Algebraic dynamics study for homotrinuclear linear spin cluster in a rotating magnetic field

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Using the method of dynamical algebras, the solution of a homotriparticle linear spin cluster (each particle with $S=1/2$) in a rotating magnetic field is obtained. We derive degeneracy energy levels and each level's Berry phase of this system. The Berry phase as a function of ω and θ has been determined by using the relation between the Berry phase and the angular velocity ω of the rotating magnetic field as well as the angle θ between the magnetic field and Z axis. We obtain the changing diagram of the Berry phase of the basis state.

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Dynamical algebras is a theory which combines the theory of dynamic symmetry with quantum mechanics [1–9]. It extends the theory of the dynamic symmetry of the stationary state of an autonomous system in nuclear physics to the theory of the time-dependent dynamic symmetry of a nonautonomous quantum system [10]. Moreover, the dynamical algebras method further emphasizes the kinetic algebraic structure, the dynamic evolvement, and the rule of evolving with time. So we can easily study the relation between conservation constant and symmetry in the system by using the method of dynamical algebras. In recent years "quantum engineering" has been used to control microscopic particles [11–14]. The method of dynamical algebras has been applied in several typical nonautonomous quantum systems, such as the particle moving in a one-dimensional Paul trap forms a SU(1,1) dynamic system [15], the polarization of spin particle in accelerator forms a SU(2) dynamic system [16], the spin particle in a rotating magnetic field and the Berry phase of a laser in helical optical fiber form a SU(2) dynamic system, etc. [17–26]. In the present work, we will use the dynamical algebras method to study a homotriparticle linear spin cluster (each particle with $S=1/2$) in a rotating magnetic field. When we input some quantum information in to the system which is formed by the unit of the homotriparticle linear spin cluster (each particle with $S=1/2$), the output information will change due to the Berry phase that is produced in the magnetic field. This system may be formed in condensed matter and solving this system may be of practical use for the understanding of the complicated energy structure and Berry phase in condensed matter. The change of the Berry phase is a very important physical question since a number of interesting phenomena have been generated by it. Up to now, a lot of studies of the Berry phase have been reported in both theoretical and experimental physics. Berry [27], Simon [28], and Aharonov and Anandan [29] have studied it theoretically. Experiments have been observed on photons [30], neutrons [31], electrons [32], nuclear quadrupole resonances [33], laser interferometry [17], and molecular energy levels [10]. When the Hamiltonian follows a closed path in parameter space in the time interval $[0,T]$ and after a period T, the initial state $|\psi(0)\rangle$ of this system will evolve to a final state $|\psi(T)\rangle=e^{-i\beta_n}e^{-i\phi_n}|\psi(0)\rangle$, where β_n is called the quantum adiabatic phase or Berry phase. It depends on the path or the path's certain geometric features: $\phi_n=\hbar^{-1}\int_0^T dtE_n(t)$.

Here ϕ_n is called the dynamical phase. It depends on the path and the rate at which the path is followed [21]. In this paper, we will study the homotriparticle (each particle with $S=1/2$) linear spin cluster in a rotating magnetic field and give the solution for the energy levels and the form of the Berry phase. The changing of the Berry phase relates to the angular velocity ω of the rotating magnetic field, as well as the angle θ between the magnetic field and Z axis. This homotriparticle linear spin cluster (each particle with $S=1/2$) system can be described by the Hamiltonian

$$\hat{H}(t)=J_{ex}\sum_i \hat{S}_i\cdot\hat{S}_{i+1}+\sum_i b_i\hat{S}_i\cdot\hat{L}_i+\sum_i(\gamma_S\hat{S}_i+\gamma_L\hat{L}_i)\cdot B(t). \tag{1}$$

Let

$$\hat{H}_{\text{int}}=J_{ex}\sum_i \hat{S}_i\cdot\hat{S}_{i+1}, \tag{2}$$

$$\hat{H}_{L-S}=\sum_i b_i\hat{S}_i\cdot\hat{L}_i, \tag{3}$$

$$\hat{H}_{Zeeman}=\sum_i(\gamma_S\hat{S}_i+\gamma_L\hat{L}_i)\cdot B(t), \tag{4}$$

so

$$\hat{H}(t)=\hat{H}_{\text{int}}+\hat{H}_{L-S}+\hat{H}_{Zeeman}. \tag{5}$$

$\hat{H}_{\text{int}}$ is the correlation interaction of adjacent particles, and J_{ex} is its coupling strength. $\hat{H}_{L-S}$ is the spin-orbit coupling interaction in a single center particle. $\hat{H}_{Zeeman}$ is the Zeeman split of a single center particle. $B(t)$ is the rotating magnetic field, and its three components are not equal to zero ($B_x\neq 0, B_y\neq 0, B_z\neq 0$).

The spin operator $\hat{S}$ and the orbital operator $\hat{L}$ satisfy the commutation rules

$$[\hat{S}_i,\hat{S}_j]=i\varepsilon_{ijk}\hat{S}_k,\quad [\hat{L}_i,\hat{L}_j]=i\varepsilon_{ijk}\hat{L}_k,\quad [\hat{S}_i,\hat{L}_j]=0. \tag{6}$$

Using the commutation rules (6), we find that the operators of Eqs. (2) and (4) satisfy the relation

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$$[\hat{H}_{\rm int},\hat{H}_{Zeeman}]=0. \tag{7}$$

The energy of the eigenwave function $|\Psi(t)\rangle$ is

$$\begin{aligned}E_n&=\langle\Psi(t)|\hat{H}(t)|\Psi(t)\rangle\\&=\langle\Psi(t)|\hat{H}_{L-S}|\Psi(t)\rangle+\langle\Psi(t)|\hat{H}_{\rm int}+\hat{H}_{Zeeman}|\Psi(t)\rangle.\end{aligned} \tag{8}$$

Let

$$E_{L-S}=\langle\Psi(t)|\hat{H}_{L-S}|\Psi(t)\rangle,\quad E_0=\langle\Psi(t)|\hat{H}_{\rm int}+\hat{H}_{Zeeman}|\Psi(t)\rangle,$$

so

$$E_n=E_{L-S}+E_0. \tag{9}$$

Let

$$\hat{S}_Z=\sum_i\hat{S}_i^Z,\quad \hat{S}_y=\sum_i\hat{S}_i^y,\quad \hat{S}_x=\sum_i\hat{S}_i^x \tag{10}$$

It is easy to show that the operators of Eqs. (2) and (10) satisfy

$$[\hat{H}_{\rm int},\hat{S}_Z]=0,\quad [\hat{H}_{\rm int},\hat{S}_y]=0,\quad [\hat{H}_{\rm int},\hat{S}_x]=0. \tag{11}$$

Using the commutation rules (6) and (11) and the SU(2) [16,17,24,25] group algebraic structure of $\hat{H}_{Zeeman}$, we can transform E_0 by the gauge transformation

$$U_g=e^{iv_3(t)(\gamma_S\hat{S}_Z+\gamma_L\hat{L}_Z)}e^{iv_2(t)(\gamma_S\hat{S}_y+\gamma_L\hat{L}_y)}, \tag{12}$$

so that

$$\begin{aligned}E_0&=\langle\Psi(t)|\hat{H}_{\rm int}+\hat{H}_{Zeeman}|\Psi(t)\rangle\\&=\langle\Psi(t)|U_gU_g^{-1}(\hat{H}_{\rm int}+\hat{H}_{Zeeman})U_gU_g^{-1}|\Psi(t)\rangle\\&=\langle\overline{\Psi}(t)|U_g^{-1}(\hat{H}_{\rm int}+\hat{H}_{Zeeman})U_g|\overline{\Psi}(t)\rangle,\end{aligned} \tag{13}$$

where $|\overline{\Psi}(t)\rangle=U_g^{-1}|\Psi(t)\rangle$. Using the identity

$$e^{-iv_i\hat{S}_i}\hat{S}_je^{-iv_i\hat{S}_i}=\hat{S}_j\cos v_i+\varepsilon_{ijk}\hat{S}_k\sin v_i, \tag{14}$$

$$e^{-iv_i\hat{L}_i}\hat{L}_je^{-iv_i\hat{L}_i}=\hat{L}_j\cos v_i+\varepsilon_{ijk}\hat{L}_k\sin v_i, \tag{15}$$

we find that, after the gauge transformation U_g, $(\hat{H}_{\rm int}+\hat{H}_{Zeeman})$ becomes ($\hbar=1$)

$$U_g^{-1}(\hat{H}_{\rm int}+\hat{H}_{Zeeman})U_g=\hat{\overline{H}}(t)+iU_g^{-1}(\partial/\partial t)U_g, \tag{16}$$

where

$$\hat{\overline{H}}(t)=\hat{H}_{\rm int}+f(t)\hat{I}(0), \tag{17}$$

$$B(t)=\Omega(\sin\theta\cos\omega t,\sin\theta\sin\omega t,\cos\theta),\theta\in(0,\pi/2), \tag{18}$$

$$v_3=-\omega t, \tag{19}$$

$$v_2=\text{const}=-\overline{\theta}, \tag{20}$$

$$\sin v_2=-\sin\theta/[1-2(\omega/\Omega)\cos\theta+(\omega/\Omega)^2]^{1/2}, \tag{21}$$

$$\overline{\Omega}=\Omega[1-2(\omega/\Omega)\cos\theta+(\omega/\Omega)^2]^{1/2}, \tag{22}$$

$$f(t)=\overline{\Omega}, \tag{23}$$

$$\hat{I}(0)=\gamma_S\hat{S}_Z+\gamma_L\hat{L}_Z=(\gamma_S-\gamma_L)\hat{S}_Z+\gamma_L\hat{J}_Z. \tag{24}$$

The basis state of the single center particle can be described as $|J^2,M,S_Z\rangle$, where M is the Z component of the total angular momentum J. S_Z is the Z component of the total spin momentum. Because there is only a spin correlation interaction among three particles, the total wave function of the spin cluster is the product of every particle basis-state wave function.

Let

$$\varphi_i^0(M_i)=|J^2,M_i,\tfrac{1}{2}\rangle,\quad \varphi_i^1(M_i)=\left|J^2,M_i,-\tfrac{1}{2}\right\rangle. \tag{25}$$

We can sort the basis-state wave function into eight classes:

$$\phi_1=\varphi_1^0(M_1)\varphi_2^1(M_2)\varphi_3^1(M_3),\quad \phi_2=\varphi_1^0(M_1)\varphi_2^0(M_2)\varphi_3^1(M_3),$$

$$\phi_3=\varphi_1^0(M_1)\varphi_2^1(M_2)\varphi_3^0(M_3),\quad \phi_4=\varphi_1^0(M_1)\varphi_2^0(M_2)\varphi_3^0(M_3),$$

$$\phi_5=\varphi_1^1(M_1)\varphi_2^1(M_2)\varphi_3^1(M_3),\quad \phi_6=\varphi_1^1(M_1)\varphi_2^1(M_2)\varphi_3^0(M_3),$$

$$\phi_7=\varphi_1^1(M_1)\varphi_2^0(M_2)\varphi_3^1(M_3),\quad \phi_8=\varphi_1^1(M_1)\varphi_2^0(M_2)\varphi_3^0(M_3).$$

Using Eqs. (13), (16), and (17), we can obtain the eigenenergy levels and the eigenwave functions of $\hat{\overline{H}}(t)$ as shown in Table I:

$$\hat{\overline{H}}(t)|\overline{\Psi}_m\rangle=E_m|\overline{\Psi}_m\rangle,\quad m\in(1,2,3,4,5,6,7,8). \tag{26}$$

The solution of the time-dependent Schrödinger equation is

$$i(\partial/\partial t)|\overline{\Psi}_m(t)\rangle=\hat{\overline{H}}(t)|\overline{\Psi}_m(t)\rangle,\quad m\in(1,2,3,4,5,6,7,8). \tag{27}$$

The solution of Eq. (26) is

$$|\overline{\Psi}_m(t)\rangle=e^{-i\Theta_m(t)}|\overline{\Psi}_m\rangle. \tag{28}$$

It is easy to compute $\Theta_m(t)$,

$$\Theta_m(t)=\int_0^t E_m dt'=E_{\rm int}^m t+E_{Zeeman}^m t, \tag{29}$$

where

$$E_{\rm int}^m=\langle\overline{\Psi}_m|\hat{H}_{\rm int}|\overline{\Psi}_m\rangle,$$

$$E_{Zeeman}^m=\langle\overline{\Psi}_m|f(t)\hat{I}(0)|\overline{\Psi}_m\rangle=\overline{\Omega}[(\gamma_S-\gamma_L)S_Z+\gamma_LM].$$

Thus the orthonormal nonadiabatic basis is

$$\begin{aligned}|\Psi_m(t)\rangle&=U_g|\overline{\Psi}_m(t)\rangle\\&=e^{iv_3(t)[(\gamma_s-\gamma_L)\hat{S}_Z+\gamma_L\hat{J}_Z]}e^{iv_2(t)[(\gamma_S-\gamma_L)\hat{S}_y+\gamma_L\hat{J}_y]}e^{-i\Theta_m(t)}|\overline{\Psi}_m\rangle\end{aligned} \tag{30}$$

and the nonadiabatic energy levels are

$$\begin{aligned}E_0^m&=\langle\Psi_m|H_{\rm int}+H_{Zeeman}|\Psi_m\rangle=\langle\overline{\Psi}_m|\hat{\overline{H}}+iU_g^{-1}(\partial/\partial t)U_g|\overline{\Psi}_m\rangle\\&=E_m-E_{\rm Zeeman}^m(\dot{v}_3\cos v_2/\overline{\Omega}).\end{aligned} \tag{31}$$

The time-dependent Schrödinger equation is

$$i(\partial/\partial t)|\Psi(t)\rangle=(\hat{H}_{\rm int}+\hat{H}_{Zeeman})|\Psi(t)\rangle. \tag{32}$$

Its solution can be expanded by the nonadiabatic basis

TABLE I. The eigenenergy levels and the eigenwave functions of $\hat{\overline{H}}(t)$, where S_Z is the Z component of the total spin momentum and M is the Z component of the total angular momentum J.

S_Z	Eigenenergy E_m	Eigenwave function $\|\overline{\Psi}_m\rangle$	$M(J_Z)$ value
1/2	$-J_{ex}+[(\gamma_S-\gamma_L)/2+\gamma_L M]\overline{\Omega}$	$\overline{\Psi}_1=\phi_2(M)-2\phi_3(M)+\phi_8(M)$	$-(3L+1/2)\sim(3L+1/2)$
−1/2	$-J_{ex}+[-(\gamma_S-\gamma_L)/2+\gamma_L M]\overline{\Omega}$	$\overline{\Psi}_2=-1/2\phi_1(M)-1/2\phi_6(M)+\phi_7(M)$	$-(3L-1/2)\sim(3L-1/2)$
1/2	$[(\gamma_S-\gamma_L)/2+\gamma_L M]\overline{\Omega}$	$\overline{\Psi}_3=-\phi_2(M)+\phi_8(M)$	$-(3L+1/2)\sim(3L+1/2)$
−1/2	$[-(\gamma_S-\gamma_L)/2+\gamma_L M]\overline{\Omega}$	$\overline{\Psi}_4=-\phi_1(M)+\phi_6(M)$	$-(3L-1/2)\sim(3L-1/2)$
1/2	$1/2J_{ex}+[(\gamma_S-\gamma_L)/2+\gamma_L M]\overline{\Omega}$	$\overline{\Psi}_5=\phi_2(M)+\phi_3(M)+\phi_8(M)$	$-(3L+1/2)\sim(3L+1/2)$
−1/2	$1/2J_{ex}+[-(\gamma_S-\gamma_L)/2+\gamma_L M]\overline{\Omega}$	$\overline{\Psi}_6=\phi_1(M)+\phi_6(M)+\phi_7(M)$	$-(3L-1/2)\sim(3L-1/2)$
−3/2	$1/2J_{ex}+[-3(\gamma_S-\gamma_L)/2+\gamma_L M]\overline{\Omega}$	$\overline{\Psi}_7=\phi_5(M)$	$-(3L-3/2)\sim(3L-3/2)$
3/2	$1/2J_{ex}+[3(\gamma_S-\gamma_L)/2+\gamma_L M]\overline{\Omega}$	$\overline{\Psi}_8=\phi_4(M)$	$-(3L+3/2)\sim(3L+3/2)$

$$
\begin{aligned}
|\Psi(t)\rangle &= \sum_m C_m|\Psi_m(t)\rangle \\
&= \sum_{mM'MS'_ZS_Z} C_m e^{\{-i\Theta_m(t)+iv_3[(\gamma_S-\gamma_L)S'_Z+\gamma_L M']\}} \\
&\quad \times D^j_{M'M}(0,-v_2,0)D^{j'}_{S'_ZS_Z}(0,-v_2,0)|\overline{\Psi}_{m'}\rangle. \quad (33)
\end{aligned}
$$

C_m is an expansion coefficient that is not dependent on time. All the dynamical information is included in the nonadiabatic basis. $D^j_{M'M}$ and $D^{j'}_{S'_zS_z}$ are the Wigner functions of j and j' order. The value of j is the total angular momentum J. The value of j' is the total spin momentum. The total angular momentum and total spin momentum of the eigenwave function $|\overline{\Psi}_{m'}\rangle$ are M' and S'_Z. So from Eqs. (12), (29), and (30) we obtain the value of E_0:

$$
E_0=\langle\Psi(t)|\hat{H}_{\rm int}+\hat{H}_{Zeeman}|\Psi(t)\rangle=\sum_m |C_m|^2E^m_0. \quad (34)
$$

The eigenenergy level of $\hat{H}_{L-S}$ is

$$
\begin{aligned}
E_{L-S} &= \langle\Psi(t)|\hat{H}_{L-S}|\Psi(t)\rangle \\
&= \sum_{mM'MS'_ZS_Z} |C_m|^2 D^{*j}_{M'M}(0,-v_2,0) \\
&\quad \times D^j_{M'M}(0,-v_2,0)D^{*j'}_{S'_ZS_Z}(0,-v_2,0) \\
&\quad \times D^{j'}_{S'_ZS_Z}(0,-v_2,0)\langle\overline{\Psi}_{m'}|\hat{H}_{L-S}|\overline{\Psi}_{m'}\rangle \\
&= \sum_{mM'MS'_ZS_Z} |C_m|^2 D^{*j}_{M'M}(0,-v_2,0) \\
&\quad \times D^j_{M'M}(0,-v_2,0)D^{*j'}_{S'_ZS_Z}(0,-v_2,0) \\
&\quad \times D^{j'}_{S'_ZS_Z}(0,-v_2,0)E^{m'}_{L-S}, \quad (35)
\end{aligned}
$$

where $E^{m'}_{L-S}=\langle\overline{\Psi}_{m'}|\hat{H}_{L-S}|\overline{\Psi}_{m'}\rangle$. Its value is determined by the total spin of the spin cluster. We have

$$
\begin{aligned}
E^{m'}_{L-S} &= (b/2)(L-1), \quad m' \in (1,3,5), \\
E^{m'}_{L-S} &= -(b/2)(L+2), \quad m' \in (2,4,6), \\
E^{m'}_{L-S} &= -(3b/2)(L+1), \quad m'=7, \\
E^{m'}_{L-S} &= (3b/2)L, \quad m'=8.
\end{aligned}
$$

Because the parameter space of the angular velocity ω of the rotating magnetic field and the angle θ between the magnetic field and Z axis determines the value of geometric phase, the Berry phase of the homotriparticle linear spin cluster (each particle with $S=1/2$) system comes from the $\hat{H}_{Zeeman}$. After the parameter of the system goes through a period $T(2\pi/\omega)$, there is only a difference of the total phase Φ^m_{total} between the initial state and the final state of the nonadiabatic basis of $\hat{H}_{Zeeman}$ and the Berry phase is obtained for this system. From Eq. (29) we can calculate the total phase Φ^m_{total} of $\hat{H}_{Zeeman}$:

$$
\begin{aligned}
\Phi^m_{total} &= -\Theta_m(T)-2\pi[(\gamma_S-\gamma_L)S_Z+\gamma_L M] \\
&= -E^m_{\rm int}T-\overline{\Omega}T[(\gamma_S-\gamma_L)S_Z+\gamma_L M] \\
&\quad -2\pi[(\gamma_S-\gamma_L)S_Z+\gamma_L M]. \quad (36)
\end{aligned}
$$

The dynamical phase is

$$
\begin{aligned}
\Phi_n &= \int_o^T (E^m_{\rm int}+E^m_{Zeeman})dt \\
&= E^m_{\rm int}T+[(\gamma_S-\gamma_L)S_Z+\gamma_L M](\overline{\Omega}T+2\pi\cos\overline{\theta}). \quad (37)
\end{aligned}
$$

The Berry phase is

$$
\beta_n=\Phi_{total}+\Phi_n=-2\pi[(\gamma_s-\gamma_L)S_Z+\gamma_L M](1-\cos\overline{\theta}). \quad (38)
$$

The nonadiabatic geometric phase is of great practical use. We can obtain different Berry phases by changing the

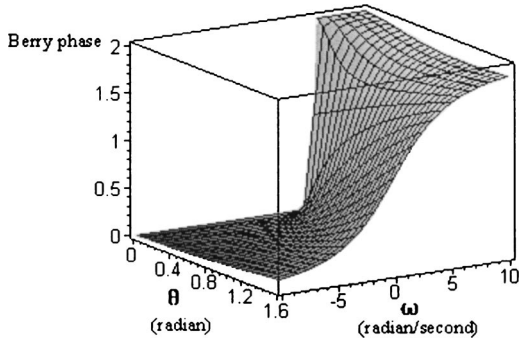

FIG. 1. The change of the Berry phase for $\Omega=5$, $\omega\in(-10\sim10)$, $\theta\in(0\sim\pi/2)$. (Unit of ω is rad/sec; unit of θ is rad.)

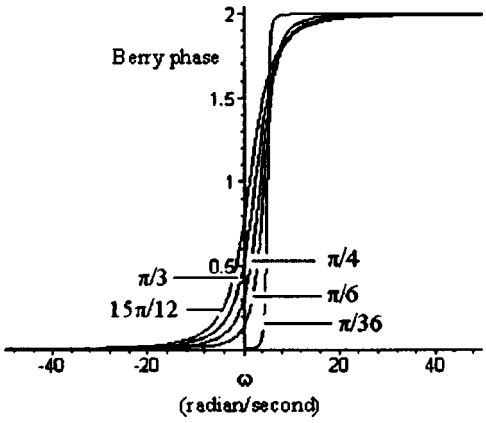

FIG. 2. The change of the Berry phase for $\Omega=5$, $\theta=\pi/36$, $\pi/6$, $\pi/4$, $\pi/3$, and $15\pi/12$. (Unit of ω is rad/sec.)

parameters and find the changing of the Berry phase as a function of parameters. It is seen from Eq. (37) that the Berry phase is altered when the values of ω and θ are different. In the formula (38), we find that the change of the Berry phase will come from the factor $(1-\cos\theta)$, as shown in Figs. 1 and 2. From Fig. 1 we can see that in the range of $|\omega|$ ($|\omega|<7.3$) the Berry phase will decrease when θ reduces, whereas in the range of $|\omega|$ ($|\omega|>7.3$) the Berry phase will increase when θ reduces. From Fig. 2 we can also note that when ω changes from negative to positive values, the Berry phase changes rapidly in a small range of $|\omega|$ ($|\omega|<20$), whereas in the large range of $|\omega|$ ($|\omega|>20$) the Berry phase will change slowly.

By using the method of dynamical algebras, we have studied the energy levels and phases of the homotriparticle (each particle with $S=1/2$) linear spin cluster in a rotating magnetic field and obtained the solution of this system. From the solution, we have derived the change of the Berry phase as a function of ω and θ. We have found that the Berry phase has a great change in a small range of $|\omega|$ and that the angle θ affects the changing speed of the phase. The results may be of practical use in applications such as quantum computers, the resonance absorption of condensed matter, and the application of phase. This work demonstrates that the method of dynamical algebras is a useful tool for the study of a nonlinear system with a bilinear term in condensed matter physics.

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