

Electron-nuclear entanglement in the cold lithium gases

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Abstract: We study the ground-state entanglement and thermal entanglement in the hyperfine interaction of the lithium atom. We present the relationship between the entanglement and both temperature and external magnetic fields.

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1 Introduction

Quantum entanglement is an important prediction of quantum mechanics and indeed constitutes a valuable resource in quantum information processing. In recent years, many important results have been obtained in both experimental and theoretical aspects [1].

The effects of temperature have been investigated and some authors used thermal entanglement to study the electron spin system or other models at finite temperature in Refs. [2-4]. For example, X.G. Wang investigated the isotropic Heisenberg XX model at finite temperature [3]. Y. Sun *et al.* investigated the thermal entanglement in the two-qubit Heisenberg XY model in nonuniform magnetic fields [4]. X.-Q. Xi *et al.* studied the entanglement of XYZ dimer [5]. On the other hand, the entanglement at the critical point is also a topic of great interest [6, 7]. For instance, Osterloh *et al.* demonstrated that for a class of one-dimensional magnetic systems, the entanglement shows scaling

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behavior in the vicinity of the transition point [6].

In this paper, we study the entanglement in the ${}^6\text{Li}$ atom. Near absolute zero, the atom shows some special properties. As we know, in ${}^6\text{Li}$ atom the 3 electrons possess spin $\frac{1}{2}$ and the nucleus has 3 protons and 3 neutrons so that the total nuclear spin is 1. The ${}^6\text{Li}$ atom obeys fermion statistics because the total number of spin-1/2 particles (i.e., electrons, protons, and neutrons) in the system is odd. As we know, two research groups have succeeded in producing a Bose-Einstein condensation of molecules made from pairs of fermion atoms [8, 9]. Note that the atoms are fermions but if considered as pairs they are bosons and therefore able to condense in Bose-Einstein fashion. So it is necessary to study the entanglement properties of the atom in the external fields at very low temperature.

In the following, the ground state entanglement of such a system is evaluated by using Rungta's concurrence. Then we use negativity to study the entanglement between the electrons and the nucleus at finite temperature.

2 The model and the Hamiltonian

In the ${}^6\text{Li}$ atom, the electron spins are coupled to the nuclear spin by the hyperfine interaction. The hyperfine line for the lithium atom has a measured frequency of 228MHz. Some calculation on the basis of first-order perturbation for the magnetic dipole interaction between the electron and the nucleus gives contribution to the coupling strength of $\mathbf{I} \cdot \mathbf{S}$ term. In this paper, we study a bipartite system, one is the nucleus which has the spin-1 and the other is the electron which has total spin-1/2. Both parts interact with external magnetic field B . Since the electrons have no orbital angular momentum ($L = 0$), there is no magnetic field at the nucleus due to the orbital motion. The Hamiltonian can be expressed as

$$H = J(I_x \cdot S_x + I_y \cdot S_y + I_z \cdot S_z) + CS_z + DI_z, \quad (1)$$

where J is the coupling constant. Throughout the paper, the constant J is set to unity. I_i is the nuclear spin which has spin-1 and S_i is electron spin. The two parameters are related to the external fields. They are given by

$$C = g\mu_B B, \quad D = -\frac{\mu}{I} B. \quad (2)$$

In the Hamiltonian (1) we study the ground state when the electronic orbital angular momentum L is zero. For the lithium atom, the nuclear magnetic moment $\mu = 0.822\mu_N$, where $\mu_N = e\hbar/(2m_p)$. Since $|C/D| \sim m_p/m_e \approx 2000$, for most applications D can be neglected. At the same level of approximation the g factor of the electron may be set equal to 2[10]. In this paper, the spin-1/2 state has the bases as $|\uparrow\rangle, |\downarrow\rangle$ and the spin-1 state has the bases as $|\uparrow\rangle, |0\rangle, |\downarrow\rangle$. In the above bases, the Hamiltonian can be rewritten

as follows,

$$\begin{pmatrix} \frac{1}{2} + \frac{C}{2} + D & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} - \frac{C}{2} + D & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{C}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{C}{2} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{2} + \frac{C}{2} - D & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} - \frac{C}{2} - D \end{pmatrix}. \quad (3)$$

From the Hamiltonian one can easily obtain the eigenvalues and eigenvectors. During the evaluation of the entanglement of the system, we will have to deal with the high-dimensional Hilbert space. Rungta *et al.* introduced *I concurrence* to measure the high-dimensional bipartite pure state[11]. For a joint pure state $|\Psi\rangle_{AB}$ in $D_1 \otimes D_2$ system, the quantity is given by

$$\mathfrak{C}(\rho) = \sqrt{2\nu_{D_1}\nu_{D_2}(1 - \text{tr}\rho_A^2)}, \quad (4)$$

where D_1 and D_2 are the dimensions of the Hilbert spaces and ν_{D_1}, ν_{D_2} are two parameter related to dimension. For pure state, the quantity is simply related to the purity of the marginal density operator. ρ_A is the reduced density matrix and $\rho_A = \text{Tr}_B \rho_{AB}$. In order to be consistent with the concurrence for qubits, a sensible choice is to set $\nu_{D_1} = \nu_{D_2} = 1$. The generalized concurrence vanishes for unentangled state. Let $X = \min\{D_1, D_2\}$. So the concurrence arranges from 0 to $\sqrt{2(X-1)/X}$. The generalized concurrence can measure the entanglement of arbitrary bipartite pure states.

3 Entanglement in the presence of non-uniform fields

We will study the ground-state entanglement of the system. Since the parameter C is much larger than D , D will be neglected in this section.

(a) When $C < 0$, the ground state energy is $(-1 - \sqrt{9 - 4C + 4C^2})/4$ and the eigenvector is given by

$$|\Psi_1\rangle = \frac{1}{N_1} \left(\frac{1 - 2C - \sqrt{9 - 4C + 4C^2}}{2\sqrt{2}} |0 \downarrow\rangle + |\downarrow \uparrow\rangle \right), \quad (5)$$

where N_1 is the normalization factor. One can use Rungta's concurrence to measure the entanglement and obtain

$$\mathfrak{C}(|\Psi_1\rangle) = \frac{4\sqrt{2}|1 - 2C - \sqrt{9 - 4C + 4C^2}|}{(1 - 2C - \sqrt{9 - 4C + 4C^2})^2 + 8}. \quad (6)$$

(b) When $C > 0$, the ground state is $(-1 - \sqrt{9 + 4C + 4C^2})/4$ and the eigenvector is given by

$$|\Psi_2\rangle = \frac{1}{N_2} \left(-\frac{1 + 2C + \sqrt{9 + 4C + 4C^2}}{2\sqrt{2}} |\uparrow \downarrow\rangle + |0 \uparrow\rangle \right), \quad (7)$$

where N_2 is the normalization factor. The concurrence is

$$\mathfrak{C}(|\Psi_2\rangle) = \frac{4\sqrt{2}|1 + 2C + \sqrt{9 + 4C + 4C^2}|}{(1 + 2C + \sqrt{9 + 4C + 4C^2})^2 + 8}. \quad (8)$$

The above results are plotted in Fig. 1 and Fig. 2. Fig. 1 shows the relationship between the ground-state energy and external magnetic fields. Fig. 2 shows the relationship between the ground-state entanglement and external magnetic fields C .

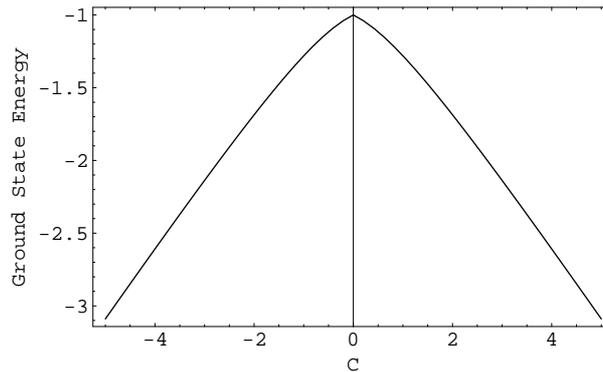


Fig. 1 Ground state energy when $D = 0$

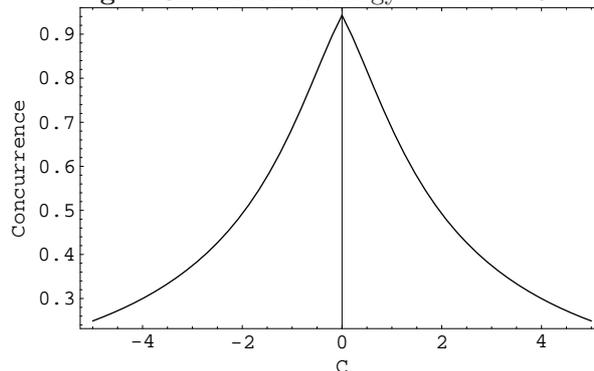


Fig. 2 Ground-state entanglement versus $C(= g\mu_B B)$.

From Fig. 2, one can see when the parameter C approaches zero, i.e., the magnetic fields is vanishing, the concurrence approaches its maximum $2\sqrt{2}/3 \approx 0.943$. In fact, when the magnetic field is absent, the ground state is degenerate, it will be discussed in the following paragraph.

(c) When $C = 0$, i.e., the magnetic field is absent, the ground state will be doubly degenerate. As we know, if the ground state is degenerate the zero-temperature ensemble becomes an equal mixture of all the possible ground states [7]. In this case, the thermal ground state may be written as

$$\rho = \frac{1}{2}|\phi_1\rangle\langle\phi_1| + \frac{1}{2}|\phi_2\rangle\langle\phi_2|, \quad (9)$$

where

$$|\phi_1\rangle = -\sqrt{\frac{1}{3}}|0\downarrow\rangle + \sqrt{\frac{2}{3}}|\downarrow\uparrow\rangle, \quad |\phi_2\rangle = -\sqrt{\frac{2}{3}}|\uparrow\downarrow\rangle + \sqrt{\frac{1}{3}}|0\uparrow\rangle.$$

One can use *negativity* to measure the entanglement of the state. The negativity was introduced by G. Vidal *et al.* [12]. The quantity is given by

$$\mathfrak{N}(\rho_{AB}) \equiv \frac{\|\rho_{AB}^{T_A}\|_1 - 1}{2}, \quad (10)$$

where the trace norm is defined by $\|M\|_1 \equiv \text{tr}\sqrt{M^\dagger M}$ and T_A denotes the partial transpose of the bipartite mixed state ρ_{AB} . Negativity vanishes for unentangled states. For a $3 \otimes 2$ bipartite mixed state, negativity is a preferred measure because a state ρ_{AB} of a $2 \otimes 2$ or $2 \otimes 3$ system is separable if and only if its partial transposition is a positive operator [13]. It is easy to show that the negativity of the state (9) is $1/3$.

4 Thermal entanglement

As we know, since thermal entanglement was introduced in 1998 [2], many efforts are devoted to study the thermal state of the qubit system. Here we want to use negativity to study the thermal entanglement of mixed-spin bipartite system at finite temperature.

Here ρ stands for the Gibbs density operator, $\rho = \frac{1}{Z} \exp(-H/kT)$, where $Z = \text{tr} \exp(-H/kT)$ is the partition function, H is the Hamiltonian, T is temperature and k is Boltzmann's constant which we henceforth will set equal to unity. In the bases $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |0\uparrow\rangle, |0\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$, the thermal state ρ can be rewritten as follows,

$$\begin{pmatrix} \omega_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \omega_2 & s_1 & 0 & 0 & 0 \\ 0 & s_1 & \omega_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & \omega_4 & s_2 & 0 \\ 0 & 0 & 0 & s_2 & \omega_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \omega_6 \end{pmatrix}. \quad (11)$$

One can use negativity to study the thermal entanglement of the state. Here the parameter D is also neglected. At various temperatures, the negativity versus C is plotted in Fig. 3. From this, one can find when the temperature is low enough, at the point $C = 0$, the negativity curve has a local minimum. However, as the temperature increases and when it is larger than a critical value $T_C = 0.107$, the local minimum changes to be a local maximum. In detail, when $T = 0.5$, at the point $C = 0$, the negativity is 0.243. This is a local maximum. When $T = 0.05$, the negativity is 0.333, but it is a local minimum. One can see that the temperature can efficiently affect the entanglement of the system.

5 Summary and acknowledgements

In this paper, we studied the entanglement of the electron-nuclear entanglement of ${}^6\text{Li}$ atoms in presence of uniform external magnetic fields. We studied the ground-state en-

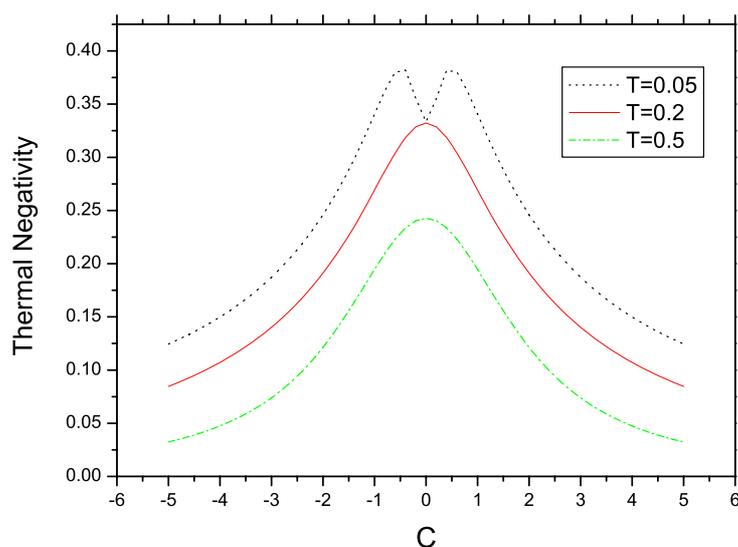


Fig. 3 Thermal negativity versus $C(= g\mu_B B)$ at various temperatures.

tanglement at zero temperature and thermal entanglement at finite temperature respectively. We have presented the relationship between the entanglement and the magnetic fields or temperature. In order to detect the entanglement of the system, the surrounding temperature should be near absolute zero.

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