General Approach to Quantum-Classical Hybrid Systems and Geometric Forces

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We present a general theoretical framework for a hybrid system that is composed of a quantum subsystem and a classical subsystem. We approach such a system with a simple canonical transformation which is particularly effective when the quantum subsystem is dynamically much faster than the classical counterpart, which is commonly the case in hybrid systems. Moreover, this canonical transformation generates a vector potential which, on one hand, gives rise to the familiar Berry phase in the fast quantum dynamics and, on the other hand, yields a Lorentz-like geometric force in the slow classical dynamics.

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Single spin detection was recently achieved with magnetic-resonance-force microscopy [1]. Technically, this remarkable experiment marks a major step in man's ability to control objects at the atomic scale and has great potential for application in future technology [2]. On the scientific side, this experiment also invokes many interesting questions of fundamental interest.

We first notice that the system used in the experiment is a hybrid system composed of a quantum subsystem (single spin) and a classical subsystem (cantilever). In Refs. [3,4], both subsystems are treated classically. Although this is adequate to address specific issues and systems related to the current experiments [1,5], this method is inadequate to treat a general hybrid system, for example, when the quantum subsystem is not a spin or when one tries to discuss phase-related issues. This kind of hybrid system was also studied by Berry and Robbins [6]. However, their formalism is not satisfying, either, as the classical dynamics never appears explicitly in the formalism and it cannot deal with the situation in which the quantum system is in a coherent noneigenstate. Then the question is how to treat adequately a general hybrid system. This question will grow more important since various techniques are being developed or explored to control objects at the atomic scale. These techniques are certainly all based on hybrid systems where a classical sensor interacts with a quantum object.

We also notice that, in the experiment of single spin detection [1], the quantum subsystem (spin) is dynamically much faster than the classical counterpart (cantilever). In other words, it is a Born-Oppenheimer-type system (one subsystem is fast and the other slow). This is, of course, typical of a hybrid system. Born-Oppenheimer-type systems have been studied by many in different settings [6–11]. One general scene in these Born-Oppenheimer-type systems is that vector potentials related to geometric phases are found to arise and generate geometric forces in the slow subsystem. It is then interesting to ask whether the geometric force can be detected with current experimental techniques in light of this successful single spin detection [1]. It is also interesting to know how to formulate the vector potential and the geometric force when the quantum subsystem is in a noneigenstate, since there is no reason to assume that the quantum subsystem is only in an eigenstate. In previous studies, the quantum subsystem is always assumed in an eigenstate [6–9].

In this Letter, we present a general theoretical framework for hybrid systems. For this kind of system, we use the well-known fact [12–14] that a quantum system possesses mathematically a canonical classical Hamiltonian structure. In this way, we can describe the hybrid system with a unified classical Hamiltonian. We emphasize that in our Hamiltonian the quantum subsystem is reduced only mathematically to a classical system and no physics is lost. This is in contrast to the Hamiltonian of Ref. [4], where the quantum subsystem is reduced physically to be classical and some physics may be lost.

We try to decipher the complicated dynamics of the hybrid system with a special canonical transformation. This transformation is particularly effective when the quantum subsystem is fast and the classical subsystem is slow. After the canonical transformation, it becomes clear that the two subsystems influence each other not only via interaction but also through a vector potential. This vector potential generates the familiar Berry phase [15] in the fast quantum subsystem while it produces a Lorentz-like geometric force in the slow classical subsystem.

We shall use a simple example, the coupling of a heavy magnetic particle with a single spin, to illustrate our theory. We also use this example to show how big the geometric force can be and whether it is detectable with current experimental techniques.

In addition, we point out that our method can also be regarded as an alternative way of deriving the Berry phase [15]. Our method has the advantage that the fast quantum subsystem need not be in an eigenstate. In other words, the Berry phase can be defined for a general quantum state. Our method can also be generalized to derive Hannay's angles [16] or the geometric phase proposed in Ref. [17] for nonlinear quantum systems. In this sense, our approach shows that these different geometric phases (Berry phase and Hannay's angles) are just different manifestations of the same mathematical concept in different dynamical systems.

We describe the aforementioned hybrid coupled system with the following Hamiltonian:

$$H = \langle \boldsymbol{\Psi} | \hat{H}_1(\mathbf{q}_2) | \boldsymbol{\Psi} \rangle + H_2(\mathbf{p}_2, \mathbf{q}_2), \tag{1}$$

where $\hat{H}_1$ is the Hamiltonian operator of the linear N-level fast quantum subsystem and $|\boldsymbol{\Psi}\rangle = (\Psi_1, \Psi_2, \ldots, \Psi_N)^T$ is its quantum state. The Hamiltonian H_2 governs a heavy classical subsystem that moves slowly and $\mathbf{p}_2$, $\mathbf{q}_2$ are its momenta and coordinates, respectively. The dependence of $\hat{H}_1$ on $\mathbf{q}_2$ indicates the coupling between the two subsystems.

We first focus on the quantum subsystem, assuming temporarily that $\mathbf{q}_2$ are just some fixed parameters. The Schrödinger equation of the quantum subsystem is $i\hbar d|\boldsymbol{\Psi}\rangle/dt = \hat{H}_1|\boldsymbol{\Psi}\rangle$, which can be rewritten as

$$i\hbar \frac{d\Psi_j}{dt} = \frac{\partial}{\partial \Psi_j^*} H_1(\boldsymbol{\Psi}, \boldsymbol{\Psi}^*, \mathbf{q}_2), \tag{2}$$

where $H_1 = \langle \boldsymbol{\Psi} | \hat{H}(\mathbf{q}_2) | \boldsymbol{\Psi} \rangle$. This shows that the quantum system has a classical Hamiltonian structure. This fact is known to many people and was discussed in detail in Refs. [12,13]. To have a more "classical" look for this quantum system, we define $p_{1j} = \sqrt{i\hbar}\Psi_j^*$, $q_{1j} = \sqrt{i\hbar}\Psi_j$ and write Eq. (2) in an apparent canonical Hamiltonian formalism

$$\frac{dq_{1j}}{dt} = \frac{\partial \tilde{H}_1}{\partial p_{1j}}, \qquad \frac{dp_{1j}}{dt} = -\frac{\partial \tilde{H}_1}{\partial q_{1j}}, \tag{3}$$

where $\tilde{H}_1 = \tilde{H}_1(\mathbf{p}_1, \mathbf{q}_1, \mathbf{q}_2) = H_1(\boldsymbol{\Psi}, \boldsymbol{\Psi}^*, \mathbf{q}_2)$. In this way, we have classically reformulated quantum systems.

The quantum state $|\boldsymbol{\Psi}\rangle$ can be expanded in terms of instantaneous eigenstates

$$|\boldsymbol{\Psi}\rangle = \sum_{n=1}^{N} a_n |\varphi_n(\mathbf{q}_2)\rangle, \tag{4}$$

where $\hat{H}_1(\mathbf{q}_2)|\varphi_n(\mathbf{q}_2)\rangle = E_n(\mathbf{q}_2)|\varphi_n(\mathbf{q}_2)\rangle$. The quantum system can be described alternatively by these expansion coefficiencies a_n's. Define $I_{1n} = \hbar|a_n|^2$ and $\Theta_{1n} = -\arg(a_n)$; one can prove readily that $\mathbf{I}_1$ and $\boldsymbol{\Theta}_1$ are another set of canonical variables for the Hamiltonian H_1. According to the standard classical theory [18], there is a canonical transformation between $\mathbf{p}_1$, $\mathbf{q}_1$ and $\mathbf{I}_1$, $\boldsymbol{\Theta}_1$, and this transformation is given by a generating function $F_1(\mathbf{q}_1, \mathbf{I}_1, \mathbf{q}_2)$ that satisfies

$$\mathbf{p}_1 = \frac{\partial F_1}{\partial \mathbf{q}_1}, \qquad \boldsymbol{\Theta}_1 = \frac{\partial F_1}{\partial \mathbf{I}_1}. \tag{5}$$

With this transformation, the Hamiltonian H_1 becomes $\mathcal{H}_1 = \mathcal{H}_1(\mathbf{I}_1, \mathbf{q}_2) = \sum_n E_n(\mathbf{q}_2) I_{1n}/\hbar$, independent of the angles $\boldsymbol{\Theta}_1$.

We go back to the hybrid coupled system, where $\mathbf{q}_2$ are dynamical variables instead of some fixed parameters. The Hamiltonian for the hybrid system can now be expressed in a pure classical formalism

$$\tilde{H} = \tilde{H}_1(\mathbf{p}_1, \mathbf{q}_1, \mathbf{q}_2) + H_2(\mathbf{p}_2, \mathbf{q}_2). \tag{6}$$

We introduce a canonical transformation from $\mathbf{p}_1$, $\mathbf{q}_1$, $\mathbf{p}_2$, $\mathbf{q}_2$ to $\mathbf{I}_1$, $\boldsymbol{\Theta}_1$, $\mathbf{P}_2$, $\mathbf{Q}_2$ with the following generating function:

$$F = F_1(\mathbf{q}_1, \mathbf{I}_1, \mathbf{q}_2) + \mathbf{q}_2 \mathbf{P}_2. \tag{7}$$

The canonical transformation is then given by

$$\mathbf{p}_1 = \frac{\partial F}{\partial \mathbf{q}_1} = \frac{\partial F_1}{\partial \mathbf{q}_1}, \qquad \boldsymbol{\Theta}_1 = \frac{\partial F}{\partial \mathbf{I}_1} = \frac{\partial F_1}{\partial \mathbf{I}_1}, \tag{8}$$

$$\mathbf{p}_2 = \frac{\partial F}{\partial \mathbf{q}_2} = \frac{\partial F_1}{\partial \mathbf{q}_2} + \mathbf{P}_2, \qquad \mathbf{Q}_2 = \frac{\partial F}{\partial \mathbf{P}_2} = \mathbf{q}_2. \tag{9}$$

The transformation does two things: (i) Since Eq. (8) is identical to Eq. (5), the transformation changes $\mathbf{p}_1$, $\mathbf{q}_1$ to $\mathbf{I}_1$, $\boldsymbol{\Theta}_1$ as if it is generated by F_1; (ii) it puts an additional vector function $\mathbf{A} = -\partial F_1/\partial \mathbf{q}_2$ in the momenta $\mathbf{p}_2$ while keeping the coordinates $\mathbf{q}_2$ unchanged. After the transformation, the total Hamiltonian in Eq. (6) becomes

$$\mathcal{H} = \mathcal{H}_1(\mathbf{I}_1, \mathbf{Q}_2) + H_2(\mathbf{P}_2 - \mathbf{A}, \mathbf{Q}_2). \tag{10}$$

In the second subsystem, $\mathbf{A}$ appears very much like a vector potential. However, it is not a true vector potential since it also depends on variables other than $\mathbf{q}_2$. For convenience, we shall call it a pseudovector potential. As we shall see, this pseudovector potential can lead to a true vector potential.

By assuming that the classical subsystem has the usual Hamiltonian $H_2 = \mathbf{p}_2^2/2M + V_2(\mathbf{q}_2)$, we write down the equations of motion for the whole system. For the quantum part, we have

$$\dot{I}_{1j} = \dot{\mathbf{q}}_2 \cdot \frac{\partial \mathbf{A}}{\partial \Theta_{1j}}, \tag{11}$$

$$\dot{\Theta}_{1j} = \frac{\partial \mathcal{H}_1}{\partial I_{1j}} - \dot{\mathbf{q}}_2 \cdot \frac{\partial \mathbf{A}}{\partial I_{1j}}. \tag{12}$$

For the classical part, we obtain

$$\dot{P}_{2j} = -\frac{\partial \mathcal{H}_1}{\partial q_{2j}} - \frac{\partial V_2}{\partial q_{2j}} + \dot{\mathbf{q}}_2 \cdot \frac{\partial \mathbf{A}}{\partial q_{2j}}, \tag{13}$$

$$\dot{Q}_{2j} = \dot{q}_{2j} = (P_{2j} - A_j)/M. \tag{14}$$

Most of the hybrid systems that we encounter in concrete problems are of Born-Oppenheimer type; that is, the quantum subsystem is much faster than the classical subsystem. We now apply the general formalism and approach to this typical type of hybrid systems. In this case, the classical variables $\mathbf{q}_2$ can be considered as the adiabatic parameters for the quantum subsystem.

We first analyze the pseudovector potential $\mathbf{A}$. To do this, we make the potential an explicit function of the new dynamical variables $\mathbf{I}_1$, $\mathbf{\Theta}_1$, $\mathbf{P}_2$, and $\mathbf{Q}_2$ $(=\mathbf{q}_2)$ by defining a new function

$$\tilde{F}_1(\mathbf{I}_1, \mathbf{\Theta}_1, \mathbf{q}_2) = F_1(\mathbf{q}_1(\mathbf{I}_1, \mathbf{\Theta}_1, \mathbf{q}_2), \mathbf{I}_1, \mathbf{q}_2). \tag{15}$$

This leads to

$$A_j = \mathbf{p}_1 \frac{\partial \mathbf{q}_1}{\partial q_{2j}} - \frac{\partial \tilde{F}_1}{\partial q_{2j}} = i\hbar \langle \mathbf{\Psi} | \frac{\partial}{\partial q_{2j}} | \mathbf{\Psi} \rangle - \frac{\partial \tilde{F}_1}{\partial q_{2j}}. \tag{16}$$

Since the variables $\mathbf{q}_2$ change very slowly compared to the dynamics of the quantum subsystem, we are allowed to apply the standard averaging technique in the study of adiabatic evolution [16,18]. It also implies that the probabilities $\mathbf{I}_1$ are conserved during the evolution according to the quantum adiabatic theorem [19]. After averaging and using the quantum adiabatic theorem, the pseudovector potential becomes

$$\begin{aligned} \bar{A}_j &= \oint \frac{d\mathbf{\Theta}_1}{(2\pi)^N} \left[i\hbar \langle \mathbf{\Psi} | \frac{\partial}{\partial q_{2j}} | \mathbf{\Psi} \rangle - \frac{\partial \tilde{F}_1}{\partial q_{2j}} \right] \\ &= i \sum_{n=1}^{N} I_{1n} \langle \varphi_n | \frac{\partial}{\partial q_{2j}} | \varphi_n \rangle - \overline{\frac{\partial \tilde{F}_1}{\partial q_{2j}}}, \end{aligned} \tag{17}$$

where the overline indicates that the average has been done for the variable. The function $\bar{\mathbf{A}}$ is now a true vector potential as it no longer depends on $\mathbf{\Theta}_1$ and at the same time $\mathbf{I}_1$ are constant. After ignoring the trivial gradient term in Eq. (17), we obtain a true vector potential

$$\bar{\mathbf{A}} = \sum_{n=1}^{N} I_{1n} \mathcal{A}_n, \qquad \mathcal{A}_n = i \langle \varphi_n | \frac{\partial}{\partial \mathbf{q}_2} | \varphi_n \rangle. \tag{18}$$

Substituting it into Eq. (12), we arrive at

$$\dot{\Theta}_{1j} = \frac{\partial \mathcal{H}_1}{\partial I_{1j}} - \mathcal{A}_j \cdot \dot{\mathbf{q}}_2, \tag{19}$$

where the integration of the last term produces exactly the Berry phase of the jth eigenstate. One can regard this as a new way to derive the Berry phase; in this new way, the quantum system does not need to be in an eigenstate.

For the slow classical subsystem, we take the averaging over Eq. (13) and rewrite it in a physically more transparent form

$$M \ddot{\bar{\mathbf{q}}}_2 = -\frac{\partial \mathcal{H}_1}{\partial \mathbf{q}_2} - \frac{\partial V_2}{\partial \mathbf{q}_2} + \dot{\bar{\mathbf{q}}}_2 \times \mathcal{B}, \tag{20}$$

where $\mathcal{B} = \nabla \times \bar{\mathbf{A}} = \sum_n I_{1n} \nabla \times \mathcal{A}_n$ is a magneticlike gauge field. Similar to the usual magnetic field, the gauge field influences the dynamics in terms of a Lorentz-like force. So the Berry phase is shown to be linked to a physical force. We shall have more discussion with this force later via an example.

We have applied our method to the cantilever-spin system in the single spin detection experiment [1,5] and recovered the theoretical result in Ref. [4]. The pity is that, since the cantilever vibrates only in one dimension, the force associated with $\bar{\mathbf{A}}$ is always zero. To have a nonzero $\mathcal{B}$, we consider an example where the classical subsystem is a magnetic particle and the quantum subsystem is a spin of 1/2 as shown in Fig. 1. The magnetic particle has a magnetic moment $\mathbf{m}_F$ and mass m; it moves freely in the xy plane. We assume that the magnetic moment $\mathbf{m}_F$ always points in the negative z direction. A single spin with magnetic moment $\boldsymbol{\mu}$ is placed below the plane at the distance d. For simplicity, we place the origin of our coordinate system in the particle plane and directly above the spin.

Because of the magnetic dipolar interaction, the spin feels a magnetic field from the classical magnetic particle. The field is given by

$$\{B_x, B_y, B_z\} = -\frac{\mu_0 m_F \{3xd, 3yd, 2d^2 - r^2\}}{4\pi (d^2 + r^2)^{5/2}}, \tag{21}$$

where $r^2 = x^2 + y^2$. So the Hamiltonian operator for the spin is

$$\hat{H}_1 = -\mu \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}. \tag{22}$$

This Hamiltonian has two eigenstates $|\pm\rangle$, whose eigenenergies are, respectively, $\mp \mu B$, with $B = \sqrt{B_x^2 + B_y^2 + B_z^2}$. The total Hamiltonian is

$$H = \langle \mathbf{\Psi} | \hat{H}_1 | \mathbf{\Psi} \rangle + \mathbf{p}^2 / 2m, \tag{23}$$

where $|\mathbf{\Psi}\rangle = (\Psi_1, \Psi_2)^T$ is the spin wave function and p is the momentum of the magnetic particle.

Following the general procedure described above, we can transform the above Hamiltonian to

$$\mathcal{H} = (|a_-|^2 - |a_+|^2) \mu B + \frac{(\mathbf{P} - \bar{\mathbf{A}})^2}{2m}, \tag{24}$$

where $|a_\pm|^2$ are the probabilities on the two spin eigenstates $|\pm\rangle$, respectively. The vector potential is given by

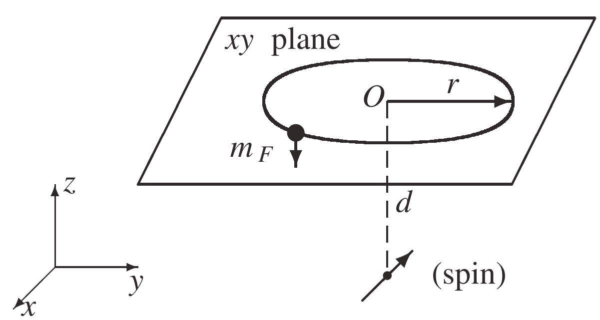

FIG. 1. A schematic setup of a magnetic particle interacting with a spin. The particle moves freely in the xy plane with a magnetic moment of $\mathbf{m}_F$ always pointing in the negative z direction. A single spin with magnetic moment $\boldsymbol{\mu}$ is placed beneath the plane with a distance of d.

$$\bar{\mathbf{A}} = i\hbar|a_+|^2\langle +|\frac{\partial}{\partial \mathbf{r}}|+\rangle + i\hbar|a_-|^2\langle -|\frac{\partial}{\partial \mathbf{r}}|-\rangle. \quad (25)$$

The equations of motion for the particle are

$$m\ddot{x} = \frac{3\mu\mu_0 m_F(5d^2+r^2)(|a_-|^2-|a_+|^2)}{4\pi\sqrt{4d^2+r^2}(d^2+r^2)^3}x + \mathcal{B}\dot{y}, \quad (26)$$

$$m\ddot{y} = \frac{3\mu\mu_0 m_F(5d^2+r^2)(|a_-|^2-|a_+|^2)}{4\pi\sqrt{4d^2+r^2}(d^2+r^2)^3}y - \mathcal{B}\dot{x}. \quad (27)$$

The magneticlike $\mathcal{B}$ field always points in the z direction. The field strength is

$$\mathcal{B} = \frac{9\hbar d^2(r^2+2d^2)}{2[(r^2+d^2)(r^2+4d^2)]^{3/2}}(|a_+|^2-|a_-|^2). \quad (28)$$

We make two observations. First, the field is geometric, depending only on the position of the magnetic particle besides $\hbar$ and independent of the strength of the dipolar interaction. Second, it curves motion in an unexpected way. For instance, if the initial conditions of the slow particle are $x(0)=0$, $y(0)=0$, $\dot{x}(0)>0$, and $\dot{y}(0)=0$, then everything in the real space is symmetric with respect to the inverse of y, including the dipolar force and the spin direction. One would then expect intuitively that the particle moves in a straight line along the x direction. However, the slow particle will curve owing to $\mathcal{B}$, breaking the left-right symmetry in the real space. What is interesting is that the force breaking of this real-space symmetry comes from the dynamics of the spin wave function's phase, a non-real-space variable.

To detect such a force experimentally, the best way may be to measure the frequency associated with this force, such as the frequency change in the single spin detection [1]. For the simple system in Fig. 1, if the spin is only an electron and $\mu<0$, we notice that the slow particle can move in a circle if $|a_+|^2<|a_-|^2$. If somehow one can fix the radius r of the circle, the frequency that the particle circulates clockwise is different from that when it circulates anticlockwise. Simple calculations show that the frequency difference is $\Delta\nu = \mathcal{B}/2\pi m$. For estimation of the value of the frequency difference, the following parameters are used: $\mu_0 m_F \sim 2.0\times10^{-21}$ T m^3, $m\sim 2.5\times10^{-15}$ kg, $r\sim 1$ nm, and $d\sim 1000$ nm. For these values of parameters, we obtain, for the case $|a_+|^2=0$ and $|a_-|^2=1$, $\mathcal{B}\sim -1.20\times10^{-22}$ kg/s (if it were for an electron, it would be equivalent to a magnetic field of 7.5×10^{-4} T) and $Bz\sim 3.2\times10^{-4}$ T. The frequency difference is $\Delta\nu\sim 0.7\times10^{-8}$ Hz, which is a challenging task for the current technique [1]. Moreover, in a real experiment, the magnetic particle needs to be attached to something such as a string so that it can oscillate in two dimensions.

A similar vector potential can also arise in connection to Hannay's angle [16]. The theoretical framework starting at Eq. (6) can be readily generalized to the cases where the fast subsystem is a classical integrable system. In this generalization, one needs only to regard $\mathbf{I}_1$ and $\mathbf{\Theta}_1$ as a set of action-angle variables. Such a coupled system was also discussed in Ref. [20]. The same extension can be done for the geometric phase proposed for nonlinear quantum systems [17].

In the general case where the two subsystems are not necessarily one fast and one slow, one may use the pseudovector potential $\mathbf{A}$ to define a "geometric" phase for nonadiabatic processes. However, this general phase may be of little use since it does not provide any insight into the dynamics. We finally note that the quantum-classical hybrid system has been studied extensively in the context of quantum measurement [21].

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