New method for calculating the Berry connection in atom–molecule systems*

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In the mean-field theory of atom–molecule systems, where the bosonic atoms combine to form molecules, there is no usual $U(1)$ symmetry, which presents an apparent hurdle for calculating the Berry connection in these systems. We develop a perturbation expansion method of Hannay's angle suitable for calculating the Berry curvature in the atom–molecule systems. With this Berry curvature, the Berry connection can be computed naturally. We use a three-level atom–molecule system to illustrate our results. In particular, with this method, we compute the curvature for Hannay's angle analytically, and compare it to the Berry curvature obtained with the second-quantized model of the same system. An excellent agreement is found, indicating the validity of our method.

Keywords: Berry phase, nonlinearity, Hannay's angle, mean field theory

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1. Introduction

In 1984, Berry discovered that in the adiabatic evolution of a quantum system, besides the dynamical phase, there exists an additional phase, which depends only on the geometric path in the parameter space[1] accompanying the evolution. This geometric phase, now called the Berry phase, along with the Berry curvature, has found wide applications in condensed matter physics[2,3] and important uses in the implementation of quantum computing gates.[4,5] Recently, the Berry phase has been generalized to nonlinear quantum systems, such as the Bose–Einstein condensates described by the nonlinear Schrödinger equations.[6] This generalization is legitimate because of the well-known fact that a quantum system has a mathematical correspondence to its classical Hamiltonian structure.[7,8]

A recent experimental development in the field of ultracold atoms is to use the Feshbach resonances[9] or the stimulated optical Raman transition[10,11] to combine two atoms into a molecule. This kind of atom–molecule systems can be well described by the mean-field theory and can become nonlinear systems when both the atom and the molecule are bosons and the number of particles in this system is large. As the nonlinearity can cause the breakdown of an adiabatic process, there has been great interest in the adiabatic evolution of the atom–molecule systems.[12−18] Naturally, there are also efforts to define the Berry connection in this type of systems.[19,20] However, even though the Berry connection is defined for these atom–molecule systems in Ref. [20], it is still difficult to compute it because of the nonlinearity, which is not the usual $U(1)$ symmetry. Thus it is not trivial to develop a convenient method suitable for computing the Berry connection in these atom–molecule systems.

In this paper, we propose a perturbation expansion method of Hannay's angle suitable for computing the Berry curvature under the mean-field theory for atom–molecule systems. With this Berry curvature, the Berry connection can be computed in the usual way. We analytically compute the curvature for Hannay's angle by using our proposed method, and numerically calculate the Berry curvature in the second-quantized model. By comparison, our method is verified. Although our approach is general, we choose a three-level Λ system[21,22] as an example to illustrate our results.

The paper is organized as follows. In Section 2, we briefly introduce our theoretical model. In Section 3, we propose our new method. In Section 4, we compute the the curvature for Hannay's angle, and compare them to the results obtained from the second-

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quantized model. The comparison shows an excellent agreement. Lastly, in Section 5, we discuss the results and conclude this paper.

2. Three level atom–molecule system

We consider an atom–molecule Λ system shown in Fig. 1. With the atomic energy level set to zero, the Hamiltonian of this atom–molecule system under the rotating-wave approximation can be written as

$$\begin{aligned}\hat{H}_N &= \hbar\omega_e\hat{\psi}_e^\dagger\hat{\psi}_e + \hbar\omega_g\hat{\psi}_g^\dagger\hat{\psi}_g + \hbar\Omega_{\rm d}\,{\rm e}^{{\rm i}\nu_{\rm d}t}\hat{\psi}_e^\dagger\hat{\psi}_g \\ &\quad +\hbar\frac{\Omega_{\rm p}\,{\rm e}^{-{\rm i}\nu_{\rm p}t}}{\sqrt{N}}\hat{\psi}_e^\dagger\hat{\psi}_a\hat{\psi}_a + {\rm h.c.}, \end{aligned} \tag{1}$$

where $\nu_{\rm d}$ is the frequency of laser pulse $\Omega_{\rm d}$, $\nu_{\rm p}$ is the frequency of laser pulse $\Omega_{\rm p}$, $\hat{\psi}_\alpha$ and $\hat{\psi}_\alpha^\dagger$ are the bosonic annihilation and creation operators for state $|\alpha\rangle$ with α being a, g, or e, and N is the total number of atoms.

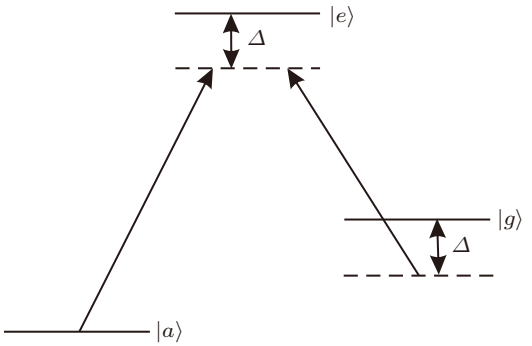


Fig. 1. Schematic diagram of an atom–molecule Λ system, where $|a\rangle$ is the atomic state, $|g\rangle$ is the molecular ground state, $|e\rangle$ is the excited molecular state, $\Omega_{\rm d}$ and $\Omega_{\rm p}$ are the Rabi frequencies of the laser pulses, and Δ is the detuning of the pump field with respect to the transition from $|a\rangle$ to $|e\rangle$.

We note that $\Omega_{\rm p}$ is set to be complex. One way to achieve this is to split the laser pulse $\nu_{\rm p}$ into two beams 1 and 2, then recombine them and focus them on the system. This will lead to a complex $\Omega_{\rm p}$ as $\Omega_{\rm p} = \varepsilon_1 + \varepsilon_2\,{\rm e}^{-{\rm i}\varphi}$, where φ is the optical path difference between the two beams.

We split the Schrödinger picture Hamiltonian into two parts, $\hat{H}_N = \hat{H}_{N0} + \hat{H}_{N1}$, where

$$\hat{H}_{N0} = \hbar\nu_{\rm p}\hat{\psi}_e^\dagger\hat{\psi}_e + \hbar(\nu_{\rm p}-\nu_{\rm d})\hat{\psi}_g^\dagger\hat{\psi}_g, \tag{2}$$

$$\begin{aligned}\hat{H}_{N1} &= \hbar(\omega_e-\nu_{\rm p})\hat{\psi}_e^\dagger\hat{\psi}_e + \hbar(\omega_g-\nu_{\rm p}+\nu_{\rm d})\hat{\psi}_g^\dagger\hat{\psi}_g \\ &\quad +\hbar\Omega_{\rm d}\,{\rm e}^{-{\rm i}\nu_{\rm d}t}\hat{\psi}_e^\dagger\hat{\psi}_g + \hbar\frac{\Omega_{\rm p}\,{\rm e}^{-{\rm i}\nu_{\rm p}t}}{\sqrt{N}}\hat{\psi}_e^\dagger\hat{\psi}_a\hat{\psi}_a \\ &\quad +{\rm h.c.}, \end{aligned} \tag{3}$$

After choosing $\omega_e = \omega_g + \nu_{\rm d}$ and using the the interaction picture Hamiltonian

$$\hat{H}_{N{\rm I}} = {\rm e}^{{\rm i}\hat{H}_{N0}t/\hbar}\hat{H}_{N1}\,{\rm e}^{-{\rm i}\hat{H}_{N0}t/\hbar}, \tag{4}$$

we obtain

$$\begin{aligned}\hat{H}_{N{\rm I}} &= \hbar\Delta\hat{\psi}_e^\dagger\hat{\psi}_e + \hbar\Delta\hat{\psi}_g^\dagger\hat{\psi}_g + \hbar Z\hat{\psi}_e^\dagger\hat{\psi}_g \\ &\quad +\hbar\frac{\varepsilon(X-{\rm i}Y)}{\sqrt{N}}\hat{\psi}_e^\dagger\hat{\psi}_a\hat{\psi}_a + {\rm h.c.}, \end{aligned} \tag{5}$$

where $\Delta = \omega_e - \nu_{\rm p}$, $Z = \Omega_{\rm d}$, and $\varepsilon(X-{\rm i}Y) = \Omega_{\rm p}$. The three parameters, εX, εY, and Z, characterize the influences of the laser beams, here ε is the Rabi frequency strength coefficient.

In the limit $N\to\infty$, this atom–molecule system becomes classical and can be described by the following mean-field Hamiltonian:

$$\begin{aligned}H_{\rm s} &= \lim_{N\to\infty}\frac{\langle\hat{H}\rangle_N}{N} \\ &= \hbar\Delta\psi_e^*\psi_e + \hbar\Delta\psi_g^*\psi_g + \hbar Z\psi_e^*\psi_g \\ &\quad +\hbar\varepsilon(X-{\rm i}Y)\psi_e^*\psi_a\psi_a + {\rm h.c.}, \end{aligned} \tag{6}$$

where ψ_i is the complex amplitude for state $|i\rangle$. The normalization condition is $2|\psi_e|^2 + 2|\psi_g|^2 + |\psi_a|^2 = 1$.

3. New method

The mean-field Berry connection for this atom–molecule system has been introduced in Ref. [20]. The nonlinear terms present an apparent difficulty in computing the Berry connection in this mean-field model. However, we notice that the mean-field Hamiltonian in Eq. (6) has a classical Hamiltonian structure. Namely, we can define three pairs of conjugate variables, $p_e = \sqrt{{\rm i}\hbar}\psi_e^*, q_e = \sqrt{{\rm i}\hbar}\psi_e$, $p_g = \sqrt{{\rm i}\hbar}\psi_g^*, q_g = \sqrt{{\rm i}\hbar}\psi_g$, and $p_a = \sqrt{{\rm i}\hbar}\psi_a^*, q_a = \sqrt{{\rm i}\hbar}\psi_a$, for this Hamiltonian. According to Ref. [6], the mean-field Berry curvature can be regarded as the curvature for Hannay's angle in this classical Hamiltonian. It means that we can obtain the mean-field Berry curvature through computing the curvature for Hannay's angle. Based on the above argument, we develop a perturbation expansion method of Hannay's angle to obtain the mean-field Berry curvature, with which the Berry connection can be computed naturally.

There is a way to justify our method, that is, through the semiclassical relation between the mean-field Berry curvature and the quantum Berry curvature which can be defined and computed with respect to the second-quantized Hamiltonian $\hat{H}_{N1}$. We can prove that[23]

$$\lim_{N\longrightarrow\infty}\Big(\frac{\boldsymbol{B}_N}{N} - \boldsymbol{B}\Big) = 0, \tag{7}$$

where $\boldsymbol{B}$ and $\boldsymbol{B}_N$ are the mean-field and the quantum Berry curvatures, respectively, and subscript N is referred to the number of atoms in the system. To prove this relation, we first notice that the mean-field Hamiltonian is actually the semiclassical limit of $\hat{H}_{N1}$. To see this clearly, we can use the three pairs of conjugate variables p_e, q_e, p_g, q_g, and p_a, q_a and quantize them as

$$[\hat{q}_e, \hat{p}_e] = [\hat{q}_g, \hat{p}_g] = [\hat{q}_a, \hat{p}_a] = \frac{\mathrm{i}\hbar}{N}\,. \tag{8}$$

As can be checked easily, this recovers the second-quantized Hamiltonian $\hat{H}_{N1}$. Since these commutators approach to zero as $N \longrightarrow \infty$, we can see that the mean-field Hamiltonian $H_{\rm s}$ is the semiclassical limit of the quantum Hamiltonian H_{N1}. Since $\boldsymbol{B}$ can also be regarded as the curvature for Hannay's angle,[6] we can then prove the above semiclassical relation by following Berry's argument.[24] Thus, if we can justify the following relation:

$$\lim_{N\longrightarrow\infty}\Big(\frac{\boldsymbol{B}_N}{N} - \boldsymbol{W}\Big) = 0, \tag{9}$$

where $\boldsymbol{W}$ is the curvature for Hannay's angle, we can confirm that our method is suitable for computing the Berry connection in the atom–molecule systems.

4. Example

In this section, we use an example to demonstrate the method introduced in the last section. We first consider the mean-field Hamiltonian

$$\begin{aligned} H_{\rm s} =\ & \hbar\Delta\psi_e^*\psi_e + \hbar\Delta\psi_g^*\psi_g + \hbar Z\psi_e^*\psi_g \\ & + \hbar\varepsilon(X - \mathrm{i}Y)\psi_e^*\psi_a\psi_a + \text{h.c}, \end{aligned} \tag{10}$$

where ε is the Rabi frequency strength coefficient, and the well known complex canonical variables (Bargmann variables) are denoted by $(\psi_e^*, \psi_g^*, \psi_a^*; \psi_e, \psi_g, \psi_a)$. The linear part of this mean-field Hamiltonian should be of the Birkhoff–Gustavson normal form, as introduced in Appendix A. However, the expression of the linear part in terms of $(\psi_e^*, \psi_g^*, \psi_a^*; \psi_e, \psi_g, \psi_a)$ obviously does not satisfy this requirement. We need to find out a linear canonical transformation to transform the linear part into the Birkhoff–Gustavson normal form. Fortunately, such a canonical transformation is not hard to find. New complex canonical variables are

$$z_1^* = \frac{(\psi_e^* + \psi_g^*)}{\sqrt{2}}, \quad z_1 = \frac{(\psi_e + \psi_g)}{\sqrt{2}}, \tag{11}$$

$$z_2^* = \frac{(\psi_e^* - \psi_g^*)}{\sqrt{2}}, \quad z_2 = \frac{(\psi_e - \psi_g)}{\sqrt{2}}. \tag{12}$$

Then we rewrite the Hamiltonian with these new canonical variables

$$\begin{aligned} H_{\rm s} =& \omega_1 z_1^* z_1 + \omega_2 z_2^* z_2 + \frac{\varepsilon(X - \mathrm{i}Y)}{\sqrt{2}}(z_1^* + z_2^* - 2z_1^{*2} z_1 \\ & - 2z_2^{*2} z_2 - 2z_1^* z_1 z_2^* - 2z_1^* z_2^* z_2) + \text{h.c}, \end{aligned} \tag{13}$$

where $\omega_1 = (\Delta + Z)$ and $\omega_2 = (\Delta - Z)$. Now we can obtain the perturbation expansion of the curvature for Hannay's angle according to the method mentioned in Appendix A. Since the Rabi frequency strength coefficient ε is usually small, we only keep the lowest order term of ε. The curvature for Hannay's angle is

$$\begin{aligned} W_{2y}(I, X, Y, Z) =& \varepsilon Y \frac{1}{\omega_2^3}\big[(1 - 2I_1 - 4I_2)^2 - 4I_2^2\big] \\ & - \varepsilon Y \frac{1}{\omega_1^3}\big[(1 - 4I_1 - 2I_2)^2 - 4I_1^2\big], \end{aligned} \tag{14}$$

$$\begin{aligned} W_{2z}(I, X, Y, Z) =& \varepsilon \frac{1}{\omega_2^2}\big[(1 - 2I_1 - 4I_2)^2 - 4I_2^2\big] \\ & + \varepsilon \frac{1}{\omega_1^2}\big[(1 - 4I_1 - 2I_2)^2 - 4I_1^2\big], \end{aligned} \tag{15}$$

where W_{2y} and W_{2z} is y and z components of the curvature for Hannay's angle, respectively.

At the same time, we have a new Hamiltonian that only keeps the lowest order term

$$H_{\rm s}' = \hbar\Delta\psi_e^*\psi_e + \hbar\Delta\psi_g^*\psi_g + \hbar Z\psi_e^*\psi_g + \text{h.c}. \tag{16}$$

Consequently, its eigenequations take the new form

$$\begin{pmatrix} \Delta & Z & 0 \\ Z & \Delta & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \psi_e \\ \psi_g \\ \psi_a \end{pmatrix} = \begin{pmatrix} 2\mu & 0 & 0 \\ 0 & 2\mu & 0 \\ 0 & 0 & \mu \end{pmatrix} \begin{pmatrix} \psi_e \\ \psi_g \\ \psi_a \end{pmatrix}. \tag{17}$$

Without loss of generality, we assume that Δ and Z are positive. For simplicity, we focus on the ground state, which can be obtained easily as

$$\psi_e = \frac{1}{2},\ \ \psi_g = -\frac{1}{2},\ \ \psi_a = 0;\ \ Z > \Delta, \tag{18}$$

$$\psi_e = 0,\ \ \psi_g = 0,\ \ \psi_a = 1;\ \ Z < \Delta. \tag{19}$$

Then adiabatical invariance I can be determined by

$$I_1 = \frac{1}{2},\ \ I_2 = 0;\ \ Z > \Delta, \tag{20}$$

$$I_1 = 0,\ \ I_2 = 0;\ \ Z < \Delta. \tag{21}$$

By inserting Eqs. (45) and (46) into the above curvature for Hannay's angle, respectively, we obtain for $Z > \Delta$,

$$W_{2y}(I, X, Y, Z) = 0, \tag{22}$$

$$W_{2z}(I, X, Y, Z) = 0, \tag{23}$$

and for $Z < \Delta$,

$$W_{2y}(I,X,Y,Z) = \varepsilon^2 Y \frac{1}{\omega_2^3} - \varepsilon^2 Y \frac{1}{\omega_1^3}, \quad (24)$$

$$W_{2z}(I,X,Y,Z) = \varepsilon^2 \frac{1}{\omega_2^2} + \varepsilon^2 \frac{1}{\omega_1^2}. \quad (25)$$

We also computed the Berry curvature with the second-quantized model $\hat{H}_N$. The second-quantized Berry curvature is compared to the curvature for Hannay's angle, as shown in Fig. 2. It is clear from the figure that these two sets of results are in very good agreement with each other. This shows that the perturbation expansion method of Hannay's angle is applicable for the Berry connection in the atom–molecule systems.

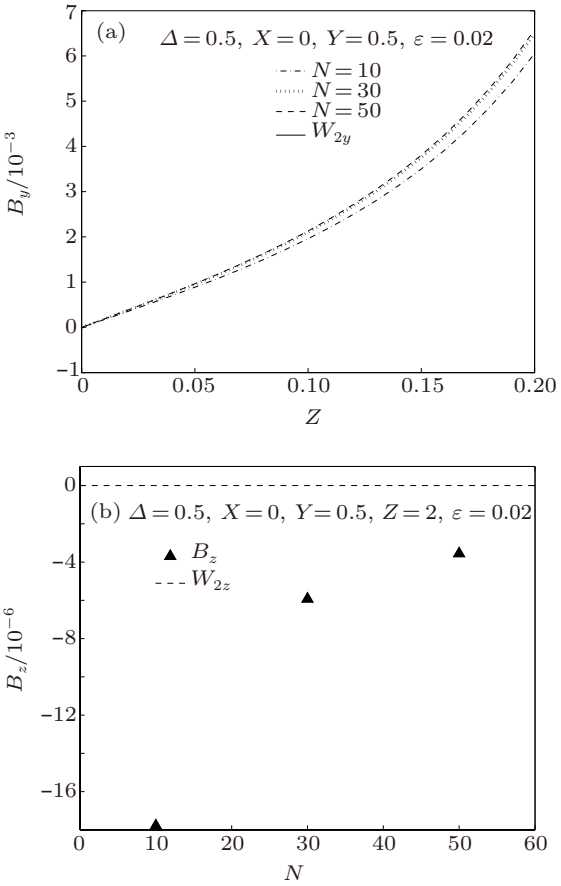


Fig. 2. (a) The y component of the Berry curvature as a function of parameters X, Y, Z, Δ, ε for $Z < \Delta$. The solid line is the curvature for Hannay's angle. (b) The z component of the Berry curvature as a function of parameters X, Y, Z, Δ, ε, N for $Z > \Delta$. The horizontal dashed line represent the curvature for Hannay's angle.

5. Conclusion

In the present work, we have developed a perturbation expansion method of Hannay's angle that is suitable for computing the Berry connection for the atom–molecule systems. We justify this method from various aspects, in particular, the relation between the mean-field Berry curvature and the Berry curvature for the corresponding quantum systems. We have used a three-level Λ atom–molecule system to illustrate our results. The results show the convenience of our method, which can used to compute the Berry connection for the atom–molecule systems. Moreover, our method can also be generalized to the other nonlinear systems.

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Appendix A: Birkhoff–Gustavson normal form and perturbation expansion method of the curvature for Hannay's angle

The classical Hamiltonian is of the Birkhoff–Gustavson normal form if it is a function of z^*z alone, where z^* and z are the complex canonical variables (Bargmann variables).[25] Here we describe the parameter-dependent canonical transformation in the context of the Lie algorithm. Let f be a specified function on the phase space consisting of $2N$ variables $(z_1^*, ..., z_N^*; z_1, ..., z_N)$, we associate a Lie operator X_f via

$$X_f = -\sum_{n=1}^{N} \Big(\frac{\partial f}{\partial z_n^*} \frac{\partial}{\partial z_n} - \frac{\partial f}{\partial z_n} \frac{\partial}{\partial z_n^*} \Big). \quad (A1)$$

The action of X_f on functions g yields the usual Poisson bracket

$$X_f g = -\{f, g\}. \quad (A2)$$

Let $(z^*, z) = (z_1^*, ..., z_N^*; z_1, ..., z_N^*)$ and $(Z^*, Z) = (Z_1^*, ..., Z_N^*; Z_1, ..., Z_N^*)$ be old and new coordinates, respectively. According to Ref. [26], the canonical mapping $Z(z, \theta)$, which depends on an additional parameter ε, has two useful properties. First, there exists a function $\omega(z, z^*, \varepsilon)$ satisfying

$$\frac{\partial Z^*}{\partial \varepsilon} = \frac{\partial \omega}{\partial z}\Big|_{Z^*(z^*,z,\varepsilon), Z(z^*,z,\varepsilon)}, \quad (A3)$$

$$\frac{\partial Z}{\partial \varepsilon} = -\frac{\partial \omega}{\partial z^*}\Big|_{Z^*(z^*,z,\varepsilon), Z(z^*,z,\varepsilon)}, \quad (A4)$$

when $\varepsilon = 0$, $Z(z^*, z, 0) = z$, and $Z^*(z^*, z, 0) = z^*$. Second, the canonical transformation t_ε obtained from the mapping (Z^*, Z) must satisfy

$$\frac{\partial t_\varepsilon}{\partial \varepsilon} = -t_\varepsilon X_\omega. \tag{A5}$$

We assume here that the original Hamiltonian H is defined by any polynomial perturbation of Bargmann variables, i.e.,

$$H = \sum_{n=1}^{N} \omega_n z_n^* z_n + \sum_{\alpha,\beta=0}^{\infty} V_{\alpha,\beta} z^{*\alpha} z^\beta, \tag{A6}$$

where α and β are multi-indices as usual, $\alpha = (\alpha_1, ..., \alpha_N)$, $\beta = (\beta_1, ..., \beta_N)$. Now the problem becomes how to find out the generating function ω to transform the original Hamiltonian into the Birkhoff–Gustavson normal form $t_\varepsilon H = H'(z^* z, \varepsilon)$. Following the derivation of Ref. [27], we have

$$\omega = \sum_{n=0}^{\infty} \varepsilon^n \omega_{n+1}, \tag{A7}$$

the coefficients in the Taylor expansion (with variables (z^*, z)) of ω_n

$$\omega_n = \sum_{\alpha,\beta=0}^{\infty} \omega_{\alpha,\beta}^{(n)} z^{*\alpha} z^\beta \tag{A8}$$

are given by

$$\omega_{\alpha,\beta}^{(n)} = \mathrm{i} \frac{V_{\alpha,\beta}^n}{\langle \omega, (\beta - \alpha) \rangle}, \ \alpha \neq \beta, \tag{A9}$$

where $V_{\alpha,\beta}^n$ represents the coefficient of the Taylor expansion of V_n, and $\langle \omega, (\beta - \alpha) \rangle$ denotes the scalar product between the n-th vector ω and $\beta - \alpha$. Moreover, $V_{\alpha,\beta}^n$ is determined by the following three recurrent equations:

$$t_n H_0 + t_{n-1} V = H_n, \ n = 1, 2, \ldots,$$

$$V = \sum_{\alpha,\beta=0}^{\infty} V_{\alpha,\beta} z^{*\alpha} z^\beta, \tag{A10}$$

$$\frac{1}{n}\{H_0, \omega_n\} + V_n = H_n, \ n = 1, 2, \ldots, \tag{A11}$$

$$V_n = t_{n-1} V + \frac{1}{n} \sum_{j=1}^{n-1} t_{n-j} X_{\omega_j} H_0, \ n = 1, 2, \ldots \tag{A12}$$

To solve these recurrent equations, we must specify the initial conditions $t_0 = I$, $H_0 = \sum_{n=1}^{N} \omega_n z_n^* z_n$, and $V_1 = V$.

In order to apply the argument of Ref. [28], we rewrite the original canonical coordinates (Z^*, Z) in terms of the canonical coordinates $(I, \theta) = (I_1, \ldots, I_N; \theta_1, \ldots, \theta_N)$. That is

$$Z^* = \left. \frac{\partial \omega}{\partial z} \right|_{z^* = \sqrt{I}\, \mathrm{e}^{-\mathrm{i}\theta}, z = \sqrt{I}\, \mathrm{e}^{\mathrm{i}\theta}}, \tag{A13}$$

$$Z = - \left. \frac{\partial \omega}{\partial z^*} \right|_{z^* = \sqrt{I}\, \mathrm{e}^{-\mathrm{i}\theta}, z = \sqrt{I}\, \mathrm{e}^{\mathrm{i}\theta}}, \tag{A14}$$

from which we obtain the perturbation expansion of Hannay's angles

$$\Delta\theta_l = - \frac{\partial}{\partial I_l} \int_{\partial A = C} W \, \mathrm{d}A, \tag{A15}$$

$$W = \frac{1}{(2\pi)^N} \oint \sum_{l=1}^{N} d\theta_l \nabla_{X,Y,Z} Z^*(I, \theta, X, Y, Z) \wedge \nabla_{X,Y,Z} Z(I, \theta, X, Y, Z). \tag{A16}$$

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