Macroscopic spin tunneling and quantum critical behavior of a condensate in double-well potential

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In a previous work [1], we have shown that a spinor condensate confined in a periodic or double-well potential exhibits ferromagnetic behavior due to the magnetic dipole-dipole interactions between different wells, and in the absence of external magnetic field, the ground state has a two-fold degeneracy. In this work, we demonstrate the possibility of observing macroscopic quantum spin tunneling between these two degenerate states and show how the tunneling rate critically depends on the strength of the transverse field.

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Tunneling, a process in which a system penetrates into a classically forbidden region (e.g., a potential barrier), is an intrinsically quantum effect with no classical counterpart. Of all tunneling effects, macroscopic quantum tunneling (MQT), the tunneling of a macroscopic variable of a macroscopic system [2], represents a particularly intriguing and interesting scenario as it touches the boundary between the classical and the quantum world and may help shed light on the quantum-classical interface. As such, it is one of the most striking manifestations of quantum mechanics. The tunneling of large magnetic spins has recently received much attention, both theoretically and experimentally [3, 4] in view of its promise as one of the few realistic candidates for an experimental demonstration of MQT, and also because of its connection to quantum computing. Despite considerable efforts, though, there are not many clear and definitive demonstrations of MQT in spin systems so far — although there have been some indications that tunneling might be the underlying reason for some observed results [5, 6]. The reasons for this difficulty are as follows: First, most theories apply to single system, while the conventional magnetic materials used in the experiments contain many domains, each possessing its own set of parameters such as magnetic anisotropy and barrier energy; second, due to the difficulty of cooling the samples down to ultracold temperatures, thermal processes cannot be completely excluded; and third, the spins in solid materials are inevitably imbedded in a crystal matrix and the spin-matrix interaction [7] complicates the physical picture. For these reasons, macroscopic spin tunneling remains one of the most anticipated, yet elusive, quantum phenomena.

In this paper, we demonstrate the possibility of observing spin tunneling in a spinor atomic condensate trapped in a double-well potential, thereby eliminating most of these difficulties. We remark at the outset that while the inter-well tunneling of condensates has been previously considered, all previous studies focused instead on the tunneling of an external degree of freedom, the condensate center-of-mass motion [7, 8, 9, 10].

In an earlier paper [1], we showed that because of the long range magnetic dipole-dipole interaction, a spinor atomic condensate trapped in a one-dimensional periodic lattice potential or a double-well potential behaves as a ferromagnet. In the absence of external magnetic fields, the ground state spins of the “mini-condensates” confined in individual wells all align parallel to each other and along the lattice direction (the z-axis), giving rise to a spontaneous magnetization along z. For the sake of simplicity, we restrict the present discussion to a double-well potential, each well containing N spin-1 condensate atoms. In the tight-binding approximation [7], they are described by the zero-temperature spin Hamiltonian [11]

\[ H = \lambda S_i^z (S_i^x + S_i^z) - 3\lambda S_i^z S_{i+1}^z + \lambda S_1 \cdot S_2 - h (S_1^x + S_2^x), \]  

where \( S_i \) is the total spin of the condensate in the \( i^{th} \) well, \( S_{i+1} \) its cartesian components. The first term in \([1]\) represents the on-site Hamiltonian of the spinor condensate. It includes short-range nonlinear spin-exchange interactions \([12]\), where the parameter \( \lambda \) is related to the s-wave scattering lengths \([12]\) and needs to be negative. The second and third terms in \([1]\) arise from the site-to-site dipole-dipole interaction \([1, 12]\), where \( \lambda \equiv 2\mu_0/(4\pi r^3) \) for pure magnetic dipolar interaction, with \( \mu_0 \) being the gyromagnetic ratio, \( \mu_0 \) the vacuum permeability and \( r \) the distance between the two wells. The value of \( \lambda \) can be greatly enhanced by the light-induced optical dipolar interaction if one chooses appropriate laser fields to form the potential well \([13, 14]\). The last term describes the effect of an external transverse magnetic field, taken to be along the x-axis without the loss of generality. Here \( h = \gamma_B B \), with \( B \) being the strength of the applied field.

In the following, we assume that the nonlinear short-range atom-atom interaction is strong enough that the first term in Hamiltonian \([1]\) dominates over the magnetic dipolar interaction \([12]\). As a result, the total spin quantum number for each mini-condensate is fixed to its maximum value \( N \) — the number of particles in each well. We can therefore neglect the first term in the Hamiltonian \([1]\), since it is a constant of motion and commutes with the remaining terms.
Before discussing quantum mechanical spin tunneling, let us first investigate the classical situation. The Hamiltonian in that limit is still given by (1), except that the spins are now c-numbers that can be represented by vectors of fixed length \(N\) in spin space. For zero field, \(h = 0\), it is easy to see that the classical ground state is two-fold degenerate with \(\mathbf{S} = \mathbf{S}_1 = \mathbf{S}_2\) pointing along either the \(z\)- or \((-z)\)-axis. Under the influence of a weak transverse field along the \(x\)-direction, the two ground states move away from the \(z\)-axis and towards the \(x\)-axis while remaining in the \(xz\)-plane, as shown in Fig. 1. For \(0 \leq h < h^{(c)}_c = 3N\lambda\), the two minima are located at
\[
\theta = \pi/2 \pm \cos^{-1}\left(\frac{h}{h^{(c)}_c}\right),
\]
where \(\theta\) is the angle between \(\mathbf{S}\) and the \(z\)-axis. For \(h \geq h^{(c)}_c\), the two minima merge along the \(x\)-axis, and the degeneracy is removed. Hence \(h^{(c)}_c\) can be regarded as the classical critical field strength.

Let us now turn to a quantum mechanical description of the system. Our goal is to investigate whether or not tunneling is present in the classically degenerate regime (i.e., when \(0 \leq h < h^{(c)}_c\)). We will present both a full numerical calculation and analytical results using the instanton technique.

A well-known consequence of the tunneling between two degenerate states is the lifting of their degeneracy: The two new eigenstates are a symmetric and an antisymmetric superposition of the original states characterized by an energy difference (or tunneling splitting) \(\Delta \varepsilon\) inversely proportional to the tunneling rate. The quantity of interest to determine the occurrence of tunneling is therefore this energy difference between the two lowest eigenstates of the Hamiltonian. We determine it by expanding the Hamiltonian \(\mathbf{H}\) onto the basis spanned by 
\[S^z_1 \otimes S^z_2,\]
and evaluate numerically the eigenvalues of the resultant \((2N+1)^2 \times (2N+1)^2\) matrix. Fig. 2(a) summarizes the result of this analysis. It shows that \(\Delta \varepsilon\) is essentially zero for small values of \(h\), but becomes finite when \(h\) exceeds a threshold value \(h^{(q)}_c\) — the quantum critical field strength. This means that for \(0 \leq h \leq h^{(q)}_c\), quantum mechanics agrees with classical mechanics in that the system is degenerate. However, for \(h^{(q)}_c < h < h^{(c)}_c\), even though the system is still degenerate in the classical picture, the presence of tunneling removes the degeneracy in the quantum treatment. Fig. 2(b) displays \(h^{(q)}_c\) as a function of \(N\), from which one sees that \(h^{(q)}_c\) increases with \(N\) and approaches \(h^{(c)}_c\) as \(N\) tends to infinity. In other words, as \(N\) increases, the system, as expected, behaves more and more classically.

To gain some analytical insight, we first notice that Hamiltonian \(\mathbf{H}\) can be rewritten as
\[
H = -\frac{3\lambda}{4}(S^z)^2 - (S^x)^2 + \frac{\lambda}{2}S^2 - hS^x
\]
where \(\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2\) and \(\mathbf{S}' = \mathbf{S}_1 - \mathbf{S}_2\). For \(h < h^{(c)}_c\), \(\mathbf{S}_1\) and \(\mathbf{S}_2\) are tightly bound together, such that \(S'^z \approx 0\) and \(\mathbf{S}\) is approximately a constant of motion with quantum number \(S = 2N\). Hence, neglecting the constant terms, the effective Hamiltonian of the system reads
\[
H_{\text{eff}} = -\frac{3\lambda}{4}(S^z)^2 - hS^x. \tag{2}
\]
Hamiltonian \(\mathbf{H}\) describes a quantum spin with the easy-axis anisotropy in a transverse field and it has been extensively studied in the context of spin tunneling. Using the instanton technique, which has been proved to
be quite accurate for $S > 5$, the tunneling splitting between the two classically degenerated ground states can be expressed as

$$\Delta \varepsilon = p \omega \sqrt{S_c/(2 \pi)} e^{-S_c},$$

(3)

where $p$ is a prefactor on the order of unity [by fitting the numerical results with Eq. (3), we find $p \approx 2.75$, $\omega = h_c^{(c)} x$ is the typical instanton frequency with $x = \sqrt{1 - (h/h_c^{(c)})^2}$, and $S_c = 2N \ln[(1 + x)(1 - x)] - 4Nx$ is the classical action. The solid curves in Fig. 2(a) represent the values calculated using Eq. (3), which agree well with the numerical results.

$$|N, N\rangle \Rightarrow \frac{1}{\sqrt{2}} (|N - 1, N\rangle + |N, N - 1\rangle) \Rightarrow |N - 1, N - 1\rangle \Rightarrow \frac{1}{\sqrt{2}} (|N - 2, N - 1\rangle + |N - 1, N - 2\rangle) \Rightarrow \ldots \Rightarrow \frac{1}{\sqrt{2}} (| - N, -N + 1\rangle + | - N + 1, -N\rangle) \Rightarrow | - N, -N\rangle.$$
results, a steady state is reached in the end (small oscillations around this steady state persists due to non-diabaticity). Fig. 3(b) is for $h_f > h_c^{(q)}$. The classical result is quite similar to that of Fig. 3(a). However, the quantum calculation clearly shows the oscillations of the system between the two macroscopically distinct states. These two states differ by a minus sign in the expectation value of $S^z$, which can be easily measured experimentally using, for example, Stern-Gerlach technique [1].

In conclusion, we have shown that the quantum macroscopic tunneling of spin is possible in a spinor condensate using, for example, Stern-Gerlach technique [9].

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