}$ of magnitude $N/2$ (see, e.g., [24]). In this identification, n is the z-component J_z of the momentum, and the tunneling term in the Hamiltonian is $-2\Delta J_x$. Since the properties of the integer and half-integer momenta are quite different, this *parity effect* makes the energy characteristics of the bosonic junction (2) dependent on the parity of N, as we show in more detail below.

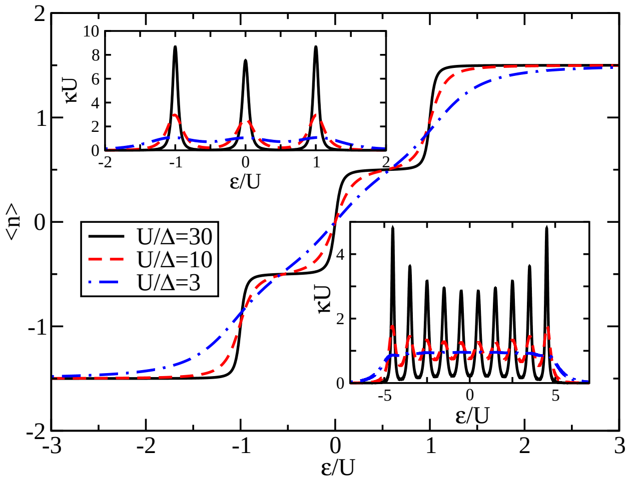

FIG. 1: Average number difference $\langle n \rangle$ in the ground state of the double-well BEC Josephson junction for $N = 3$ as a function of the energy difference ϵ between the two wells, for several values of the ratio of interaction energy versus tunnel amplitude U/Δ. Curves with $U/(N\Delta) \gg 1$ show the single-atom staircase, which is smeared with increasing tunneling strength. Left inset: Compressibility $\kappa = \partial\langle n \rangle/\partial\epsilon$ showing the peak structure associated with the single-atom resonances. For odd N, there is a resonance in the unbiased junction $\epsilon \simeq 0$. Right inset: κ for $N = 10$ bosons in the two wells. With increasing tunneling strength, κ changes from sharp single-atom resonances to a quasiclassical behavior with constant large-scale compressibility $\simeq 1/U$ and weak sinusoidal single-atom oscillations.

To see this quantitatively, we start with the regime of strong interaction, $U \gg N\Delta$. In this case, the tunnel coupling $\lambda \equiv \Delta[(N/2+n+1)(N/2-n)]^{1/2}$ of the states n and $n+1$ that differ by the transfer of one atom in the junction, is small, $\lambda \ll U$. This means that these states are coupled effectively only in the vicinity of certain values of the energy bias $\epsilon \approx \epsilon_n$,

$$\epsilon_n \equiv (n + 1/2)U\;, \tag{3}$$

when the interaction energy difference between them is suppressed and atoms can tunnel across the junction. Since these resonances are uniformly spaced by U, the average number difference $\langle n \rangle$ in the ground state of the junction shows a regular *staircase-like structure* (Fig. 1) similar to the corresponding structure in the Cooper-pair box [7, 8]. The curves in Fig. 1 are obtained by straightforward numerical diagonalization of the Hamiltonian (2) and show also the smearing of the staircase by tunneling when it is increased to the level $\Delta \sim U/N$. At $U \gg N\Delta$, the system dynamics reduces in the vicinity of each step to the two states n and $n+1$, and one can find directly the shape of the steps in the staircase:

$$\langle n \rangle = n + \frac{1}{2}\left(1 + \frac{\epsilon - \epsilon_n}{[(\epsilon-\epsilon_n)^2 + \lambda^2]^{1/2}}\right)\,. \tag{4}$$

The shape of each of the single-atom transitions is seen more clearly in the resonant peaks in the compressibility $\kappa = \partial\langle n \rangle/\partial\epsilon$ of the ground state. In particular, Eq. (4) shows that the maximum of each peak reflects directly the effective tunnel coupling of the two states:

$$\kappa = \frac{1}{2\lambda} = \frac{1}{2\Delta}[(N/2+n+1)(N/2-n)]^{-1/2}\,. \tag{5}$$

This equation agrees with the curve for strongest interaction in the right inset to Fig. 1, and shows that the enhancement of the tunneling amplitude from the single-particle value Δ to the multi-particle value $\lambda \sim N\Delta$ by the BEC coherence manifests itself even in the regime of single-atom tunneling. The modulation (5) is a quantum consequence of the dependence of the critical current of the BEC junction on the population imbalance between the two wells that also leads to "self-trapping" of the condensate in the case of classical Josephson dynamics [12, 14, 25].

The main qualitative feature of the staircase that reflects the parity effect is that the steps (4) occur at half-integer values of energy bias ϵ (in units of interaction energy U) for even N and integer ϵ/U for odd N, see Eq. (3). In particular, the tunneling is always suppressed for even N in the symmetric unbiased junction, when $\epsilon \simeq 0$, but there is a tunneling resonance at $\epsilon = 0$ for odd N (Fig. 1). This resonance at $\epsilon = 0$ has an obvious interpretation in the single-atom regime with strong interaction energy, $U \gg N\Delta$: the interaction energy of N atoms is degenerate with respect to the last atom out of an odd total number N being placed in the left or right well.

This simple interpretation is not valid in junctions with large N, when $U \ll N\Delta$, but the parity effect exists even in this case, provided the interaction energy still plays a role in the junction dynamics, $U \gg \Delta/N$. (If $U \ll \Delta/N$, the interaction is not essential and the junction represents a collection of N independent two-state systems of individual atoms.) In this regime, the number-difference fluctuations δn around the average value $\langle n \rangle = \epsilon/U$ have the magnitude (estimated from the Hamiltonian (6) below) $1 \ll \delta n \simeq (N\Delta/U)^{1/4} \ll \sqrt{N}$. If $\langle n \rangle$ is not too close to the boundaries $\pm N/2$ of the allowed interval for n, this means that effectively there are no restrictions on the values of n, and variations of the tunneling amplitude λ are negligible. As a result, one can define a phase $\phi \in [0, 2\pi]$ conjugate to n and the Hamiltonian (2) takes a form that essentially coincides with that of the "solid-state" Josephson junction:

$$H = -\frac{\epsilon^2}{U} - U\frac{\partial^2}{\partial \phi^2} - 2\lambda(\epsilon)\cos\phi\,, \tag{6}$$

where $\lambda(\epsilon) = \Delta[(N/2)^2 - (\epsilon/U)^2]^{1/2}$. The boundary conditions on the wavefunctions $\psi(\phi)$, however, depend on the bias ϵ and the parity of N:

$$\psi(\phi + 2\pi) = (-1)^N e^{-i2\pi\epsilon/U}\psi(\phi)\,. \tag{7}$$

Using the known result [6] for the Hamiltonian (6) we see that the ground state energy of the bosonic junction is

$$E_0 = -(\epsilon^2/U) - (-1)^N \delta_0 \cos(2\pi\epsilon/U)\,, \tag{8}$$

where $\delta_0 \simeq (1/\pi)(\lambda U)^{1/2}\exp[-8(\lambda/U)^{1/2}]$. The first term in (8) describes the large-scale, mean-field compressibility $\kappa = -(1/2)\partial^2 E_0/\partial\epsilon^2 = 1/U$ for ϵ within the range $[-NU/2, NU/2]$ (right inset to Fig. 1). Qualitatively, this compressibility is dominated by the interaction, since the total interaction energy scales as N^2 as opposed to the tunneling energy which is proportional to N. The second term in (8) describes the sinusoidal single-atom oscillations of small amplitude which increase at the ends of the range of ϵ because of the decrease of λ (right inset to Fig. 1). These oscillations represent what is left of the single-atom resonances when they are washed out by strong tunneling, i.e., describe the discreteness of the BEC flow in this quasiclassical regime. The position of the oscillations as a function of the bias ϵ depends on the parity of N, with a minimum in κ at $\epsilon \simeq 0$ for even N and a maximum for odd N.

The sensitivity of the bosonic JJ to individual atoms makes it interesting to consider the situation with one extra "foreign" atom in the junction. Motivated by experiments on Bose-Fermi mixtures [26], we assume that this extra particle is a "fermion", although its statistics does not play a role in our discussion. Besides the bosonic part H_0 (1), the junction Hamiltonian includes then a fermionic part H_f of the same structure with the tunnel amplitude Δ_f, the number operator n_{fi}, on-site interaction U_f, and a boson-fermion interaction term:

$$H = H_0 + H_f + U_{bf}(n_1 n_{f1} + n_2 n_{f2})\,, \tag{9}$$

The boson-fermion interaction energy U_{bf} can be positive or negative [26]. The difference ϵ in on-site energies is assumed to be the same for bosons and the fermion.

One can follow separately the dynamics of the two types of particles, and we limit our brief discussion to the behavior of the bosons. The average boson number difference $\langle n \rangle$ is shown in Fig. 2 for $N = 3$. In the case of vanishing boson-fermion interaction, $U_{bf} = 0$, we obtain the familiar three steps of height 1. For strong attraction, $U_{bf} \ll -U$, or repulsion, $U_{bf} \gg U$, minimization of the interaction energy requires that the bosons are moving all together, and $\langle n \rangle$ shows only one step of height 3 at $\epsilon = 0$. In our example of 3 bosons, this case is realized already for $|U_{bf}| \geq 2U$. In the intermediate region $|U_{bf}| \leq 2U$, we find a more complex behavior: for $U_{bf} < 0$ and $U_{bf} > 0$ the bosonic steps are shifted, respectively, to and away from the region $\epsilon = 0$. Moreover, for $U_{bf} > 0$ (i.e., for antiferromagnetic coupling between the angular momenta representing bosonic and fermionic parts of the junction), the system is frustrated and the steps have regions with negative slope, see the curves for $U_{bf}/U = 0.5$ and 1. In the "single-atom" regime of small tunneling amplitudes, and for odd N, the region of the negative slope around $\epsilon \simeq 0$ corresponds to the range $\epsilon \in [-U_{bf}/2, U_{bf}/2]$, where $\langle n \rangle$ is described by the following general relation:

$$\langle n \rangle = \frac{1}{2}\frac{\epsilon(\Delta_f^2 - \lambda^2)}{[\epsilon^2(\Delta_f^2 - \lambda^2)^2 + \lambda^2\Delta_f^2 U_{bf}^2]^{1/2}}\,. \tag{10}$$

Note that the slope depends of the relation between the effective boson and fermion tunneling amplitudes.

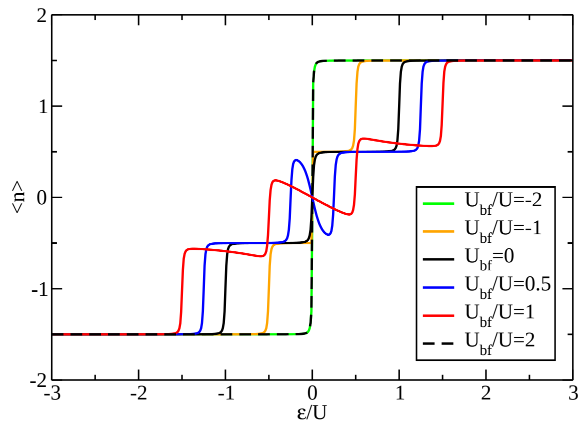

FIG. 2: (color online) Steps in $\langle n \rangle$ as a function of ϵ for $N = 3$ bosons, $N_f = 1$ fermions, $\Delta/U = 0.01$, and $\Delta_f/U = 0.004$.

One way of studying the effects discussed in this work would be to measure the interference pattern of the expanding atomic cloud after switching off an optical lattice of appropriately spaced uncoupled double-well junctions. Such arrays of double wells have already been realized experimentally [27]. The interference of particles within each junction will produce a cosine modulation of the average atom intensity I. The visibility of this modulation pattern is given [28] by the average kinetic (tunneling) energy per boson in units of Δ:

$$v = (I_{max} - I_{min})/(I_{max} + I_{min}) = \langle a_1^\dagger a_2 + a_2^\dagger a_1 \rangle / N \,.$$

In the single-atom regime of the bosonic junction (2), the visibility is modulated by the bias ϵ and reaches its maximum at the resonances (4)

$$v = (\lambda/N)[(\epsilon - \epsilon_n)^2 + \lambda^2]^{-1/2} \,, \qquad (11)$$

where the states of the two wells deviate most strongly from pure number states. For the Bose-Fermi junction (9), v shows a rich dependence on ϵ and U_{bf} that is also related to the staircase structure, see Fig. 3.

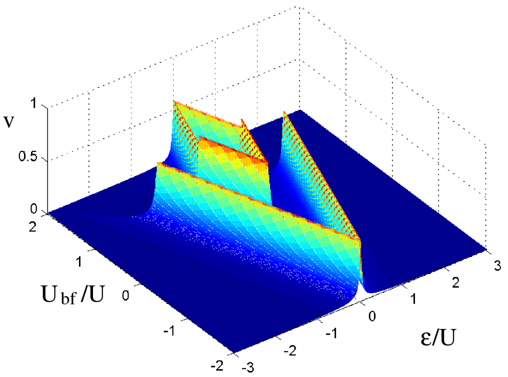

FIG. 3: (color online) Visibility v of the bosonic interference pattern in the Bose-Fermi junction. All the parameters are chosen as in Fig. 2.

In conclusion, we have shown that a Josephson junction formed by two tunnel-coupled BECs shows single-atom effects similar to those in solid-state Josephson junctions. In addition to periodically spaced resonances as a function of the difference in on-site energy leading to a single-atom staircase, there are modulations of the strength of the resonances and parity effects that can be traced back to the fixed total number of bosons N in the BEC junction. A different, e.g. fermionic, additional particle in the junction leads to non-trivial modifications of the staircase, that can be experimentally observed in the visibility of the interference pattern.

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