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# Berry phase and Hannay's angle in the Born–Oppenheimer hybrid systems

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## HIGHLIGHTS

- We have derived the Berry phase and Hannay's angle in BO hybrid systems.
- The Berry phase contains a novel term brought by the effective gauge potential.
- This mechanism can be used to generate artificial gauge potentials for neutral atoms.
- The relation between Hannay's angles and Berry phases is established.

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## ABSTRACT

In this paper, we investigate the Berry phase and Hannay's angle in the Born–Oppenheimer (BO) hybrid systems and obtain their algebraic expressions in terms of one form connection. The semiclassical relation of Berry phase and Hannay's angle is discussed. We find that, besides the usual connection term, the Berry phase of quantum BO composite system also contains a novel term brought forth by the coupling induced effective gauge potential. This quantum modification can be viewed as an effective Aharonov–Bohm effect. Moreover, the similar phenomenon is founded in Hannay's angle of classical BO composite system, which indicates that the Berry phase and Hannay's angle possess the same relation as the usual one. An example is used to illustrate our theory. This scheme can be used to generate artificial gauge potentials for neutral atoms. Besides, the quantum–classical hybrid BO system is also studied to compare with the results in full quantum and full classical composite systems.



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## 1. Introduction

It is known that quantum eigenstates will acquire an additional geometric phase factor in cyclic adiabatic processes [1]. This phase, now called Berry phase, has become a central unifying concept in quantum mechanics [2–4] and found wide applications in fields ranging from chemistry to condensed matter physics [5,6]. The Berry phase has two key properties that make it special [7]. First, it has a beautiful analogy in differential geometry. The Berry phase can be regarded as the holonomy in a Hermitian line bundle [8]. Second, the evolution of the parameters driving the quantum system is adiabatic which naturally defines a connection in the bundle. In a subsequent development of this idea, Hannay found that the angle variable of classical integrable system [9] also acquires an additional angle shift as the system adiabatically cycles in phase space [10]. It was later proved by Berry that this Hannay's angle possesses a natural relation with the Berry phase under semiclassical approximation [11]. As a matter of course, this quantum–classical correspondence gives rise to a great number of impressive works [12–15].

The early works of the geometric phase were mainly focus on simply quantum system. However, as the rapid development of atoms physics and quantum physics, the geometric phases in many kinds of composite systems has been attracting renewed attention [5,6,16]. Specifically, if one subsystem is much 'heavier' and 'slower' than the other subsystem in the composite system, the system is dominant by Born–Oppenheimer (BO) approximation, which has been widely used in physics and quantum chemistry and becomes a fundamental tool in these fields [5,17] (Here we call the composite systems BO composite system). With this approximation, one can first resolve the eigenvalue problem of the fast Hamiltonian by treating the slow variables as parameters, and then add the slow variables dependent eigenvalue to the slow subsystem to get an effective Hamiltonian. In particular, if the fast subsystem carries a Berry connection, the effective Hamiltonian will contain an effective gauge potential [18]. Its influence on the dynamics of the BO composite system has also been discussed in several interesting works [19–24]. However, the Berry phase associated with the adiabatic evolution of an effective eigenstate in the BO composite system is still unresolved and the role of effective gauge potential in it has not been studied yet. Furthermore, in Ref. [11], a semiclassical connection was established between Berry phase and Hannay's angle. One may imagine that if the same relation exists between the Berry phase in BO system and its classical correspondent Hannay's angle. All of this calls for a further investigation.

In the present paper, we have made a systematic analysis of the Berry phase and Hannay's angle for BO system driven by adiabatic parameters. We find that the Berry phase can still be well defined by the one form connections in which the effective gauge potential induces an effective connection via an effective Aharonov–Bohm effect. Moreover, Hannay's angles in the correspondent classical BO system are proved to be related to the Berry phase by the derivative form as the usual one [11]. Furthermore, the Berry phase and Hannay's angle in quantum–classical BO hybrid system are also related with the one in full quantum or full classical BO system. This means that the quantum–classical correspondence is also kept under BO approximations.

Our paper is organized as follows. The Berry phase and Hannay's angle in BO system are analytically studied in Sections 2 and 3, respectively. In Section 4, the relations between the Berry phase and Hannay's angle are established. An electromagnetic model driven by a harmonic field model is used to illustrate our theory in Section 5. In Section 6, we investigate the Berry phase and Hannay's angle in BO system and compare the result with the full quantum and full classical one. Section 7 presents our conclusion.

## 2. Berry phase in BO composite system

The Hamiltonian of a quantum composite system with coordinates and momenta $(\boldsymbol{q}, \boldsymbol{p})$ and $(\boldsymbol{Q}, \boldsymbol{P})$ can be written as $\hat{H} = \hat{H}(\hat{\boldsymbol{p}}, \hat{\boldsymbol{q}}, \hat{\boldsymbol{P}}, \hat{\boldsymbol{Q}}; \boldsymbol{X})$. Suppose the subsystem with $(\boldsymbol{Q}, \boldsymbol{P})$ is much 'heavier' and 'slower' than the one with $(\boldsymbol{q}, \boldsymbol{p})$, $\hat{H}$ becomes

$$\hat{H} = \hat{H}_1(\hat{\boldsymbol{p}}, \hat{\boldsymbol{q}}; \hat{\boldsymbol{Q}}, \boldsymbol{X}) + \hat{H}_2(\hat{\boldsymbol{P}}, \hat{\boldsymbol{Q}}; \boldsymbol{X}) \tag{1}$$

where $\hat{H}_1$ and $\hat{H}_2$ describes the fast and slow subsystem driven by varying parameters $\boldsymbol{X} = (X, Y, \ldots)$, respectively.

According to BO approximation, we first solves the eigenvalue problem for $H_1$ and obtains its eigenvalues $E_n(\boldsymbol{Q}, \boldsymbol{X})$ as functions of the eigenvalues $\boldsymbol{Q}$ of the operator $\hat{\boldsymbol{Q}}$, and then add $E_n$ to $\hat{H}_2$ as an additional potential (the detailed proof can be found in Ref. [5]). Thus, the effective Hamiltonian of the slow subsystem reads

$$\hat{H}_n^{\text{eff}} = \hat{H}_2(\boldsymbol{P} - \hbar \boldsymbol{A}^{\text{eff}}, \boldsymbol{Q}; \boldsymbol{X}) + E_n(\boldsymbol{Q}, \boldsymbol{X}), \tag{2}$$

where

$$\boldsymbol{A}^{\text{eff}}(n; \boldsymbol{Q}, \boldsymbol{X}) \equiv i \int dq \psi_n^*(\boldsymbol{q}; \boldsymbol{Q}, \boldsymbol{X}) \frac{\partial \psi_n(\boldsymbol{q}; \boldsymbol{Q}, \boldsymbol{X})}{\partial \boldsymbol{Q}} \tag{3}$$

is the gauge potential introduced by Mead [18]. Since $\boldsymbol{A}^{\text{eff}}(n; \boldsymbol{Q}, \boldsymbol{X})$ is not explicitly time-dependent, it will give rise to an effective Aharonov–Bohm (AB) effect [25] like those in Molecular systems [18]. From this, we perform the following gauge transformation on the eigenfunctions $\varphi_m^n$ of $\hat{H}_n^{\text{eff}}$

$$\varphi_m^n(\boldsymbol{Q}; \boldsymbol{X}) \to \tilde{\varphi}_m^n(\boldsymbol{Q}; \boldsymbol{X}) = e^{-i\Phi} \varphi_m^n(\boldsymbol{Q}; \boldsymbol{X}) \tag{4}$$

where $\Phi(n; \boldsymbol{Q}, \boldsymbol{X}) \equiv \int^{C(\boldsymbol{Q})} \boldsymbol{A}^{\text{eff}}(n; \boldsymbol{Q}, \boldsymbol{X}) \cdot d\boldsymbol{Q}$, and the line integral is evaluated along an arbitrary curve $C(\boldsymbol{Q})$. This transformation removes the gauge potential $\boldsymbol{A}^{\text{eff}}$ from the expression for the Hamiltonian in (2). Therefore, the transformed wave function $\tilde{\varphi}_m^n(\boldsymbol{Q}; \boldsymbol{X})$ satisfies

$$\left[\hat{H}_2(\boldsymbol{P}, \boldsymbol{Q}; \boldsymbol{X}) + E_n(\boldsymbol{Q}, \boldsymbol{X})\right] \tilde{\varphi}_m^n = E_{mn}^{\text{eff}}(\boldsymbol{X}) \tilde{\varphi}_m^n. \tag{5}$$

After these treatments, the eigenvalues $E_{mn}^{\text{eff}}(\boldsymbol{X})$ of $\hat{H}_n^{\text{eff}}$ can be taken as the eigenvalues of $\hat{H}$, and the eigenfunctions of $\hat{H}$ can be defined as the product of $\varphi_m^n$ and the eigenfunctions $\psi_n$ of the fast subsystem:

$$\Psi_{mn}^{\text{tot}}(\boldsymbol{q}, \boldsymbol{Q}; \boldsymbol{X}) \approx \varphi_m^n(\boldsymbol{Q}; \boldsymbol{X}) \psi_n(\boldsymbol{q}; \boldsymbol{Q}, \boldsymbol{X}). \tag{6}$$

Therefore, the Berry phase of the whole system can be calculated straightforwardly by [1]

$$\begin{aligned} \gamma_{mn} &= i \iint dq dQ \oint \psi_n^*(\boldsymbol{q}; \boldsymbol{Q}, \boldsymbol{X}) \varphi_m^{n*}(\boldsymbol{Q}; \boldsymbol{X}) d_{\boldsymbol{X}} [\varphi_m^n(\boldsymbol{Q}; \boldsymbol{X}) \psi_n(\boldsymbol{q}; \boldsymbol{Q}, \boldsymbol{X})] \\ &= \oint \left[\langle A_1(n; \boldsymbol{Q}, \boldsymbol{X}) \rangle_m + A_2(m, n; \boldsymbol{X})\right], \end{aligned} \tag{7}$$

where

$$\begin{aligned} A_1(n; \boldsymbol{Q}, \boldsymbol{X}) &\equiv i \int dq \psi_n^*(\boldsymbol{q}; \boldsymbol{Q}, \boldsymbol{X}) d_{\boldsymbol{X}} \psi_n(\boldsymbol{q}; \boldsymbol{Q}, \boldsymbol{X}) \\ A_2(m, n; \boldsymbol{X}) &\equiv i \int dQ \tilde{\varphi}_m^{n*}(\boldsymbol{Q}; \boldsymbol{X}) d_{\boldsymbol{X}} \tilde{\varphi}_m^n(\boldsymbol{Q}; \boldsymbol{X}) - \langle d_{\boldsymbol{X}} \Phi(n; \boldsymbol{Q}, \boldsymbol{X}) \rangle_m \end{aligned} \tag{8}$$

are the quantum one-form connections of the fast and slow subsystems (hereafter referred to as fast and slow phase one-form), respectively. The brackets $\langle \cdots \rangle_m$ denote an averaging over the eigenvector $\tilde{\varphi}_m : \int dQ \tilde{\varphi}_m^{n*} \cdots \tilde{\varphi}_m^n$, and $d_{\boldsymbol{X}}$ is defined as $d_{\boldsymbol{X}} F(\boldsymbol{X}) = \frac{\partial F(\boldsymbol{X})}{\partial \boldsymbol{X}} \cdot d\boldsymbol{X}$. It means that the Berry phase of the whole system can still be well defined by the slow phase one-form and the average value of the fast phase one-form in the slow subsystem. Note that, the term $A_2^{\text{eff}}(m, n; \boldsymbol{X}) \equiv -\langle d_{\boldsymbol{X}} \Phi(n; \boldsymbol{Q}, \boldsymbol{X}) \rangle_m$ in the slow phase one-form is brought by the effective gauge potential (3) which is induced by the coupling between the slow variables $Q$ and the fast variables. Thus, it can be treated as the result of an effective AB effect mentioned above, and is not found in the usual quantum systems.

## 3. Hannay's angle in BO composite system

According to the quantum–classical correspondence theory, Hannay's angles are classical analogues of the quantum Berry phase [11,24]. Therefore, it is of interest to extend to consider the classical counterpart of the above form of Berry phase. The classical version of Hamilton (1) can be written as

$$H = H_1(\boldsymbol{p}, \boldsymbol{q}; \boldsymbol{X}, \boldsymbol{Q}) + H_2(\boldsymbol{P}, \boldsymbol{Q}; \boldsymbol{X}). \tag{9}$$

Performing the canonical transformation $(\boldsymbol{q}, \boldsymbol{p}) \to (\boldsymbol{\theta}, \boldsymbol{I})$ to the fast subsystem as $Q$ is a constant and averaging over all $\boldsymbol{\theta}$ [24], and then transform $\boldsymbol{P}$ into $\boldsymbol{P}' = \boldsymbol{P} + \boldsymbol{\mathscr{A}}^{\text{eff}}(\boldsymbol{I}; \boldsymbol{Q}, \boldsymbol{X})$ [23], we have

$$H^{\text{eff}} = \mathscr{H}_1(I; \boldsymbol{Q}, \boldsymbol{X}) + H_2(\boldsymbol{P}' - \boldsymbol{\mathscr{A}}^{\text{eff}}, \boldsymbol{Q}; \boldsymbol{X}) + \dot{\boldsymbol{X}} \cdot \left\langle \sum_i p_i \frac{\partial q_i}{\partial \boldsymbol{X}} \right\rangle_\theta , \tag{10}$$

where the first two terms is the effective Hamiltonian under BO approximation and $\mathscr{A}_1(\boldsymbol{I}; \boldsymbol{Q}, \boldsymbol{X}) \equiv \dot{\boldsymbol{X}} \cdot \left\langle \sum_i p_i \frac{\partial q_i}{\partial \boldsymbol{X}} \right\rangle_\theta dt$ is the one-form connection brought by the time-dependent canonical transformation [11]. The vector function $\boldsymbol{\mathscr{A}}^{\text{eff}}(\boldsymbol{I}; \boldsymbol{Q}, \boldsymbol{X}) \equiv \left\langle \sum_i p_i \frac{\partial q_i}{\partial \boldsymbol{Q}} \right\rangle_\theta$ acts as an effective potential. Since the action $I$ can be treated as constant, the effective Hamiltonian only contains the variables of slow subsystem. Taking the canonical transformation $(\boldsymbol{Q}, \boldsymbol{P}) \to (\boldsymbol{\phi}, \boldsymbol{J})$ and averaging over all $\phi$, we get the action dependent Hamiltonian under averaging principles [9,11,24]

$$\begin{aligned} \langle H_{av} \rangle &= \mathscr{H}(\boldsymbol{I}, \boldsymbol{J}; \boldsymbol{X}) - \langle \tilde{\mathscr{A}}_1(\boldsymbol{I}; \boldsymbol{Q}, \boldsymbol{X}) \rangle_\phi - \tilde{\mathscr{A}}_2(\boldsymbol{I}; \boldsymbol{J}, \boldsymbol{X}) \\ &= \mathscr{H}(\boldsymbol{I}, \boldsymbol{J}; \boldsymbol{X}) - \dot{\boldsymbol{X}} \cdot \left[ \left\langle \sum_i p_i \frac{\partial q_i}{\partial \boldsymbol{X}} \right\rangle_{\theta,\phi} + \left\langle \sum_l P_l \frac{\partial Q_l}{\partial \boldsymbol{X}} \right\rangle_\phi + \left\langle \sum_l \mathscr{A}_l^{\text{eff}} \frac{\partial Q_l}{\partial \boldsymbol{X}} \right\rangle_\phi \right], \end{aligned} \tag{11}$$

where

$$\begin{aligned} \mathscr{A}_1(\boldsymbol{I}; \boldsymbol{Q}, \boldsymbol{X}) &= \tilde{\mathscr{A}}_1(\boldsymbol{I}; \boldsymbol{Q}, \boldsymbol{X}) dt = \left\langle \sum_i p_i d_{\boldsymbol{X}} q_i \right\rangle_\theta , \\ \mathscr{A}_2(\boldsymbol{I}, \boldsymbol{J}; \boldsymbol{X}) &\equiv \tilde{\mathscr{A}}_2(\boldsymbol{I}; \boldsymbol{J}, \boldsymbol{X}) dt = \left\langle \sum_l P_l d_{\boldsymbol{X}} Q_l \right\rangle_\phi + \left\langle \sum_l \mathscr{A}_l^{\text{eff}} d_{\boldsymbol{X}} Q_l \right\rangle_\phi \end{aligned} \tag{12}$$

are the classical one-form connections of the fast and slow subsystems (hereafter referred to as fast and slow angle one-form), respectively, and $\langle \cdots \rangle_\phi$ denote averaging over all angles $\boldsymbol{\phi}$. Comparing $\mathscr{A}_2$ with the regular definition of the angle one-form [11], we find that the effective vector potential $\boldsymbol{\mathscr{A}}^{\text{eff}}$ gives rise to an additional term $\mathscr{A}_2^{\text{eff}}(\boldsymbol{I}, \boldsymbol{J}; \boldsymbol{X}) \equiv \left\langle \sum_l \mathscr{A}_l^{\text{eff}} d_{\boldsymbol{X}} Q_l \right\rangle_\phi$ which is analogue to the one brought by the effective AB effect in the quantum BO composite system. Thus, Hannay's angles of the whole system read

$$\Delta\theta_j = -\frac{\partial}{\partial I_j} \oint \left( \langle \mathscr{A}_1 \rangle_\phi + \mathscr{A}_2 \right), \qquad \Delta\phi_k = -\frac{\partial}{\partial J_k} \oint \left( \langle \mathscr{A}_1 \rangle_\phi + \mathscr{A}_2 \right). \tag{13}$$

It can be seen that Hannay's angles (13) are defined by the similar one-form connection with the Berry phase in Eq. (7).

## 4. Semiclassical relation between Berry phase and Hannay's angle

To figure out the relation between the Berry phase and Hannay's angle above, we follow the procedure in Ref. [11]. In semiclassical theory, the eigenfunction $\psi_n$ of the fast subsystem is associated with a classical action by the corrected Bohr–Sommerfeld quantized condition

$$I_j = (n_j + \sigma_j)\hbar, \tag{14}$$

where $\sigma_j$ is Maslov index whose values are unimportant here. Its semiclassical expression [11] reads

$$\psi_n(\boldsymbol{q};\boldsymbol{Q},\boldsymbol{X}) = \sum a_\alpha(\boldsymbol{q},\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X}) e^{iS^{(\alpha)}(\boldsymbol{q},\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X})/\hbar} \tag{15}$$

where $a_\alpha^2 = (d\theta^{(\alpha)}/dq)(1/2\pi)^N$, and $\alpha$ labels different branches of the multivalued classical generating function $S^{(\alpha)}(\boldsymbol{q},\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X})$. Substituting Eq. (15) into Eq. (8) and transforming the variables of integration from $q$ to $\theta$, we have

$$\begin{aligned} A_1(n;\boldsymbol{Q},\boldsymbol{X}) &= \frac{-1}{\hbar}\int dq \frac{1}{(2\pi)^N}\sum_\alpha \frac{d\theta^{(\alpha)}}{dq} d_{\boldsymbol{X}} S^{(\alpha)} \\ &= \frac{1}{\hbar}\left[-\langle d_{\boldsymbol{X}}\mathscr{S}\rangle_\theta + \mathscr{A}_1(\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X})\right], \end{aligned} \tag{16}$$

where $\mathscr{S} \equiv S(\boldsymbol{q}(\boldsymbol{\theta},\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X}),\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X})$ is a single-valued function. Thus, the fast phase one-form is related to the fast angle one-form. By the quantized condition (14), we suppose $E_n(\boldsymbol{Q},\boldsymbol{X}) = \mathscr{H}_1(I;\boldsymbol{Q},\boldsymbol{X})$, and then the effective Hamiltonian in Eq. (5) is just the quantum version of the classical effective Hamiltonian (10) without the additional term $\dot{\boldsymbol{X}}\cdot\left\langle\sum_i p_i \frac{\partial q_i}{\partial \boldsymbol{X}}\right\rangle_\theta$. Therefore, these two effective Hamiltonians can also be connected by a quantized condition $J_k = (m_k + \sigma_k')\hbar$, and the eigenfunction $\tilde{\varphi}_m$ in Eq. (5) has the semiclassical expression:

$$\tilde{\varphi}_m^n(\boldsymbol{Q};\boldsymbol{X}) = \sum_{\alpha'} a'_{\alpha'}(\boldsymbol{Q},\boldsymbol{J};\boldsymbol{X}) e^{iS'^{(\alpha')}(\boldsymbol{Q},\boldsymbol{J};\boldsymbol{X})/\hbar} \tag{17}$$

where $a'^2_{\alpha'} = (d\phi^{(\alpha')}/dQ)(1/(2\pi)^N)$, and $\alpha'$ labels different branches of the multivalued classical generating function $S'^{(\alpha')}(\boldsymbol{Q},\boldsymbol{J};\boldsymbol{X})$. Making a change of coordinates from $Q$ to $\phi$ in the average value $\langle A_1\rangle_m$, we can prove that

$$\begin{aligned} \langle A_1(n;\boldsymbol{Q},\boldsymbol{X})\rangle_m &= \int dQ \frac{1}{(2\pi)^N}\sum_{\alpha'}\frac{d\phi^{(\alpha')}}{dQ} A_1(n;\boldsymbol{Q},\boldsymbol{X}) \\ &= \langle A_1(n;\boldsymbol{Q},\boldsymbol{X})\rangle_\phi. \end{aligned} \tag{18}$$

This means the quantum average value of the fast phase one-form in the effective slow subsystem is equal to its angle average in the classical effective slow subsystem. Furthermore, By substituting Eq. (17) into Eq. (8), we get the relation between the slow phase one-form and the slow angle one-form:

$$\begin{aligned} A_2(m,n;\boldsymbol{X}) &= \frac{-1}{\hbar(2\pi)^N}\int dQ \sum_{\alpha'}\frac{d\phi^{(\alpha')}}{dQ} d_{\boldsymbol{X}} S'^{(\alpha)}(\boldsymbol{Q},J;\boldsymbol{X}) \\ &= \frac{1}{\hbar}\left[-\left\langle d_{\boldsymbol{X}}\mathscr{S}'\right\rangle_\phi + \mathscr{A}_2(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X})\right], \end{aligned} \tag{19}$$

and

$$\begin{aligned} A_2^{\text{eff}}(m,n;\boldsymbol{X}) &= \frac{-1}{(2\pi)^N}\int dQ \sum_{\alpha'}\frac{d\phi^{(\alpha')}}{dQ} d_{\boldsymbol{X}}\Phi^{(C)} \\ &= \frac{1}{\hbar}\left[-\langle d_{\boldsymbol{X}}\mathscr{D}\rangle_\phi + \mathscr{A}_2^{\text{eff}}(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X})\right] \end{aligned} \tag{20}$$

where $\mathscr{S}'$ and $\mathscr{D}$ are single-valued functions like $\mathscr{S}$. Since $\mathscr{S}$, $\mathscr{S}'$ and $\mathscr{D}$ have no contribution to cyclic evolution, this relation, together with (16), (18) and (19) immediately gives out the connection between the Berry phase of Quantum BO system and the Hannay angle of Classical BO system

$$\Delta\theta_j = -\hbar\frac{\partial\gamma_{mn}}{\partial I_j} = -\frac{\partial\gamma_{mn}}{\partial n_j}, \qquad \Delta\phi_k = -\hbar\frac{\partial\gamma_{mn}}{\partial J_k} = -\frac{\partial\gamma_{mn}}{\partial m_k}. \tag{21}$$

Comparing Eq. (21) with Ref. [11], we find that the Berry phase and Hannay's angle in BO composite system possess the same semiclassical relation with those without BO approximation.

## 5. Example

To illustrate our theory, we now consider an example, where a fast particle coupled with a slow one (e.g. electron and nucleus) driven by a vector potential and a harmonic potential. This type of system can be modelled by the coupled generalized harmonic oscillators [11]. Its quantum Hamilton reads

$$\hat{H} = \frac{1}{2}\left[X\hat{q}^2 + Y(\hat{p}\hat{q} + \hat{q}\hat{p}) + Z\hat{p}^2\right] + K_2\hat{p}\hat{Q} + K_1\hat{q}\hat{Q} + \frac{1}{2}\left[X\hat{Q}^2 + Y(\hat{P}\hat{Q} + \hat{Q}\hat{P}) + Z\hat{P}^2\right]. \quad (22)$$

where $K_1, K_2$ are the coupling constant and $\boldsymbol{X} = (X, Y, Z)$ is the slow varying parameters. The Hamiltonian for the light particle is

$$\hat{H}_1 = \frac{1}{2}\left[X\hat{q}^2 + Y(\hat{p}\hat{q} + \hat{q}\hat{p}) + Z\hat{p}^2\right] + K_1\hat{q}\hat{Q} + K_2\hat{p}\hat{Q}, \quad (23)$$

which includes the free Hamiltonian of the fast subsystem and the subsystem–subsystem coupling. Its eigenfunctions $\psi_n(q; Q, \boldsymbol{X})$ and eigenvalues $E_n(Q, \boldsymbol{X})$ are obtained as functions of the eigenvalues $Q$ of $\hat{Q}$

$$\begin{aligned} E_n &= \left(n + \frac{1}{2}\right)\hbar\omega - \frac{(Z^2K_1^2 + \omega^2K_2^2)Q^2}{2Z\omega^2}, \\ \psi_n &= \sqrt{\alpha}\chi_n\left(\alpha\left(q + \frac{K_1ZQ}{\omega^2}\right)\right)\exp\left[-i\left(\frac{Yq^2 + 2K_2Qq}{2Z\hbar} - \frac{K_1YQq}{\omega^2\hbar}\right)\right], \end{aligned} \quad (24)$$

with $\omega = \sqrt{XZ - Y^2}$, $\alpha = \sqrt{\frac{\omega}{Z\hbar}}$ and the normalized Hermite functions $\chi_n(\xi)$. Note that $E_n(Q)$ enters into the Hamiltonian for the heavy particle as a potential, thus the Hamiltonian for the heavy particle takes the form

$$\hat{H}_n^{\mathrm{eff}} = \frac{1}{2}\left\{XQ^2 + Y\left[(\hat{P}' - \hbar A^{\mathrm{eff}})Q + Q(\hat{P}' - \hbar A^{\mathrm{eff}})\right] + Z(\hat{P}' - \hbar A^{\mathrm{eff}})^2\right\} + E_n(Q, \boldsymbol{X}) \quad (25)$$

where $A^{\mathrm{eff}}(n; Q, \boldsymbol{X}) = -\frac{(K_1K_2\omega^2 - K_1^2YZ)Q}{\hbar\omega^4}$ is the effective vector potential. Its eigenvalues and eigenfunctions can be calculated straightforwardly,

$$\begin{aligned} E_{mn}^{\mathrm{eff}}(\boldsymbol{X}) &= \left(m + \frac{1}{2}\right)\hbar\Omega + \left(n + \frac{1}{2}\right)\hbar\omega, \\ \varphi_m(Q; \boldsymbol{X}) &= \tilde{\varphi}(Q; \boldsymbol{X})e^{i\Phi} \\ &= \sqrt{\alpha}\chi_m(\alpha Q)\exp\left[\frac{-i(Y\omega^2 + K_1K_2\omega^2Z - K_1^2YZ^2)Q^2}{2Z\hbar\omega^4}\right], \end{aligned} \quad (26)$$

where $\Omega = [\frac{(Z\omega^2X - Z^2K_1^2 - \omega^2K_2^2)}{\omega^2} - Y^2]^{1/2}$. $E_{mn}^{\mathrm{eff}}(\boldsymbol{X})$ are taken as the eigenvalues of the total Hamiltonian, the corresponding eigenvectors are

$$\Psi_{mn}^{\mathrm{tot}}(q, Q; \boldsymbol{X}) \approx \varphi_m(Q; \boldsymbol{X})\psi_n(q; Q, \boldsymbol{X}). \quad (27)$$

Therefore, the Berry phase of the total system is given by

$$\begin{aligned} \gamma_{mn} &= \oint\iint dqdQ\,\psi_n^*(q; Q, \boldsymbol{X})\varphi_m^*(Q; \boldsymbol{X}) \cdot d_{\boldsymbol{X}}[\varphi_m(Q; \boldsymbol{X})\psi_n(q; Q, \boldsymbol{X})] \\ &= \oint\left\{\left[\frac{(2n+1)Z}{4\omega} + \frac{(2m+1)K_1^2Z^3}{4\omega^4\Omega}\right]d\left(\frac{Y}{Z}\right)\right. \\ &\quad \left. + \frac{(2m+1)Z}{4\Omega}\left[\frac{2K_1K_2}{\omega^2}d\left(\ln\frac{Z}{\omega}\right) + d\left(\frac{Y}{Z}\right)\right]\right\}. \end{aligned} \quad (28)$$

The Hamiltonian of the classical version of this model is

$$H = \frac{1}{2}(Xq^2 + 2Ypq + Zp^2) + K_1 qQ + K_2 pQ + \frac{1}{2}(XQ^2 + 2YPQ + ZP^2), \tag{29}$$

where $\boldsymbol{X} = (X, Y, \ldots)$ is time dependent parameters of the fast subsystem governed by $H_1 = \frac{1}{2}(Xq^2+2Ypq+Zp^2)+K_1qQ+K_2pQ$, and the slow subsystem described by $H_2 = \frac{1}{2}(XQ^2+2YPQ+ZP^2)$. Taking $Q$ as a parameter of $H_1$, the canonical transformation $(q, p) \to (\theta, I)$ can be obtained directly

$$\begin{aligned} q &= \left(\frac{2ZI}{\omega}\right)^{\frac{1}{2}} \cos\theta - \frac{ZK_1Q}{\omega^2}, \\ p &= -\left(\frac{2I}{Z\omega}\right)^{\frac{1}{2}} (Y\cos\theta + \omega\sin\theta) + \left(\frac{YK_1}{\omega^2} - \frac{K_2}{Z}\right) Q, \end{aligned} \tag{30}$$

with $\omega = \sqrt{XZ - Y^2}$. Therefore, the effective Hamiltonian can be written as

$$H^{\text{eff}} = \frac{1}{2}[XQ^2 + 2Y(P' - \mathcal{A}^{\text{eff}})Q + Z(P' - \mathcal{A}^{\text{eff}})^2] + I\omega - \frac{(Z^2K_1^2 + \omega^2K_2^2)Q^2}{2Z\omega^2} + \frac{A_1}{dt}, \tag{31}$$

where

$$\mathcal{A}_1 = \frac{-Y}{2Z}\left[Id\left(\frac{Z}{\omega}\right) + K_1^2Q^2d\left(\frac{Z^2}{\omega^4}\right)\right] + \frac{K_1K_2Q^2}{Z}d\left(\frac{Z}{\omega^2}\right) \tag{32}$$

is the classical one-form connections of the fast subsystem (here we drop the zero contribution terms), and $\mathcal{A}^{\text{eff}}(I; Q, X) = \frac{(K_1K_2\omega^2 - K_1^2YZ)Q}{\omega^4}$ is the effective gauge potential. Since action $I$ is invariant, there are only $Q$ and $P$ left of the variables.

After the canonical transformation $(Q, P) \to (\phi, J)$

$$\begin{aligned} Q &= \left(\frac{2ZJ}{\Omega}\right)^{1/2} \cos\phi, \\ P &= -\left(\frac{2ZJ}{\Omega}\right)^{1/2} \left(\frac{Y}{Z}\cos\phi + \frac{\Omega}{Z}\sin\phi\right) + \mathcal{A}^{\text{eff}}, \\ \Omega &= \left[\frac{(Z\omega^2X - Z^2K_1^2 - \omega^2K_2^2)}{\omega^2} - Y^2\right]^{1/2}, \end{aligned} \tag{33}$$

and substituting Eq. (33) into Eq. (31) as well as averaging over $\phi$, the Hamiltonian of the whole system becomes

$$\langle H_{av}\rangle = I\omega + J\Omega + \langle\tilde{\mathcal{A}}_1\rangle_\phi + \tilde{\mathcal{A}}_2 \tag{34}$$

where

$$\begin{aligned} \langle\mathcal{A}_1\rangle_\phi &= \langle\tilde{\mathcal{A}}_1\rangle_\phi\, dt = -\frac{Y}{2Z}\left[Id\left(\frac{Z}{\omega}\right) + \frac{K_1^2ZJ}{\Omega}d\left(\frac{Z^2}{\omega^4}\right)\right] + \frac{K_1K_2ZJ}{Z\Omega}d\left(\frac{Z}{\omega^2}\right), \\ \mathcal{A}_2 &= \tilde{\mathcal{A}}_2 dt = \left[-\frac{YJ}{2Z} - \frac{K_1^2YZJ}{2\omega^4} + \frac{K_1K_2J}{2\omega^2}\right] d\left(\frac{Z}{\Omega}\right). \end{aligned} \tag{35}$$

Therefore, Hannay's angle can be given by

$$\begin{aligned} \Delta\theta &= -\oint \frac{Z}{2\omega}d\left(\frac{Y}{Z}\right), \\ \Delta\phi &= -\oint \left[\frac{Z}{2\Omega}d\left(\frac{Y}{Z}\right) + \frac{K_1^2Z^3}{2\omega^4\Omega}d\left(\frac{Y}{Z}\right) + \frac{K_1K_2Z}{\omega^2\Omega}d\left(\ln\frac{Z}{\omega}\right)\right]. \end{aligned} \tag{36}$$

Compare with Eq. (28), the relation (21) has been exactly proved: $\Delta\theta = -\partial\gamma_{mn}/\partial n$, $\Delta\phi = -\partial\gamma_{mn}/\partial m$.

## 6. Berry phase and Hannay angle in BO hybrid system

The systems we have studied is either full quantum or full classical. However, sometime the composite system is neither pure quantum nor pure classical and described by a quantum–classical hybrid model under mean field approximation [23,24] (we call it BO hybrid system here) in which the quantum–classical hybrid version of Hamilton (1) can be written as

$$H_{\text{hybrid}} = \langle\psi|\hat{H}_1(\boldsymbol{Q},\boldsymbol{X})|\psi\rangle + H_2(\boldsymbol{P},\boldsymbol{Q};\boldsymbol{X}), \tag{37}$$

where $|\psi\rangle$ is the quantum state of the Hamiltonian operator $\hat{H}_1$. The Hamiltonian $H_2$ Corresponds to the slow classical Hamiltonian in Eq. (9). If we take a mathematical transformation, the quantum subsystem can be reduced to a classical system without loss of physics [23,24]. The hybrid system can be described by a classical Hamiltonian:

$$H = H_1(\boldsymbol{p},\boldsymbol{q};\boldsymbol{Q},\boldsymbol{X}) + H_2(\boldsymbol{P},\boldsymbol{Q};\boldsymbol{X}). \tag{38}$$

Following the procedure in Ref. [24], this Hamiltonian can be transformed into a effective Hamiltonian which only contains the variables of the slow subsystem by a canonical transformation $(\boldsymbol{q},\boldsymbol{p}) \to (\boldsymbol{\theta},\boldsymbol{I})$ and $\boldsymbol{P}' = \boldsymbol{P} + \mathscr{A}^{\text{eff}}_{\text{hyb}}(\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X})$:

$$\begin{aligned} H^{\text{hyb}}_{\text{eff}} &= \mathscr{H}_1(\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X}) + H_2(\boldsymbol{P}' - \mathscr{A}^{\text{eff}}_{\text{hyb}},\boldsymbol{Q};\boldsymbol{X}) - \sum_n I_n\tilde{A}^{\text{hyb}}_1(n;\boldsymbol{Q},\boldsymbol{X}) \\ &= \mathscr{H}_1(\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X}) + H_2(\boldsymbol{P}' - \mathscr{A}^{\text{eff}}_{\text{hyb}},\boldsymbol{Q};\boldsymbol{X}) - \dot{\boldsymbol{X}}\cdot i\sum_n I_n\int dq\psi_n^*\frac{\partial\psi_n}{\partial\boldsymbol{X}} \end{aligned} \tag{39}$$

where

$$\mathscr{H}_1(\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X}) = \sum_n I_n E_n(\boldsymbol{Q},\boldsymbol{X})/\hbar, \tag{40}$$

and the vector function

$$\mathscr{A}^{\text{eff}}_{\text{hyb}}(\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X}) \equiv \left\langle\sum_i p_i\frac{\partial q_i}{\partial\boldsymbol{Q}}\right\rangle_\theta = i\sum_n I_n\int dq\psi_n^*(\boldsymbol{q};\boldsymbol{Q},\boldsymbol{X})\frac{\partial\psi_n(\boldsymbol{q};\boldsymbol{Q},\boldsymbol{X})}{\partial\boldsymbol{Q}} \tag{41}$$

acts as an effective potential. The angle one-form brought by the canonical transformation equals to $\sum_n I_n A^{\text{hyb}}_1(n;\boldsymbol{Q},\boldsymbol{X})$, where

$$A^{\text{hyb}}_1(n;\boldsymbol{Q},\boldsymbol{X}) = \tilde{A}^{\text{hyb}}_1(n;\boldsymbol{Q},\boldsymbol{X})dt = i\int dq\psi_n^*(\boldsymbol{q};\boldsymbol{Q},\boldsymbol{X})d_{\boldsymbol{X}}\psi_n(\boldsymbol{q};\boldsymbol{Q},\boldsymbol{X}) \tag{42}$$

is the quantum one-form connection for the Hamiltonian $\hat{H}_1$ in Eq. (37), and $E_n(\boldsymbol{Q},\boldsymbol{X})$ is the eigenvalue of the $\hat{H}_1$ with corresponding eigenfunction $\psi_n(\boldsymbol{q};\boldsymbol{Q},\boldsymbol{X})$. Taking the canonical transformation $(\boldsymbol{P},\boldsymbol{Q}) \to (\boldsymbol{\phi},\boldsymbol{J})$ and average over all $\phi$, we have the averaged Hamiltonian for the hybrid system

$$\begin{aligned} \langle H^{\text{hyb}}_{av}\rangle &= \mathscr{H}^{\text{hyb}}(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X}) - \left\langle\sum_n I_n\tilde{A}^{\text{hyb}}_1(n;\boldsymbol{Q},\boldsymbol{X})\right\rangle_\phi - \tilde{\mathscr{A}}^{\text{hyb}}_2(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X}) \\ &= \mathscr{H}^{\text{hyb}}(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X}) + \dot{\boldsymbol{X}}\cdot\left[i\left\langle\sum_n I_n\int dq\psi_n^*\frac{\partial\psi_n}{\partial\boldsymbol{X}}\right\rangle_\phi - \left\langle\sum_l[P_l + (\mathscr{A}^{\text{eff}}_{\text{hyb}})_l]\frac{\partial Q_l}{\partial\boldsymbol{X}}\right\rangle_\phi\right], \end{aligned} \tag{43}$$

where

$$\begin{aligned} A^{\text{hyb}}_1(n;\boldsymbol{Q},\boldsymbol{X}) &= i\int dq\psi_n^*(\boldsymbol{q};\boldsymbol{Q},\boldsymbol{X})d_{\boldsymbol{X}}\psi_n(\boldsymbol{q};\boldsymbol{Q},\boldsymbol{X}) \\ \mathscr{A}^{\text{hyb}}_2(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X}) &\equiv \tilde{\mathscr{A}}^{\text{hyb}}_2(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X}) = \left\langle\dot{\boldsymbol{X}}\cdot\sum_l[P_l + (\mathscr{A}^{\text{eff}}_{\text{hyb}})_l]\frac{\partial Q_l}{\partial\boldsymbol{X}}\right\rangle_\phi dt. \end{aligned} \tag{44}$$

are the quantum and classical one-form connections of the hybrid system. Thus, the Berry phase $\gamma_n^{\mathrm{hyb}}$ and Hannay's angle $\Delta\phi_k^{\mathrm{hyb}}$ can be defined as [24]

$$\begin{aligned}\gamma_n^{\mathrm{hyb}} &= \frac{\partial}{\partial I_n}\oint\left(\sum_n I_n\langle A_1^{\mathrm{hyb}}(n;\boldsymbol{Q},\boldsymbol{X})\rangle_\phi + \mathcal{A}_2^{\mathrm{hyb}}(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X})\right),\\ \Delta\phi_m^{\mathrm{hyb}} &= -\frac{\partial}{\partial J_m}\oint\left(\sum_n I_n\langle A_1^{\mathrm{hyb}}(n;\boldsymbol{Q},\boldsymbol{X})\rangle_\phi + \mathcal{A}_2^{\mathrm{hyb}}(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X})\right).\end{aligned} \tag{45}$$

Using Eqs. (16), (18) and (19), we find that

$$\begin{aligned}\gamma_n^{\mathrm{hyb}} &= \oint\langle A_1(n;\boldsymbol{Q},\boldsymbol{X})\rangle_m + \frac{\partial}{\partial\alpha_n}\oint A_2^{\mathrm{hyb}}(m,n;\boldsymbol{X}),\\ \Delta\phi_m^{\mathrm{hyb}} &= \left\langle -\frac{\partial}{\partial J_m}\oint\langle\mathcal{A}_1(\boldsymbol{I};\boldsymbol{Q},\boldsymbol{X})\rangle_\phi\right\rangle - \frac{\partial}{\partial J_m}\oint\mathcal{A}_2^{\mathrm{hyb}}(\boldsymbol{I},\boldsymbol{J};\boldsymbol{X}),\end{aligned} \tag{46}$$

where $A_2^{\mathrm{hyb}}(m,n;\boldsymbol{X}) \equiv \hbar\mathcal{A}_2^{\mathrm{hyb}}(m,n;\boldsymbol{X})$ can be seen as the quantum one-form for the quantum version of $H_{\mathrm{eff}}^{\mathrm{hyb}}$, $\alpha_n \equiv I_n/\hbar = |\langle\psi_n|\psi\rangle|^2$ are the occupation probabilities of different fast eigenfunction and the brackets $\langle\cdots\rangle$ denote an averaging over the quantum state $\psi$ : $\langle\psi|\cdots|\psi\rangle$. It is interesting to note that the contributions of the quantum subsystem to $\gamma_n^{\mathrm{hyb}}$ are just the contributions of the quantum fast system to $\gamma_{mn}$ in Eq. (7) and the partial of $A_2$ with respect to $\alpha_j$ is a result of the mean field treatment of the quantum subsystem [26]. For the same reason, the contribution of the fast quantum subsystem to $\Delta\phi_k$ is written as the mean value of the one in Eq. (13). For $\mathcal{A}_2^{\mathrm{hyb}}(m,n;\boldsymbol{X})$, different with the full quantum phase one-form or classical angle one-form, the part $\left\langle\sum_l(\mathcal{A}_{\mathrm{hyb}}^{\mathrm{eff}})_l d_{\boldsymbol{X}} Q_l\right\rangle_\phi$ have contribution to the fast quantum subsystem as $\partial_{I_n}\left\langle\sum_l(\mathcal{A}_{\mathrm{hyb}}^{\mathrm{eff}})_l d_{\boldsymbol{X}} Q_l\right\rangle_\phi = A_2^{\mathrm{eff}}(m,n;\boldsymbol{X})$.

As an example, For the quantum–classical hybrid version of the Hamiltonian (22), after a straightforward calculation, the Berry phase and Hannay's angle takes the form

$$\begin{aligned}\gamma_n^{\mathrm{hyb}} &= \oint\frac{(2n+1)Z}{4\omega}d\left(\frac{Y}{Z}\right) + \frac{K_1^2Z^3J}{2\hbar\omega^4\Omega}d\left(\frac{Y}{Z}\right) + \frac{K_1K_2ZJ}{\hbar\omega^2\Omega}d\left(\ln\frac{Z}{\omega}\right),\\ \Delta\phi^{\mathrm{hyb}} &= -\oint\left[\frac{Z}{2\Omega}d\left(\frac{Y}{Z}\right) + \frac{K_1^2Z^3}{2\omega^4\Omega}d\left(\frac{Y}{Z}\right) + \frac{K_1K_2Z}{\omega^2\Omega}d\left(\ln\frac{Z}{\omega}\right)\right].\end{aligned} \tag{47}$$

Compare with Eqs. (28) and (36), it satisfies $\Delta\phi^{\mathrm{hyb}} = -\partial\gamma_{mn}/\partial m$.

## 7. Conclusion

To sum up, we have investigated the Berry phase and Hannay's angle in quantum and classical system with BO approximation, respectively. For full quantum BO composite system, the acquired Berry phase is defined by two parts: the slow one-form connection and the average value of fast one-form in the slow subsystem. Interestingly, compared with the system without BO approximation, the Berry phase is found to be modified by the effective gauge potential induced by the coupling between the slow and fast variables. This modification can be treated as the result of an effective AB effect. Therefore, this mechanism can be used to generate artificial gauge potentials for neutral atoms [27]. We will discuss this application in detail in another paper. Furthermore, the classical correspondent Hannay's angles of the Berry phase are analytically derived and the similar effects are found. Using semiclassical theory, we prove that Hannay's angles are related to the Berry phase by the derivative form as the usual one [11]. Two coupled generalized harmonic oscillators has been taken as an example to illustrate our theory. Besides, the Berry phase and Hannay's angle in quantum–classical hybrid BO system is studied to compare with the phase and angle in full quantum and full classical systems.

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