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A new concept of geometric phase in parameter space: coupling as a parameter

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Abstract
We have obtained the geometric phase of the tripartite spin-1/2 system with spin–spin coupling and discussed the influence of this coupling on the geometric phase. We have discovered the *coupling-independent geometric phase* and explained it. Based on this work, we propose the concept of quasimagnetic field and assimilate the coupling into the parameter space. By this theory, the relation between the geometric phase and the solid angle in parameter space still holds for a system with spin–spin coupling if the concept of the parameter is properly revised in the way we have elucidated.

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1. Introduction

Since 1984, the concept of geometric phase [1] has attracted a large amount of interest from various branches of modern physical research. The geometric phases of different backgrounds, such as in mixed states [2], for open systems [3–11] and with a quantized field driving [12], have been actively researched.

One of the most important applications of geometric phase is quantum computation [13]. The basic idea is to let one sub-system undergo a coherent evolution that depends on the quantum state of other sub-systems. After the evolution, the evolving sub-system will acquire a conditional phase shift, which is a combination of the dynamic phase shift and geometric phase shift. If the unwanted dynamic phase is offset by some methods [14] and the geometric phase shift is measured, then this quantal system will become a quantum computer operation unit. Because geometric phases depend only on the geometry of the path executed, they are resilient to certain types of errors. This fault-tolerant feature is very attractive.

As the carrier of geometric phase in the evolving field, spin systems are an important model in the realization of the solid-state quantum computer [15] because they each only have two levels and thereby are a natural representation of a quantum bit (qubit). Besides, unusually

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long spin coherence time in doped semiconductors, exceeding 100 ms, has been revealed by magneto-optical experiments [16].

The basic picture in this paper is as follows: there are n ($n \geqslant 2$) spin-1/2 particles in a slowly rotating magnetic field with one particle driven by the field. After a cyclic process, a geometric phase is generated. This model is labelled as a one-site magnetic drive n-particle system.

Generally, spin particles have internal exchange coupling, which comes from virtual tunnelling of electrons from one quantum dot to the other and back, and is subject to several external physical parameters (gate voltages, magnetic field, etc) [17]. Because the spin–spin coupling can affect the state of the quantal system and therefore affect the geometric phase shift, a study on this influence is of great significance.

So far, there have been several papers [18] discussing the case $n = 2$, i.e. two spin-1/2 particles. They found that the coupling remarkably affects the geometric phase. However, a more complicated system, i.e. $n \geqslant 3$, has not been discussed and the mechanisms of the influence of spin coupling on geometric phase remain unexplored. In this paper, we investigate the geometric phase of the three-particle system ($n = 3$). We also carefully discuss the influence of coupling on geometric phase and propose a new perspective on the parameter space.

2. The geometric phase of tripartite spin-1/2 system

To begin with, we briefly review the case of one quantum spin driven by a slowly rotating magnetic field [1, 19]. In particular, we consider the case in which the direction of the magnetic field precesses around a fixed axis which we take as the 3-axis (z-axis) of our laboratory coordinate frame in space R^3. We suppose that the direction rotates slowly (i.e. adiabatically). The Hamiltonian is $H(\vec{B}) = \frac{e\hbar}{2mc}\vec{\sigma}_1 \cdot \vec{B}$, e and m being the charge and mass of the particle, respectively. After a cyclic process, a geometric phase shift is generated. The phase shift is defined by the Berry formula [19] as

$$\gamma = \mathrm{i}\int_0^T \mathrm{d}t \langle\psi(t)|\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \frac{1}{2}\Omega. \tag{1}$$

Here, $|\psi(t)\rangle$ is a single-valued energy eigenvector and Ω is the solid angle subtended by the loop Γ traversed by $\vec{B}$ in the parameter space. Traditionally, $\hat{n}$, the direction of $\vec{B}$, acts as the parameter vector; it is equivalent to regard $\vec{B}$ as a parameter vector here.

However, when this spin is the component of a spin system, the spin–spin coupling will influence the geometric phase. Here, we discuss the geometric phase of the tripartite model in detail.

The tripartite spin systems are widely studied in chemical spectroscopy by NMR [20]. For example, trichloroethane, CCl_3–CH_3, is a system of three spins placed at the apices of an equilateral triangle [21]. The value of coupling constant J often lies between 1 and 10 Hz [22]. Practically, the one-site magnetic drive is routinely realized in NMR by using spins of nuclei of different isotopes, such as those of different species of atoms, as the sub-systems. These spins usually have precession frequencies that differ from each other by many megahertz; a resonant magnetic field for one spin then has little effect on the others [14]. Supposing that spins 2 and 3 belong to the same type of particles and spin 1 belongs to another type, we can write the Hamiltonian as follows:

$$H(\vec{B}) = \frac{e\hbar}{2mc}\vec{\sigma}_1 \cdot \vec{B}(t) + J_z\left(\sigma_1^z\sigma_2^z + \sigma_1^z\sigma_3^z\right) + J_z'\sigma_2^z\sigma_3^z, \tag{2}$$

where $\hat{n} = \{\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\}$ and θ is a constant. We suppose that the spin coupling constant between spins 1 and 2 (or 3) is J_i and between 2 and 3 is J_i', where $i = x, y, z$ (generally $J_i \neq J_i'$). For simplicity, here we only consider the coupling in the z-direction, i.e. $J_x = J_y = 0$, $J_x' = J_y' = 0$.

In the space spanned by $|\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\downarrow\downarrow\rangle, |\downarrow\uparrow\uparrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle, |\uparrow\downarrow\uparrow\rangle$ and the unit $\frac{e\hbar}{2mc} = 1$, we present the Hamiltonian in equation (2) as

$$H = \begin{bmatrix} B\cos\theta + J_z' + 2J_z & 0 & 0 & 0 & B\sin\theta\,\mathrm{e}^{-\mathrm{i}\varphi} & 0 & 0 & 0 \\ 0 & B\cos\theta - J_z' & 0 & 0 & 0 & B\sin\theta\,\mathrm{e}^{-\mathrm{i}\varphi} & 0 & 0 \\ 0 & 0 & B\cos\theta + J_z' - 2J_z & B\sin\theta\,\mathrm{e}^{-\mathrm{i}\varphi} & 0 & 0 & 0 & 0 \\ 0 & 0 & B\sin\theta\,\mathrm{e}^{\mathrm{i}\varphi} & -B\cos\theta + J_z' + 2J_z & 0 & 0 & 0 & 0 \\ B\sin\theta\,\mathrm{e}^{\mathrm{i}\varphi} & 0 & 0 & 0 & -B\cos\theta + J_z' - 2J_z & 0 & 0 & 0 \\ 0 & B\sin\theta\,\mathrm{e}^{\mathrm{i}\varphi} & 0 & 0 & 0 & -B\cos\theta - J_z' & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & B\sin\theta\,\mathrm{e}^{-\mathrm{i}\varphi} & B\cos\theta - J_z' \\ 0 & 0 & 0 & 0 & 0 & 0 & -B\cos\theta - J_z' & B\sin\theta\,\mathrm{e}^{\mathrm{i}\varphi} \end{bmatrix}. \tag{3}$$

Evaluating the matrix yields the eigenvalues E_i, $i = 1, 2, \ldots, 8$:

$$\begin{aligned} &E_1 = -B - J_z', \qquad E_2 = -B - J_z', \qquad E_3 = B - J_z', \qquad E_4 = B - J_z', \\ &E_5 = J_z' - \sqrt{B^2 + 4J_z^2 - 4BJ_z\cos\theta}, \qquad E_6 = J_z' + \sqrt{B^2 + 4J_z^2 - 4BJ_z\cos\theta}, \\ &E_7 = J_z' - \sqrt{B^2 + 4J_z^2 + 4BJ_z\cos\theta}, \qquad E_8 = J_z' + \sqrt{B^2 + 4J_z^2 + 4BJ_z\cos\theta}. \end{aligned} \tag{4}$$

The corresponding eigenstates are

$$\begin{aligned} |\psi_1\rangle &= -\mathrm{e}^{\mathrm{i}\varphi}\cot(\theta/2)|\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle, \\ |\psi_2\rangle &= -\mathrm{e}^{-\mathrm{i}\varphi}\tan(\theta/2)|\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle, \\ |\psi_3\rangle &= \mathrm{e}^{\mathrm{i}\varphi}\tan(\theta/2)|\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle, \\ |\psi_4\rangle &= \mathrm{e}^{-\mathrm{i}\varphi}\cot(\theta/2)|\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle, \\ |\psi_5\rangle &= \frac{\mathrm{e}^{-\mathrm{i}\varphi}\left(-2J_z + B\cos\theta - \sqrt{B^2 + 4J_z^2 - 4BJ_z\cos\theta}\right)\csc\theta}{B}|\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\downarrow\rangle, \\ |\psi_6\rangle &= \frac{\mathrm{e}^{-\mathrm{i}\varphi}\left(-2J_z + B\cos\theta + \sqrt{B^2 + 4J_z^2 - 4BJ_z\cos\theta}\right)\csc\theta}{B}|\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\downarrow\rangle, \\ |\psi_7\rangle &= \frac{\mathrm{e}^{-\mathrm{i}\varphi}\left(2J_z + B\cos\theta - \sqrt{B^2 + 4J_z^2 + 4BJ_z\cos\theta}\right)\csc\theta}{B}|\uparrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle, \\ |\psi_8\rangle &= \frac{\mathrm{e}^{-\mathrm{i}\varphi}\left(2J_z + B\cos\theta + \sqrt{B^2 + 4J_z^2 + 4BJ_z\cos\theta}\right)\csc\theta}{B}|\uparrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle. \end{aligned} \tag{5}$$

Here $|\psi_i\rangle$ $(i = 1, 2, \ldots, 8)$ is a single-valued energy eigenvector and we only consider the geometric phase of the pure state evolving adiabatically and cyclically. By the definition of

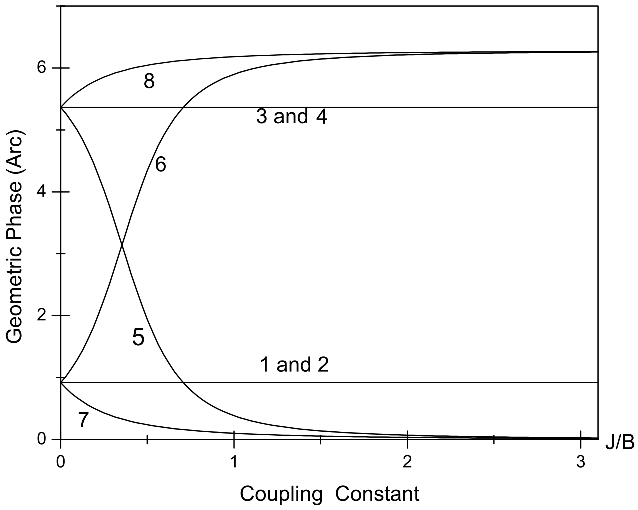

Figure 1. The relation between geometric phase and coupling constant J_z of the one-site drive tripartite model, where $\theta = \pi/4$. It is seen that the phases of states 1–4 are constants independent of coupling constant. The geometric phase of the other states will tend to a fixed value when the coupling approaches infinity.

Berry, we get the geometric phases of these states by the formula $\gamma = \mathrm{i}\int \langle\psi|\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle \mathrm{d}t$ as follows:

$$\begin{aligned}
\gamma_1 &= \gamma_2 = \pi(1-\cos\theta), \\
\gamma_3 &= \gamma_4 = \pi(1+\cos\theta), \\
\gamma_{5,6} &= \pi\left(1 \mp \frac{B\cos\theta - 2J_z}{\sqrt{B^2+4J_z^2-4BJ_z\cos\theta}}\right), \\
\gamma_{7,8} &= \pi\left(1 \mp \frac{B\cos\theta + 2J_z}{\sqrt{B^2+4J_z^2+4BJ_z\cos\theta}}\right).
\end{aligned} \tag{6}$$

These are the final result. Now we are in a position to discuss the influence of the spin coupling on geometric phase.

3. Influence of spin coupling on geometric phase

To further the discussion, we plot the geometric phases of these states in figure 1 and the relationship of the geometric phase of the state 6, coupling constant and cone angle of the magnetic field in figure 2. It is noted that the geometric phases of the states from 1 to 4 are exactly the case of a single spin driven by a rotating magnetic field with no coupling. In other words, the spin coupling has no influence on the geometric phases of these states. We label these phases as *coupling-independent geometric phase*. On the other hand, the phases of states 5–8 are markedly affected by the coupling from figure 1. It is worth noting that as the coupling approaches infinity, the phases all tend to a fixed value—multiple of 2π. This is called the *quenching effect*, which was pointed out by Yi and Sjoqvist [23]. Although the effect is obvious from the figure, a sound explanation is, however, still open to us. Here, we carefully discuss the origin of such an effect.

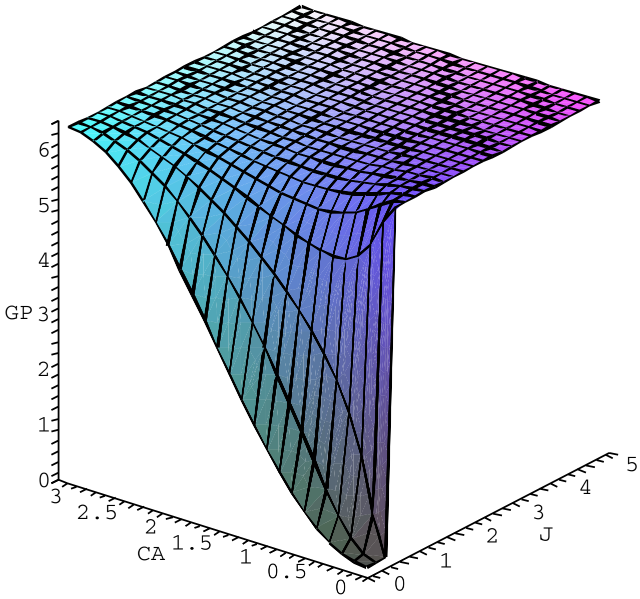

Figure 2. The relation between coupling constant J_z, cone angle (CA) θ and geometric phase (GP) in state 6. The magnetic field strength is chosen as unity because GP is a function of J/B and θ. (This figure is in colour only in the electronic version)

First, let us review the form of equation (6). After careful observation, we may find that the phases of states 5–8 can be rewritten in the following way:

$$\gamma_{5,6} = \pi(1 \mp \cos\beta) \qquad \text{and} \qquad \gamma_{7,8} = \pi(1 \mp \cos\eta), \tag{7}$$

where

$$\begin{aligned} \cos\beta &= \frac{B\cos\theta - 2J_z}{\sqrt{B^2 + 4J_z^2 - 4BJ_z\cos\theta}} = \frac{\Delta y_1}{r_1}, \\ \cos\eta &= \frac{B\cos\theta + 2J_z}{\sqrt{B^2 + 4J_z^2 + 4BJ_z\cos\theta}} = \frac{\Delta y_2}{r_2}. \end{aligned} \tag{8}$$

Why do we use the notation $\frac{\Delta y}{r_i}$ $(i = 1, 2)$? The reason can be found by examining the geometry relation in figure 3. By virtue of this simple triangle in figure 3, we can instantly understand that η (or β) is actually the internal angle of the triangle constructed by $2J_z$ and B with separation angle θ. So it is obvious that the cosine of β or η is $\frac{\Delta y}{r_i}$, where r_i is the amplitude of a new vector $\vec{K}$. Using this geometry relation, we find that the geometric phase in the form of equation (7) can also be viewed as half the solid angle subtended by the loop Γ traversed by the vector $\vec{K}$ in figure 3.

4. The new parameter vector and quasimagnetic field

One may wonder why the coupling has no influence on the geometric phases of states 1–4 according to equation (6). In answering this question, we propose the concept of *quasimagnetic* field in this section. First, we may write the form of the one-site drive

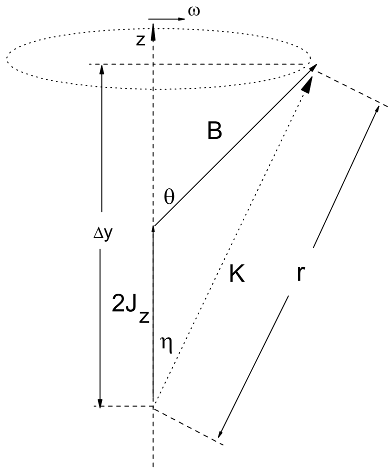

Figure 3. The implicit geometry relation in equation (6). We find what equation (6) implies is actually this basic triangle with $2J_z$, B and K being its sides. The coupling and magnetic field constitute the vector K.

tripartite system in the aforementioned unit $\frac{e\hbar}{2mc} = 1$. For generality, we take account of the anisotropic spin coupling existent in all directions:

$$H(\vec{B}) = \vec{\sigma}_1 \cdot \vec{B}(t) + \left(J_x\sigma_1^x\sigma_2^x + J_y\sigma_1^y\sigma_2^y + J_z\sigma_1^z\sigma_2^z\right) + \left(J_x\sigma_1^x\sigma_3^x + J_y\sigma_1^y\sigma_3^y + J_z\sigma_1^z\sigma_3^z\right) + J_x'\sigma_2^x\sigma_3^x + J_y'\sigma_2^y\sigma_3^y + J_z'\sigma_2^z\sigma_3^z. \quad (9)$$

It is worth noting that equation (2) is actually the special case of this Hamiltonian on the condition that we omit the coupling in x, y directions, i.e. $J_x = J_y = 0$, $J_x' = J_y' = 0$. In the following, we make a substitution. First, we introduce two new vectors $\vec{D}_2 = \left\{D_2^x, D_2^y, D_2^z\right\}$ and $\vec{D}_3 = \left\{D_3^x, D_3^y, D_3^z\right\}$, which satisfy

$$\begin{aligned} D_2^x &= J_x\sigma_2^x, \quad D_2^y = J_y\sigma_2^y, \quad D_2^z = J_z\sigma_2^z, \\ D_3^x &= J_x\sigma_3^x, \quad D_3^y = J_y\sigma_3^y, \quad D_2^z = J_z\sigma_3^z. \end{aligned} \quad (10)$$

Then we transform equation (9) into

$$\begin{aligned} H(\vec{B}) &= \vec{\sigma}_1 \cdot \vec{B}(t) + \vec{\sigma}_1 \cdot \vec{D}_2 + \vec{\sigma}_1 \cdot \vec{D}_3 + \sum_{i=x,y,z} J_i'\sigma_2^i\sigma_3^i \\ &= \vec{\sigma}_1 \cdot [\vec{B}(t) + \vec{D}_2 + \vec{D}_3] + \sum_{i=x,y,z} J_i'\sigma_2^i\sigma_3^i, \end{aligned} \quad (11)$$

where $\vec{K}(t) = \vec{B}(t) + \vec{D}_2 + \vec{D}_3$ is a new parameter vector. We note that $\vec{D}_2 + \vec{D}_3$ can be viewed as a magnetic field. We term it as *quasimagnetic field*. So the new parameter vector is the vector superposition of the original magnetic field and the newcomer—quasimagnetic field.

After the introduction of $\vec{K}(t)$, the Hamiltonian can be expressed as $H(\vec{K})$. For the convenience of plotting and discussion, we still use the simplified case previously discussed, i.e. $J_x = J_y = 0$, $J_x' = J_y' = 0$. In this case, there only exists coupling in the z-direction, so $\vec{D}_2 = \left\{0, 0, J_z\sigma_2^z\right\}$,$\vec{D}_3 = \left\{0, 0, J_z\sigma_3^z\right\}$. By equation (11), we can get the Hamiltonian with the coupling present only in the z-direction:

$$H = \vec{\sigma}_1 \cdot \left[\vec{B}(t) + J_z\left(\sigma_2^z + \sigma_3^z\right)\hat{k}\right] + J_z'\sigma_2^z\sigma_3^z, \quad (12)$$

where $\hat{k}$ is the unit vector in the z-direction.

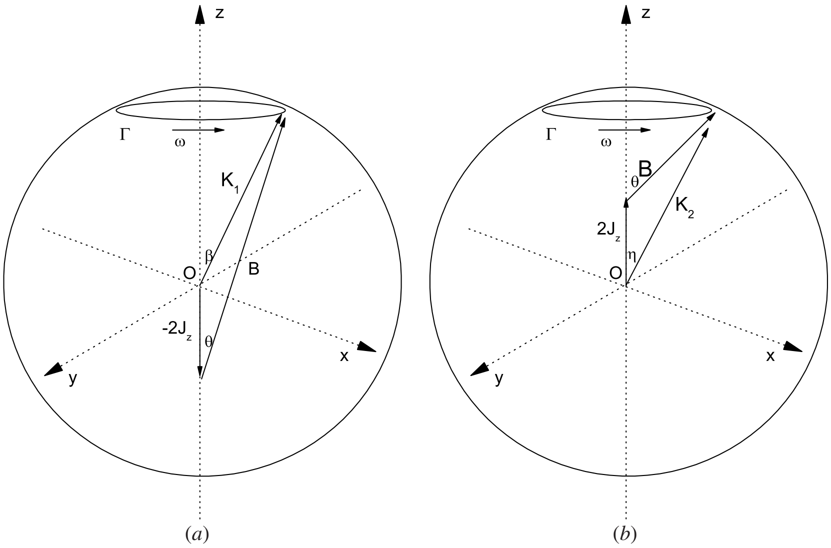

Figure 4. The new parameter space. (*a*) The superposition relation for states 5 and 6. (*b*) The superposition relation for states 7 and 8. The new parameter vector $\vec{K}_i, i = 1, 2$, is the superposition of $\vec{B}$ and $\pm 2J_z$ where the sign is dependent on the eigenvalues of $(\sigma_2^z + \sigma_3^z)$ in equation (12). The geometric phase is half the solid angle subtended by the loop Γ which is traversed by $\vec{K}_i$.

All the following discussion and figures are based on this simplified case. We plot the parameter space of $\vec{K}$ in figure 4. It is clearly seen that if $\vec{K}$ replaces the previous $\vec{B}$, then the geometric phase shift equals in value half the solid angle subtended by the loop traversed by $\vec{K}$ rather than $\vec{B}$. In [23], it is demonstrated that the relation between the geometric phase and the solid angle enclosed by the magnetic field is broken by the spin–spin coupling. But we find that, if the parameter itself is properly revised, the relation between the phase and the solid angle still holds.

By this new parameter space theory, we can straightforwardly explain the origin of *coupling-independent geometric phase* and the *quenching effect*. First, from equation (5) in states 1–4, we find that spins 2 and 3 in these states have opposite direction. For example, in state 1 $|\psi_1\rangle = -\mathrm{e}^{\mathrm{i}\varphi}\cot(\theta/2)|\downarrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle$, spin 2 is down and spin 3 is up. By equation (12), the counteracting spins lead to offset coupling effect and $\vec{K}$ reverts to the magnetic field $\vec{B}$. This is the case of single spin in the magnetic field. Second, in the states where spins 2 and 3 have the same direction, the coupling effect will be reinforced. States 5–8 have such a property, so they have the geometric phases subject to the influence of spin–spin coupling. In addition, it is worth noting that the derived formula (equation (12)) from the original form of the Hamiltonian has prophesied that some eigenvectors will be irrelevant of the spin coupling in the state satisfying $\sigma_2^z + \sigma_3^z = 0$. Therefore, the *coupling-independent geometric phase* will be present in the state of other spin systems where the spins interacting with that in the magnetic field can be counteracted.

From figure 4, we roughly deduce the solid angle from basic geometry relations as follows:

$$\Omega \approx \frac{2\pi B^2(1 - \cos\theta)}{(2J_z + B)^2}, \qquad J_z \gg B. \tag{13}$$

When the coupling increases to infinity, the geometric phase will tend to 0 (multiple of 2π), i.e.

$$\lim_{J\to+\infty} \Omega = 0. \tag{14}$$

This is the origin of the quenching effect. However, we should state here that the quenching effect is not peculiar to the tripartite system. Because the geometric phase is dependent on the evolution of the time-dependent part in the Hamiltonian, the coupling term defines a fixed preferred quantization axis that makes the eigenstates essentially unaffected by a weak magnetic field. Therefore, as long as the coupling of the spin affected by magnetic field approaches infinity, the geometric phase of multi-spin system will tend to 0 or a multiple of 2π.

Now we have well explained the *coupling-independent geometric phase* and the *quenching effect*. By our theory, except the magnetic field, only the quasimagnetic field $(\vec{D}_2 + \vec{D}_3)$ can influence the geometric phase. Consequently, we infer that the omission of $J_z'\sigma_2^i \cdot \sigma_3^i$ will not affect any change in the final geometric phase. This can be verified by equation (6), from which we find that J_z' does not occur in the final form of the geometric phase. Therefore, we reach the conclusion: not all couplings exert the influence on the geometric phase although they may usually affect the eigenvalues or eigenvectors of Hamiltonian; only those coupling terms that contain the spin(s) simultaneously interacting with the (magnetic) drive field can affect the final geometric phase.

Here we add some comments on this method. Although our concept that coupling is viewed as a parameter and combined with the magnetic field term is new, the idea that several parameters can be combined into a new parameter has been used or mentioned in several papers. For example, in [24], Berry studied two examples about the generalized harmonic oscillator and rotated rotator. In dealing with generalized harmonic oscillator, he regarded the three parameters X, Y, Z as the components of the new vector $\boldsymbol{X}$. Furthermore, in [25], the author also used a similar method in the study of the gauge field structure. Besides, [26] discusses the selection of parameter's space by using a nonrelativistic charged spinless particle evolving in the superposition of the fields produced by a Penning trap and a rotating magnetic field and has excellently obtained the relation between the geometric phase and the symmetry of the binding potential. But we find that although these papers excellently resolved the problems each focuses on by virtue of the concept of parameter, they are fundamentally different from our construction of a new parameter, where coupling is introduced into the parameter space rather than merely combined with other parameter vectors. Most importantly, in the conclusion section of [26], the authors explicitly left the search for '*a parameter's space* $X(t)$ *such that* $\alpha(X(t)) = B(t)$' as an open question, which is just what we deal with in our paper.

The spirit of the above treatment is to include coupling into the parameter space and view it as a component of the new constructed vector. Because of the innate deficiency of the geometry method, we must admit that albeit this method is very clear and straightforward in explaining the influence of spin coupling on geometric phase and predicting new phenomena, the precise calculation of the geometric phase by this method is complicated and time consuming.

Because the coupling discussed here is time independent, one may wonder whether the coupling can become time dependent and uniquely serve as the driving force of evolution? Recently, intra-variable coupling has become an active research area [27, 28]. Spin–orbit coupling during quantum gate operations can be changed by using time-symmetric pulse shapes for the coupling between the spins. The attention to this time-dependent coupling perhaps arises from the ambition for the universal quantum computation just by the exchange interaction alone.

In conclusion, we have obtained the geometric phase of the one-site magnetic drive tripartite spin system and discovered the phenomenon of *coupling independent of geometric phase*. After discussing the influence of coupling on geometric phase, we proposed the concept of quasimagnetic field and updated the concept of parameter vector. This treatment has satisfactorily explained the discovered phenomenon in this paper. We also found that only certain couplings have relevance for the value of geometric phase. The prospect of intra-variable coupling is also mentioned. A more complicated case, i.e. $n \geqslant 4$, is still open to us.

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