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Invariance of the generalised Berry phase under unitary transformations: application to the time-dependent generalised harmonic oscillator

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Abstract. A generalisation of the Berry phase, which reduces to the usual Berry phase in the adiabatic and cyclic case, is derived in a gauge-invariant way. This generalised Berry phase, unlike the Berry phase, is invariant under unitary transformations. A time-dependent generalised harmonic oscillator with a cross term in the Hamiltonian is taken as an example. The Hamiltonian of this system is not in general the energy. An energy, the time derivative of which is the power, is obtained from the equation of motion. When the system is quantised, the generalised Berry phase is zero, and remains invariant under unitary transformations. On the other hand, if the energy is chosen to be the Hamiltonian, a non-zero generalised Berry phase is obtained, but the power is given incorrectly. In this case the total phase, which includes the dynamical phase and the generalised Berry phase, is equal in the adiabatic limit to the correct total phase.

1. Introduction

It has been stated in recent papers [1, 2] that the Berry phase [3] can be removed by a unitary transformation. Nevertheless, it has been shown that in the adiabatic case the total phase, which is the sum of the dynamical phase and the Berry phase, is invariant [4]. Since energy differences are observable through spectroscopic methods and the Berry phase is separately observable through interference experiments [5,6], it seems strange that a unitary transformation should change either. Indeed, one of the requirements of quantum mechanics is that observable effects should be invariant under unitary transformations.

In this paper we show that a generalised Berry phase, called the Yang phase after K-H Yang [7], who first introduced it in a gauge-invariant formulation of quantum mechanics, is invariant under unitary transformations. The Yang phase is defined in general for non-adiabatic and non-cyclic processes, but reduces to the Aharonov and Anandan [8, 9] phase for cyclic, but not adiabatic, processes. For adiabatic and cyclic processes, it reduces to the Berry phase [3]. In time-dependent problems the Hamiltonian is not necessarily the energy operator, and each transforms differently under time-dependent unitary transformations. The energy, defined in a gauge-invariant way [10], is also invariant under unitary transformations. The total phase is therefore

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invariant under unitary transformations, not only for adiabatic processes, but in general for non-adiabatic and non-cyclic processes.

As an application of the general formalism developed here, a time-dependent generalised harmonic oscillator [11, 12] is considered. By generalised we mean that, in addition to the squared terms in the Hamiltonian, there is a cross term involving a product of the coordinate and the canonical momentum. All the terms are multiplied by time-dependent coefficients. In time-dependent problems, the Hamiltonian is not necessarily the energy [13]. From Hamilton's equations the equation of motion may be obtained. The equation of motion can be used to obtain an energy, which has the property that its time derivative is the power supplied to (or removed from) the system due to the time variation of the parameters of the system. This energy can be canonically quantised and the energy operator eigenvalue problem can be solved. When the energy eigenstates are used to calculate the Yang phase for this time-dependent generalised harmonic oscillator the result is zero. Therefore, in the special case of adiabatic and cyclic variation of the parameters, the Berry phase is likewise zero. The total phase is just the dynamical phase. This result is invariant under unitary transformations.

On the other hand, if the energy of the time-dependent generalised harmonic oscillator is chosen to be equal to the Hamiltonian [1, 2, 11, 12], the corresponding Yang phase or Berry phase is non-zero. This result is also invariant under unitary transformations when the different transformation properties of the Hamiltonian and the energy are used. The choice of the energy of the generalised harmonic oscillator to be equal to the Hamiltonian is, however, not consistent with the physical principle that the time derivative of the energy should be the power supplied to (or removed from) the system. The difficulty with [1, 2] is that they assume that the energy is always the Hamiltonian, even if a time-dependent canonical (or unitary) transformation is made.

The total phase is, in general, different for the two choices of energy. In the adiabatic limit, however, the total phases calculated with different energy operators are equal. It is not correct to assume *a priori* that a given Hamiltonian is the energy in a time-dependent problem, without first obtaining the equations of motion. From the equations of motion, the energy can be constructed such that its time derivative is the power supplied to (or removed from) the system. In general the energy is different from the Hamiltonian.

In section 2 a gauge-invariant derivation of the Yang phase is given. For processes that are adiabatic and cyclic the Yang phase reduces to the Berry phase. Both the energy and the Yang phase are separately invariant under unitary transformations as shown in section 3. The time-dependent generalised harmonic oscillator is considered in section 4 from both a classical and quantum mechanical viewpoint. In section 5 the energy of the generalised harmonic oscillator is chosen to be the Hamiltonian, and a non-zero Yang phase is derived. In section 6 the results are compared and discussed. A general analysis of the total phase is given in section 7. Finally, section 8 gives the conclusion.

2. Gauge-invariant generalised Berry phase

In this section a generalised Berry phase, or Yang phase, is derived in a gauge-invariant way [7, 10] for situations which are not necessarily adiabatic or cyclic. When the time-dependent parameters are varying cyclically, the Yang phase reduces to the phase

of Aharonov and Anandan [8, 9], which is generalisation of the Berry phase to the non-adiabatic case. In the adiabatic case the phase of Aharonov and Anandan reduces to the usual Berry phase [3].

2.1. The Yang phase

The Schrödinger equation for a single particle is

$$H\psi = \mathrm{i}\partial\psi/\partial t \tag{2.1}$$

where natural units such that $\hbar = c = 1$ are used. If the particle of mass m and charge q is in an (non-conservative) electromagnetic field characterised by the vector potential $\boldsymbol{A}$ and scalar potential A_0, the Hamiltonian is

$$H = \frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A})^2 + V(\boldsymbol{r}) + qA_0(\boldsymbol{r}, t). \tag{2.2}$$

The (conservative) potential energy $V(\boldsymbol{r})$ in equation (2.2) must be specified, but it can be of gravitational, nuclear or electrostatic origin. The kinetic momentum is $m\boldsymbol{v} = \boldsymbol{p} - q\boldsymbol{A}$, where $\boldsymbol{p}$ is the canonical momentum operator $\boldsymbol{p} = -\mathrm{i}\nabla$. For this time-dependent problem, the Hamiltonian is not in general the energy. The energy operator is defined as the sum of the kinetic and the (conservative) potential energies:

$$\mathscr{E} = \frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A})^2 + V(\boldsymbol{r}). \tag{2.3}$$

When equations (2.2) and (2.3) are compared it can be seen that the energy operator is

$$\mathscr{E} = H - qA_0 \tag{2.4}$$

i.e. the Hamiltonian minus the scalar potential of the external time-dependent (non-conservative) electromagnetic field [13]. The energy eigenvalue problem is [7]

$$\mathscr{E}\psi_n = \varepsilon_n\psi_n \tag{2.5}$$

where ε_n is the energy eigenvalue and ψ_n is the corresponding energy eigenstate. Since the vector potential in equation (2.3) of the external electromagnetic field can depend on the time, the energy operator, eigenstates, and eigenenergies generally depend on the time as a parameter.

The probability amplitude for finding the system in an energy eigenstate at time t is

$$c_n(t) = \langle\psi_n(t)|\psi(t)\rangle \tag{2.6}$$

which is the inner product between the energy eigenstate $\psi_n(t)$ and the solution to the Schrödinger equation $\psi(t)$ at time t. If equation (2.6) is multiplied by ψ_n and summed over n, we obtain

$$\psi = \sum_n c_n\psi_n \tag{2.7}$$

where the completeness of the energy eigenstates is used. When equation (2.7) is substituted into the Schrödinger equation in (2.1) and equations (2.4) and (2.5) are used, the equation of motion obtained for the probability amplitude c_n is

$$\mathrm{i}\dot{c}_n - \varepsilon_n c_n + \dot{\gamma}_n c_n = -\sum_{k\neq n}\langle\psi_n|(\mathrm{i}\partial/\partial t - qA_0)\psi_k\rangle c_k \tag{2.8}$$

where

$$\dot{\gamma}_n(t) = \langle \psi_n | (\mathrm{i}\partial/\partial t - qA_0)\psi_n \rangle \tag{2.9}$$

is the time derivative of the generalised Berry phase or Yang phase $\gamma_n(t)$. From equation (2.8) we can see that the time dependence of the Hamiltonian has three effects. (i) It gives in general a time-dependent energy eigenvalue $\varepsilon_n(t)$. (ii) It induces transitions from the energy eigenstate ψ_k to the state ψ_n. (iii) It gives a Yang phase $\gamma_n(t)$ if the operator which induces transitions has a diagonal element.

We can define the amplitude C_n in the interaction picture by

$$c_n(t) = \exp\left(-\mathrm{i}\int_0^t \mathrm{d}t'\, \varepsilon_n(t') + \mathrm{i}\gamma_n(t)\right) C_n(t) \tag{2.10}$$

where the gauge-invariant Yang phase is

$$\gamma_n(t) = \int_0^t \mathrm{d}t' \langle \psi_n | (\mathrm{i}\partial/\partial t' - qA_0)\psi_n \rangle \tag{2.11}$$

by integration of equation (2.9). When equation (2.10) is substituted into equation (2.8), the result is

$$\mathrm{i}\dot{C}_n = -\sum_{k\neq n} \langle \psi_n | (\mathrm{i}\partial/\partial t - qA_0)\psi_k \rangle \times C_k \exp\left(-\mathrm{i}\int_0^t \mathrm{d}t' (\varepsilon_k(t') - \varepsilon_n(t')) + \mathrm{i}(\gamma_k(t) - \gamma_n(t))\right). \tag{2.12}$$

The right-hand side of equation (2.12) describes transitions from other states. In the non-degenerate case the matrix element in equation (2.12) can be written for $n \neq k$ as

$$\langle \psi_n | (\mathrm{i}\partial/\partial t - qA_0)\psi_k \rangle = -\mathrm{i}(\varepsilon_n - \varepsilon_k)^{-1} \langle \psi_n | P \psi_k \rangle \tag{2.13}$$

where the power operator P is in general defined as

$$P = [\partial/\partial t + \mathrm{i}qA_0, \mathscr{E}]. \tag{2.14}$$

When equation (2.13) is substituted into equation (2.12) for the amplitude in the interaction picture, we obtain

$$\mathrm{i}\dot{C}_n = \sum_{k\neq n} \mathrm{i}(\varepsilon_n - \varepsilon_k)^{-1} \langle \psi_n | P \psi_k \rangle \times C_k \exp\left(-\mathrm{i}\int_0^t \mathrm{d}t' (\varepsilon_k(t') - \varepsilon_n(t')) + \mathrm{i}(\gamma_k(t) - \gamma_n(t))\right). \tag{2.15}$$

It is thus not necessary to restrict our attention to the adiabatic case, where transitions between states are neglected, because the Yang phase occurs in equation (2.10) for the probability amplitude, and differences of the Yang phase $\gamma_k(t) - \gamma_n(t)$ also enter on the right-hand side of equation (2.15). The total phase in equation (2.10) is the sum of the dynamical phase, the Yang phase, and arg $C_n(t)$. In some cases, including the adiabatic case, the phase arg $C_n(t)$ is independent of the time.

If the particle is an electromagnetic field, the power operator in equation (2.14) becomes [7, 10]

$$P = \tfrac{1}{2}q(\boldsymbol{v}\cdot\boldsymbol{E} + \boldsymbol{E}\cdot\boldsymbol{v}) \tag{2.16}$$

where $\boldsymbol{E}$ is the electric field

$$\boldsymbol{E} = -\nabla A_0 - \partial \boldsymbol{A}/\partial t. \tag{2.17}$$

The velocity operator $\boldsymbol{v}$ in equation (2.16) is

$$\boldsymbol{v} = m^{-1}(\boldsymbol{p} - q\boldsymbol{A}) \tag{2.18}$$

where $\boldsymbol{p}$ is the canonical momentum operator. Equation (2.16) is the Hermitian form of the classical expression for the power in this case.

2.2. The Berry phase

The dependence on time in this problem can be due to the time dependence of parameters $\boldsymbol{X}(t) = \{X_1(t), X_2(t), X_3(t), \dots\}$. These parameters can be varied through a cycle, so that after one period T they return to their original values $\boldsymbol{X}(T) = \boldsymbol{X}(0)$. In this case the Yang phase in equation (2.11) becomes

$$\gamma_n(T) = \int_0^T \mathrm{d}t' \langle \psi_n | (\mathrm{i}\partial/\partial t' - qA_0)\psi_n \rangle \tag{2.19}$$

which is the phase obtained by Aharonov and Anandan [8, 9]. They consider, however, the case where the energy operator in equation (2.3) consists only of the kinetic energy. Here the eigenstate in equation (2.19) is an eigenstate of the full energy operator in equation (2.3), which also includes the conservative potential energy $V(\boldsymbol{r})$.

We now specialise to a gauge in which the scalar potential $A_0 = 0$, so that the energy operator in equation (2.4) is equal to the Hamiltonian. Equation (2.19) then becomes

$$\gamma_n(T) = \mathrm{i}\int_0^T \mathrm{d}t' \langle \psi_n | \dot{\psi}_n \rangle \tag{2.20}$$

where the overdot denotes the partial time derivative. Equation (2.20) has the form of the phase obtained by Berry [3], but it applies also in the non-adiabatic case.

If the energy eigenfunction $\psi_n(x, t; \boldsymbol{X}(t))$ in equation (2.20), where x are the particle coordinates, depends on the time through the external parameters $\boldsymbol{X}(t)$ and also has explicit time dependence, equation (2.20) can be written as

$$\gamma_n(T) = \oint \mathrm{d}\boldsymbol{X} \cdot \boldsymbol{a} - \int_0^T \mathrm{d}t\, a_0. \tag{2.21}$$

The 'vector potential' in parameter space is defined as

$$\boldsymbol{a}(\boldsymbol{X}, t) = \langle \psi_n | \mathrm{i}\partial\psi_n/\partial\boldsymbol{X} \rangle \tag{2.22}$$

and the 'scalar potential' in parameter space is

$$a_0(\boldsymbol{X}, t) = -\langle \psi_n | \mathrm{i}\partial_t \psi_n \rangle. \tag{2.23}$$

The ∂_t in equation (2.23) acts only on the *explicit* time dependence of ψ_n. Equation (2.21) can be written in a more compact form as

$$\gamma_n(T) = -\oint_\Gamma \mathrm{d}X^\mu\, a_\mu \tag{2.24}$$

where $X^\mu = (t, -\boldsymbol{X})$ and $a_\mu = (a_0, \boldsymbol{a})$. The path Γ in the space $\{X^\mu\}$ goes from $\{0, \boldsymbol{X}(0)\}$ to $\{T, \boldsymbol{X}(T)\}$, where $\boldsymbol{X}(T) = \boldsymbol{X}(0)$ and the time T of one period is identified with the time zero. The path Γ in equation (2.24) is therefore closed, and the integral is over one cycle. The metric in parameter space used here is $g^{\mu\nu} = \mathrm{diag}(1, -1, -1, \dots, -1)$.

Equations (2.21) and (2.24) are invariant under gauge transformations *in parameter space*

$$a'_\mu = a_\mu + \partial g / \partial X^\mu \tag{2.25}$$

where g is a differentiable function of X^ν satisfying

$$\oint_\Gamma \mathrm{d}X^\mu \, \partial g / \partial X^\mu = 0. \tag{2.26}$$

The gauge transformations in parameter space in equation (2.25) on the connection a_μ are different from gauge transformations on the electromagnetic scalar and vector potentials $A_\mu = (A_0, \boldsymbol{A})$ under which the Schrödinger equation in (2.1) is form invariant. By Stokes' theorem in parameter space the generalised Berry phase in equation (2.24) can be written as the surface integral

$$\gamma_n(T) = -\int_S \mathrm{d}\sigma^{\mu\nu} \mathscr{F}_{\mu\nu} \tag{2.27}$$

where the boundary of the surface S is the closed path Γ in the space $\{X^\mu\}$. The curvature $\mathscr{F}_{\mu\nu}$ is an antisymmetric tensor defined as

$$\mathscr{F}_{\mu\nu} = \partial a_\mu / \partial X^\nu - \partial a_\nu / \partial X^\mu \tag{2.28}$$

which can be written as a 2-form. The curvature in equation (2.28) is invariant under gauge transformations in parameter space in equation (2.25). The formulation given here is similar to that of Ralston [14], except that the a_0 term in equation (2.21) is not related to the dynamical phase, and to that of Bhattacharjee and Sen [15] for the case of Hannay's angle.

The total phase of the probability amplitude in equation (2.10) in the cyclic case is

$$\arg c_n(T) = -\int_0^T \mathrm{d}t' \, \varepsilon_n(t') + \gamma_n(T) + \arg C_n(T). \tag{2.29}$$

The first term on the right-hand side is the dynamical phase, the second term is the Yang phase (or generalised Berry phase), and the third term $\arg C_n(t)$ is the phase which can be obtained from the solution of equation (2.15). If the parameters $\boldsymbol{X}(t)$ vary adiabatically and there is no explicit time dependence in ψ_n, the matrix elements on the right-hand side in equation (2.12) or (2.15) can be neglected. The result is that $C_n(t)$ is a constant, $C_n(0)$. Therefore, equation (2.10) becomes

$$c_n(T) = \exp\left(-\mathrm{i}\int_0^T \mathrm{d}t' \, \varepsilon_n(t') + \mathrm{i}\gamma_n(T)\right) c_n(0) \tag{2.30}$$

where $\gamma_n(T)$ is the usual Berry phase.

In the adiabatic case we can always prepare our system at time $t = 0$ in a given eigenstate $\psi(0) = \psi_k(0)$, where $c_n(0) = \delta_{nk}$. From equation (2.30) the expansion for $\psi(T)$ in equation (2.7) collapses to one term, which is

$$\psi(T) = \exp\left(-\mathrm{i}\int_0^T \mathrm{d}t' \, \varepsilon_k(t') + \gamma_k(T)\right) \psi(0) \tag{2.31}$$

where the energy eigenstate in equation (2.5) is $\psi_k(T) = \psi_k(0)$ because the parameters $\boldsymbol{X}(t)$ are carried through a complete cycle. Equation (2.31) is the adiabatic theorem which includes the Berry phase. The derivation here shows how the Yang phase in the general case reduces to the Berry phase for adiabatic and cyclic variation of the time-dependent parameters.

3. Invariance under unitary transformations

The equations of section 2 are form invariant under unitary transformations, which cannot change the physical content of the theory. Observables, like the energy and the Berry phase, must be separately invariant under unitary transformations. Energy differences can be measured spectroscopically, and the Berry phase can be measured by interference experiments. The idea that a unitary transformation can change the dynamical phase and also the Berry phase is due to using the Hamiltonian, instead of the energy operator, to obtain the energy eigenvalues [11, 12].

Under a unitary transformation U, which can in general depend on the spatial coordinates, momentum operator, and the time, the wavefunction transforms as

$$\psi' = U\psi. \tag{3.1}$$

When U depends only on the spatial coordinates and the time, equation (3.1) is a gauge transformation on the wavefunction. The Schrödinger equation in (2.1) is transformed to

$$H'\psi' = \mathrm{i}\partial\psi'/\partial t \tag{3.2}$$

where the new Hamiltonian H' is related to the old Hamiltonian H by

$$H' = UHU^{\dagger} - \mathrm{i}U(\partial U^{\dagger}/\partial t). \tag{3.3}$$

The Hamiltonian in equation (2.2) can be used in equation (3.3) to obtain

$$H' = \frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A}')^2 + V'(\boldsymbol{r}) + qA'_0. \tag{3.4}$$

The (conservative) potential energy transforms as

$$V' = UVU^{\dagger} \tag{3.5}$$

which reduces to $V' = V$ when U is a gauge transformation that does not depend on the momentum operator. The potentials in equation (3.4) transform as

$$A'_{\mu} = UA_{\mu}U^{\dagger} - (\mathrm{i}/q)U(\partial_{\mu}U^{\dagger}) \tag{3.6}$$

for $\mu = 0, 1, 2, 3$. The derivative is defined as $\partial_{\mu} = \partial/\partial x^{\mu}$, where $x^{\mu} = (x^0, x^1, x^2, x^3)$ and $x^0 = t$. The metric used here is $g^{\mu\nu} = \mathrm{diag}(1, -1, -1, -1)$. Equation (3.6) has the same form as the transformation law for potentials in a non-Abelian gauge field theory, but here the non-commutativity arises because U can depend on the momentum operator. If U depends only on the spatial variables and the time, equation (3.6) reduces to the usual gauge transformation of electromagnetism.

On the other hand, the energy operator in equation (2.3) transforms under unitary transformations as

$$\mathscr{E}' = U\mathscr{E}U^{\dagger} = \frac{1}{2m}(\boldsymbol{p} - q\boldsymbol{A}')^2 + V'(\boldsymbol{r}). \tag{3.7}$$

The energy eigenvalue problem in equation (2.5) transforms to

$$\mathscr{E}'\psi'_n = \varepsilon_n\psi'_n \tag{3.8}$$

where the energy eigenvalue ε_n is invariant. The energy eigenstate transforms as

$$\psi'_n = U\psi_n \tag{3.9}$$

which is the same as equation (3.1) for ψ'. The probability amplitude $c_n(t)$ in equation (2.6) is therefore invariant under the transformations in equations (3.1) and (3.9):

$$c_n(t) = \langle \psi_n(t) | \psi(t) \rangle = \langle \psi'_n(t) | \psi'(t) \rangle \tag{3.10}$$

as long as U is unitary. The equation of motion for C_n in equation (2.12) is invariant under the unitary transformation, because the matrix element

$$\langle \psi_n | (i\partial/\partial t - qA_0)\psi_k \rangle = \langle \psi'_n | (i\partial/\partial t - qA'_0)\psi'_k \rangle \tag{3.11}$$

in equation (2.12) is invariant. From equation (3.11) it follows that the Yang phase in equation (2.11) is also invariant under the unitary transformation

$$\gamma_n(t) = \int_0^t dt' \langle \psi'_n | (i\partial/\partial t' - qA'_0)\psi'_n \rangle \tag{3.12}$$

where A'_0 is given in equation (3.6). Therefore, under a unitary transformation the energy eigenvalue and the Yang phase in equations (3.8) and (3.12), respectively, are separately invariant. This invariance also holds for the adiabatic and cyclic case where the Yang phase reduces to the Berry phase.

4. Generalised time-dependent harmonic oscillator

The generalised time-dependent harmonic oscillator has been previously treated as an example [11, 12]. It has been shown that the Berry phase, defined in the usual way, can be removed by a unitary transformation [1, 2]. The unitary transformation also changes the dynamical phase in the adiabatic case in such a way that the total phase is unchanged [4]. We apply the analysis of section 3 and show that when the energy operator, instead of the Hamiltonian, is used to obtain the energy eigenstates, both the Yang phase and the energy eigenvalues are separately invariant under unitary transformations. This conclusion is still valid in the adiabatic and cyclic case, where the Yang phase reduces to the Berry phase. The Yang phase, and consequently the Berry phase, is zero for this problem.

4.1. Hamiltonian and equations of motion

The classical Hamiltonian for the generalised time-dependent harmonic oscillator is

$$H = \tfrac{1}{2}(a(t)p^2 + 2b(t)px + c(t)x^2) \tag{4.1}$$

where x is a generalised coordinate, p is the canonical momentum conjugate to x, and a, b, c are parameters all of which depend on the time t. From Hamilton's equations, the velocity is

$$\dot{x} = \frac{\partial H}{\partial p} = ap + bx \tag{4.2}$$

and the time derivative of the canonical momentum is

$$\dot{p} = -\frac{\partial H}{\partial x} = -bp - cx. \tag{4.3}$$

When equation (4.2) is solved for p and substituted into equation (4.3), the resulting equation of motion is

$$m\ddot{x} = -\dot{m}\dot{x} - kx \tag{4.4}$$

where $m = a^{-1}$ is the time-dependent mass and the overdot denotes differentiation with respect to time. The spring 'constant' k is a function of time defined as

$$k = c - \frac{b^2}{a} - \frac{d}{dt}\left(\frac{b}{a}\right) > 0 \tag{4.5}$$

and must be positive. The term $-\dot{m}\dot{x}$ on the right-hand side of equation (4.4) is a 'fictitious force' which comes from the time rate of change of the momentum $\mathrm{d}(m\dot{x})/\mathrm{d}t = m\ddot{x} + \dot{m}\dot{x}$. If $\dot{m} < 0$ the term $-\dot{m}\dot{x}$ in equation (4.4) is positive. It is like the thrust for a rocket in which the relative velocity between the mass m and the mass expelled is $\dot{x}$ (i.e. the mass expelled is at rest). If $\dot{m} > 0$ the term $-\dot{m}\dot{x}$ in equation (4.4) is negative. It is like a friction force for a dampled harmonic oscillator. The mass increase of the oscillator could be due, for example, to the absorption of a gas. Equation (4.4) shows that the Hamiltonian of equation (4.1) describes the motion of a harmonic oscillator with a time-dependent mass $m = a^{-1}$ and spring 'constant' k.

4.2. Energy

The energy $\mathscr{E}$ can be constructed, as in the time-independent case, by multiplying the equation of motion in equation (4.4) by the velocity $\dot{x}$. If the energy is chosen to be

$$\mathscr{E} = \tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}kx^2 \tag{4.6}$$

which is the sum of kinetic and potential energies, its time rate of change is

$$\frac{\mathrm{d}\mathscr{E}}{\mathrm{d}t} = \tfrac{1}{2}\dot{m}\dot{x}^2 + \tfrac{1}{2}\dot{k}x^2 + (-\dot{m}\dot{x})\dot{x} = P. \tag{4.7}$$

The right-hand side of equation (4.7) is the total power P which is supplied to (or removed from) the particle. The first term on the right-hand side of equation (4.7) is the power supplied to the oscillator due to the change in the mass at constant velocity, the second term is the power supplied due to the change in the spring 'constant' at constant displacement, and the last term is the power $F_f\dot{x}$ due to the 'fictitious force' $F_f = -\dot{m}\dot{x}$. When the time-dependent parameters a, b and c in the Hamiltonian in equation (4.1) become constants, the power in equation (4.7) is zero and the energy is conserved.

The energy in equation (4.6) can be expressed in terms of the canonical momentum in equation (4.2), which gives

$$\mathscr{E} = \frac{1}{2m}(p + bx/a)^2 + \tfrac{1}{2}kx^2. \tag{4.8}$$

When the system is quantised, this expression is used to obtain the energy operator.

4.3. Lagrangian

The Lagrangian L for the system may be obtained from

$$L = p\dot{x} - H. \tag{4.9}$$

When equations (4.1) for the Hamiltonian and (4.2) for the canonical momentum are used in equation (4.9), the result can be written as

$$L = \tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}kx^2 - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{bx^2}{2a}\right). \tag{4.10}$$

The total time derivative in equation (4.10) does not change the dynamics. A new Lagrangian can be defined as

$$L' = L + \frac{d\Lambda}{dt} \tag{4.11}$$

where

$$\Lambda = bx^2/2a \tag{4.12}$$

which is a gauge (or canonical) transformation. From equations (4.10)-(4.12) the new Lagrangian L' is

$$L' = \tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}kx^2 \tag{4.13}$$

which is the standard Lagrangian for a harmonic oscillator. The Euler-Lagrange equation with the Lagrangian in either equation (4.10) or (4.13) gives the equation of motion in (4.4).

4.4. New Hamiltonian

The new Hamiltonian H' corresponding to the new Lagrangian L' in equation (4.13) can be constructed by the usual procedure. The new canonical momentum p' is

$$p' = \frac{\partial L'}{\partial \dot{x}} = m\dot{x} \tag{4.14}$$

which is the same as the kinetic momentum. The new Hamiltonian H' is

$$H' = p'\dot{x} - L' \tag{4.15}$$

which with equations (4.13) and (4.14) gives

$$H' = \frac{1}{2m}p'^2 + \tfrac{1}{2}kx^2. \tag{4.16}$$

Equation (4.16) is the standard Hamiltonian of a harmonic oscillator with a (time-dependent) mass $m = a^{-1}$ and spring 'constant' k.

The energy is still given by equation (4.6), which in terms of the new canonical momentum p' in equation (4.14) is

$$\mathscr{E} = \frac{1}{2m}p'^2 + \tfrac{1}{2}kx^2. \tag{4.17}$$

Equation (4.17) for the energy is the same as the new Hamiltonian in equation (4.16)

$$H' = \mathscr{E} \tag{4.18}$$

so that we may identify them in this gauge. The new canonical momentum p' in equation (4.14) is related to the old canonical momentum p in equation (4.2) by

$$p' = p + bx/a. \tag{4.19}$$

When equation (4.19) is substituted into equation (4.17), the energy in equation (4.8) is obtained.

4.5. Canonical quantisation

The particle can be canonically quantised by replacing the canonical momentum p by the operator $\hat{p} = -i\partial/\partial x$. Then the energy in equation (4.8) becomes an operator $\mathscr{E}$ which satisfies the eigenvalue problem

$$\mathscr{E}\psi_n = \varepsilon_n \psi_n. \tag{4.20}$$

Equation (4.20) is form invariant under a unitary transformation

$$\mathscr{E}'\psi'_n = \varepsilon_n \psi'_n \tag{4.21}$$

where the eigenvalue ε_n is invariant. The energy eigenfunction transforms as in equation (3.9)

$$\psi'_n = \exp(i\Lambda)\psi_n \tag{4.22}$$

and the energy operator transforms as in equation (3.7)

$$\mathscr{E}' = \exp(i\Lambda)\mathscr{E}\exp(-i\Lambda) \tag{4.23}$$

with $U = \exp(i\Lambda)$. If Λ is given by equation (4.12), then $\mathscr{E}'$ is the same as the standard Hamiltonian for a harmonic oscillator

$$\mathscr{E}' = \frac{1}{2m}p^2 + \tfrac{1}{2}kx^2 \tag{4.24}$$

but here m and k depend on the time as a parameter. The solutions to equation (4.21) are *real* eigenfunctions with eigenenergies

$$\varepsilon_n = (n + \tfrac{1}{2})\omega \tag{4.25}$$

for $n = 0, 1, 2, 3, \ldots$, where the time-dependent angular frequency is $\omega = (k/m)^{1/2}$.

4.6. The Yang phase

The Yang phase can be calculated for the canonically transformed problem, in which the new Hamiltonian in equation (4.16) is equal to the energy in equation (4.17). In this case the scalar potential in equation (2.4) is $qA'_0 = H' - \mathscr{E} = 0$ because of equation (4.18). The Yang phase in equation (3.12) is therefore

$$\gamma_n(t) = \int_0^t dt' \langle \psi'_n | (i\partial/\partial t')\psi'_n \rangle = 0 \tag{4.26}$$

which may be proved as follows. The quantity $\langle \psi'_n | \dot{\psi}'_n \rangle$, where the overdot denotes the partial time derivative, is real because ψ'_n in equation (4.21) is real. On the other hand, since ψ'_n is normalised to unity, we have

$$\langle \psi'_n | \dot{\psi}'_n \rangle = -\langle \psi'_n | \dot{\psi}'_n \rangle^* \tag{4.27}$$

so $\langle \psi'_n | \dot{\psi}'_n \rangle$ is pure imaginary. The only way that a quantity can be both real and imaginary is if it is zero. Therefore, the Yang phase in equation (4.26) is zero. If the parameters are varied adiabatically and cyclically, the Yang phase reduces to the Berry phase, which is also zero. In general, if the scalar potential is zero and the wavefunction is real, the Yang or Berry phase is zero.

If we use the expression in equation (2.11) for the Yang phase, we also get zero, because the Yang phase is invariant under unitary transformations. In this case the scalar potential A_0 in equation (2.4) is the difference between the Hamiltonian H in equation (4.1) and the energy $\mathscr{E}$ in equation (4.8), which gives

$$qA_0 = \frac{1}{2}\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{b}{a}\right)\right]x^2 = \frac{\partial \Lambda}{\partial t} \tag{4.28}$$

where Λ is given by equation (4.12). The quantity $\langle \psi_n | \mathrm{i}\dot{\psi}_n \rangle$ in equation (2.11) can be calculated using the energy eigenfunction in equation (4.22), which gives

$$\langle \psi_n | (\mathrm{i}\partial/\partial t)\psi_n \rangle = \langle \psi_n | (\partial \Lambda/\partial t)\psi_n \rangle + \langle \psi'_n | (\mathrm{i}\partial/\partial t)\psi'_n \rangle. \tag{4.29}$$

The last term on the right-hand side of equation (4.29) is zero because it is both real and imaginary. The Yang phase in equation (2.11) is thus

$$\begin{aligned} \gamma_n(t) &= \int_0^t \mathrm{d}t' (\langle \psi_n | (\partial \Lambda/\partial t')\psi_n \rangle - \langle \psi_n | (\partial \Lambda/\partial t')\psi_n \rangle) \\ &= 0 \end{aligned} \tag{4.30}$$

because of equation (4.28). Therefore, the Yang phase $\gamma_n(t)$ is zero regardless of whether the old or new energy eigenfunctions and scalar potentials are used. The total phase in equation (2.10) is given by the sum of the dynamical phase plus $\arg C_n(t)$. The dynamical phase is also the same for both the old and new eigenfunctions because the energy in equation (4.25) is invariant under a unitary transformation on equation (4.20). The phase $\arg C_n(t)$ is also invariant under unitary transformations because of equation (3.11).

4.7. Probability amplitudes

The equation for the probability amplitudes C_n in the interaction picture in equation (2.10) is given by equation (2.12). The matrix elements in that equation can be evaluated explicitly for the generalised harmonic oscillator, and are

$$\begin{aligned} &\langle \psi_n | (\mathrm{i}\partial/\partial t - qA_0)\psi_k \rangle \\ &\quad = \frac{\mathrm{i}}{4}\frac{\mathrm{d}}{\mathrm{d}t}\ln(m\omega)\{[(n+1)(n+2)]^{1/2}\delta_{n+2,k} - [n(n-1)]^{1/2}\delta_{n-2,k}\}. \end{aligned} \tag{4.31}$$

When $k = n$, the matrix element is zero, which shows that the Yang phase indeed vanishes.

When equation (4.31) is substituted into equation (2.12), we obtain a differential difference equation for the probability amplitudes

$$\begin{aligned} \mathrm{i}\dot{C}_n = \frac{\mathrm{i}}{4}[\mathrm{d}\ln(m\omega)/\mathrm{d}t]\Bigg[&[n(n-1)]^{1/2} C_{n-2} \exp\left(2\mathrm{i}\int_0^t \mathrm{d}t'\omega(t')\right) \\ &- [(n+1)(n+2)]^{1/2} C_{n+2} \exp\left(-2\mathrm{i}\int_0^t \mathrm{d}t'\omega(t')\right)\Bigg] \end{aligned} \tag{4.32}$$

where $C_{-1}, C_{-2}, \ldots$ are all zero. In the case where the parameter $m\omega$ is varying slowly in time, the right-hand side of equation (4.32) can be neglected. Then C_n is a constant, and the probability amplitude $c_n(T)$ varies as in equation (2.30) with $\gamma_n(T) = 0$. In the non-adiabatic case, the probability amplitude for the state n is coupled to the probability amplitudes for the states $n \pm 2$, and so, in general, $\arg C_n(t)$ depends on the time.

5. Energy chosen equal to the Hamiltonian

In this section the energy of the generalised time-dependent harmonic oscillator is chosen to be equal to the Hamiltonian in equation (4.1). With this choice the Yang phase (or generalised Berry phase) is different from zero. The energy eigenvalues are also different from those in equation (4.25). The energy operator and the Hamiltonian are still two distinct operators, which transform under unitary transformations as in equations (3.7) and (3.3), respectively. After a time-dependent unitary transformation, the new energy operator and the new Hamiltonian are no longer equal. The energy eigenvalues and the Yang phase (or generalised Berry phase) nevertheless remain invariant under unitary transformations.

5.1. Hamiltonian and energy

In this approach the generalised time-dependent harmonic oscillator is *assumed* to describe a physical situation such that the Hamiltonian H in equation (4.1) is equal to the energy $\tilde{\mathscr{E}}$ of the particle. Whether or not this assumption is consistent is discussed in subsection 6.1. The Hamiltonian H in equation (4.1) can be expressed in terms of the velocity by using equation (4.2) for p, which gives the energy $\tilde{\mathscr{E}}$,

$$H = \tilde{\mathscr{E}} = \tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}\tilde{k}x^2 \tag{5.1}$$

where the mass is $m = a^{-1}$. The time-dependent spring 'constant' $\tilde{k}$ is

$$\tilde{k} = c - \frac{b^2}{a} > 0 \tag{5.2}$$

which is different from k in equation (4.5), but reduces to it when b/a is independent of the time. The energy $\tilde{\mathscr{E}}$ can be written in terms of the canonical momentum in equation (4.2) as

$$\tilde{\mathscr{E}} = \frac{1}{2m}(p + bx/a)^2 + \tfrac{1}{2}\tilde{k}x^2 \tag{5.3}$$

which is necessary for canonical quantisation.

The energy operator is obtained by replacing the canonical momentum p with the operator $\hat{p} = -\mathrm{i}\partial/\partial x$. The energy eigenvalue problem is thus

$$\tilde{\mathscr{E}}\tilde{\psi}_n = \tilde{\varepsilon}_n\tilde{\psi}_n. \tag{5.4}$$

If we make the unitary transformation of equations (4.22) and (4.23) on $\tilde{\psi}_n$ and $\tilde{\mathscr{E}}$, respectively, we obtain the new eigenvalue problem

$$\tilde{\mathscr{E}}'\tilde{\psi}'_n = \tilde{\varepsilon}_n\tilde{\psi}'_n \tag{5.5}$$

where the energy eigenvalue $\tilde{\varepsilon}_n$ is invariant. The unitarily transformed energy operator is

$$\tilde{\mathscr{E}}' = \frac{p^2}{2m} + \tfrac{1}{2}\tilde{k}x^2 \tag{5.6}$$

from equation (4.23). The solutions to equation (5.5) are *real* eigenfunctions with energies

$$\tilde{\varepsilon}_n = (n + \tfrac{1}{2})\tilde{\omega} \tag{5.7}$$

where $n = 0, 1, 2, \ldots$, and the time-dependent angular frequency is $\tilde{\omega} = (\tilde{k}/m)^{1/2}$.

The Hamiltonian H in equation (4.1) transforms under unitary transformations as in equation (3.3). When the unitary transformation $U=\exp(i\Lambda)$, where Λ is given by equation (4.12), is used in equation (3.3), the new Hamiltonian is

$$H'=\frac{p^2}{2m}+\tfrac{1}{2}\left[\tilde{k}-\frac{d}{dt}\left(\frac{b}{a}\right)\right]x^2 \tag{5.8}$$

which is the same as equation (4.24). Equation (5.8) differs from equation (5.6). After a time-dependent unitary transformation, the new Hamiltonian and the new energy are not equal, even though the old ones were.

5.2. The Yang phase

The Yang phase in equation (2.11) in this case reduces to

$$\tilde{\gamma}_n(t)=\int_0^t dt'\langle\tilde{\psi}_n|(i\partial/\partial t')\tilde{\psi}_n\rangle \tag{5.9}$$

because the scalar potential in equation (2.4) is $q\tilde{A}_0=H-\tilde{\mathscr{E}}=0$ from equation (5.1). The energy eigenfunction $\tilde{\psi}_n$ transforms as in equation (4.22), where Λ is given by equation (4.12). The Yang phase in equation (5.9) can be calculated in a way similar to equations (4.29) and (4.30), and is

$$\tilde{\gamma}_n(t)=\int_0^t dt'\frac{1}{2}\left[\frac{d}{dt'}\left(\frac{b}{a}\right)\right]\langle\tilde{\psi}_n|x^2\tilde{\psi}_n\rangle. \tag{5.10}$$

The expectation value in equation (5.10) is

$$\langle\tilde{\psi}_n|x^2\tilde{\psi}_n\rangle=(m\tilde{\omega})^{-1}(n+\tfrac{1}{2}). \tag{5.11}$$

The Yang phase in equation (5.10) is therefore

$$\tilde{\gamma}_n(t)=(n+\tfrac{1}{2})\int_0^t dt'\frac{(a\dot{b}-b\dot{a})}{2a(ca-b^2)^{1/2}} \tag{5.12}$$

when equations (5.2) and (5.11) are used. Equation (5.12) is the result of Berry [11].

The Yang phase is invariant under a unitary transformation. When equation (3.12) is used to calculate the Yang phase, we obtain

$$\tilde{\gamma}_n(t)=\int_0^t dt'\langle\tilde{\psi}'_n|(-q\tilde{A}'_0)\tilde{\psi}'_n\rangle \tag{5.13}$$

because $\langle\tilde{\psi}'_n|\dot{\tilde{\psi}}'_n\rangle$ is zero from equation (4.27). The new scalar potential $\tilde{A}'_0$ given by equation (3.6) for $\mu=0$ is

$$q\tilde{A}'_0=Uq\tilde{A}_0U^+-iU(\partial U^+/\partial t)=-\frac{\partial\Lambda}{\partial t} \tag{5.14}$$

because $\tilde{A}_0=0$ and $U=\exp(i\Lambda)$. When equation (5.14) is substituted into equation (5.13), the same Yang phase as given in equations (5.10) and (5.12) is obtained because Λ is given by equation (4.12). Therefore, the Yang phase (or generalised Berry phase) is invariant under the unitary transformation. In the adiabatic and cyclic case the Yang phase reduces to the Berry phase, so the Berry phase is also invariant under unitary transformations.

5.3. Probability amplitudes

The equation for the probability amplitudes C_n in the interaction picture in equation (2.10) is given by equation (2.12). The matrix elements in that equation can be evaluated explicitly for the generalised harmonic oscillator in this case, and are

$$\langle\tilde{\psi}_n|(\mathrm{i}\partial/\partial t - q\tilde{A}_0)\tilde{\psi}_k\rangle$$
$$= \left(\frac{\mathrm{i}}{4}\frac{\mathrm{d}}{\mathrm{d}t}\ln(m\tilde{\omega}) + \dot{\tilde{\gamma}}_0\right)[(n+1)(n+2)]^{1/2}\delta_{n+2,k}$$
$$+\left(-\frac{\mathrm{i}}{4}\frac{\mathrm{d}}{\mathrm{d}t}\ln(m\tilde{\omega}) + \dot{\tilde{\gamma}}_0\right)[n(n-1)]^{1/2}\delta_{n-2,k} + 2\dot{\tilde{\gamma}}_0(n+\tfrac{1}{2})\delta_{nk} \tag{5.15}$$

where

$$\dot{\tilde{\gamma}}_0(t) = (4m\tilde{\omega})^{-1}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{b}{a}\right) \tag{5.16}$$

is the time derivative of the Yang phase in equation (5.10) for $n=0$. When $n=k$ equation (5.15) gives the time derivative of the Yang phase in equation (5.12).

When equation (5.15) is substituted into equation (2.12) we obtain a differential difference equation for the probability amplitudes

$$\mathrm{i}\dot{\tilde{C}}_n = \left(\frac{\mathrm{i}}{4}\frac{\mathrm{d}}{\mathrm{d}t}\ln(m\tilde{\omega}) - \dot{\tilde{\gamma}}_0\right)[n(n-1)]^{1/2}\tilde{C}_{n-2}\exp\left(2\mathrm{i}\int_0^t \mathrm{d}t'\,\tilde{\omega}(t') - 4\mathrm{i}\tilde{\gamma}_0(t)\right)$$
$$+\left(-\frac{\mathrm{i}}{4}\frac{\mathrm{d}}{\mathrm{d}t}\ln(m\tilde{\omega}) - \dot{\tilde{\gamma}}_0\right)[(n+1)(n+2)]^{1/2}C_{n+2}$$
$$\times\exp\left(-2\mathrm{i}\int_0^t \mathrm{d}t'\,\tilde{\omega}(t') + 4\mathrm{i}\tilde{\gamma}_0(t)\right) \tag{5.17}$$

where $\tilde{C}_{-1}, \tilde{C}_{-2}, \ldots$ are all zero. In the non-adiabatic case, the probability amplitude for the state n is coupled to the probability amplitudes for the states $n\pm 2$. The solution of equation (5.17) gives $\tilde{C}_n$, which can be used in equation (2.10) for the probability amplitude $\tilde{c}_n(t)$. The total phase of $\tilde{c}_n(t)$ in equation (2.10) is

$$\arg\tilde{c}_n(t) = -\int_0^t \mathrm{d}t'\,\tilde{\varepsilon}_n(t') + \tilde{\gamma}_n(t) + \arg\tilde{C}_n(t). \tag{5.18}$$

In the case where the parameters $m\tilde{\omega}$ and $\tilde{\gamma}_0$ are varying slowly in time, the right-hand side of equation (5.17) can be neglected. The solution of equation (5.17) is then $\tilde{C}_n(t) = \tilde{C}_n(0)$, so $\arg\tilde{C}_n(t)$ in equation (5.18) is independent of the time.

Equation (5.17) reduces to equation (4.32) for C_n when $\tilde{\gamma}_0 = 0$ and $\tilde{\omega}$ is replaced by ω. The solution of equation (5.17) is different from the solution of equation (4.32) because the coupling terms in equation (5.17) are complex, while in equation (4.32) they are imaginary.

6. Comparison

In this section a comparison between the approaches used in sections 4 and 5 is made. First the energies are examined, and then the phases.

6.1. Energy

In the approach of section 5 the energy $\tilde{\mathscr{E}}$ is assumed to be equal to the Hamiltonian H in equation (4.1). If the time derivative of the energy $\tilde{\mathscr{E}}$ in equation (5.1) is taken, we obtain

$$\frac{\mathrm{d}\tilde{\mathscr{E}}}{\mathrm{d}t}=\tfrac{1}{2}\dot{m}\dot{x}^2+\tfrac{1}{2}\dot{k}x^2+(-\dot{m}\dot{x})\dot{x}+\frac{\mathrm{d}}{\mathrm{d}t}[\tfrac{1}{2}(\tilde{k}-k)x^2]. \tag{6.1}$$

The total time derivative on the right-hand side of equation (6.1) can be taken to the left-hand side, which gives

$$\frac{\mathrm{d}}{\mathrm{d}t}[\tilde{\mathscr{E}}+\tfrac{1}{2}(k-\tilde{k})x^2]=P \tag{6.2}$$

where P is the total power in equation (4.7) which is supplied to (or removed from) the particle. Equation (6.2) is the same as equation (4.7) because the quantity in square brackets on the left-hand side is the energy $\mathscr{E}$ in equation (4.6)

$$\mathscr{E}=\tilde{\mathscr{E}}+\tfrac{1}{2}(k-\tilde{k})x^2 \tag{6.3}$$

from equation (5.1). Only the first three terms on the right-hand side of equation (6.1) have a physical interpretation in terms of power. The total time derivative on the right-hand side of equation (6.1) shows that the energy $\tilde{\mathscr{E}}$ used in section 5 is not the total energy. The total energy $\mathscr{E}$ is used in section 4.

6.2. Total phases

In this subsection the total phases of the probability amplitudes in sections 4 and 5 are compared.

The total phase Φ_n of the probability amplitude $c_n(t)$ in equation (2.10) is the sum of the dynamical phase, Yang phase, and arg $C_n(t)$:

$$\Phi_n=\arg c_n(t)=-\int_0^t \mathrm{d}t'\,\varepsilon_n(t')+\gamma_n(t)+\arg C_n(t). \tag{6.4}$$

For the quantised particle in section 4, the Yang phase in equation (4.26) is zero. From equation (4.25) the total phase in equation (6.4) is

$$\Phi_n=-(n+\tfrac{1}{2})\int_0^t \mathrm{d}t'\,\omega(t')+\arg C_n(t). \tag{6.5}$$

In the adiabatic case arg $C_n(t)=\arg C_n(0)$, which can be chosen to be zero as an initial condition.

In section 5 the total phase $\tilde{\Phi}_n$ for the quantised particle whose energy is the Hamiltonian in equation (5.1) is

$$\tilde{\Phi}_n=\arg \tilde{c}_n(t)=-(n+\tfrac{1}{2})\int_0^t \mathrm{d}t'\,\tilde{\omega}(t')+(n+\tfrac{1}{2})\int_0^t \mathrm{d}t'\,\frac{1}{2}\left(\frac{\omega^2}{\tilde{\omega}}\right)z(t')+\arg \tilde{C}_n(t) \tag{6.6}$$

from equation (5.7) for the energy and equation (5.10) for the Yang phase. The time-dependent dimensionless parameter $z(t)$ in equation (6.6) is defined as

$$z(t)=\frac{a}{\omega^2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{b}{a}\right). \tag{6.7}$$

The frequency $\tilde{\omega}$ of this oscillator is

$$\tilde{\omega} = \omega(1+z)^{1/2} \tag{6.8}$$

from equations (5.2) and (4.5). Equation (6.6) can be rewritten as

$$\tilde{\Phi}_n = -(n+\tfrac{1}{2}) \int_0^t \mathrm{d}t'\, \omega(t')[(1+z)^{1/2} - \tfrac{1}{2}z(1+z)^{-1/2}] + \arg \tilde{C}_n(t). \tag{6.9}$$

In equation (6.9) the first term in the square brackets is due to the dynamical phase and the second term is due to the Yang phase.

If the parameter $z \ll 1$, which would be the case for an adiabatic variation in the parameter a/b, the square roots in equation (6.9) can be expanded. The total phase in equation (6.9) then becomes

$$\tilde{\Phi}_n = -(n+\tfrac{1}{2}) \int_0^t \mathrm{d}t'\, \omega(t')(1+\tfrac{1}{8}z^2 - \tfrac{1}{8}z^3 + \dots) + \arg \tilde{C}_n(t). \tag{6.10}$$

In the adiabatic limit the phase $\tilde{\Phi}_n$ is equal to the phase Φ_n in equation (6.5)

$$\tilde{\Phi}_n = \Phi_n \tag{6.11}$$

because the terms of order z^2 and higher are negligible and in the adiabatic limit $\arg \tilde{C}_n(t) = \arg \tilde{C}_n(0) = 0$ and $\arg C_n(t) = \arg C_n(0) = 0$ by an appropriate choice of the initial conditions. If the parameters a, b and c are not varying adiabatically, the total phase Φ_n of section 4 in equation (6.5) is not in general equal to the total phase $\tilde{\Phi}_n$ of section 5 in equation (6.6). The correct total phase is Φ_n because the correct energy operator is used in section 4.

7. General analysis of the total phase

In this section we give a general proof of the equality in the adiabatic case of the total phases calculated using eigenstates of the energy operator and the Hamiltonian.

7.1. Gauge-dependent and gauge-invariant phases

It is usually assumed [1, 2] that the Hamiltonian H is the energy operator for the system, and that it satisfies the eigenvalue problem

$$H\varphi_n = E_n\varphi_n \tag{7.1}$$

where E_n is the eigenvalue and φ_n is the eigenstate. The Hamiltonian H depends on the time, so that the total phase $\tilde{\Phi}_n$ in equation (2.10) is

$$\tilde{\Phi}_n = -\int_0^t \mathrm{d}t' E_n(t') + \int_0^t \mathrm{d}t' \langle \varphi_n | (\mathrm{i}\partial/\partial t')\varphi_n \rangle + \arg \tilde{C}_n(t) \tag{7.2}$$

in the general case which is not necessarily adiabatic or cyclic. This expression for the total phase is not invariant under time-dependent unitary transformations on the eigenstates and operators, because the Hamiltonian transforms by equation (3.3).

The gauge-invariant total phase Φ_n is based on using the energy operator $\mathscr{E}$ in equation (2.3), which satisfies the eigenvalue problem of equation (2.5). The gauge-invariant total phase Φ_n in equation (2.10) is the sum of the dynamical phase, the Yang phase and arg $C_n(t)$

$$\Phi_n = -\int_0^t \mathrm{d}t'\, \varepsilon_n(t') + \int_0^t \mathrm{d}t' \langle \psi_n | (\mathrm{i}\partial/\partial t' - qA_0)\psi_n \rangle + \arg C_n(t). \tag{7.3}$$

In section 3 the terms in this phase are shown to be separately invariant under unitary transformations. The relationship between the gauge-dependent total phase in equation (7.2) and the gauge-invariant one in equation (7.3) can be investigated by perturbation theory.

7.2. Perturbation expansion of the gauge-dependent total phase

The total Hamiltonian H can be written as an unperturbed Hamiltonian H_0 and a perturbation $\mathscr{V}$ as

$$H = H_0 + \mathscr{V}. \tag{7.4}$$

The unperturbed Hamiltonian satisfies the eigenvalue problem

$$H_0 \varphi_n^0 = E_n^0 \varphi_n^0 \tag{7.5}$$

where E_n^0 is the unperturbed eigenvalue and φ_n^0 is the unperturbed eigenstate. If we choose the unperturbed Hamiltonian H_0 to be the energy operator $\mathscr{E}$ in equation (2.3), then by equation (2.4) the perturbation is $\mathscr{V} = qA_0$. By equation (2.5) the unperturbed eigenvalue $E_n^0 = \varepsilon_n$ is the energy eigenvalue, and the unperturbed eigenstate $\varphi_n^0 = \psi_n$ is the energy eigenstate.

The perturbation expansion of the eigenvalue E_n of the Hamiltonian in equation (7.1) in first order is

$$\begin{aligned} E_n &= E_n^0 + \langle \varphi_n^0 | \mathscr{V} \varphi_n^0 \rangle + \dots \\ &= \varepsilon_n + \langle \psi_n | qA_0 \psi_n \rangle + \dots . \end{aligned} \tag{7.6}$$

The perturbation expansion in zero order of the eigenstate for the second term in the total phase of equation (7.2) is

$$\int_0^t \mathrm{d}t' \langle \varphi_n | (\mathrm{i}\partial/\partial t') \varphi_n \rangle = \int_0^t \mathrm{d}t' \langle \varphi_n^0 | (\mathrm{i}\partial/\partial t') \varphi_n^0 \rangle + \dots = \int_0^t \mathrm{d}t' \langle \psi_n | (\mathrm{i}\partial/\partial t') \psi_n \rangle + \dots \tag{7.7}$$

where only the lowest-order term is explicitly shown. Therefore, the perturbation expansion of the phase in equation (7.2) is

$$\begin{aligned} \tilde{\Phi}_n = &-\int_0^t \mathrm{d}t' (\varepsilon_n(t') + \langle \psi_n | qA_0 \psi_n \rangle + \dots) \\ &+ \int_0^t \mathrm{d}t' (\langle \psi_n | (\mathrm{i}\partial/\partial t') \psi_n \rangle + \dots) + (\arg C_n(t) + \dots). \end{aligned} \tag{7.8}$$

The 'energy correction' in equation (7.8) can be associated with the second integral to give the gauge-invariant Yang phase. Equation (7.8) can then be expressed in terms of Φ_n in equation (7.3), so that [4]

$$\tilde{\Phi}_n = \Phi_n + \dots \tag{7.9}$$

where the dots denote higher-order terms in perturbation theory. If the perturbation qA_0 vanishes in the adiabatic limit, then the two phases in equation (7.9) are equal.

In section 6.2 the perturbation qA_0 is given by equation (4.28), which can be written as

$$qA_0 = \frac{\omega^2}{2a} z(t) x^2 \tag{7.10}$$

from equation (6.7) for z. Since the perturbation is proportional to z, which vanishes in the adiabatic limit, we can now understand the equality of phases in equation (6.11). The difference between the two phases in equation (6.10) is of *second* order in the parameter $z(t)$.

8. Conclusion

It has been shown that the energy and the Yang phase (generalised Berry phase) are separately invariant under unitary transformations. The invariance is required because both energy differences and phase differences can be separately observed. Energy differences can be measured spectroscopically, while phase differences can be measured by doing an interference experiment.

As an example, the time-dependent generalised harmonic oscillator is considered, both classically and quantum mechanically. A proper choice of energy in this problem gives a zero Yang phase (or generalised Berry phase) and this result is invariant under unitary transformations. On the other hand, if the energy is chosen to be the original Hamiltonian, with a cross term between the coordinate and the canonical momentum, a non-zero Yang phase or generalised Berry phase is obtained, which is also invariant under unitary transformations. This choice of the energy, however, does not lead to a proper expression for the power.

The Hamiltonian, which governs the time development of the system, is in general different from the energy. The energy has to be defined on physical grounds as the quantity whose time derivative is equal to the power supplied to (or removed from) the system due to the time variation of the external parameters. Just as the quantum mechanical Hamiltonian is obtained from the classical Hamiltonian by the canonical quantisation of the canonical momentum, the energy operator is obtained from the classical energy by canonical quantisation. The energy and the Hamiltonian transform differently under unitary (or canonical) transformations. Under a unitary transformation the energy operator transforms in such a way that the energy eigenvalues are invariant, while the Hamiltonian transforms so that the Schrödinger equation is form invariant. The Yang phase (or generalised Berry phase) is defined here so that it is also invariant under unitary transformations. When the time variation is adiabatic and cyclic, the Yang phase reduces to the Berry phase.

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