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Macroscopic quantum tunnelling of magnetization in spinor Bose-Einstein condensates

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Abstract. We investigate macroscopic quantum tunneling of magnetization in a a spinor Bose-Einstein condensate trapped in a double-well potential. Using the mean field theory applicable for large condensates, and employing the single spatial mode approximation we derive dynamical equations for magnetization, independent from density mode, for certain initial conditions. We show that they can be reduced to standard Josephson junction dynamics equations under certain conditions.

1. Introduction

Quantum tunnelling is a pure quantum phenomena which is described by leakage of a particle in a classically forbidden region. In terms of particle interpretation of quantum physics, one can explain how it happens using Heisenberg time-energy uncertainty. During the tunnelling, one may assume the particle has strong energy fluctuations which might overcome the potential energy barrier trapping the particle and forbidden zone become accessible. In terms of the wave interpretation of quantum physics, one simply assumes there is a certain probability for the particle to be in the forbidden zone associated with a finite potential energy barrier as the wave function of the particle would not vanish there. This fascinating effect cannot happen in our daily life which would otherwise rather strange. Using both of these interpretations one could argue that quantum tunnelling cannot happen in macroscopic systems at high temperatures. Wave associated with a particle of mass m is characterized by thermal de Broglie wavelength given by $\lambda = \sqrt{h^2/3mk_BT}$ which would be negligibly small at high temperatures. Furthermore, in the thermodynamical limit it is known that fluctuations are also negligible relative to the energy of the particle such that $\Delta E/E \to 0$. Hence, the tunnelling o the particle is prohibited completely. One might wonder whether a macroscopic system could exhibit tunnelling at low temperatures. To answer that question, we first note that macroscopic tunnelling should be a coherent effect that is a collective behavior of the particles constituting the system[1, 2, 3]. The interactions (scattering) among the particles at such large system would severely limit the coherence and thus it is not expected to observe any macroscopic quantum coherent tunnelling. A promising situation however may arise if one can consider tunnelling associated with internal degrees of freedom (such as their spin) of the particles rather than their external degrees of freedom (such as center of mass coordinate). Possibility of such an event has already been

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known in the context of superfluid ^{3}He systems and demonstrated via Josephson oscillations. Macroscopic quantity associated with internal spin degree of freedom or the atomic magnetic moment is the magnetization. Indeed magnetism is based upon quantum principles and perhaps a good place to look for signatures of pure quantum effects at a macroscopic scale. Macroscopic tunnelling of magnetization has attracted much interest recently[4, 5, 6] in the context of molecular nanomagnets of Mn_{12}-acetate, Fe_8 compounds[7, 8], and iron storage protein ferritin[9]. Understanding and controlled realization of MQTM would make strong impact to spintronics and spin based information processing. Storing and processing quantum information for quantum computation and communication is a rapidly developing subject nowadays. Atomic ground states are considered to be good places to encode quantum information as it is highly delicate and suffers strongly from decoherence. Realization of MQTM in an atomic system would be rather useful for such reasons. Quite recently advances in atom trapping and cooling technology allowed for bringing atoms to ultra-cold temperatures, in the order of nano-Kelvins, where they all condense into a same single particle ground state, if they are bosonic composite atoms. This new form of matter is called as Bose-Einstein condensate (BEC), which is described by a macroscopic quantum wave function. Their coherence properties has been demonstrated using atomic external Josephson effect in magnetic trap as a double-well potential[10, 11]. More recently, realization of an all-optical trapping method allowed for removing restriction of frozen internal degree of freedom [12, 13]. Novel condensates with free hyperfine spin variable have created and called as spinor BECs as their macroscopic wave function is given by a three component spinor (for hyperfine spin = 1). One can look for possibility of tunnelling associated with this additional degree of freedom[14]. In this paper, we also investigate such a possibility.

2. Model System

A spin-1 condensate in a double-well potential is described by the Hamiltonian

$$\begin{aligned} H &= \int d\vec{r}\Psi^\dagger(\vec{r})(T+V)\Psi(\vec{r}) \\ &+ \frac{1}{2}\int d\vec{r_1}\int d\vec{r_2}\Psi^\dagger(\vec{r_1})\Psi^\dagger(\vec{r_2})U(\vec{r_1},\vec{r_2})\Psi(\vec{r_1})\Psi(\vec{r_2}), \end{aligned}$$

where $V(\vec{r})$ is all optically created single particle double-well potential independent of the internal degree of freedom. $\Psi(\vec{r})$ $[\Psi(\vec{r})^\dagger]$ is the annihilation(creation) operator of the bosonic atom field, T the single particle kinetic energy and $U(\vec{r_1},\vec{r_2})$ is an effective low energy atom-atom scattering interaction[15, 16]

$$U(\vec{r}_1,\vec{r}_2) == \delta(\vec{r}_1-\vec{r}_2)(\lambda_S+\lambda_A\vec{F}_1\cdot\vec{F}_2), \tag{1}$$

where $g_{0,2}=4\pi\hbar^2 a_{0,2}/M$, $\lambda_S=(g_0+2g_2)/3$ and $\lambda_A=(g_2-g_0)/3$. $a_{0,2}$ the $s-$wave scattering lengths in the corresponding spin channels. For bosonic atoms, $F=0,2$. $F_{j=x,y,z}$ are spin-1 matrices. Corresponding to the three internal spin states (Zeeman levels), the order parameter Ψ has three components ψ_i, $i=+,0,-$. In order to study tunnelling between two spatially distinguishable wells, it is natural to write $\psi_i=\psi_{Li}+\psi_{Ri}$ when the perturbation due to the potential barrier is weak[17].. In a mean field approach, together with the assumption of space-time separability of the wave functions, we write $\psi_i(\vec{r},t)=\phi_{Li}(\vec{r})\xi_i(t)+\phi_{Ri}(\vec{r})\eta_i(t)$, where ϕ_{Li} and ϕ_{Ri} are the ground state wave functions of the i-th spin component in left and right wells respectively when tunnelling is neglected. For ferromagnetic type interactions ($\lambda_a<0$), we recently showed that the ground state wave functions of each component are identical [18], hence $\phi_{Li}=\sqrt{n_L(\vec{r})}$ and $\phi_{Ri}=\sqrt{n_R(\vec{r})}$ with $n_{L,R}(\vec{r})$ the atomic density. For anti-ferromagnetic interactions this becomes the so-called single mode approximation (SMA) [19, 20]. We rewrite the field operators as

$$\Psi(\vec{r},t)=\sqrt{n_L(\vec{r})}\,\vec{\xi}(t)+\sqrt{n_R(\vec{r})}\,\vec{\eta}(t). \tag{2}$$

After integrating over the spatial variables we get[20]

$$\begin{aligned} H_S &= \epsilon_L \vec{\xi}^\dagger \vec{\xi} + \epsilon_R \vec{\eta}^\dagger \vec{\eta} + \frac{\Lambda_L}{2} \vec{\xi}^\dagger \vec{\xi} \vec{\xi}^\dagger \vec{\xi} + \frac{\Lambda_R}{2} \vec{\eta}^\dagger \vec{\eta} \vec{\eta}^\dagger \vec{\eta} \\ &\quad + J(\vec{\xi}^\dagger \vec{\eta} + \vec{\eta}^\dagger \vec{\xi}) \qquad (3) \\ H_A &= \frac{u_L}{2} \sum_{j=x,y,z} \vec{\xi}^\dagger F_j \, \vec{\xi} \vec{\xi}^\dagger F_j \, \vec{\xi} \\ &\quad + \frac{u_R}{2} \sum_{j=x,y,z} \vec{\eta}^\dagger F_j \, \vec{\eta} \vec{\eta}^\dagger F_j \, \vec{\eta}. \qquad (4) \end{aligned}$$

There barrier induced tunnel coupling related coefficients are

$$\begin{aligned} \Lambda_\nu &= \lambda_S \int d\vec{r} \, n_\nu^2(\vec{r}), \qquad (5) \\ u_\nu &= \lambda_A \int d\vec{r} n_{L,R}^2(\vec{r}), \qquad (6) \\ \epsilon_\nu &= \int d\vec{r} \left(\frac{\hbar^2}{2M} \left[\nabla \sqrt{n_\nu} \right]^2 + \sqrt{n_\nu} \, V \sqrt{n_\nu} \right), \qquad (7) \\ J &= \int d\vec{r} \left(\frac{\hbar^2}{2M} \nabla \sqrt{n_L} \cdot \nabla \sqrt{n_R} + \sqrt{n_L} \, V \sqrt{n_R} \right), \qquad (8) \end{aligned}$$

The tunnel coupling is identical for all spin components as the optical potential is spin independent.

Density oscillations between the wells could be studied starting from

$$\begin{aligned} i\hbar \frac{d\vec{\xi}}{dt} &= [\epsilon_L + (\Lambda_L + u_L) \left| \vec{\xi} \right|^2 - u_L H_L] \vec{\xi} + J\vec{\eta}, \\ i\hbar \frac{d\vec{\eta}}{dt} &= J\vec{\xi} + [\epsilon_R + (\Lambda_R + u_R) \left| \vec{\eta} \right|^2 - u_R H_R] \vec{\eta}, \qquad (9) \end{aligned}$$

where

$$\begin{aligned} H_L &= \vec{\xi'}^* \vec{\xi'}^T \equiv \vec{\xi'}^* \otimes \vec{\xi'}^T, \qquad (10) \\ H_R &= \vec{\eta'}^* \vec{\eta'}^T \equiv \vec{\eta'}^* \otimes \vec{\eta'}^T, \qquad (11) \\ \vec{\xi'} &= \begin{pmatrix} \xi_- \\ -\xi_0 \\ \xi_+ \end{pmatrix}; \quad \vec{\eta'} = \begin{pmatrix} \eta_- \\ -\eta_0 \\ \eta_+ \end{pmatrix}, \qquad (12) \\ \left| \vec{\xi} \right|^2 - H_L &= \sum_{j=x,y,z} F_j \vec{\xi} \vec{\xi}^\dagger F_j, \qquad (13) \\ \left| \vec{\eta} \right|^2 - H_R &= \sum_{j=x,y,z} F_j \vec{\eta} \vec{\eta}^\dagger F_j. \qquad (14) \end{aligned}$$

For a symmetric double-well, the numbers of atoms in each well can be kept constant by choosing appropriate initial states. For magnetization tunnelling separated from density oscillations, we consider a special initial state where $\eta_+ = \xi_-$, $\eta_0 = \xi_0$, and $\eta_- = \xi_+$. Focusing on the left well only, density matrix of the system becomes

$$\begin{aligned} \rho &= \vec{\xi}^* \otimes \vec{\xi}^T, \qquad (15) \\ \rho_{ij} &= \xi_i^* \xi_j, \quad i,j = +,0,-. \qquad (16) \end{aligned}$$

Dynamical variables to describe magnetization dynamics are

$$\begin{aligned} M &= \rho_{++} - \rho_{--}; \quad n_0 = \rho_{00}; \\ R_\pm &= \frac{\rho_{+0} \pm \rho_{0-} + c.c}{2}; \quad R_0 = \frac{\rho_{+-} + \rho_{-+}}{2}; \\ I_\pm &= \frac{\rho_{+0} \pm \rho_{0-} - c.c}{2i}; \quad I_0 = \frac{\rho_{+-} - \rho_{-+}}{2i}. \end{aligned} \tag{17}$$

The associated Heisenberg equations become ($\hbar = 1$)

$$\dot{M} = 4JI_0, \tag{18}$$
$$\dot{n_0} = -2u(R_+I_- - R_-I_+), \tag{19}$$
$$\dot{R_+} = 0, \tag{20}$$
$$\dot{R_0} = -2uI_0M + u(R_+I_- + R_-I_+), \tag{21}$$
$$\dot{R_-} = -uI_-M - 2u(R_0I_+ + R_+I_0) + [2J - u(3n_0 - 1)]I_+, \tag{22}$$
$$\dot{I_+} = -2JR_-, \tag{23}$$
$$\dot{I_0} = 2uR_0M - JM - u(R_+R_- - I_+I_-), \tag{24}$$
$$\dot{I_-} = uR_-M - 2u(R_+R_0 + I_+I_0) + u(3n_0 - 1)R_+. \tag{25}$$

We notice $R_0^2 + I_0^2 = (1 - n_0^2)^2 - M^2)/4$, which comes directly from the definition of R_0, I_0, M and normalization of $\vec{\xi}$. For a particular initial state $\xi_0 = 0$ we find a simple situation analogous to the standard Josephson Junction case [17]

$$\dot{M} = 4JI_0, \tag{26}$$
$$\dot{R_0} = -2uI_0M, \tag{27}$$
$$\dot{I_0} = 2uR_0M - JM. \tag{28}$$

In this case the identity becomes $R_0^2 + I_0^2 = (1 - M^2)/4$. Defining $\tan\Phi = I_0/R_0$ we find

$$\dot{M} = 2J\sqrt{1 - M^2}\sin\Phi \tag{29}$$
$$\dot{\Phi} = 2uM - 2J\frac{M}{\sqrt{1 - M^2}}\cos\Phi. \tag{30}$$

With $2J \to -2J \equiv t$ or with $2J \equiv t, \Phi \to -\Phi$ these equations are identical with standard Josephson equations. Classical mechanical interpretation is also possible in terms of an inverted pendulum.

3. Conclusion

We have shown that for certain initial conditions in a symmetric double-well potential MQTM is possible. When $n_0 = 0$ macroscopic tunnelling is identical to standard Josephson junction system which is capable to exhibit self-trapping, Josephson and Rabi regimes. When $n_0 \neq 0$ more rich behaviors within MQTM emerge in comparison to scalar or spin-$\frac{1}{2}$ systems.

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