Effects of a single fermion in a Bose Josephson junction

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We consider the tunneling properties of a single fermionic impurity immersed in a Bose-Einstein condensate in a double-well potential. For strong boson-fermion interaction, we show the existence of a tunnel resonance where a large number of bosons and the fermion tunnel simultaneously. We give analytical expressions for the line shape of the resonance using degenerate Brillouin-Wigner theory. We finally compute the time-dependent dynamics of the mixture. Using the fermionic tunnel resonances as a beam splitter for wave functions, we construct a Mach-Zehnder interferometer that allows complete population transfer from one well to the other by tilting the double-well potential and only taking into account the fermion's tunnel properties.

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I. INTRODUCTION

Bose-Einstein condensates (BEC) have become a valuable resource in current research on many-body physics [1]. Loaded into an optical lattice, the low-energy regime realizes a Bose-Hubbard Hamiltonian [2] whose parameters can be tuned over a wide range by adjusting the optical lattice or engineering particle interactions via Feshbach resonances.

A simpler, although not less interesting, variant of BEC in an optical lattice is obtained when in the Mott insulator regime, the lattice is modulated by an additional laser beam to create local double-well potentials at each lattice site. When tunneling between the local double-well potentials is negligible compared to tunneling inside the double-well potential, the system is well described by a *two-site* Hubbard Hamiltonian. BECs in double-well potentials have received considerable attention in recent years [3]. In [4], the dynamics are discussed both on a mean-field level, where the nonlinear Schrödinger equation becomes the discrete self-trapping equation [5], and in a quantum mechanically exact way. For large enough particle numbers, the two-site Hubbard Hamiltonian can be approximated by the Josephson Hamiltonian [6], which is the reason for these systems to be called Bose Josephson Junctions. A BEC in a double-well potential defines a representation of the rotation group and hence a pseudospin, which can be utilized for quantum information processing and studies of decoherence [7]. Other applications exploit the regime of weak tunneling, where the system behaves similarly to a quantum nanostructure in the sequential tunneling limit [8,9].

A related branch of research is constituted by the investigation of Bose-Fermi mixtures. These have been studied mostly on the mean-field level by solving nonlinear Schrödinger equations for one [10] or two wells [11] or by composite-fermion methods on an optical lattice [12–14]. Phase diagrams have been computed for Bose-Fermi mixtures in three [15] or one dimensions [16–18].

In this paper, we want to study the adiabatic dynamics of a Bose-Einstein condensate in a double-well potential when a single fermionic impurity is added to the system. As these dynamics are accessible by evaluating an appropriate observable in the numerically computed exact ground state of the Hamiltonian, the problem is a static one. Here the notion of tunneling refers to the mixing of two eigenstates of the isolated wells by the tunneling term in the Hamiltonian. This causes a broadening in the steplike profile of the expectation value of the number operator, as does tunneling in Coulomb-blockade systems. Since the derivative of these steps with respect to the energy differences is a Lorentzian, they are termed tunnel resonances [8]. With an additional particle in the system, the main question that comes into mind refers to the tunneling properties of that particle: Does the BEC leave the fermion's tunnel properties unaffected, or does the BEC expel the fermion to the other well against the potential gradient? Obviously, the answer depends on the relative interactions between the two species. In our work, we consider the ground-state properties in the weak-tunneling limit. We discuss the different regimes in the parameter space defined by the particle interactions and the implications of large repulsion between the two species on the adiabatic and quasiadiabatic dynamics.

In Sec. II, we introduce the Hamiltonian and its basic properties. Then, in Sec. III, we compute the expectation value of the relative number operators indicating that the ground state shows different phases defined by the repulsive forces. In particular, we find an avoided crossing between two states that are not connected directly by the tunneling Hamiltonian. We calculate the splitting by an application of Brillouin-Wigner perturbation theory in Sec. IV. In Sec. V, we consider time-dependent dynamics and show that by using the avoided crossings due to the tunneling of the fermion as "beam splitters," we can construct a Mach-Zehnder interferometer that allows us to transfer all populations from one well into the other on a time scale that is only defined by the tunneling properties of the fermion.

II. MODEL

The starting point for our discussion is the standard Bose Josephson junction [4]: a Bose-Einstein condensate is loaded into an optical double-well potential such that only the ground state of each well is occupied. Defining the relative number operator $n_{\mathrm{B}} := \frac{1}{2}(n_{\mathrm{R}} - n_{\mathrm{L}})$ as the difference between the number of bosons in the right and the left wells, the

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Hamiltonian is, up to a constant depending on the total number of particles $N = n_R + n_L$, [8]

$$H_B = -2\varepsilon n_B + U_B n_B^2 - \Delta_B (b_L^\dagger b_R + \text{H.c.}). \tag{1}$$

The double-well potential can be tilted, generating an energy difference 2ε between the two wells' ground states. The interparticle repulsion of the bosons is of strength U_B, and tunneling between the two wells occurs with amplitude Δ_B. The operators b_i and $b_i^\dagger$ annihilate and create a boson in the respective well. The two most prominent regimes of the Bose Josephson junction are the superfluid-like regime $U_B \ll \Delta_B$, where the particles are delocalized over the two wells, and the Mott-like regime $\Delta_B \ll U_B$, where the particles are localized. In the latter case, tunneling is considered a perturbation to the Hamiltonian, which is diagonal in the relative number-state representation. Tilting the double-well potential by adjusting ε, the bosons will tunnel into the other well one by one, leading to a staircase profile for the expectation value $\langle n_B \rangle(\varepsilon)$ [8,9].

We now consider an additional single fermion or, since in that case the particle statistics do not matter at all, an atom of a different species than the constituents of the condensate. Its dynamics are governed by the very same Hamiltonian without the repulsive term:

$$H_F = -2\varepsilon n_F - \Delta_F (c_L^\dagger c_R + \text{H.c.}), \tag{2}$$

with appropriately labeled constants and c_i and $c_i^\dagger$ being the fermion's annihilation and creation operators, respectively. We assume that the mutual interaction of both species is proportional to $\sum_{\alpha=L,R} n_B^\alpha n_F^\alpha$ [8], which in the relative number representation reads

$$H_{B-F} = 2U_{B-F} n_B n_F \tag{3}$$

plus a constant. The full Hamiltonian of our system is thus

$$H = H_B + H_F + H_{B-F}. \tag{4}$$

The double-well potential in the two-mode approximation defines a representation of the rotation group SU(2), hence a pseudospin on the Bloch sphere whose length is the number of particles. The z direction of this spin encodes the position information of the particles and is given by the relative number operator n_B (n_F) with eigenvalues m_B (m_F) [4].

III. PHASE DIAGRAM

As shown in [8,9], by adjusting ε adiabatically and thereby tilting the double-well potential, the Bose Josephson junction shows single-particle tunneling and a staircase profile of the expectation value of the relative number operator. In our case, where an additional species, albeit only a single particle of it, is present in the system, we expect the same behavior in the tunneling regime $U_B, U_{B-F} \gg \Delta_B, \Delta_F$: tilting the potential makes the particles tunnel from one well to the other. Since there are two species of atoms present in the potential, the obvious question to ask is, which species will tunnel?

In general, transitions will be shown to be interaction mediated; that is, the relative magnitude of the repulsive interactions will determine the tunneling species. If there are no interactions as, for instance, in the case $N = 1$, or at the exact threshold where the tunneling species changes, $U_B = U_{B-F}$, the profile of the transitions in $\langle n_B \rangle$ and $\langle n_F \rangle$ is heavily influenced by the kinetic energy.

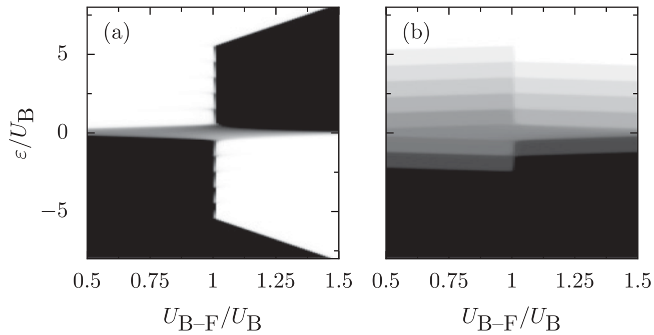

FIG. 1. Number expectation for a single fermion and $N_{\text{bosons}} = 11$. (left) $\langle n_F \rangle$ and (right) $\langle n_B \rangle$. The parameters are $\Delta_F = 0.01\, U_B$ and $\Delta_B = 0.05\, U_B$. The color code is white-gray-black for negative-zero-positive.

In Fig. 1, we show numerical results for $\langle n_B \rangle$ and $\langle n_F \rangle$ as a function of interspecies interaction U_{B-F} and tilt ε. The most obvious characteristic is the change of the tunneling species at the first resonance for $U_{B-F} = U_B$. Close to this point, the fermionic expectation values show traces of attempted tunneling [Fig. 1(a)]. For larger interspecies interaction, the bosonic expectation values are shifted by 1 due to the presence of the fermion in the well with higher energy [Fig. 1(b)]. For larger fermionic tunnel amplitude (not shown), the bosons will also show negative compressibility $\kappa_B = d\langle n_B \rangle / d\varepsilon$ close to zero tilt. In the following, we shall discuss and explain these phenomena in detail.

Since we are in the tunneling regime with well-separated resonances, we begin by restricting the bosonic Hilbert space at each resonance to the subspace spanned by the eigenstates of $n_B|m\rangle = m|m\rangle$: $|m\rangle$ and $|m+1\rangle$. The fermionic Hilbert space is also two-dimensional, such that we have

$$H_B = \begin{pmatrix} U_B m^2 - 2\varepsilon m & -\lambda_m \\ -\lambda_m & U_B (m+1)^2 - 2\varepsilon(m+1) \end{pmatrix}, \tag{5a}$$

$$H_F = \begin{pmatrix} \varepsilon & -\Delta_F \\ -\Delta_F & -\varepsilon \end{pmatrix}, \tag{5b}$$

$$H_{B-F} = 2U_{B-F} n_B n_F \tag{5c}$$

in the respective basis. The off-diagonal elements of H_B are the tunnel amplitudes times the matrix element of the bosonic operators b_α, $b_\alpha^\dagger$: $\lambda_m := \Delta_B \sqrt{(\frac{1}{2}N_B + m + 1)(\frac{1}{2}N_B - m)}$ [8]. In the same basis, the relative number operators take the form

$$n_B = \begin{pmatrix} m & 0 \\ 0 & m+1 \end{pmatrix}, \quad n_F = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \tag{6}$$

In the absence of tunneling, the Hamiltonian is already diagonal with energies

$$E_{|m;\pm\frac{1}{2}\rangle} = U_B m^2 \pm U_{B-F} m - 2\varepsilon\left(m \pm \tfrac{1}{2}\right). \tag{7}$$

If we place the system at a point, where tunneling of a particle should occur, we have either the states $|m; \pm\frac{1}{2}\rangle$ and

$|m+1;\pm\frac{1}{2}\rangle$, which are degenerate for a bosonic resonance, or $|m;\frac{1}{2}\rangle$ and $|m;-\frac{1}{2}\rangle$, which have the same energy for a fermionic resonance. Equating the unperturbed energies of the Hamiltonian, we find that the fermion can tunnel for $\varepsilon = mU_{\mathrm{B-F}}$, and the boson can tunnel for $\varepsilon = U_{\mathrm{B}}(m+\frac{1}{2}) \pm \frac{1}{2}U_{\mathrm{B-F}}$, depending on the position of the fermion. In particular, if we consider two values of the boson-fermion interaction, $U_{\mathrm{B-F},\pm}$ with $\frac{1}{2}(U_{\mathrm{B-F},+}+U_{\mathrm{B-F},-}) = U_{\mathrm{B}}$, at $U_{\mathrm{B-F}} = U_{\mathrm{B-F},+}$, the state $|m;-\frac{1}{2}\rangle$ has the same energy as $|m-1;\frac{1}{2}\rangle$ has at $U_{\mathrm{B-F}} = U_{\mathrm{B-F},-}$. This property is seen in Fig. 1(b), where the bosonic resonances at equal distances to the left and right of $U_{\mathrm{B-F}} = U_{\mathrm{B}}$ differ by one boson exactly.

Approaching the first resonance of the system from large negative ε, the ground state is $|m=-N/2;-\frac{1}{2}\rangle$. If the fermion tunnels first, we have to equate its energy with $E_{-N/2;1/2}$; otherwise, we equate its energy with $E_{-N/2+1;-1/2}$. From the above formula for the energy, we see that the difference between the positions of these resonances is $\varepsilon_{\mathrm{F}} - \varepsilon_{\mathrm{B}} = \frac{1}{2}[(1-N)(U_{\mathrm{B-F}} - U_{\mathrm{B}})]$. Hence, if $U_{\mathrm{B-F}} > U_{\mathrm{B}}$, the fermion will tunnel first, and a boson will tunnel first otherwise. Repeating this calculation for arbitrary m shows that this condition is independent of the resonance in question: for large enough interspecies repulsion, the fermion will tunnel first; otherwise, it will tunnel last.

This result is intuitively clear, as the condition states that for $U_{\mathrm{B-F}} > U_{\mathrm{B}}$, keeping the fermion together with the bosons costs more energy than keeping the additional boson. Hence, the fermion will be expelled to the other well. Noting that such behavior occurs for finite ε, the fermion will move to the potential well with higher energy, hence against the potential gradient.

Directly at the degenerate point $U_{\mathrm{B-F}} = U_{\mathrm{B}}$, which particle will tunnel first cannot be decided from the atomic interactions alone. In this situation, we have to include the tunnel Hamiltonian, as now the kinetic energy of the particles will decide. At $\varepsilon = mU_{\mathrm{B}} = mU_{\mathrm{B-F}}$, the unperturbed Hamiltonian's ground state is fourfold degenerate:

$$\left|m-1;\tfrac{1}{2}\right\rangle, \quad \left|m;-\tfrac{1}{2}\right\rangle, \quad \left|m;\tfrac{1}{2}\right\rangle, \quad \left|m+1;-\tfrac{1}{2}\right\rangle,$$

all have the same energy. Including the tunneling, the Hamiltonian in this basis reads

$$\tilde{H} = \begin{pmatrix} 0 & 0 & -\lambda_{m-1} & 0 \\ 0 & 0 & -\Delta_{\mathrm{F}} & -\lambda_m \\ -\lambda_{m-1} & -\Delta_{\mathrm{F}} & 0 & 0 \\ 0 & -\lambda_m & 0 & 0 \end{pmatrix} \tag{8}$$

plus a constant. This Hamiltonian has a biquadratic characteristic polynomial, which can be solved explicitly, leading to the ground-state expectation values

$$\langle n_{\mathrm{F}}\rangle = \frac{\Delta_{\mathrm{B}}^2 m}{\sqrt{\Delta_{\mathrm{F}}^4 + 4\Delta_{\mathrm{B}}^4 m^2 + \Delta_{\mathrm{B}}^2\Delta_{\mathrm{F}}^2[-4m^2 + N(N+2)]}} \tag{9a}$$

$$\langle n_{\mathrm{B}}\rangle = m - \langle n_{\mathrm{F}}\rangle. \tag{9b}$$

For the first resonance from positive (negative) ε, only three states have to be considered because the state $|\pm|N/2+1|;\mp\frac{1}{2}\rangle$ does not exist, and the expression simplifies to

$$\langle n_{\mathrm{F}}\rangle = \pm\frac{1}{2}\frac{\Delta_{\mathrm{B}}^2 N}{\Delta_{\mathrm{B}}^2 N + \Delta_{\mathrm{F}}^2} \tag{10a}$$

$$\langle n_{\mathrm{B}}\rangle = \pm\frac{N}{2}\left(1 - \frac{\Delta_{\mathrm{B}}^2}{\Delta_{\mathrm{F}}^2 + \Delta_{\mathrm{B}}^2 N}\right). \tag{10b}$$

Note that these are discrete values evaluated at $\varepsilon = mU_{\mathrm{B-F}}$ and are *not* continuous in m.

From these expressions, we directly infer that at the first resonance, a fast tunneling species, i.e., one with large Δ_i, will hamper the other and restrict its number expectation value to the asymptotic value of $\pm\frac{1}{2}$ or $\pm N/2$, respectively.

By considering the limit of large and small tunneling amplitudes, we can significantly simplify expressions (9a) and (9b). Also, as for $U_{\mathrm{B-F}} < U_{\mathrm{B}}$, only single-particle processes are present, and the situation at $U_{\mathrm{B-F}} = U_{\mathrm{B}}$ can be used as a good approximation for the ground-state properties in that regime. For $U_{\mathrm{B-F}} > U_{\mathrm{B}}$ we observe processes where a larger number of particles tunnels simultaneously. This will be discussed in Sec. IV. In the present case $U_{\mathrm{B-F}} = U_{\mathrm{B}}$, the asymptotic expectation values at the resonances are

$$\langle n_{\mathrm{F}}\rangle \to \begin{cases} 0 & \text{for } \Delta_{\mathrm{B}}/\Delta_{\mathrm{F}} \to 0 \\ \frac{m}{\sqrt{1+N(N+2)}} & \text{for } \Delta_{\mathrm{B}} = \Delta_{\mathrm{F}} \\ \frac{1}{2}\mathrm{sgn}(m) & \text{for } \Delta_{\mathrm{B}}/\Delta_{\mathrm{F}} \to \infty \end{cases}$$

and

$$\langle n_{\mathrm{B}}\rangle \to \begin{cases} m & \text{for } \Delta_{\mathrm{B}}/\Delta_{\mathrm{F}} \to 0 \\ m\left(1 - \frac{1}{\sqrt{1+N(N+2)}}\right) & \text{for } \Delta_{\mathrm{B}} = \Delta_{\mathrm{F}} \\ m - \frac{1}{2}\mathrm{sgn}(m) & \text{for } \Delta_{\mathrm{B}}/\Delta_{\mathrm{F}} \to \infty. \end{cases}$$

For $\Delta_{\mathrm{B}} = \Delta_{\mathrm{F}}$, shown in Fig. 2 (top panels), the fermionic expectation value shows steps linear in the resonance number m. For $\Delta_{\mathrm{B}} < \Delta_{\mathrm{F}}$, Fig. 2 (middle panels), the fermionic expectation shows oscillations about $\langle n_{\mathrm{F}}\rangle = 0$. In the other case, $\Delta_{\mathrm{B}} > \Delta_{\mathrm{F}}$, shown in Fig. 2 (bottom panels), we see that the presence of the fermion and, in particular, its tunnel amplitude do influence the bosons in such a way that for $\Delta_{\mathrm{B}} \gg \Delta_{\mathrm{F}}$, i.e., a strongly localized fermion, the relative number expectation value approaches $m - \frac{1}{2}\mathrm{sgn}(m)$, which is the same as in the case $U_{\mathrm{B-F}} < U_{\mathrm{B}}$. Also, the expectation value of the fermionic relative number operator approximates a step function.

In the case of low fermionic tunnel amplitude, the resonance at zero tilt $\varepsilon = 0$, with $m = 0$, will also show negative compressibility $\kappa_{\mathrm{B}} = d\langle n_{\mathrm{B}}\rangle/d\varepsilon < 0$ because in the limit $\Delta_{\mathrm{F}} = 0$, $\lim_{m\nearrow 0}\langle n_{\mathrm{B}}\rangle = \frac{1}{2}$ and $\lim_{m\searrow 0}\langle n_{\mathrm{B}}\rangle = -\frac{1}{2}$; see Fig. 3. A quantitative result is given in [8] for $0 \leqslant \varepsilon \ll U_{\mathrm{B-F}} < U_{\mathrm{B}}$.

IV. ZERO-BIAS SPIN FLIP

Due to the symmetries of the Hamiltonian without tunneling, $\Delta_{\mathrm{B}} = \Delta_{\mathrm{F}} = 0$, at $\varepsilon = 0$, the states $|m_{\mathrm{B}};m_{\mathrm{F}}\rangle$ and $|-m_{\mathrm{B}};-m_{\mathrm{F}}\rangle$ are degenerate. In particular, this holds for the ground state of the noninteracting system. In general, such a degeneracy for the ground state always occurs at a resonance. In our system, however, the degenerate states do not only

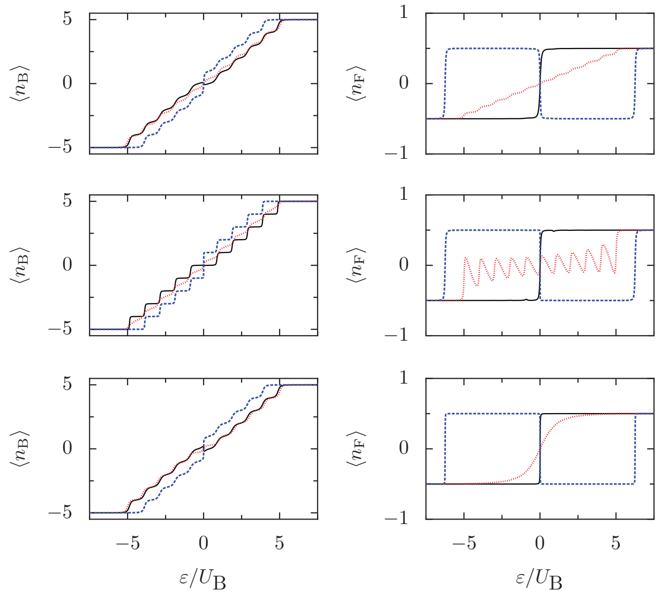

FIG. 2. (Color online) Occupation number difference $\langle n_i\rangle$ (left, bosons; right, fermions) for a mixture of 10 bosons and one fermion. The plots are for different values of the Bose-Fermi repulsion $U_b - -F/UB \in 0.75, 1, 1.25$ in solid black, dotted red, and dashed blue. The tunneling amplitudes are (top) $\Delta_{\rm B} = \Delta_{\rm F} = 0.05\, U_{\rm B}$, (middle) $\Delta_{\rm B} = 0.01\, U_{\rm B}, \Delta_{\rm F} = 0.05\, U_{\rm B}$, and (bottom) $\Delta_{\rm B} = 0.05\, U_{\rm B}$, $\Delta_{\rm F} = 0.01\, U_{\rm B}$.

differ by a single particle having changed its position, but rather correspond to the exchange of positions for two species and, depending on the interspecies repulsion $U_{\rm B-F}$, a larger number of bosons. Since, as we have mentioned before, the relative number operators are equivalent to the z components of the pseudospin defined by the double-well potential, this transition corresponds to a flip of the combined pseudospin of bosons and fermion.

A. Higher-order degenerate perturbation theory

In contrast to the single-particle resonance, whose physics is that of an avoided crossing and degenerate perturbation

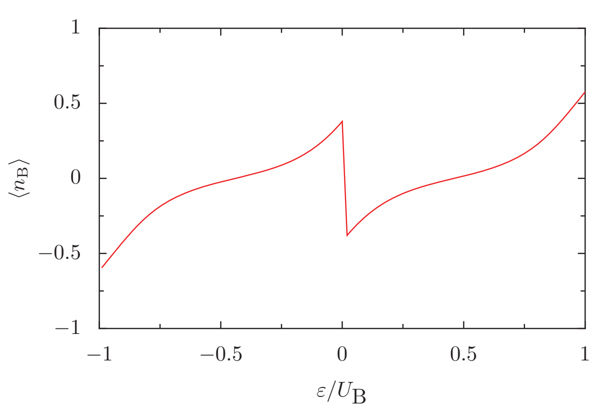

FIG. 3. (Color online) Negative compressibility $\kappa_{\rm B} = d\langle n_{\rm B}\rangle/d\varepsilon$ due to low fermionic tunnel amplitude $\Delta_{\rm F} = 10^{-4}\, U_{\rm B}$, $\Delta_{\rm B} = 0.05\, U_{\rm B}$, and $U_{\rm B-F}/U_{\rm B} = 0.9$.

theory, the zero-bias spin flip is not easily amenable to degenerate perturbation theory because the involved states are not directly connected by the tunneling term in the Hamiltonian. Although a numerical treatment of the problem is straightforwardly implemented, perturbation theory allows for a simple analytical approach to the resonance and provides a very good approximation for the line shape.

For general considerations, let $|m\rangle$ and $|-m\rangle$ be eigenstates of the unperturbed Hamiltonian with energies $E_{\pm m} = \varepsilon_0 \pm \epsilon$ such that they are degenerate for $\epsilon = 0$. Let ξV be a perturbation, with a scalar ξ to keep track of orders of magnitude, and $\langle -m \mid V \mid m\rangle = 0$. Assume the shortest chain of matrix elements of V that connects the two degenerate states via intermediate states $|n_j\rangle$ has length k. Brillouin-Wigner perturbation theory to lowest order in ξ yields, for the splitting [19],

$$\Delta E_m = 2\xi^k V_{m,n_1} \frac{1}{E_{n_1} - E_m} V_{n_1,n_2} \frac{1}{E_{n_2} - E_m} \cdots \cdots \frac{1}{E_{n_k} - E_m} V_{n_k,-m}. \quad (11)$$

The line shape of the expectation value of the relative occupation number $n = m(|m\rangle\langle m| - |-m\rangle\langle -m|)$ restricted to the degenerate subspace as a function of ϵ is thus, to lowest order in ξ, $\langle n\rangle(\epsilon) \approx |m|\epsilon/\sqrt{\frac{1}{4}\Delta E_m^2 + \epsilon^2}$.

B. Application to the Bose-Fermi mixture

Let us apply this reasoning to the spin flip at zero bias of a Bose-Fermi mixture in a double-well potential when the perturbation V is the tunneling of single particles. In the regime with $U_{\rm B-F} > U_{\rm B}$, the spin-flip transition is $|-m; \frac{1}{2}\rangle \mapsto |m; -\frac{1}{2}\rangle$. To construct the chain of intermediate states connecting the two degenerate states by single-particle processes, we climb up the angular-momentum ladder in m. At a certain $m = m_0$, the fermion jump is included. Then, due to the different repulsion energies, the energy denominators are different, and the chain naturally splits into two products. Consider the energy differences

$$G_<^{-1}(n) := E_{n,\frac{1}{2}} - E_{-m,\frac{1}{2}} = (n^2 - m^2)U_{\rm B} + (n+m)U_{\rm B-F} \quad (12a)$$

$$G_>^{-1}(n) := E_{n,-\frac{1}{2}} - E_{-m,\frac{1}{2}} = (n^2 - m^2)U_{\rm B} - (n-m)U_{\rm B-F} \quad (12b)$$

for bosonic transitions left ($G_<^{-1}$) and right ($G_>^{-1}$) of m_0. The fermionic jump is given by $G_>^{-1}(m_0)$, which leads to the result

$$\Delta E = 2\Delta_{\rm F} \left(\prod_{k=-m}^{m} \lambda_k\right) \sum_{m_0=-m}^{m} \left[\prod_{n=m+1}^{m_0} G_<(n) \prod_{n=m_0}^{m-1} G_>(n)\right]. \quad (13)$$

The fermionic jump is included as the first factor of the last product. Here we use the convention that a product without factors, eg., $\prod_m^n$ with $n < m$, is unity.

As an example, we consider the smallest nontrivial mixture: $N = 2$. For $U_{\rm B-F} > U_{\rm B}$, the spin-flip transition at zero bias

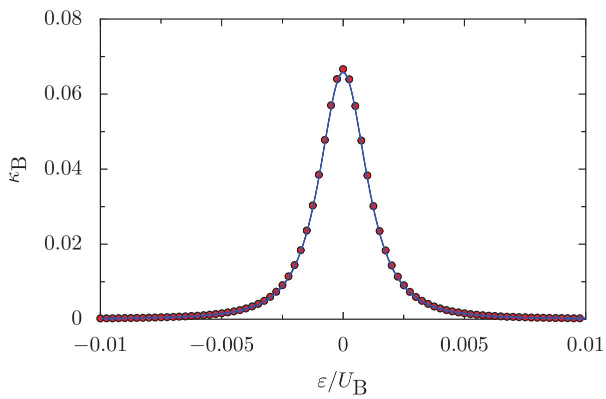

FIG. 4. (Color online) The Brillouin-Wigner result (dots) and the numerically obtained line shape (solid line) for the compressibility $\kappa_B = d\langle n_B\rangle/d\varepsilon$ of the zero-bias spin flip. Note that the energy scales have to be separated by about two orders of magnitude $J/U \sim 10^{-2}$. Here $U_B = 1$, $U_{B-F} = 2$, $\Delta_B = 0.1$, and $\Delta_F = 0.05$, such that $\Delta E = 6\Delta_B^2\Delta_F$.

is $|-1;1/2\rangle \mapsto |1;-1/2\rangle$, which are connected by three paths:

$$\left|-1;\tfrac{1}{2}\right\rangle \mapsto \left\{\begin{array}{c} \left|0;\tfrac{1}{2}\right\rangle \mapsto \left|1;\tfrac{1}{2}\right\rangle \\ \left|0;\tfrac{1}{2}\right\rangle \mapsto \left|0;-\tfrac{1}{2}\right\rangle \\ \left|-1;-\tfrac{1}{2}\right\rangle \mapsto \left|0;-\tfrac{1}{2}\right\rangle \end{array}\right\} \mapsto \left|1;-\tfrac{1}{2}\right\rangle. \tag{14}$$

The level splitting is thus

$$\Delta E = 4\Delta_B^2\Delta_F\frac{1}{U_B - U_{B-F}}\left[\frac{-1}{U_{B-F}} + \frac{1}{U_B - U_{B-F}}\right], \tag{15}$$

and since $m = 1$, as a function of the tilt ε, $\langle n_B\rangle(\varepsilon) = \varepsilon/\sqrt{\varepsilon^2 + \frac{1}{4}\Delta E^2}$. In Fig. 4, we show the numerical data for $\kappa_B = d\langle n_B\rangle/d\varepsilon$ as well as the line shape computed with Brillouin-Wigner perturbation theory.

Of course, the result is not absolutely accurate, as in the tails of the resonance, we do *not* recover the asymptotic states with well-defined occupation numbers, but rather the exact eigenstates of the full Hamiltonian. If we look at the numbers of Fig. 4, Brillouin–Wigner theory gives $\Delta E = 3 \times 10^{-3}\, U_B$, whereas the numerically evaluated splitting is approximately $2.88 \times 10^{-3}\, U_B$.

V. LANDAU-ZENER DYNAMICS

In the previous sections, we have focused on the adiabatic dynamics of population transfer from one well into the other by increasing the tilt ε of the potential. In a realistic scenario, however, we will always adjust the tilt within finite time and hence with finite velocity $d\varepsilon/dt$. This means that we have to take into account Landau-Zener physics of quasiadiabatic transitions [20–25]. Depending on the velocity and the splitting of the states at a resonance, the population transfer is thus heavily influenced.

In the regime $U_{B-F} > U_B$ of our model, the zero-bias spin-flip resonance is so narrow that it is very difficult to traverse it adiabatically as the necessary velocities, which depend on the splitting, are very small. In [26], such an effect is also seen and successfully exploited to achieve the population transfer sought for. Let us choose a velocity α for the change of $\varepsilon(t) = \alpha t$ in time that allows to pass the single-particle resonances adiabatically. The expectation values of the respective relative number operator as a function of ε are shown in Fig. 5(a), and the corresponding spectrum of the Hamiltonian is plotted in Fig. 6. Starting at infinite negative time, where the system is in its ground state, the fermion tunnels from left to right at finite negative ε (point A in Fig. 6), as expected for $U_{B-F} > U_B$. The spin-flip resonance (point B in Fig. 6) is, however, passed completely diabatically, such that all particles stay where they are and do not exchange places. At this point, the system is no longer in its ground state but is in the first excited state. Further tilting of the potential causes the bosons to tunnel to the lower-lying well step by step. Finally, the system adiabatically passes an avoided crossing of two excited states, where, again, the fermion changes sides and tunnels back into the *left*, i.e., higher-lying well, as is seen in Fig. 5(a). The avoided crossing labeled A′ in Fig. 6 is passed adiabatically in the *excited* state, where the system stays until other processes than those described by our Hamiltonian cause it to relax to the ground state and hence cause the fermion to change sides again. The diabatic traversing of the spin-flip resonance thus causes the transition of the system from its

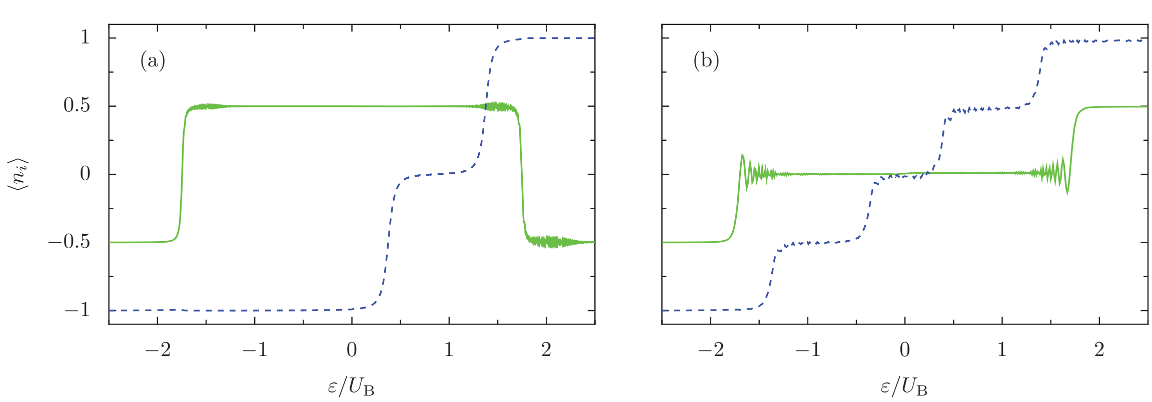

FIG. 5. (Color online) Expectation values $\langle n_i\rangle$ of the relative number operator for fermions (solid green line) and bosons (blue dashed line) in a numerical Landau-Zener experiment on the Bose-Fermi mixture. $\Delta_B = 0.05\, U_B$, $\Delta_F = 0.025\, U_B$, $U_{B-F} = 1.72\, U_B$, and (a) $\alpha = \frac{1}{4000}\, U_B^2$ and (b) $\alpha \approx \frac{11}{4000}\, U_B^2$. The velocity α with which we can use the constructive interferences is about 10 times as large as the one with which the zero-bias spin flip is still passed diabatically and the system is kept in an excited state.

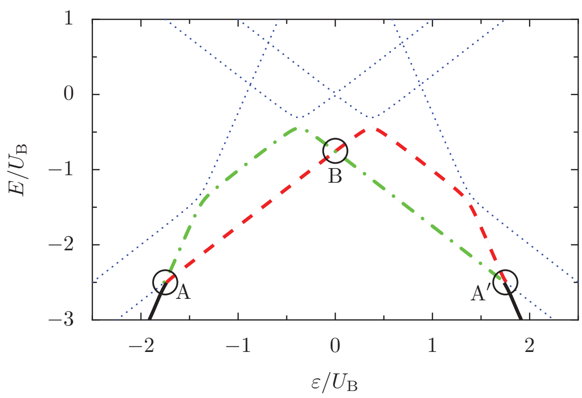

FIG. 6. (Color online) Spectrum of the Bose-Fermi mixture and the path that is traversed by a linear scan of ε. The branches that define the two equivalent arms of the Mach-Zender interference are the red dashed and the green dash-dotted line. The black solid lines denote the incoming and outgoing beams, respectively. The fermionic resonances, where the wave function is split into halves, are labeled A and A′, and the zero-bias spin flip is labeled B. The parameters are the same as in Fig. 5.

ground state at $t \to -\infty$ to the first excited state at $t \to \infty$. Lowering the velocity allows us to pass to the adiabatic regime also for the zero-bias spin flip, but the more bosons we have in the condensate, the slower we would have to adjust $\varepsilon(t)$.

In spite of the difficulties introduced by the narrow zero-bias spin-flip resonance, we are able to facilitate adiabatic population transfer from one well to the other by employing a constructive interference effect, the result of which is shown in Fig. 5(b). The spectrum of the Bose-Fermi mixture, as shown in Fig. 6, is symmetric about $\varepsilon = 0$. If we adjust the tunnel amplitudes such that $\Delta_\mathrm{F} < \Delta_\mathrm{B}$, we can control the Landau-Zener physics of the fermionic jump and still pass all other bosonic resonances almost adiabatically. This allows us to restrict the problem to only consider the ground state $|g\rangle$ and the first excited state $|e\rangle$ of the Hamiltonian, as depicted in Fig. 6 for the case of $N = 2$. Passing the first avoided crossing by adjusting the tilt $\varepsilon(t)$ amounts to a unitary transformation of the asymptotic states

$$U = \begin{pmatrix} \cos\Theta & \sin\Theta \\ -\sin\Theta & \cos\Theta \end{pmatrix},$$

with the angle Θ depending on the velocity α and the splitting ΔE of the two states $\cos^2\Theta = 1 - \exp(-\frac{2\pi}{\hbar}\frac{\Delta E^2}{\alpha})$ [20]. The zero-bias spin-flip transition is very narrow, such that we traverse it diabatically, hence exchanging ground and excited states, which corresponds to the unitary transformation σ_x. The second avoided crossing is identical to the first; however, it is passed in the opposite direction, when the invoked unitary is $U^\dagger$. Since both arms of the interferometer are identical, i.e., they can be mapped by $\varepsilon \mapsto -\varepsilon$ onto each other, the accumulated dynamical phase is the same and amounts to a global phase factor, which is of no importance for our purpose.

With these assumptions, the constructed Mach-Zehnder interferometer is the map

$$U\sigma_x U^\dagger = \sigma_x \cos(2\Theta) - \sigma_z \sin(2\Theta).$$

For $\Theta = \pi/4$, $U\sigma_x U^\dagger = -\sigma_z$: the ground state of the full Hamiltonian will again be mapped onto the ground state and the population can be transferred completely. Considering the avoided crossings as a beam splitter for an incoming ground-state wave function [23], this choice of Θ amounts to a velocity α for which the Landau-Zener transition splits the wave function exactly into two halves $|g\rangle \mapsto \frac{1}{\sqrt{2}}(|g\rangle + |e\rangle)$.

In the numerical data in Fig. 5(b), the achieved population transfer is almost perfect. The expectation values of the relative number operators show some oscillations in the fermionic part, which are due to the coherent superposition created by the Landau-Zener transition. The remainder of the profile is, however, well in accordance with the adiabatic picture for atom counting, except that since the wave function is split by the avoided crossing, the time-dependent evaluation of $\langle n_i \rangle$ does not count full atoms like in the adiabatic regime. Instead, we pass twice as many resonances for which $\langle n_i \rangle$ only changes by a half integer.

The important advantage of this approach over a completely adiabatic transfer is that with this interferometer, we only need to adjust the Landau-Zener transition of the single fermionic resonance. This, however, is independent of the number of bosons in the system, and we can use a much higher velocity than in the purely adiabatic regime where the Landau-Zener physics of the spin-flip transition are taken fully into account.

VI. CONCLUSION

In this paper, we have investigated a Bose-Fermi mixture in a double-well potential with the restriction that while the number of bosons is arbitrary, the number of fermions is fixed at 1. We thus discussed the influence of a single fermionic impurity on the ground-state properties of the Bose Josephson junction when the potential was allowed to be tilted. It has turned out that rather than the bosons, it is the fermion that is affected most by the boson-fermion interactions. We have separated the dynamics into two regimes: one where the bosons and the fermion live side by side and one where the fermion is expelled from the BEC toward the higher-lying well. In this regime, we have found a zero-bias spin flip where the fermion and a large number of bosons change places. The physics of this process, in particular the level splitting and the line shape of the observed resonance in the relative particle number, are well accessible by Brillouin-Wigner perturbation theory. Since many particles are involved in this transition, complete population transfer of all particles from the left well to the right well upon tilting the potential is hardly possible any longer when we assume the realistic case of slow but not infinitely slow adjustment of the potential tilt ε. Instead, we have shown how the fermionic resonance in the regime $U_{\mathrm{B-F}} > U_\mathrm{B}$ can be employed as a beam splitter of a Mach-Zehnder interferometer to achieve population transfer at much higher tilting speeds than would be necessary to traverse the zero-bias spin-flip resonance adiabatically.

There are several directions in which we want to extend our investigation. In the case of very large N, the Gross-Pitaevskii equation provides a much simpler description of the BEC than can be achieved by numerical diagonalization of the two-site Bose-Hubbard Hamiltonian. We will therefore ask for the lowest-order corrections of the dynamics of a Bose Josephson junction with large N in the presence of a single fermionic impurity. The trade-off for the reduction to the Gross-Pitaevskii equation is, however, the extension to the study of nonlinear eigenvalue problems [11].

The second direction relates to the number of fermions in the double-well potential. Experiments of two fermions with opposite spin in such a system without a BEC have been conducted by Trotzky *et al.* [27]. The orbital wave function of two fermions with opposite spin in a double-well potential is decomposed into a singlet and three triplet states with respect to the pseudospin defined by the double-well potential. Interestingly, the singlet does not couple to the bosons at all. On the contrary, the state $|\uparrow,\downarrow\rangle$, that is, a configuration with *definite* position of the spin-up fermion in the left well and the spin-down particle in the right well, is a superposition of the singlet and the $J_z = 0$ triplet, which, however, does couple to the BEC. In this configuration we expect the time-dependent dynamics to show very interesting phenomena, which could be observed experimentally.

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