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# Entanglement in the supermolecular dimer $[Mn_4]_2$*

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This paper investigates the entanglement in the supermolecular dimer $[Mn_4]_2$ consisting of a pair of single molecular magnets with antiferromagnetic exchange-coupling $J$. The conventional von Neumann entropy as a function of the exchange-coupling is calculated explicitly for all eigenstates with the quantum number range from $M = M_1 + M_2 = -9$ to 0. It is shown that the von Neumann entropy is not a monotonic function of the coupling strength. However, it is significant that the entropy of entanglement has the maximum values and the minimum values for most eigenstates, which is extremely useful in the quantum computing. It also presents the time-evolution of entanglement from various initial states. The results are useful in the design of devices based on the entanglement of two molecular magnets.

**Keywords:** entanglement, supermolecular dimer $[Mn_4]_2$, exchange-coupling, time-evolution of entanglement
**PACC:** 0365

## 1. Introduction

The entanglement as a fundamental quantum property in quantum transport of information proposed by Bennett *et al*[1] has attracted growing interest.[2−8] Besides the conceptual importance in quantum theory the entanglement which lies at the heart of the difference between the quantum and classical worlds has assumed a role of quantum information theory complementary in many ways to the role of classical information and is therefore regarded as a physical resource to perform numerous tasks in quantum computation.[9−13] On other hand various specialized applications of magnets particularly in quantum information require monodisperse, small magnetic particles, and thus the discovery of molecules that can function as nanoscale magnets was an important development in this regard. Recently several quantum-computing schemes are suggested by using molecular magnets[14−16] and a two-qubit quantum logic gate with molecular magnets has been proposed.[17] It is demonstrated by Leuenberger and Loss[14] that molecular magnets such as $Fe_8$ and $Mn_{12}$ may be the most promising candidates to build dense and efficient memory devices based on the Grover algorithm. Wernsdorfer *et al*[18] recently pointed out that the supermolecular dimer $[Mn_4]_2$ consisting of two molecule magnets $Mn_4$ with antiferromagnetic exchange-coupling exhibits a quite different quantum behaviour from two individual $Mn_4$ molecules without coupling,[18−21] it is this coupling which is the essential ingredient in a quantum device and enables encoding of data via arbitrary superpositions of pure quantum states. This result is of great importance if such systems are to be used for quantum computation. Quantum tunnelling of magnetization in molecule magnets is k one of the well known macroscopic quantum phenomena and has the advantage of providing the quantum superposition of states required for quantum computation, however it has a disadvantage in information storage, where it leads to information loss. The antiferromagnetic coupling between the $Mn_4$ units in $[Mn_4]_2$ dimer makes this dimer an excellent candidate for studying quantum tunnelling.[19] Thus it is important to both understand and control the quantum properties of the $[Mn_4]_2$ dimer. The quantum tunnelling transitions via entangled states of $[Mn_4]_2$ dimer have been also identified showing the evidence for quantum mechanical entanglement. In this paper, we study the entanglement in the supermolecular dimer $[Mn_4]_2$ with respect to energy eigenvectors

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which are obtained in terms of the high-order perturbation method. The conventional von Neumann entropy as the entanglement measure of pure quantum states is calculated for all eigenstates in the quantum number range from $M = M_1 + M_2 = -9$ to 0. We pay more attention to the dependence of the entanglement on the coupling $J$ and the dynamics of entanglement as well. We believe that the theoretical analyses can suggest a means of tuning the quantum tunnelling of magnetization in $[Mn_4]_2$ dimer and provide useful information for the design of quantum computing devices.

## 2. Entanglements of the energy eigenstates

For the supermolecular dimer $[Mn_4]_2$ with antiferromagnetic coupling the Hamiltonian is written as[22,23]

$$\hat{H} = [\hat{H}_1 + \hat{H}_2 + J_z \hat{S}_{1z} \widehat{S}_{2z}] + \frac{1}{2} J_{xy} (\widehat{S}_{1+} \widehat{S}_{2-} + \widehat{S}_{1-} \widehat{S}_{2+}), \quad (1)$$

and

$$\hat{H}_i = -D \widehat{S}_{iz}^2 - B \widehat{S}_{iz}^4 + g_z \mu_B B_z \widehat{S}_{iz}, \quad (2)$$

with $i = 1, 2$ labelling the two $Mn_4$ molecules in the dimer, and $\widehat{S}_{\pm} = \widehat{S}_x \pm \mathrm{i} \widehat{S}_y$, where $J_z$ and $J_{xy}$ denote the strengths of exchange coupling. Here we consider only the isotropic case that $J_z = J_{xy} = J > 0$ which has been verified experimentally.[20] We furthermore assume that the exchange coupling $J$ is much less than the anisotropy constant $D$. In the case, the electron paramagnetic resonance (EPR) transitions in the supermolecular dimer $[Mn_4]_2$ have been studied, and the high-order corrections of level splitting have been obtained employing the high-order perturbation method.[23] The corresponding eigenstates are listed in Appendix A in Ref.[23] (where $|M_1, M_2\rangle_{\mathrm{S}}$ and $|M_1, M_2\rangle_{\mathrm{A}}$ denote the symmetric and antisymmetric states respectively) with parameter values $D = 0.72$ K, $B = 1.8 \times 10^{-3}$ K, $J = 0.10$ K which give rise to the best fit between theoretical and measured level splitting.[22,23]

The means to create, manipulate, and characterize quantum states is becoming an increasingly important area of research due to the technological applications in quantum computing, quantum cryptography, and communications where entanglement plays a central role and is a phenomenon facilitating quantum information and quantum computing with many qubits. It is therefore of a great importance to explore the entanglement of eigenstate basis of the supermolecular dimer $[Mn_4]_2$. Obviously, all eigenvectors listed in Appendix A in Ref.[23] are entangled states of two molecules $Mn_4$. The standard entanglement measure of a bipartite system is the von Neumann entropy of the reduced density operator which is obtained by tracing out the other subsystems. For the supermolecular dimer $[Mn_4]_2$ the orthonormal basis of a single-molecule magnet $|M_i\rangle$ $(i = 1, 2)$ forms a ten dimensional Hilbert space. All eigenvectors $|\Psi\rangle$ (see Appendix A in Ref.[23]) of the supermolecular dimer $[Mn_4]_2$ can be written in the general form,

$$|\Psi\rangle = \sum_{M_1, M_2 = -9/2}^{9/2} C_{M_1 M_2} |M_1, M_2\rangle, \quad (3)$$

where $\sum |C_{M_1 M_2}|^2 = 1$. The reduced density operator with respect to the subsystem 1 is defined by

$$\rho_1 = \mathrm{Tr}_2(\rho) = \sum_{M_1 = -9/2}^{9/2} C_{M_1}^2 |M_1\rangle\langle M_1|, \quad (4)$$

where $Tr_2$ is the partial trace over subsystem 2, $\rho = |\Psi\rangle\langle\Psi|$ is the density operator and $C_{M_1} = C_{M_2} = C_{M_1 M_2}$ for the present case.

The von Neumann entropy of either $\rho_1$ or $\rho_2$, is determined by the squares of the Schmidt coefficients[24–26] such that

$$E = -\mathrm{Tr}\rho_1 \log_2 \rho_1 = -\mathrm{Tr}\rho_2 \log_2 \rho_2 = -\sum_{M_1 = -9/2}^{9/2} C_{M_1}^2 \log_2 C_{M_1}^2. \quad (5)$$

The value of entropy $E$ varies between 0 and the maximum value $E_{\max} = \log_2 d = 3.322$ for the maximally entangled state, where $d$ is the dimension of the Hilbert space of the subsystem.[27] Making use of Eqs.(4) and (5), we can calculate entanglements of all eigenstates given in Appendix A in Ref.[23] and result is shown in Table 1 with the exchange coupling $J = 0.1$ K. The entanglement of eigenstate $|\Psi_{29}\rangle_{\mathrm{A}}$ is 1.9068 which is the largest value. The ground state $|\Psi_1\rangle_{\mathrm{S}} = |-\frac{9}{2}, -\frac{9}{2}\rangle$ in a wide range of the longitudinal magnetic field $B_z$ is non-entangled with vanishing von Neumann entropy $E(|\Psi_1\rangle_{\mathrm{S}}) = 0$ while in a small range of longitudinal magnetic field $|\Psi_{26}\rangle$ is the lowest energy state of the dimer instead with non-vanishing entropy $E(|\Psi_{26}\rangle) = 1.0129$.

**Table 1.** Entanglement in a supermolecular dimer $[Mn]_2$.

| States | entanglement | states | entanglement | states | Entanglement |
|---|---|---|---|---|---|
| $\|\psi_1\rangle_S$ | 0 | $\|\psi_2\rangle_S$ | 1 | $\|\psi_2\rangle_A$ | 1 |
| $\|\psi_3\rangle_S$ | 1.5006 | $\|\psi_3\rangle_A$ | 1 | $\|\psi_4\rangle_S$ | 03478 |
| $\|\psi_5\rangle_S$ | 1.1556 | $\|\psi_5\rangle_A$ | 1.3093 | $\|\psi_6\rangle_S$ | 1.2303 |
| $\|\psi_6\rangle_S$ | 1.2303 | $\|\psi_7\rangle_S$ | 1.1578 | $\|\psi_7\rangle_A$ | 1.1388 |
| $\|\psi_8\rangle_S$ | 1.6721 | $\|\psi_8\rangle_A$ | 1.1443 | $\|\psi_9\rangle_S$ | 0.7034 |
| $\|\psi_{10}\rangle_S$ | 1.0992 | $\|\psi_{10}\rangle_A$ | 1.1001 | $\|\psi_{11}\rangle_S$ | 1.3328 |
| $\|\psi_{11}\rangle_A$ | 1.6528 | $\|\psi_{12}\rangle_S$ | 1.5262 | $\|\psi_{12}\rangle_A$ | 1.5262 |
| $\|\psi_{13}\rangle_S$ | 1.0681 | $\|\psi_{13}\rangle_A$ | 1.0680 | $\|\psi_{14}\rangle_S$ | 1.3475 |
| $\|\psi_{14}\rangle_A$ | 1.2969 | $\|\psi_{15}\rangle_S$ | 1.6396 | $\|\psi_{15}\rangle_A$ | 1.2499 |
| $\|\psi_{16}\rangle_S$ | 0.9637 | $\|\psi_{17}\rangle_S$ | 1.0452 | $\|\psi_{17}\rangle_A$ | 1.0452 |
| $\|\psi_{18}\rangle_S$ | 1.2045 | $\|\psi_{18}\rangle_A$ | 1.2085 | $\|\psi_{19}\rangle_S$ | 1.4265 |
| $\|\psi_{19}\rangle_A$ | 1.8472 | $\|\psi_{20}\rangle_S$ | 1.5350 | $\|\psi_{20}\rangle_A$ | 1.5350 |
| $\|\psi_{21}\rangle_S$ | 1.0274 | $\|\psi_{21}\rangle_A$ | 1.0274 | $\|\psi_{22}\rangle_S$ | 1.1289 |
| $\|\psi_{22}\rangle_A$ | 1.1287 | $\|\psi_{23}\rangle_S$ | 1.4500 | $\|\psi_{23}\rangle_A$ | 1.3756 |
| $\|\psi_{24}\rangle_S$ | 1.5914 | $\|\psi_{24}\rangle_A$ | 1.3075 | $\|\psi_{25}\rangle_S$ | 1.0952 |
| $\|\psi_{26}\rangle_{SA}$ | 1.0129 | $\|\psi_{26}\rangle_{SA}$ | 1.0129 | $\|\psi_{27}\rangle_S$ | 1.0723 |
| $\|\psi_{27}\rangle_A$ | 1.0723 | $\|\psi_{28}\rangle_S$ | 1.2399 | $\|\psi_{28}\rangle_A$ | 1.2442 |
| $\|\psi_{29}\rangle_S$ | 1.4558 | $\|\psi_{29}\rangle_A$ | 1.9068 | $\|\psi_{30}\rangle_{BA}$ | 1.5753 |

The supramolecular approach to materials design is particularly attractive, since it affords control over many key parameters required for basis states of viable qubits which may be realized through the choice of exchange couplings selectively designed into crystalline arrays of these molecules. It is of interest to see the variation of the von Neumann entropy with the coupling and is useful for future design strategies with optical control of the exchange coupling between the halves of a dimer. To this end we begin with the explicit dependence of all eigenstates on the exchange coupling $J$ listed in Appendix A in Ref [23]. For example, the eigenstate $|\Psi_{26}\rangle_{SA}$ as a function of $J$ is written as

$$|\Psi_{26}\rangle_{SA} = \Big|-\frac{9}{2},\frac{9}{2}\Big\rangle_{SA} - 0.3395J\Big|-\frac{7}{2},\frac{7}{2}\Big\rangle_{SA} + 0.1186J^2\Big|-\frac{5}{2},\frac{5}{2}\Big\rangle_{SA} - 0.04268J^3\Big|-\frac{3}{2},\frac{3}{2}\Big\rangle_{SA} + (1.395\times10^{-2}J^4 - 6.146\times10^{-3}J^5)\Big|-\frac{1}{2},\frac{1}{2}\Big\rangle_{SA}. \quad (6)$$

The eigenstate $|\Psi_5\rangle_S$ as a function of $J$ is written as

$$|\Psi_5\rangle_S = \Big|-\frac{9}{2},-\frac{3}{2}\Big\rangle_S - C\Big|-\frac{7}{2},-\frac{5}{2}\Big\rangle_S = \Big|-\frac{9}{2},-\frac{3}{2}\Big\rangle_S - (1.9714J - 4.523J^2)\Big|-\frac{7}{2},-\frac{5}{2}\Big\rangle_S. \quad (7)$$

The $J$ dependences of the non-vanishing entropy for various eigenstates are shown in Fig.1, which are divided into six types: (a) for eigenstates $|\Psi_5\rangle_S$ and $|\Psi_7\rangle_A$; (b) $|\Psi_3\rangle_S$, $|\Psi_8\rangle_S$, $|\Psi_{15}\rangle_S$ and $|\Psi_{24}\rangle_S$; (c) $|\Psi_4\rangle_S$, $|\Psi_8\rangle_A$, $|\Psi_9\rangle_S$, $|\Psi_{15}\rangle_A$, $|\Psi_{16}\rangle_S$, $|\Psi_{20}\rangle_{SA}$, $|\Psi_{24}\rangle_A$, $|\Psi_{25}\rangle_S$ and $|\Psi_{30}\rangle_{SA}$; (d) $|\Psi_{10}\rangle_S$, $|\Psi_{11}\rangle_S$, $|\Psi_{13}\rangle_A$, $|\Psi_{14}\rangle_A$, $|\Psi_{18}\rangle_S$, $|\Psi_{19}\rangle_S$, $|\Psi_{22}\rangle_A$, $|\Psi_{23}\rangle_A$, $|\Psi_{28}\rangle_S$ and $|\Psi_{29}\rangle_S$; (e) $|\Psi_5\rangle_A$, $|\Psi_6\rangle_{SA}$, $|\Psi_7\rangle_S$, $|\Psi_{10}\rangle_A$, $|\Psi_{11}\rangle_A$, $|\Psi_{12}\rangle_{SA}$, $|\Psi_{13}\rangle_S$, $|\Psi_{14}\rangle_S$, $|\Psi_{18}\rangle_A$, $|\Psi_{19}\rangle_A$, $|\Psi_{22}\rangle_S$, $|\Psi_{23}\rangle_S$, $|\Psi_{28}\rangle_A$ and $|\Psi_{29}\rangle_A$; (f) $|\Psi_{17}\rangle_S$, $|\Psi_{17}\rangle_A$, $|\Psi_{21}\rangle_S$, $|\Psi_{21}\rangle_A$, $|\Psi_{26}\rangle_{SA}$, $|\Psi_{27}\rangle_S$ and $|\Psi_{27}\rangle_A$.

From Eq.(7) and Fig.1 we see that the entangled state $|\Psi_5\rangle_S$ is a superposition of the states $|-\frac{9}{2},-\frac{3}{2}\rangle_S$ and $|-\frac{7}{2},-\frac{5}{2}\rangle_S$ depending on the parameter $C = 1.9714J - 4.523J^2$ which is not a monotonous function of the coupling parameter $J$ and gives rise to the similar $J-$dependence of entanglement. The entropy of entanglement for eigenstate $|\Psi_5\rangle_S$ has two maximum

values at $J = 0.218$ K , 0.736 K, and a minimum value ($E = 1$) at $J = 0.436$ K. The entropy increases with the coupling parameter $J$ and therefore $C$ in the region from $J$ =0 K to 0.218 K, and reaches the first maximum value when $C = 0.215$, and $J = 0.218$ K. Then the entropy decreases from $J$ =0.218 K due to the decrease of the parameter $C$ and becomes minimum ($E = 1$) at $J = 0.436$ K which leads to vanishing $C = 0$ where only the state $|-\frac{9}{2},-\frac{3}{2}\rangle_S$ contributes the entanglement; it increases again starting from $J$ =0.436 K and reaching the second maximum at $J = 0.736$ K where $|C| = 1$ and thus both states $|-\frac{7}{2},-\frac{5}{2}\rangle_S$ and $|-\frac{9}{2},-\frac{3}{2}\rangle_S$ have equal contributions on the entropy of entanglement of eigenstate $|\Psi_5\rangle_S$. When $J > 0.736$ K, $|C| > 1$, the contribution of state $|-\frac{9}{2},-\frac{3}{2}\rangle_S$ decreases again. When $J > 2$ K, the effect of $|-\frac{7}{2},-\frac{5}{2}\rangle_S$ dominates the entanglement of $|\Psi_5\rangle_S$, and thus the entropy approaches an asymptotic value ($E = 1$).

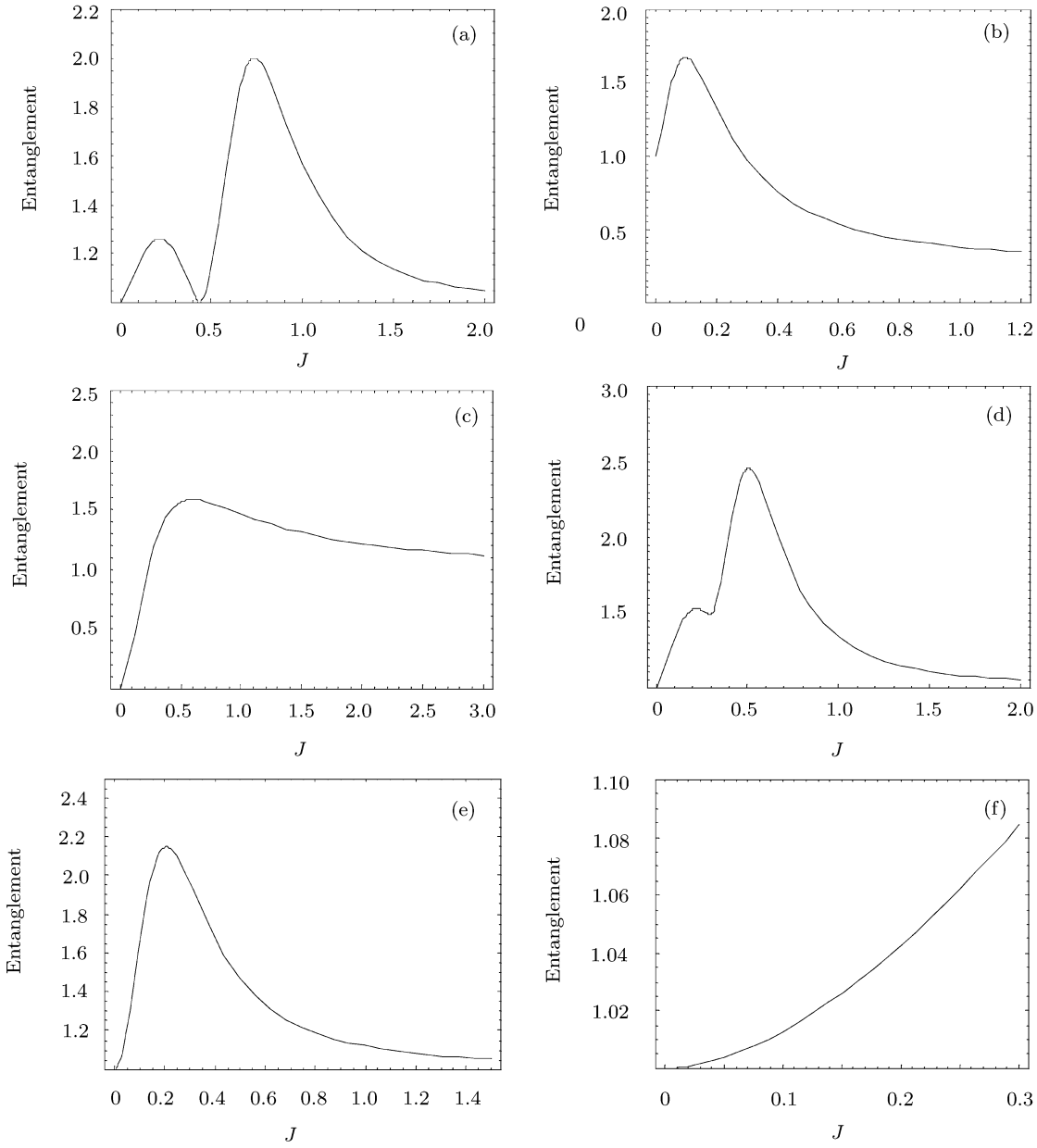



**Fig.1.** The dependence of the entanglement measure on the coupling parameter $J$ with (a), (b), (c), (d), (e) and (f) relating to the eigenstate$|\Psi_5\rangle_S$, $|\Psi_8\rangle_S$, $|\Psi_4\rangle_S$, $|\Psi_{11}\rangle_S$, $|\Psi_{11}\rangle_A$ and $|\Psi_{26}\rangle_{SA}$ respectively.

The entropy measure of the entanglement for eigenstate $|\Psi_8\rangle_{\rm S}$ has only one maximum value at $J = 0.1$ K and approaches asymptotic value $E = 0.25$ with increase of $J$. The entropy measure of the entanglement for eigenstate $|\Psi_{11}\rangle_{\rm S}$ has two maximum values at $J = 0.22$ K, 0.52 K, and one minimum value at $J = 0.3$ K and approaches asymptotic value $E = 1$ when the coupling parameter $J$ continuously increases similar to that of the state $|\Psi_5\rangle_{\rm S}$. The explanation of the entropy of entanglement for other eigenstates are similar to that of the state $|\Psi_5\rangle_{\rm S}$ too. The dependence of entanglement on the coupling parameter may be useful in the logical-gate design with molecular magnets.

## 3. Dynamics of entanglement

One of the most interesting aspects of the dynamics of the composite quantum system is the time evolution of entanglement which is necessary in quantum information processing. The dynamics of quantum state is governed by the Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

with an initial condition

$$|\Psi(0)\rangle = \sum_k C_k|\Phi_k\rangle,$$

where $|\Phi_k\rangle$ are chosen from the energy eigenstates listed in Appendix A in Ref.[23] with an equal quantum number $M = M_1 + M_2$. The time-dependent state can be expressed as

$$|\Psi(t)\rangle = \sum_k C_k \exp\Big(-\frac{\mathrm{i}}{\hbar}E_k t\Big)|\Phi_k\rangle, \tag{8}$$

where $E_k$ is the eigenvalue corresponding to the eigenstate $|\Phi_k\rangle$. The time evolution of the reduced density operator is seen to be

$$\rho_1(t) = \mathrm{Tr}_2(\rho) = \sum_{n,k,l} C_k C_l A_{k,n} A_{l,n} \times \exp\Big[-\frac{\mathrm{i}}{\hbar}(E_k - E_l)t\Big]\xi_n, \tag{9}$$

where $\xi_n = |M_1(n)\rangle\langle M_1(n)|$ and $A_{k,n}$ is defined by

$$|\Phi_k\rangle = \sum_n A_{k,n}|M_1(n), M_2\rangle.$$

$n = 1, \ldots, 10$ denotes the state order with $M_1 = -\frac{9}{2}, \frac{9}{2}, \ldots -\frac{1}{2}, \frac{1}{2}$ respectively. The time evolution of the von Neumann entropy for the state $|\Psi(t)\rangle$ is given by

$$E(t) = -\sum_n \Big\{\sum_{k,l} C_k C_l A_{k,n} A_{l,n} \times \exp\Big[-\frac{\mathrm{i}}{\hbar}(E_k - E_l)t\Big]\Big\} \times \log_2\Big\{\sum_{k,l} C_k C_l A_{k,n} A_{l,n} \times \exp\Big[-\frac{\mathrm{i}}{\hbar}(E_k - E_l)t\Big]\Big\}. \tag{10}$$

For the initial state with $M = -7$, i.e.

$$|\Psi(0)\rangle = \frac{1}{\sqrt{3}}(|\Psi_3\rangle_{\rm S} + |\Psi_3\rangle_{\rm A} + |\Psi_4\rangle_{\rm S}), \tag{11}$$

we have

$$\xi_1 = \Big|-\frac{9}{2}\Big\rangle\langle-\frac{9}{2}\Big|, \quad \xi_2 = \Big|-\frac{7}{2}\Big\rangle\Big\langle-\frac{7}{2}\Big|, \quad \xi_3 = \Big|-\frac{5}{2}\Big\rangle\Big\langle-\frac{5}{2}\Big|,$$

and

$$|\Phi_1\rangle = \Big|\Psi_3\Big\rangle_{\rm S} = 0.64013\Big|-\frac{9}{2},-\frac{5}{2}\Big\rangle - 0.42482\Big|-\frac{7}{2},-\frac{7}{2}\Big\rangle + 0.64013\Big|-\frac{5}{2},-\frac{9}{2}\Big\rangle. \tag{12}$$

Figure 2(a) displays the evaluated time-evolution of entanglement for the state with initial condition Eq.(11). The time evolutions of entanglements for the initial states $|\Psi(0)\rangle = \frac{1}{\sqrt{3}}(|\Psi_5\rangle_{\rm S} + |\Psi_5\rangle_{\rm A}) + \frac{1}{\sqrt{6}}(|\Psi_6\rangle_{\rm S} + |\Psi_6\rangle_{\rm A})$ with $M = -6$, $\frac{1}{\sqrt{5}}(|\Psi_7\rangle_{\rm S} + |\Psi_7\rangle_{\rm A} + |\Psi_8\rangle_{\rm S} + |\Psi_8\rangle_{\rm A} + |\Psi_9\rangle_{\rm S})$ with $M = -5$, $\frac{1}{2}(|\Psi_{10}\rangle_{\rm S} + |\Psi_{10}\rangle_{\rm A}) + \frac{1}{\sqrt{5}}(|\Psi_{11}\rangle_{\rm S} + |\Psi_{11}\rangle_{\rm A}) + \frac{1}{\sqrt{20}}(|\Psi_{12}\rangle_{\rm S} + |\Psi_{12}\rangle_{\rm A})$ with $M = -4$, $\frac{1}{\sqrt{7}}(|\Psi_{13}\rangle_{\rm S} + |\Psi_{13}\rangle_{\rm A} + |\Psi_{14}\rangle_{\rm S} + |\Psi_{14}\rangle_{\rm A} + |\Psi_{15}\rangle_{\rm S} + |\Psi_{15}\rangle_{\rm A} + |\Psi_{16}\rangle_{\rm S})$ with $M = -3$, $\frac{1}{\sqrt{8}}(|\Psi_{17}\rangle_{\rm S} + |\Psi_{17}\rangle_{\rm A} + |\Psi_{18}\rangle_{\rm S} + |\Psi_{18}\rangle_{\rm A} + |\Psi_{19}\rangle_{\rm S} + |\Psi_{19}\rangle_{\rm A} + |\Psi_{20}\rangle_{\rm S} + |\Psi_{20}\rangle_{\rm A})$ with $M = -2$, $\frac{1}{3}(|\Psi_{21}\rangle_{\rm S} + |\Psi_{21}\rangle_{\rm A} + |\Psi_{22}\rangle_{\rm S} + |\Psi_{22}\rangle_{\rm A} + |\Psi_{23}\rangle_{\rm S} + |\Psi_{23}\rangle_{\rm A} + |\Psi_{24}\rangle_{\rm S} + |\Psi_{24}\rangle_{\rm A} + |\Psi_{25}\rangle_{\rm S})$ with $M = -1$, and $\frac{1}{\sqrt{10}}(|\Psi_{26}\rangle_{\rm S} + |\Psi_{26}\rangle_{\rm A} + |\Psi_{27}\rangle_{\rm S} + |\Psi_{27}\rangle_{\rm A} + |\Psi_{28}\rangle_{\rm S} + |\Psi_{28}\rangle_{\rm A} + |\Psi_{29}\rangle_{\rm S} + |\Psi_{29}\rangle_{\rm A} + |\Psi_{30}\rangle_{\rm S} + |\Psi_{30}\rangle_{\rm A})$ with $M = 0$ are shown in Fig.2(b), 2(c), 2(d), 2(e), 2(f), 2(g), 2(h) respectively. From Fig.2 we see that the entanglement oscillates with different periods for different quantum number $M$ and the oscillation of the entanglement is different for another initial state. The time-evolution of entanglement, useful in the design of devices based on the entanglement of two molecular magnets, is basically periodic for the initial states of given quantum number $M$ which are seen to be superposition of energy eigenstates.

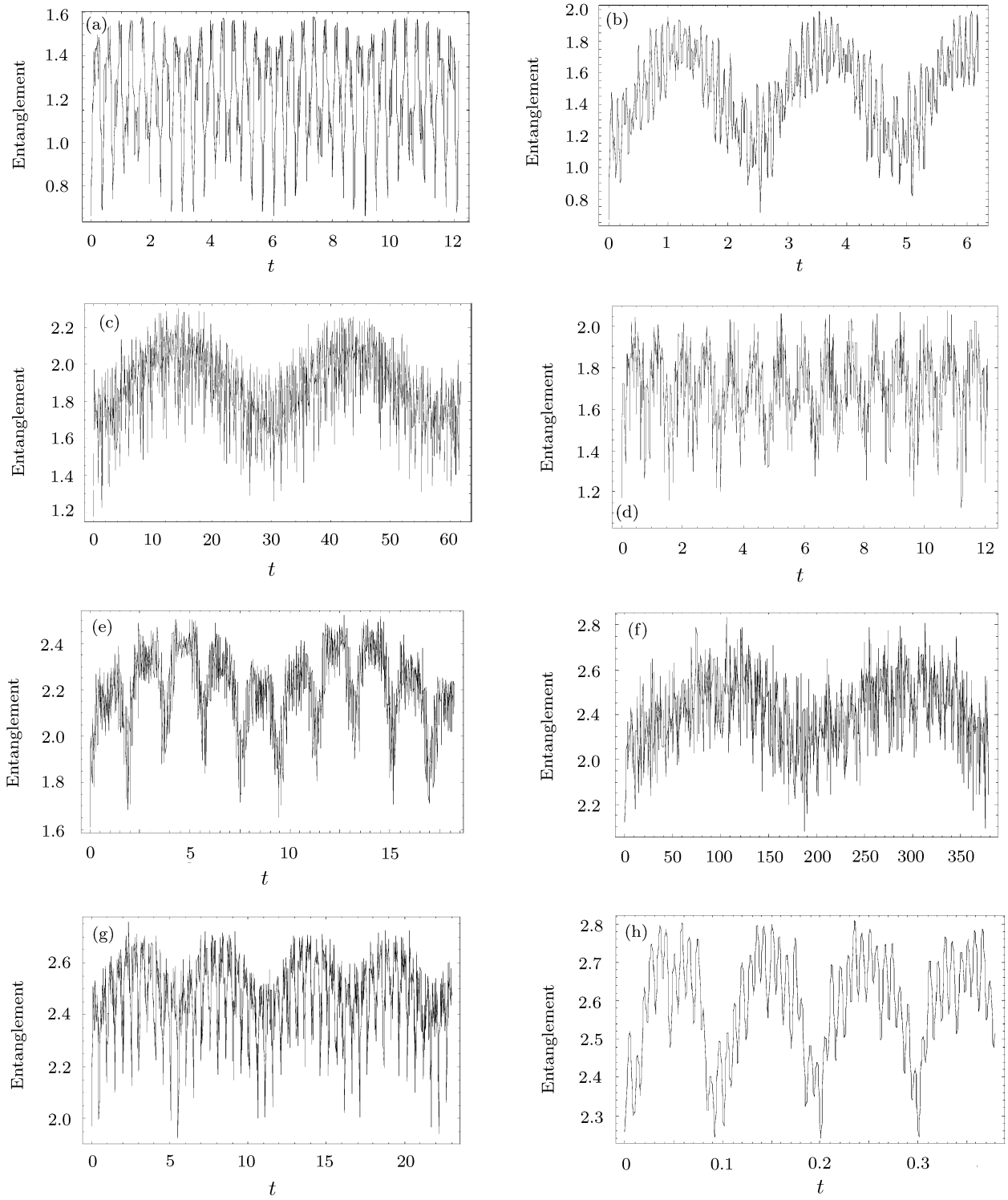



**Fig.2.** Time evolution of entanglements for the initial states being the superposition of energy eigenstates with quantum number $M = -7$ (a), $M = -6$ (b), $M = -5$ (c), $M = -4$ (d), $M = -3$ (e), $M = -2$ (f), $M = -1$ (g), and $M = 0$ (h). Where the unit of time $t$ is nanosecond (ns).

# 4. Conclusion

The entanglement in the supermolecular dimer $[Mn_4]_2$ with the antiferromagnetic exchange-coupling is studied in terms of energy eigenvectors which are entangled states. The entanglement measures of the von Neumann entropy are obtained for all eigenstates in the quantum number range from $M = M_1 + M_2 = -9$

to 0. The dependence of the entanglement on the coupling parameter $J$ is not a monotonic function for most of the eigenstates. However, it is of great importance that the entropy of entanglement for most eigenstates has the maximum values and the minimum values. We also show the dynamics of the entanglement for initial states which are superposition of those energy eigenstates with the equal quantum number $M$. It is observed that the entanglement oscillates with different periods. These findings are useful for a better understanding of the dynamics of such systems and highlight the potential utility of supermolecular magnets in the design of future quantum devices.

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