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Cyclic states, Berry phases and the Schrödinger operator

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Abstract. An evolution of a quantum mechanical system under a non-adiabatic external perturbation at the time interval $[0, T]$ is considered. It is shown that all the cyclic states of the system, $|\Psi(T)\rangle = e^{i\phi}|\Psi(0)\rangle$, are determined by the eigenvalues ε (quasi-energies) and associated eigenvectors $|\varphi_\varepsilon(t)\rangle$ of the Schrödinger operator $S_q(t) = H(t) - i\hbar(\partial/\partial t)$ acting on some Hilbert space. The set of linearly independent cyclic (quasi-energy) states possess some properties similar to the properties of the stationary states of a closed system. The Berry phases of the states associated with eigenvectors of the discrete spectrum of $S_q(t)$, which are single-valued functions of $\omega = 2\pi/T$, are supplied by the partial derivatives of the corresponding eigenvalues (quasi-energies) with respect to ω . The approach developed is illustrated by several applications to time-dependent systems: the system under an adiabatic perturbation, the forced harmonic oscillator, and the two-level system. Even in the case of a system with a time-independent Hamiltonian there exist non-stationary quasi-energy states that have non-trivial Berry phases ($\beta/2\pi$ not an integer). The criterion of existence of such states is formulated in terms of the energies of the system, and the corresponding expression for the Berry phases is obtained. Some examples of non-stationary cyclic states of closed systems, including the coherent states of a force-free oscillator and the Wannier states of electrons in the parabolic band, are considered.

1. Introduction

This paper is based on the early works [1-5] on the quasi-energy approach to time-dependent systems. It is shown that although the notions of the 'quasi-energy' and the 'quasi-energy state' were originally introduced for systems with T -periodic Hamiltonians, they can be applied to the description of any system considered in the time interval $[0, T]$.

The language of the quasi-energy approach is well suited for the description of cyclic states and Berry phases of non-adiabatic quantum systems. The results of exploiting this language are presented below. They are grouped into sections as follows.

It is shown in section 2 that the problem of determining all possible cyclic states $\Psi_n(T) = \Psi_n(0) e^{i\phi}$ of a quantum system with an arbitrary Hamiltonian $H(t)$ can be reduced to an eigenvalue problem for the Schrödinger operator $S_q(t) = H(t) - i\hbar(\partial/\partial t)$ on some Hilbert space \mathcal{H} . Any cyclic state can be presented in the form

$$|\Psi_\varepsilon(t)\rangle = \exp(-i\varepsilon t/\hbar)|\varphi_\varepsilon(t)\rangle \quad |\varphi_\varepsilon(T)\rangle = |\varphi_\varepsilon(0)\rangle$$

where ε is an eigenvalue and $|\varphi_\varepsilon(t)\rangle$ is the corresponding eigenvector of $S_q(t)$. The

expression for the evolution operator of the system in terms of the cyclic states is obtained for the case where $\{|\varphi_e(t)\rangle\}$ is complete in \mathcal{H} .

The connection is established in section 3 between the cyclic states of a system considered in the time interval $[0, T]$ and the quasi-energy states of a T -periodic system, closely related to the former. It is shown that the quasi-energy approach [1-5] can be applied to the description of the system in the time interval $[0, T]$, even if $H(T) \neq H(0)$.

In section 4 Berry phases and dynamical phases of the system are expressed in terms of the inner product of the Hilbert space \mathcal{H} . It is shown that the Berry phases of the states associated with eigenvectors of the discrete spectrum of $S(t)$, which are single-valued functions of $\omega = 2\pi/T$ in some interval, are supplied by the partial derivatives of the corresponding eigenvalues (quasi-energies) with respect to ω . It is shown that some linear combinations of the quasi-energy states become cyclic for certain isolated values of the frequency ω of the external perturbation (multiphoton resonance). The Berry phases for this case are also considered.

An expression for the quasi-energy of the quasi-energy state corresponding to a cyclic adiabatic evolution of a quantum system is obtained in section 5. In the adiabatic approximation $\varepsilon(\omega)$ is a linear function of ω with a gradient $-\beta\hbar/2\pi$, where β is the corresponding Berry phase.

In section 6 the two-level system is considered. It is shown that in the rotating-wave approximation the shift (with respect to the unperturbed value) of a quasi-energy is proportional to the corresponding Berry phase. Since the quasi-energies determine the spectral characteristics of the system, this shift can be measured. It is shown that in the case of the multiphoton resonance all states of the system are cyclic and the corresponding Berry phases are calculated.

It is shown in section 7 that the complete set of quasi-energy states of a forced harmonic oscillator can be obtained from the set of stationary states of a force-free oscillator by means of the unitary transformation which belongs to a representation of the Heisenberg-Weyl group W_1 . The set of all cyclic generalized coherent states of the oscillator coincides with the set of the quasi-energy states, if $\omega_0 \neq l\omega$ (ω is the frequency of the external perturbation, ω_0 is the resonance frequency of the oscillator). The Berry phases of bound cyclic states are calculated. The behaviour of the oscillator under a perturbation applied at $0 \leq t \leq T$ is considered.

In section 8 the system with a time-independent Hamiltonian is considered. The criterion of existence of states with non-trivial Berry phases ($\beta/2\pi$ is non-integer) is formulated in terms of the energies of the system, and the corresponding expression for the Berry phases is obtained. Some examples of non-stationary cyclic states, including the coherent states of a force-free oscillator and the Wannier states of electrons in the parabolic band, are considered.

2. Cyclic states and the Schrödinger operator

Let us consider the evolution of a quantum system in the time interval $[0, T]$. Let $H(t)$ be the Hamiltonian of the system acting on a Hilbert space \mathcal{R} . States of the system are described by vector-valued functions $|\Psi\rangle: [0, T] \rightarrow \mathcal{R}$. The set of functions $L^2([0, T]; \mathcal{R})$, which satisfy the condition

$$\int_0^T \langle g(t) | g(t) \rangle dt < \infty$$

is a Hilbert space with the inner product

$$\langle\langle g_1(t) | g_2(t) \rangle\rangle_t = \frac{1}{T} \int_0^T \langle g_1(t) | g_2(t) \rangle dt. \quad (2.1)$$

The Schrödinger equation may be written in the form

$$S(t)|\Psi(t)\rangle = 0 \quad (2.2)$$

where

$$S(t) = H(t) - i\hbar \frac{\partial}{\partial t}$$

is the Schrödinger operator [3] acting on $L^2([0, T]; \mathcal{R})$.

Let us consider the case where the system returns to its original state at the moment T . The wavevector $|\Psi(t)\rangle$, corresponding to such a cyclic evolution, satisfies the condition

$$|\Psi(T)\rangle = e^{i\phi} |\Psi(0)\rangle \quad (2.3)$$

where ϕ is some real number. It was first pointed out by Zel'dovich [1] that a function satisfying the condition (2.3) may be presented in the form

$$|\Psi_\varepsilon(t)\rangle = \exp(-i\varepsilon t/\hbar) |\varphi_\varepsilon(t)\rangle \quad (2.4)$$

where

$$\varepsilon = -\phi\hbar/T \quad (2.5)$$

and

$$|\varphi_\varepsilon(T)\rangle = |\varphi_\varepsilon(0)\rangle. \quad (2.6)$$

Although the form (2.4) was stated for the systems with T -periodic Hamiltonians it is easy to see that a wavevector of an arbitrary system at the time interval $[0, T]$ may be presented in the form (2.4) provided this vector satisfies (2.3). Note that

$$\langle\Psi_\varepsilon(t) | \Psi_\varepsilon(t)\rangle = \langle\varphi_\varepsilon(t) | \varphi_\varepsilon(t)\rangle. \quad (2.7)$$

It follows from (2.4), (2.6) and (2.7) that $|\varphi_\varepsilon(t)\rangle \in \mathcal{H}$, where \mathcal{H} is the subspace of $L^2([0, T]; \mathcal{R})$ formed by the functions $|g\rangle: [0, T] \rightarrow \mathcal{R}$ such that $|g(T)\rangle = |g(0)\rangle$.

The substitution of (2.4) into (2.2) gives the equation for $|\varphi_\varepsilon(t)\rangle$,

$$S(t)|\varphi_\varepsilon(t)\rangle = \varepsilon|\varphi_\varepsilon(t)\rangle. \quad (2.8)$$

The equation (2.8) with the boundary condition (2.6) is an eigenvalue problem for the Schrödinger operator $S(t)$. Therefore, $|\varphi_\varepsilon(t)\rangle$ is an eigenvector of $S(t)$ with the real eigenvalue ε . Note that $S(t)$ is not Hermitian on $L^2([0, T]; \mathcal{R})$, consequently, it may have complex eigenvalues. Since all $|\varphi_\varepsilon(t)\rangle \in \mathcal{H}$ this complication can be removed by restricting $S(t)$ to the space \mathcal{H} . This restriction, denoted by $S_q(t)$, is a Hermitian operator and its eigenvalues are real.

Thus, it is shown that the problem of finding all cyclic solutions of the Schrödinger equation, which belong to $L^2([0, T]; \mathcal{R})$, may be reduced to the eigenvalue problem

$$S_q(t)|\varphi_\varepsilon(t)\rangle = \varepsilon|\varphi_\varepsilon(t)\rangle. \quad (2.9)$$

on \mathcal{H} . All the possible values of the phase ϕ are determined by the eigenvalue ε by means of (2.5). The corresponding cyclic wavevectors are given by (2.4). The correspondence between the solutions of the eigenvalue problem (2.9) and cyclic states is not, however, one-to-one. Indeed, if $(\varepsilon, |\varphi_\varepsilon(t)\rangle)$ is a solution of the eigenvalue problem (2.9), then for any integer p

$$\varepsilon' = \varepsilon + p\hbar\omega \quad |\varphi_{\varepsilon'}(t)\rangle = e^{ip\omega t} |\varphi_\varepsilon(t)\rangle \quad (2.10)$$

is also a solution. The corresponding cyclic solutions of the Schrödinger equation are, however, identical:

$$|\Psi_{\varepsilon'}(t)\rangle = \exp\left(-\frac{i}{\hbar} \varepsilon' t\right) |\varphi_{\varepsilon'}(t)\rangle = \exp\left(-\frac{i}{\hbar} \varepsilon t\right) |\varphi_\varepsilon(t)\rangle = |\Psi_\varepsilon(t)\rangle.$$

In other words, all the solutions $\{(\varepsilon', |\varphi_{\varepsilon'}(t)\rangle)\}$ given by (2.10) are physically equivalent and correspond to the state $|\Psi_\varepsilon(t)\rangle$. Any solution from the equivalence class $\{(\varepsilon', |\varphi_{\varepsilon'}(t)\rangle)\}$ may be chosen to represent the state $|\Psi_\varepsilon(t)\rangle$. If the dimension of the eigensubspace belonging to the eigenvalue ε is more than one, a set of the linear independent eigenvectors $\{|\varphi_{m\varepsilon}\rangle\}$ will be chosen in such a way that

$$\langle\langle \varphi_{k\varepsilon} | \varphi_{m\varepsilon} \rangle\rangle_t = \delta_{km}.$$

The number of equivalence classes corresponding to the eigenvalue ε is equal to the dimension of the eigensubspace associated with ε .

The eigenvectors of $S_q(t)$ will be labelled by two indexes j and p . The index j will label different equivalence classes of eigenvectors, the index p will label eigenvectors inside each class in such a way that

$$|\varphi_{\varepsilon_j p}(t)\rangle = e^{ip\omega t} |\varphi_{\varepsilon_j}(t)\rangle \quad (2.11)$$

where $|\varphi_{\varepsilon_j}(t)\rangle$ is one of the eigenvectors of the class number j and ε_j is the eigenvalue associated with this eigenvector. The cyclic state corresponding to the class number j will be denoted by $|\Psi_{\varepsilon_j}(t)\rangle$. Since $S_q(t)$ is Hermitian in \mathcal{H}

$$\langle\langle \varphi_{\varepsilon_j p'} | \varphi_{\varepsilon_j p} \rangle\rangle_t = \delta_{jj'} \delta_{pp'}. \quad (2.12)$$

Substituting (2.11) into (2.12) and using the definition (2.1) we obtain

$$\langle \varphi_{\varepsilon_j p'}(t) | \varphi_{\varepsilon_j p}(t) \rangle = \delta_{jj'} \quad (2.13)$$

and

$$\langle \Psi_{\varepsilon_j'}(t) | \Psi_{\varepsilon_j}(t) \rangle = \delta_{jj'}$$

for any $t \in [0, T]$. The equation (2.13) together with (2.11) gives

$$\langle \varphi_{\varepsilon_j p'}(t) | \varphi_{\varepsilon_j p}(t) \rangle = \delta_{jj'} e^{i(p-p')\omega t}.$$

Thus it is shown that periodic functions which belong to different equivalence classes are orthogonal in the inner product of \mathcal{R} while functions which belong to the same equivalence class are not.

Consider the case where the set $\{|\varphi_{\varepsilon_j p}\rangle\}$ is complete in \mathcal{H} . Then the set $\{|\Psi_\varepsilon(t)\rangle\}$ is complete in \mathcal{R} at any $t \in [0, T]$. In order to prove this we proceed as follows. Let us take $|h\rangle \in \mathcal{R}$. The vector function $|h(t)\rangle \equiv |h\rangle$ belongs to \mathcal{H} , therefore

$$|h\rangle = \sum_{jp} |\varphi_{\varepsilon_j p}(t)\rangle \frac{1}{T} \int_0^T \langle \varphi_{\varepsilon_j p}(t') | h \rangle dt'. \quad (2.14)$$

Substitution of (2.11) into (2.14) and integration gives

$$|h\rangle = \sum_j |\varphi_{\varepsilon_j}(t)\rangle \langle \varphi_{\varepsilon_j}(t) | h \rangle.$$

This relation is equivalent to

$$|h\rangle = \sum_j |\Psi_{\varepsilon_j}(t)\rangle \langle \Psi_{\varepsilon_j}(t) | h \rangle.$$

Therefore sets $\{|\varphi_{\varepsilon_j}(t)\rangle\}$ and $\{|\Psi_{\varepsilon_j}(t)\rangle\}$ are complete in \mathcal{R} . Note that in the set $\{|\varphi_{\varepsilon_j}(t)\rangle\}$ only one representative of each equivalence class of solutions of (2.9) is included. Let us take the value of a solution of the Schrödinger equation, $|\Psi(t)\rangle$, at the moment t in place of $|h\rangle$:

$$|\Psi(t)\rangle = \sum_j |\Psi_{\varepsilon_j}(t)\rangle \langle \Psi_{\varepsilon_j}(t) | \Psi(t) \rangle. \tag{2.15}$$

The inner product of any two exact solutions of the Schrödinger equation does not depend on time [1]. Therefore the expansion coefficients in (2.15) do not depend on time, namely

$$\langle \Psi_{\varepsilon_j}(t) | \Psi(t) \rangle = \langle \Psi_{\varepsilon_j}(t_0) | \Psi(t_0) \rangle = a_j$$

for any $t_0 \in [0, T]$. The expansion (2.15) may also be written in the form

$$|\Psi(t)\rangle = \sum_j b_j \exp\left(-\frac{i}{\hbar} \varepsilon_j(t - t_0)\right) |\varphi_{\varepsilon_j}(t)\rangle \quad b_j = \langle \varphi_{\varepsilon_j}(t_0) | \Psi(t_0) \rangle. \tag{2.16}$$

The following expressions for the evolution operator of the system can be easily obtained from (2.15) and (2.16),

$$U(t, t_0) = \sum_j |\Psi_{\varepsilon_j}(t)\rangle \langle \Psi_{\varepsilon_j}(t_0) | = \sum_j \exp\left(-\frac{i}{\hbar} \varepsilon_j(t - t_0)\right) |\varphi_{\varepsilon_j}(t)\rangle \langle \varphi_{\varepsilon_j}(t_0) |.$$

Note that each cyclic state, taken at $t = 0$, is an eigenvector of the evolution operator $U(T, 0)$,

$$U(T, 0) |\Psi_{\varepsilon}(0)\rangle = \rho_{\varepsilon} |\Psi_{\varepsilon}(0)\rangle$$

where $\rho_{\varepsilon} = \exp(-i\varepsilon T/\hbar)$ is the corresponding eigenvalue. Any eigenvector of $U(T, 0)$ corresponds to some cyclic state of the system. In the case $H(T) = H(0)$ the states $|\Psi_{\varepsilon}(0)\rangle = |\varphi_{\varepsilon}(0)\rangle$ are identical with the ‘cyclic initial states’ discussed by Moore and Stedman [10] and by Moore [7, 9].

In the particular case of a time-independent Hamiltonian each eigenvector $|\varphi_{E_j}\rangle$ of the Hamiltonian is an eigenvector of $S_a(t)$. The equivalence classes of solutions of (2.9) may be generated by the solutions $(E_j, |\varphi_{E_j}\rangle)$, where $|\varphi_{E_j}\rangle$ is an eigenvector of Hamiltonian and E_j is the associated eigenvalue. If $|\varphi_{E_j}\rangle$ is chosen as a representative of the class j for each j then the expansion (2.16) reads

$$|\Psi(t)\rangle = \sum_j b_j \exp\left(-\frac{i}{\hbar} E_j(t - t_0)\right) |\varphi_{E_j}\rangle \quad b_j = \langle \varphi_{E_j} | \Psi(t_0) \rangle.$$

This is the familiar expansion of a state of a closed system in stationary states of discrete spectrum. Thus the solutions of the form (2.4), which describe the stable behaviour of the system under a non-adiabatic perturbation, provide a natural extension of the notion of stationary states of a closed system.

For finite-dimensional systems the existence of the complete set of cyclic states is provided by Floquet theory [14], because in this case the Schrödinger equation in a finite interval $[0, T]$ is equivalent to a system of ordinary linear differential equations with piecewise-continuous T -periodic coefficients (see the next section).

For infinite-dimensional systems one cannot always expect solutions of (2.9) to belong to \mathcal{H} . In a number of cases the solutions of interest do not belong to \mathcal{H} , and it is useful to consider, instead of the Hilbert space \mathcal{H} , the rigged Hilbert space $\mathcal{H} \supset \mathcal{H}$. The latter case takes place when S_q has a continuous spectrum.

3. Cyclic states and quasi-energy states

In this section the connection is established between the cyclic states of a system considered in the time interval $[0, T]$ (system I) and the quasi-energy states of a T -periodic system (system II), closely related to the first one.

The Hamiltonian of the system II, $H_{II}(t)$, is defined as follows: $H_{II}(t) = H_I(t)$ for $t \in [0, T)$, $H_{II}(t+T) = H_{II}(t)$ for $t \in (-\infty, \infty)$, where $H_I(t) = H(t)$ is the Hamiltonian of the system I. The Schrödinger equation for the system II has piecewise-continuous T -periodic coefficients.

Consider the problem of finding quasiperiodic solutions

$$|\Psi_\varepsilon(t)\rangle = \exp\left(-\frac{i}{\hbar} \varepsilon t\right) |\varphi_\varepsilon(t)\rangle$$

$$|\varphi_\varepsilon(t+T)\rangle = |\varphi_\varepsilon(t)\rangle$$

of the Schrödinger equation with the Hamiltonian $H_{II}(t+T) = H_{II}(t)$ for all real t . In the case of T -periodic systems the real parameter ε , which determines spectral characteristics of the system, is called the quasi-energy [1, 5] and the state $|\Psi_\varepsilon(t)\rangle$ is called the quasi-energy state.

It is clear that any quasi-energy state $|\Psi_\varepsilon(t)\rangle$ of the system II satisfies the condition (2.3). Therefore, it coincides with one of the cyclic states of the system I in the interval $[0, T]$. On the other hand, if the vector $|\varphi_\varepsilon(t)\rangle$, corresponding to a cyclic state of the system I, is periodically extended for all real t , then $|\Psi_\varepsilon(t)\rangle = \exp(-i\varepsilon t/\hbar) |\varphi_\varepsilon(t)\rangle$ coincides with the wavefunction of one of the quasi-energy states of the system II. Thus it is shown that the eigenvalue problem (2.9) for the $S_q(t)$ is equivalent to the problem of finding quasi-energy states of the corresponding T -periodic system. In what follows the terms 'the quasi-energy state', and 'quasi-energy' will be used for the description of cyclic states of the system I as well as the system II.

The set $\{|\varphi_{np}(t)\rangle : |\varphi_{np}(t)\rangle = e^{i\rho\omega t} |g_n\rangle\}$, where $\{|g_n\rangle\}$ is a basis of \mathcal{R} , is a complete orthonormal set in \mathcal{H} . The matrix form of the equation (2.9) in this basis set of \mathcal{H} is:

$$\sum_1 \sum_k (H_{np, lk} + p\hbar\omega\delta_n\delta_{kp}) F_{\varepsilon, l}^{(k)} = \varepsilon_j F_{\varepsilon, j}^{(p)}. \quad (3.1)$$

The matrix elements of $H(t)$ in the basis $\{|\varphi_{np}\rangle\}$, are equal to the definite Fourier coefficients of the matrix elements of $H(t)$ in the basis $\{|g_n(t)\rangle\}$, namely

$$H_{np, lk} = \langle \varphi_{np} | H(t) | \varphi_{lk} \rangle_t = \frac{1}{T} \int_0^T e^{-i(p-k)\omega t} H_{n,l}(t) dt \equiv H_{nl}^{(p-k)}$$

where $H_{n,l}(t) = \langle g_n(t) | H(t) | g_l(t) \rangle$. The expansion coefficients of the vector $|\varphi_\varepsilon(t)\rangle$ in

the basis $\{|\varphi_{np}(t)\rangle\}$ are equal to the Fourier coefficients of $\langle g_n(t) | \varphi_{e_j}(t) \rangle$, namely,

$$F_{\epsilon_j n}^{(p)} = \langle \varphi_{np}(t) | \varphi_{e_j}(t) \rangle_t = \frac{1}{T} \int_0^T e^{-ip\omega t} \langle g_n(t) | \varphi_{e_j}(t) \rangle dt.$$

It is shown above that to any system, considered at a finite time interval $[0, T]$, there corresponds a system with T -periodic Hamiltonian, which may in general have discontinuities. The Fourier series for a function $F(t)$ is convergent in the interval $[0, T]$ and its sum is equal to $(F(t+0) + F(t-0))/2$ if it satisfies the Dirichlet conditions (see, for example, chapter VI of [13]). One of the conditions is to have a finite number of discontinuities of the first kind. If the series is convergent in the interval $[0, T]$ then it is convergent for all real t and its sum is T -periodic function. Therefore, if the difference $H_{1n,l}(T) - H_{1n,l}(0)$ is finite the Fourier series for the matrix element $H_{1n,l}(t)$ is convergent in the interval $[0, T]$. The sum of the series is equal to $(H_{1n,l}(t+0) + H_{1n,l}(t-0))/2$ for all real t . Consequently, the condition on $H(t)$, $H(T) = H(0)$ can be relaxed to the requirement that $H_{n,l}(t)$ should have a finite number of discontinuities of the first kind in the interval $[0, T]$.

Thus, the eigenvalue problem (2.9) is reduced to that (3.1) of an infinite matrix with constant coefficients. This matrix has certain regularity in its block structure for a suitable ordering of indices. For some systems the eigenvalue problem (3.1) may be reduced to that of a finite block [4, 8].

The eigenvalue problem (2.9) for the case $S_q(0) = S_q(T)$ was considered by Sambe [2] and Okuniewicz [3]. The composite Hilbert space introduced in [2, 3] is identical with \mathcal{H} . The matrix form (3.1) of the problem was first considered by Shirley [4] for the case of finite-dimensional systems with T -periodic Hamiltonians.

4. Berry phases

In this section the language of the quasi-energy approach will be applied to the description of the Berry phases of a quantum-mechanical system. In order to do this we begin with the generalization of the Berry phase by Aharonov and Anandan [12]. In this formulation the wavevector of the cyclic state $|\Psi(t)\rangle$ is presented in the form

$$|\Psi(t)\rangle = e^{if(t)} |\varphi(t)\rangle$$

where

$$f(T) - f(0) = \phi \tag{4.1}$$

$$|\varphi(T)\rangle = |\varphi(0)\rangle. \tag{4.2}$$

The phase ϕ is expressed as a sum of two terms $\phi = \beta + \gamma$, where

$$\gamma = -\frac{1}{\hbar} \int_0^T \langle \Psi(t) | H(t) | \Psi(t) \rangle dt$$

is called the ‘dynamical phase’ and

$$\beta = i \int_0^T \left\langle \varphi(t) \left| \frac{\partial}{\partial t} \right| \varphi(t) \right\rangle dt$$

is the Berry or ‘geometrical’ phase. Note that the conditions (4.1) and (4.2) define $f(t)$ and $|\varphi(t)\rangle$ up to the transformation

$$f(t) \rightarrow f(t) + g(t) \quad |\varphi(t)\rangle \rightarrow \exp[-ig(t)] |\varphi(t)\rangle$$

where $g(T) = g(0)$, and β is invariant under this transformation. Thus $|\Psi(t)\rangle$ may be taken in the quasi-energy form (2.4). This form corresponds to the choice of $f(t)$ to be a linear function of time:

$$f(t) = -\varepsilon t / \hbar.$$

In the framework of the quasi-energy approach, the cyclic evolution is described by the quasi-energy state and represented by the ray of the Hilbert space \mathcal{H} , while in terms of the Hilbert space \mathcal{R} the cyclic evolution is considered as 'propagation of the state of the system along the closed curve in the projective Hilbert space \mathcal{P} of rays of \mathcal{R} ' [12].

The phases γ and β can be expressed in terms of the inner product of the Hilbert space \mathcal{H}

$$\beta = T \left\langle \left\langle \varphi_\varepsilon \left| i \frac{\partial}{\partial t} \right| \varphi_\varepsilon \right\rangle \right\rangle, \quad \gamma = -\frac{T}{\hbar} \langle \langle \varphi_\varepsilon | \mathbf{H} | \varphi_\varepsilon \rangle \rangle. \quad (4.3)$$

Thus, the Berry phases of the system differ only by the factor T from the corresponding diagonal elements of the matrix of the operator $i(\partial/\partial t)$ in the basis $\{|\varphi_\varepsilon(t)\rangle\}$ of the appropriate subspace of \mathcal{H} . Similarly, the dynamical phases differ only by the factor $-T/\hbar$ from the corresponding diagonal elements of the matrix of the Hamiltonian in the same basis.

Note that the change of timescale,

$$\tau = \omega t \quad \text{where } \omega = 2\pi/T$$

transforms the Hilbert space \mathcal{H} into the space \mathcal{H}' independent of T [3]. The Schrödinger operator in \mathcal{H}' is given by

$$S'_q(\tau, \omega) = \mathbf{H}'(\tau) - i\hbar\omega \frac{\partial}{\partial \tau} \quad (4.4)$$

where $\mathbf{H}'(\tau) \equiv \mathbf{H}(\tau/\omega)$. Let us represent the Hamiltonian as a Fourier series

$$\mathbf{H}(t) = \sum_k \mathbf{H}^{(k)} e^{ik\omega t}.$$

If we consider \mathbf{H} as a function of the parameters $\{\mathbf{H}^{(k)}\}$ and ω , then $\mathbf{H}'(\tau)$, represented as a Fourier series, does not depend explicitly on ω :

$$\frac{\partial \mathbf{H}'(\{\mathbf{H}^{(k)}\}, \tau)}{\partial \omega} = 0. \quad (4.5)$$

Taking the partial derivative of (4.4) with respect to ω we obtain:

$$-i\hbar \frac{\partial}{\partial \tau} = \frac{\partial S'_q(\tau, \omega)}{\partial \omega}.$$

Now the Berry phase may be rewritten as

$$\beta_\varepsilon = 2\pi \left\langle \left\langle \varphi'_\varepsilon(\tau) \left| i \frac{\partial}{\partial \tau} \right| \varphi'_\varepsilon(\tau) \right\rangle \right\rangle_\tau = -\frac{2\pi}{\hbar} \left\langle \left\langle \varphi'_\varepsilon(\tau) \left| \frac{\partial S'_q(\tau, \omega)}{\partial \omega} \right| \varphi'_\varepsilon(\tau) \right\rangle \right\rangle_\tau \quad (4.6)$$

where $\varphi'_\varepsilon(\tau) \equiv \varphi_\varepsilon(t)$ and

$$\langle \langle \varphi'_1(\tau) | \varphi'_2(\tau) \rangle \rangle_\tau = \frac{1}{2\pi} \int_0^{2\pi} \langle \varphi'_1(\tau) | \varphi'_2(\tau) \rangle d\tau = \langle \langle \varphi_1(t) | \varphi_2(t) \rangle \rangle_t.$$

The eigenvalues and eigenvectors of S_q depend on the parameters $\{H^{(k)}\}$ and ω . If the eigenvector $|\varphi_\varepsilon(t)\rangle$ of the discrete spectrum of S_q is a single-valued function of ω in some interval Λ , and the associated eigenvalue ε is a differentiable function of ω in this interval, we can apply the Hellman-Feynman theorem [2, 18] to obtain

$$\left\langle\left\langle \varphi'_\varepsilon(\tau) \left| \frac{\partial S'_q(\tau, \omega)}{\partial \omega} \right| \varphi'_\varepsilon(\tau) \right\rangle\right\rangle_\tau = \frac{\partial}{\partial \omega} \langle\langle \varphi_\varepsilon(t) | S_q(t, \omega) | \varphi_\varepsilon(t) \rangle\rangle_t = \frac{\partial \varepsilon}{\partial \omega}. \quad (4.7)$$

It follows from (4.6) and (4.7) that the Berry phase of the state $|\Psi_\varepsilon(t)\rangle$ for any $\omega \in \Lambda$ is given by

$$\beta_\varepsilon = -\frac{2\pi}{\hbar} \frac{\partial \varepsilon(\omega, \{H^{(k)}\})}{\partial \omega}. \quad (4.8)$$

Let us now examine the case where (4.8) is not applicable. Let the quasi-energies of some subset of quasi-energy states $\{|\Psi_n(t)\rangle\}$ satisfy the condition

$$\varepsilon_n = \varepsilon_0 + k_n \hbar \omega_0 \quad (4.9)$$

where k_n are integers, ω_0 is a positive real number. For the frequency $\omega = \omega_0$ this subset is degenerate, because according to (2.10) all the quasi-energies of the states $\{|\Psi_n(t)\rangle\}$ may be chosen to be ε_0 . Any superposition of the corresponding quasi-energy states

$$|\Psi(t)\rangle = \sum_n a_n |\Psi_n(t)\rangle \quad (4.10)$$

is the quasi-energy state with the frequency ω_0 and the quasi-energy ε_0 . Indeed,

$$|\Psi(t)\rangle = \exp\left(-\frac{i\varepsilon_0 t}{\hbar}\right) \sum_n a_n |\varphi_n(t)\rangle = \exp\left(-\frac{i\varepsilon_0 t}{\hbar}\right) |\varphi_0(t)\rangle$$

where each $|\varphi_n(t)\rangle$ is the T -periodic part of $|\Psi_n(t)\rangle$ associated with the value of the quasi-energy ε_0 , and

$$|\varphi_0(t)\rangle = \sum_n a_n |\varphi_n(t)\rangle \quad (4.11)$$

is the T -periodic part of $|\Psi(t)\rangle$. The Berry phases of the states (4.10) with more than one non-zero a_n cannot be found by means of (4.8), because these states are cyclic for the isolated value of $\omega = \omega_0$ only. Substitution of (4.11) into (4.3) gives an expression for the Berry phase of $|\Psi(t)\rangle$:

$$\beta = T \sum_{n,m} a_m^* a_n \left\langle\left\langle \varphi_m(t) \left| i \frac{\partial}{\partial t} \right| \varphi_n(t) \right\rangle\right\rangle_t. \quad (4.12)$$

5. The adiabatic approximation

Let us now illustrate the above approach by the case of the adiabatic approximation. Let the initial state of the system be an eigenstate of $H(0)$. If the Hamiltonian of the system is slowly altered, then, according to the adiabatic theorem, at any instant the system will be in an eigenstate of the instantaneous $H(t)$. If the Hamiltonian is returned to its original form, the system returns to its original state. The wavefunction in this case is [11]

$$|\Psi(t)\rangle = \exp\left(\frac{-i}{\hbar} \int_0^t E_n(R(t')) dt'\right) \exp(i\beta(t)) |n(R)\rangle \quad (5.1)$$

where $E_n(R)$ and $|n(R)\rangle$ are the instant eigenvalues and eigenvectors of the Hamiltonian $H(R)$, $R = R(t)$ is some parameter and $R(T) = R(0)$. The wavefunction (5.1) satisfies the condition (2.3), and the corresponding ϕ is given by

$$\phi = \frac{-1}{\hbar} \int_0^T E_n(R(t')) dt' + \beta \quad \beta = \beta(C) = i \int_C \langle n(R) | \nabla_R | n(R) \rangle dR \quad (5.2)$$

where $C = \{R(t): 0 \leq t \leq T\}$ is a closed curve in the parameter space. According to the results of sections 2 and 3, the state (5.1) is a quasi-energy state and its quasi-energy for a given T is

$$\varepsilon(\omega, \{H^{(k)}\}) = \frac{1}{2\pi} \int_0^{2\pi} E_n(R'(\tau)) d\tau - \frac{\beta}{2\pi} \hbar\omega \quad (5.3)$$

where $R'(\tau) \equiv R(\tau/\omega)$ and $\omega = 2\pi/T$. It follows from (4.5) that $\partial E_n(R'(\tau))/\partial\omega = 0$. The first term in the right-hand side of (5.3) does not depend explicitly on the frequency ω . The Berry phase β does not depend on the parametrization of the curve C and, consequently, does not depend on ω . Thus, we can see that the expression (5.2) for the quasi-energy of the cyclic state in the adiabatic approximation is in agreement with the general formula (4.8). The expression (5.3) is the expansion of $\varepsilon(\omega, \{H^{(k)}\})$ in powers of ω in the vicinity of $\omega = 0$,

$$\varepsilon(\omega, \{H^{(k)}\}) = \varepsilon(0, \{H^{(k)}\}) - \frac{\beta}{2\pi} \hbar\omega.$$

Thus, in the adiabatic approximation, $\varepsilon(\omega, \{H^{(k)}\})$ is a linear function of ω .

Let us now imagine two identical systems in the same initial state, which is an eigenstate of the Hamiltonian $H(0)$ with an eigenvalue E_0 . Let the Hamiltonians of these systems be slowly and independently altered in such a way that at $t = T$ they return to their initial value $H(0)$, and then remain time-independent. For any $t \geq T$ the wavefunctions of these systems will have the phase difference

$$\Delta\phi = (\varepsilon_1 - \varepsilon_2)T/\hbar. \quad (5.4)$$

Thus, for the fixed T , the difference between the phases of the wavefunctions acquired in the process of the adiabatic perturbation is proportional to the difference between the quasi-energies of the states of the systems.

Let us note that $H(0) = H(T')$ for any $T' \geq T$. Therefore, any $T' \geq T$ may be taken instead of T . Consequently, the phase difference $\Delta\phi$ given by (5.4) should not depend on T' . To see this, let us consider ϕ' corresponding to T' :

$$\phi' = \frac{-1}{\hbar} \int_0^{T'} E_n(R(t')) dt' + \beta = \phi - \frac{1}{\hbar} E_0(T' - T).$$

The corresponding quasi-energy is given by

$$\varepsilon' \equiv -\frac{\phi' \hbar}{T'} = \varepsilon \frac{T}{T'} + \frac{E_0(T' - T)}{T'}.$$

The phase difference $\Delta\phi'$, according to (5.4), is

$$\Delta\phi' = (\varepsilon'_1 - \varepsilon'_2)T'/\hbar = \Delta\phi.$$

6. The two-level system

In this section we will illustrate the general approach developed above by the example of the two-level system. For simplicity we consider the rotating-wave approximation. The Hamiltonian of the system is given by

$$H(t) = \begin{pmatrix} E_2 & F e^{-i\omega t} \\ F^* e^{i\omega t} & E_1 \end{pmatrix}. \tag{6.1}$$

The solutions of the Schrödinger equation with the Hamiltonian (6.1) are well known (see, for example, Landau and Lifshitz [15], problem at the end of section 40). There exist two linearly independent quasi-energy solutions:

$$|\Psi_1(t)\rangle = \exp\left(-\frac{i}{\hbar} \varepsilon_1 t\right) |\varphi_1(t)\rangle \quad |\Psi_2(t)\rangle = \exp\left(-\frac{i}{\hbar} \varepsilon_2 t\right) |\varphi_2(t)\rangle. \tag{6.2}$$

The quasi-energies of the states $|\Psi_1(t)\rangle$ and $|\Psi_2(t)\rangle$ are given by

$$\varepsilon_1 = E_1 - \hbar(\Omega - \Delta\omega)/2 \quad \varepsilon_2 = E_2 + \hbar(\Omega - \Delta\omega)/2 \tag{6.3}$$

and the corresponding T -periodic functions in the basis

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

are

$$|\varphi_1(t)\rangle = \begin{pmatrix} b_{12} e^{-i\omega t} \\ b_{11} \end{pmatrix} \quad |\varphi_2(t)\rangle = \begin{pmatrix} b_{22} \\ b_{21} e^{i\omega t} \end{pmatrix} \tag{6.4}$$

where

$$b_{11} = \sqrt{\frac{(\Delta\omega + \Omega)}{2\Omega}} \quad b_{12} = -e^{i\varphi} \sqrt{\frac{(\Omega - \Delta\omega)}{2\Omega}}$$

$$b_{21} = -e^{-i\varphi} b_{12} \quad b_{22} = e^{i\varphi} b_{11} \quad \Delta\omega = \omega_0 - \omega$$

and

$$\omega_0 = \frac{E_2 - E_1}{\hbar} \quad \Omega = \sqrt{(\Delta\omega)^2 + 4|\eta|^2} \quad \eta \equiv |\eta| e^{i\varphi} = \frac{F}{\hbar}.$$

It is an interesting fact that

$$\varepsilon_2 - \varepsilon_1 = \hbar\omega + \hbar\Omega.$$

Hence the frequency $\omega + \Omega$ is a resonance frequency of the system.

Let us now consider the limit case $F \rightarrow 0$ (ω is kept constant). For small enough η we have

$$\Omega = |\Delta\omega|(1 + 2|\eta|^2/(\Delta\omega)^2).$$

The limit values of the quasi-energies (6.3) and of the T -periodic functions (6.4) depend on the sign of $\Delta\omega$.

If $\Delta\omega > 0$,

$$\varepsilon_1 \rightarrow E_1 \quad \varepsilon_2 \rightarrow E_2$$

$$|\varphi_1(t)\rangle \rightarrow |1\rangle \quad |\varphi_2(t)\rangle \rightarrow e^{i\varphi}|2\rangle.$$

If $\Delta\omega < 0$,

$$\begin{aligned} \varepsilon_1 &\rightarrow E_2 - \hbar\omega & \varepsilon_2 &\rightarrow E_1 + \hbar\omega \\ |\varphi_1(t)\rangle &\rightarrow -e^{-i\omega t} e^{i\varphi}|2\rangle & |\varphi_2(t)\rangle &\rightarrow e^{i\omega t}|1\rangle. \end{aligned}$$

Thus, we have shown that the quasi-energy states $|\Psi_1(t)\rangle$ and $|\Psi_2(t)\rangle$ tend to the stationary states of the system if $F \rightarrow 0$. At first glance it may seem strange that in the case $\Delta\omega < 0$ the quasi-energies do not tend to the energies of the unperturbed states. This is due to the fact that the quasi-energy and the T -periodic part of the wavefunction of a quasi-energy state are defined up to the transformation (2.10).

Let us now consider the Berry phases of the states (6.2). For $F \neq 0$ the functions (6.4) are continuous functions of ω , and the quasi-energies (6.3) are differentiable functions of ω . Therefore, the Berry phases of the states $|\Psi_1(t)\rangle$, $|\Psi_2(t)\rangle$ can be calculated by means of (4.8):

$$\beta_1 = \pi(1 - \Delta\omega/\Omega) \quad \beta_2 = -\beta_1. \quad (6.5)$$

The quasi-energies (6.3) and the T -periodic functions (6.4) can be neatly expressed in terms of the Berry phases:

$$\begin{aligned} \varepsilon_1 &= E_1 - \frac{\beta_1}{2\pi} \hbar\Omega = E_1 - \bar{\beta} \hbar\Omega & \varepsilon_2 &= E_2 - \frac{\beta_2}{2\pi} \hbar\Omega = E_2 + \bar{\beta} \hbar\Omega \\ \varphi_1(t) &= \begin{pmatrix} -e^{i\varphi} e^{-i\omega t} \sqrt{\bar{\beta}} \\ \sqrt{1-\bar{\beta}} \end{pmatrix} & \varphi_2(t) &= \begin{pmatrix} e^{i\varphi} \sqrt{1-\bar{\beta}} \\ e^{i\omega t} \sqrt{\bar{\beta}} \end{pmatrix} \end{aligned}$$

where

$$\bar{\beta} = \frac{|\beta_1|}{2\pi} = \frac{|\beta_2|}{2\pi}.$$

Thus, it has been shown that the shift (with respect to the case $F = 0$) of a quasi-energy of a two-level system caused by a non-adiabatic periodic perturbation is proportional to the Berry phase of the corresponding quasi-energy state. Since the quasi-energies determine the spectral characteristics of the system, this shift can be measured.

Consider now the case of resonance where

$$\varepsilon_2 - \varepsilon_1 = l\hbar\omega$$

for some integer l . The multiphoton resonance frequencies of the system, ω_l , can be found from the equation

$$\hbar\omega_l + \hbar\Omega = l\hbar\omega_l. \quad (6.6)$$

$l = 1 \Rightarrow$ the equation (6.6) has no solutions if $F \neq 0$, the system has no exact one-photon resonance

$$l = 2 \Rightarrow \omega_2 = \frac{\omega_0}{2} + \frac{2|\eta|^2}{\omega_0}$$

$$l > 2 \Rightarrow \omega_l = \frac{-\omega_0 + \sqrt{\omega_0^2(l-1)^2 + 4|\eta|^2 l(l-2)}}{l(l-2)}$$

if $\omega_0 \gg |\eta|$ then

$$\omega_l = \frac{\omega_0}{l} + \frac{2|\eta|^2}{\omega_0(l-1)}.$$

At the frequency of the external field $\omega = \omega_l$ the quasi-energy states (6.2) are degenerate. Let us equalize the quasi-energies of both states in the following way:

$$\varepsilon'_1 = \varepsilon_1 \quad \varepsilon'_2 = \varepsilon_2 - l\hbar\omega_0 = \varepsilon_1.$$

The corresponding T -periodic functions are

$$|\varphi'_1(t)\rangle = |\varphi_1(t)\rangle \quad |\varphi'_2(t)\rangle = e^{-i\omega_0 t} |\varphi_2(t)\rangle. \quad (6.7)$$

The Berry phase of a normalized mixed quasi-energy state $a_1|\Psi_1(t)\rangle + a_2|\Psi_2(t)\rangle$ can be obtained from (4.12). Substitution of (6.4) into (6.7) and direct calculation shows that

$$\langle\langle \varphi'_1 | i(\partial/\partial t) | \varphi'_2(t) \rangle\rangle_t = 0$$

which gives

$$\beta = |a_1|^2 \beta_1 + |a_2|^2 (\beta_2 + 2\pi l).$$

In the case where $F = 0$ and $\omega_0 \geq \omega$, $\beta_1 = \beta_2 = 0$. The Berry phase of a mixed cyclic state is given by

$$\beta = 2\pi l |a_2| \quad (6.8)$$

in agreement with (8.4).

Finally, we note that the Berry phases of non-adiabatic two-level systems were considered previously by Moore [9], who employed the Floquet Hamiltonian method [4] for finding cyclic states. The expressions for the Berry phases (6.5) are equivalent to that obtained in [9]. However, the case of resonance, where all states are cyclic, was not considered in [9].

7. The forced harmonic oscillator

In this section the general approach developed above will be applied to the forced harmonic oscillator. The Hamiltonian in this case is given by

$$H(t) = \frac{1}{2}(p^2 + \omega_0^2 x^2) - f(t)x$$

where x and p are the coordinate and momentum operators, ω_0 is the resonance frequency of the oscillator ($\hbar = m = 1$ in this section). It was shown by Popov and Perelomov [16, 17] that the quasi-energy states of an harmonic oscillator subjected to an action of a T -periodic force can be expressed in terms of a periodic solution of the classical equation of motion

$$\ddot{\eta}(t) + \omega_0^2 \eta(t) = f(t) \quad (7.1)$$

and the stationary states $\{|n(\omega_0, t)\rangle\}$ of the force-free oscillator:

$$|n(\omega_0, t)\rangle = e^{-iE_n t} |n(\omega_0)\rangle \quad E_n = (n + \frac{1}{2})\omega_0$$

$$\langle x | n(\omega_0) \rangle = \left(\frac{1}{2^n n!} \sqrt{\frac{\omega_0}{\pi}} \right)^{1/2} \exp\left\{ -\frac{\omega_0 x^2}{2} \right\} H_n(\sqrt{\omega_0} x)$$

where $H_n(x)$ is a Hermite polynomial. If $\omega_0 \neq l\omega$, where l is an integer, the equation (7.1) has a unique periodic solution given by

$$\eta(t) = \sum_{k=-\infty}^{\infty} \frac{f^{(k)} e^{ik\omega t}}{\omega_0^2 - k^2 \omega^2} \quad (7.2)$$

where $\{f^{(k)}\}$ are the Fourier coefficients of $f(t)$. Since $f(t)$ is real, $f^{(k)} = f^{(-k)*}$. In the case $\omega_0 \neq l\omega$ there exists a set of quasi-energy solutions $\{ \langle x | \Psi_n(t) \rangle \}$ of the Schrödinger equation [16, 17]:

$$\langle x | \Psi_n(t) \rangle = \exp\left(i\dot{\eta}(t)(x - \eta(t)) + \frac{i}{2} \dot{\eta}(t)\eta(t) + \frac{i}{2} \int_0^t \eta(\tau)f(\tau) d\tau \right) \times e^{i\phi_n} \langle x - \eta(t) | n(\omega_0, t) \rangle$$

where

$$\phi_n = -\frac{1}{2} \dot{\eta}(0)\eta(0)$$

and $\eta(t)$ is given by (7.2). The quasi-energy ϵ_n of the state $|\Psi_n(t)\rangle$ is

$$\begin{aligned} \epsilon_n &= E_n + \Delta\epsilon \\ \Delta\epsilon &= -\frac{1}{2T} \int_0^T f(t)\eta(t) dt = -\frac{|f^{(0)}|^2}{2\omega_0^2} + \sum_{k=1}^{\infty} \frac{|f^{(k)}|^2}{k^2\omega^2 - \omega_0^2}. \end{aligned} \tag{7.3}$$

It is not difficult to verify that the set $\{|\Psi_n(t)\rangle\}$ can be obtained by a unitary transformation of the set $\{|n(\omega_0, t)\rangle\}$, namely

$$|\Psi_n(t)\rangle = e^{i\theta_n(t)} D(\alpha_\eta(t)) |n(\omega_0, t)\rangle \tag{7.4}$$

where

$$\theta_\eta(t) = \phi_n + \frac{1}{2} \int_0^t \eta(\tau)f(\tau) d\tau$$

$D(\alpha) = \exp(\alpha a^+ - \alpha^* a)$ is the displacement operator and

$$\alpha_\eta(t) = \frac{\omega_0 \eta(t) + i\dot{\eta}(t)}{\sqrt{2\omega_0}}$$

Thus if $\omega_0 \neq l\omega$, where l is an integer, the set $\{|\Psi_n(t)\rangle\}$ is complete in \mathcal{R} at any moment of time.

If $\omega_0 = l\omega$ for some integer l the equation (7.1) has periodic solutions if, and only if, $f^{(l)} = 0$. If $\omega_0 = l\omega$ and $f^{(l)} = 0$ for some l any solution of the classical equation is periodic. The set $\{|\Psi_n(t)\rangle\}$ given by the particular solution (7.2) is complete. The quasi-energy states $|\Psi_n(t)\rangle$ are degenerate, because, according to (2.10), all the quasi-energies ϵ'_n may be chosen to be the same:

$$\epsilon'_n = \epsilon_n - nl\omega = \epsilon_0.$$

Any superposition of the states $|\Psi_n(t)\rangle$ is a quasi-energy state with the quasi-energy ϵ_0 . In the case of resonance, where $\omega_0 = l\omega$, the classical equation (7.1) has periodic solutions and the Schrödinger equation has bound solutions if, and only if, $f^{(\neq l)} = 0$.

Let us consider an oscillator subjected to the action of an arbitrary force $f(t)$ for $0 \leq t \leq T$. If $f(T) \neq f(0)$ the periodic extension of $f(t)$ has discontinuities in the points kT where k is an integer. Nevertheless any solution $\xi(t)$ of the classical equation (7.1) has a continuous derivative. The continuity of $\xi(t)$, and $\dot{\xi}(t)$ can be easily verified if one takes into account that any solution $\xi(t)$, including the periodic solution $\eta(t)$, can be presented in the form:

$$\xi(t) = \frac{1}{\sqrt{2\omega_0}} (e^{i\omega_0 t} d^*(t) + e^{-i\omega_0 t} d(t)) \tag{7.5}$$

where

$$d(t) = d(0) + \frac{i}{\sqrt{2}\omega_0} \int_0^t e^{i\omega_0\tau} f(\tau) d\tau$$

and $d(0)$ is a constant. Consequently if the classical equation (7.1) has the periodic solution $\eta(t)$ then functions $\{|\Psi_n(t)\rangle\}$ and the corresponding periodic functions

$$|\varphi_n(t)\rangle = e^{i\varepsilon_n t} |\Psi_n(t)\rangle \quad |\varphi_n(T)\rangle = |\varphi_n(0)\rangle$$

are continuous functions of time. Thus, apart from the case where $\omega_0 = l\omega$ and $f^{(l)} \neq 0$ for some l , an oscillator subjected to an action of an arbitrary force $f(t)$ for $0 \leq t \leq T$ has a complete set of quasi-energy states given by (7.4).

Note that the transformation

$$W = e^{-iE_n t} e^{i\theta_\eta(t)} D(\alpha_\eta(t)) \tag{7.6}$$

belongs to a representation of the Heisenberg-Weyl group W_1 [6]. It follows from (7.4) that the quasi-energy state

$$|\Psi_n(t)\rangle = W|n(\omega_0)\rangle$$

is a generalized coherent state with the starting vector $|n(\omega_0)\rangle$ (see section 1.2 in [6]). Since the displacement operator $D(\alpha)$ preserves the dispersions Δp and Δq the uncertainty relation for the state $|\Psi_n(t)\rangle$ is

$$\Delta p \Delta q = n + \frac{1}{2}.$$

In particular, the ground quasi-energy state $|\Psi_0(t)\rangle$ is a standard coherent state.

Now we can see that if a force-free harmonic oscillator is in the generalized coherent state with the starting vector $|n(\omega_0)\rangle$ and the amplitude $\alpha_\eta(0) e^{-i\omega_0 t}$ at $t < 0$, and a non-adiabatic external perturbation, such that if $\omega_0 = l\omega$ then $f^{(l)} = 0$, is applied on $[0, T]$, then the state of the system on this interval is the quasi-energy state $|\Psi_n(t)\rangle$. For $t > T$ the oscillator is in the generalized coherent state with the amplitude $\alpha_\eta(0) e^{-i\omega_0(t-T)}$. Let us imagine another oscillator identical with the first one in the same initial state with no perturbation applied on $[0, T]$. For $t > T$ the state of the second oscillator will have the amplitude $\alpha_\eta(0) e^{-i\omega_0 t}$. Therefore the states of the oscillators will be the same for $t > T$ only in the case of resonance, $\omega_0 = l\omega$, $f^{(l)} = 0$. In this case for any $t \geq T$ the wavefunctions of the systems will have the phase difference

$$\Delta\phi = \Delta\varepsilon T \tag{7.7}$$

where $\Delta\varepsilon$ is given by (7.3). On the other hand in the case of resonance any state of the perturbed harmonic oscillator is cyclic as well as any state of a force-free oscillator being cyclic with the frequency ω_0 (see section 9). Thus if we take two identical oscillators in the same states at $t < 0$, one of them subjected to an external perturbation on $[0, T]$ such that $\omega_0 = l\omega$, $f^{(l)} = 0$, the states of the oscillators will be the same for $t > T$ and the phase difference of the wavefunctions, $\Delta\phi$, will be given by (7.7). Note that $\Delta\phi$ does not depend on the initial state.

Let us now calculate the Berry phases for the cyclic states of the forced oscillator. In the case $\omega_0 \neq l\omega$, where l is an integer, all the cyclic states are given by (7.4). The Berry phases of these states can be obtained from (4.8) and (7.3)

$$\beta_n = 4\pi\omega \sum_{k=1}^{\infty} \frac{|f^{(k)}|^2}{(k^2\omega^2 - \omega_0^2)^2} \equiv \beta_0.$$

The Berry phase β_0 can also be expressed in terms of the periodic solution $\eta(t)$ of the classical equation

$$\beta_0 = - \int_0^T \eta(t) \ddot{\eta}(t) dt.$$

If $\omega_0 = l\omega, f^{(l)} = 0$ for some integer l the quasi-energy states $|\Psi_n(t)\rangle$ are degenerate, namely

$$\begin{aligned} |\Psi_n(t)\rangle &= e^{-i\varepsilon_0 t} |\varphi_n^l(t)\rangle \\ |\varphi_n^l(t)\rangle &= e^{-inl\omega t} |\varphi_n(t)\rangle. \end{aligned}$$

Any superposition of the states $|\Psi_n(t)\rangle$ is a quasi-energy state with the quasi-energy ε_0 . The Berry phases of mixed states cannot be found by means of (4.8), because these states are cyclic for the isolated value of $\omega = \omega_0/l$ only. The Berry phases of mixed states will be obtained from (4.12). The diagonal matrix elements of the operator $i(\partial/\partial t)$ are given by

$$\left\langle \left\langle \varphi_n^l(t) \left| i \frac{\partial}{\partial t} \right| \varphi_n^l(t) \right\rangle \right\rangle_t = \beta_0 + nl\omega. \quad (7.8)$$

Let us consider non-diagonal matrix elements of $i(\partial/\partial t)$. It is not difficult to see that for $m \neq n$

$$\left\langle \left\langle \varphi_m^l(t) \left| i \frac{\partial}{\partial t} \right| \varphi_n^l(t) \right\rangle \right\rangle_t = \left\langle \left\langle m(\omega_0) \left| e^{il(m-n)\omega t} \mathbf{D}^+(\alpha_\eta) i \frac{\partial}{\partial t} \mathbf{D}(\alpha_\eta) \right| n(\omega_0) \right\rangle \right\rangle_t. \quad (7.9)$$

Taking the derivative of the displacement operator we obtain

$$\mathbf{D}^+(\alpha_\eta) \frac{\partial \mathbf{D}(\alpha_\eta)}{\partial t} = \mathbf{A} + i \operatorname{Im}(\dot{\alpha}_\eta \alpha_\eta^*) \quad (7.10)$$

where

$$\mathbf{A} = \dot{\alpha}_\eta \mathbf{a}^+ - \dot{\alpha}_\eta^* \mathbf{a}. \quad (7.11)$$

Substitution of (7.10) and (7.11) into (7.9) gives for $m \neq n$

$$\left\langle \left\langle \varphi_m^l(t) \left| i \frac{\partial}{\partial t} \right| \varphi_n^l(t) \right\rangle \right\rangle_t = \frac{1}{T} \int_0^T e^{il(m-n)\omega t} \langle m(\omega_0) | \mathbf{A} | n(\omega_0) \rangle dt. \quad (7.12)$$

Let us show that the matrix element (7.12) equals zero. In order to do this consider the matrix elements of \mathbf{A} in the basis $\{|n(\omega_0)\rangle\}$ of \mathcal{R} ,

$$\langle m(\omega_0) | \mathbf{A} | n(\omega_0) \rangle = \dot{\alpha}_\eta \sqrt{n+1} \delta_{m,n+1} - \dot{\alpha}_\eta^* \sqrt{n} \delta_{m,n-1} \quad (7.13)$$

and the Fourier series for α_η ,

$$\alpha_\eta(t) = \frac{1}{\sqrt{2\omega_0}} \sum_{k=-\infty}^{\infty} \frac{f^{(k)} e^{ik\omega t}}{\omega_0 + k\omega}. \quad (7.14)$$

The subsequent substitutions of (7.13) and (7.14) into (7.12) give the matrix element (7.12) as a sum of terms containing factors of the type:

$$f^{(k)} \int_0^T e^{\pm il\omega t} e^{ik\omega t} dt. \quad (7.15)$$

If $k = \pm l$, (7.15) equals zero, because $f^{(\pm l)} = 0$. If $k \neq \pm l$, the expression (7.15) equals zero, because the integral equals zero. Therefore,

$$\left\langle \left\langle \varphi_m^l(t) \left| i \frac{\partial}{\partial t} \right| \varphi_n^l(t) \right\rangle \right\rangle_t = 0 \quad \text{for } m \neq n. \quad (7.16)$$

Substitution of (7.8) and (7.16) into (4.12) gives the Berry phase of an arbitrary state of a forced oscillator in the case of resonance, $\omega_0 = l\omega, f^{(l)} = 0$,

$$\beta = \beta_0 + 2\pi l \sum_n n |\alpha_n|^2. \tag{7.17}$$

The first term in the right-hand side of (7.17) is due to the dependence of the quasi-energy on the frequency of the external perturbation. The second term is due to the degeneracy of the quasi-energy in the case of resonance.

It is well known that if the initial state of a forced oscillator is a coherent state then this state will be coherent at any time $t \geq 0$. Let us obtain the Berry phase of a standard coherent state $|\Psi_\alpha(t)\rangle$ with the initial amplitude α ,

$$|\Psi_\alpha(0)\rangle = D(\alpha)|0(\omega_0)\rangle. \tag{7.18}$$

Substituting

$$D(\alpha) = D(\alpha_\eta(0))D(\alpha_q) \exp\{i \operatorname{Im}(\alpha_q \alpha_\eta^*(0))\}$$

where

$$\alpha_q = \alpha - \alpha_\eta(0)$$

into (7.18) and taking (7.4) into account we obtain the expansion of the state $|\Psi_\alpha(0)\rangle$ in quasi-energy states $\{|\Psi_n(0)\rangle\}$,

$$|\Psi_\alpha(0)\rangle = e^{i\delta} \exp\left(-\frac{|\alpha_q|^2}{2}\right) \sum_{n=0}^{\infty} \frac{(\alpha_q)^n}{\sqrt{n!}} |\Psi_n(0)\rangle \tag{7.19}$$

where $\delta = \alpha_q \alpha_\eta^*(0) - \phi_\eta$.

The quantity α_q can be interpreted as the amplitude of the coherent state $|\Psi_\alpha(t)\rangle$ in the quasi-energy states basis. Indeed, the expansion coefficients of any solution of the Schrödinger equation in the quasi-energy states basis do not depend on time, consequently the expansion coefficients of $|\Psi_\alpha(t)\rangle$ in $\{|\Psi_n(t)\rangle\}$ can be obtained from (7.19)

$$a_n = e^{i\delta} \exp\left(-\frac{|\alpha_q|^2}{2}\right) \frac{(\alpha_q)^n}{\sqrt{n!}} \tag{7.20}$$

and we have

$$|\Psi_\alpha(t)\rangle = e^{i\delta} \exp\left(-\frac{|\alpha_q|^2}{2}\right) \sum_{n=0}^{\infty} \frac{(\alpha_q)^n}{\sqrt{n!}} |\Psi_n(t)\rangle.$$

This expansion is similar to the expansion of a standard coherent state of a force-free oscillator in the stationary states basis $\{|n(\omega_0, t)\rangle\}$.

Substitution of (7.20) into (7.17) gives the Berry phase of a standard coherent state in the case of resonance

$$\beta_\alpha = \beta_0 + 2\pi l |\alpha_q|^2. \tag{7.21}$$

Note that the Berry phases of standard coherent states in the particular case of resonance, where $l = 1$, were considered previously by Moore [7]. The equation (7.21) is different from Moore's equation (52) because in Moore the Berry phase of a standard coherent state is expressed in terms of its time-dependent amplitude $z(t)$ relevant to the basis $\{|n(\omega_0)\rangle\}$, while in this paper the Berry phase of a standard coherent state is expressed in terms of its time-independent amplitude α_q relevant to the quasi-energy states basis $\{|\Psi_n(t)\rangle\}$.

8. The time-independent Hamiltonian

A time-independent Hamiltonian is a particular case of a T -periodic Hamiltonian with an arbitrary period T . Let the Hamiltonian have a discrete spectrum. The equivalence classes of solutions of (2.9) can be generated by the solutions $(E_j, |\varphi_{E_j}\rangle)$, where $|\varphi_{E_j}\rangle$ is an eigenvector of Hamiltonian and E_j is the associated eigenvalue. The Berry phases of stationary states $|\Psi_j\rangle = \exp[-iE_j(t)/\hbar]|\varphi_{E_j}\rangle$ are trivial, $\beta = 2\pi k$, where k is an integer.

Let us note now, that even in the case of a closed system, for some values of the frequency ω there are quasi-energy states which are not eigenstates of the Hamiltonian. The Berry phases of these states are non-trivial in general. In order to show this, let us consider the case where the energies $\{E_n\}$ of a subset of the stationary states, $\{|\Psi_n(t)\rangle\}$, of a closed system are given by

$$E_n = E_0 + k_n \hbar \omega_0 \quad (8.1)$$

where k_n are integers, ω_0 and E_0 are real numbers, $\omega_0 > 0$. The condition (8.1) is a particular case of the condition (4.9). Clearly, any two energy levels $E_i < E_l$ of any system satisfy this condition when $E_0 = E_i$, $k_i = 0$, $k_l = 1$, and ω_0 is equal to the resonance frequency of the system $\omega_{li} = (E_l - E_i)/\hbar$. For some systems all the energy levels satisfy the condition (8.1), e.g. harmonic oscillators, spin- j particles in an homogeneous magnetic field.

Taking (8.1) into account $|\Psi_n(t)\rangle$ can be written down as

$$|\Psi_n(t)\rangle = \exp\left(-\frac{i}{\hbar} E_0 t\right) |\varphi_n(t)\rangle \quad |\varphi_n(t)\rangle = \exp(-ik_n \omega_0 t) |\varphi_{E_n}\rangle$$

where $|\varphi_n(t)\rangle$ is a periodic function with the period $T_0 = 2\pi/\omega_0$. An arbitrary superposition of the quasi-energy states from the subset $\{|\Psi_n(t)\rangle\}$,

$$|\Psi(t)\rangle = \exp\left(-\frac{i}{\hbar} E_0 t\right) \sum_n a_n |\varphi_n(t)\rangle \quad (8.2)$$

is also a quasi-energy state with the quasi-energy E_0 . On the other hand, if more than one a_n differs from zero, then $|\Psi(t)\rangle$ is not a stationary state.

It is easy to prove that the converse is also true, namely, if some non-stationary state $|G(t)\rangle$ of a closed system is cyclic, i.e. $|G(0)\rangle = e^{i\phi_s} |G(T_g)\rangle$, then a subset of the energy levels satisfies the condition (8.1). Thus, we have obtained a criterion of existence of non-stationary cyclic states of a closed system.

The Berry phase of a non-stationary cyclic state can be obtained from the general expression (4.12). Substitution of

$$\left\langle\left\langle \varphi_m(t) \left| i \frac{\partial}{\partial t} \right| \varphi_n(t) \right\rangle\right\rangle_t = k_n \omega_0 \delta_{mn}$$

into (4.12) gives

$$\beta = 2\pi \sum_n k_n |a_n|^2. \quad (8.3)$$

If only one of the coefficients a_n in (8.2) is not zero, then $|\Psi(t)\rangle$ is a stationary state. We can see from (8.3) that in this case $\beta = 2\pi k_n$, i.e. it is trivial. For the case of two energy levels $E_i < E_l$, considered above, the Berry phase is given by

$$\beta = 2\pi |a_l|^2 \quad (8.4)$$

in agreement with (6.8). The expression (8.4) identical with the result obtained by Moore ([7], equation 8) for a time-independent two-level system. Formula (8.4) reproduces the result of Aharonov and Anandan [12] for the case of a spin- $\frac{1}{2}$ particle in an homogeneous magnetic field.

Let us now turn our attention to a force-free harmonic oscillator. Its energy levels are given by the formula (8.1) with $E_0 = \hbar\omega_0/2$ and $k_n = 1$, where ω_0 is its resonance frequency. All its states are cyclic, with the frequency ω_0 . Let us derive an expression for the Berry phase of the coherent state with the initial amplitude α . Its expansion coefficients a_n are given by

$$a_n = \exp\left(-\frac{|\alpha|^2}{2}\right) \frac{\alpha^n}{\sqrt{n!}}.$$

The Berry phase of the coherent state $|\alpha\rangle$ is

$$\beta_\alpha = 2\pi|\alpha|^2.$$

This expression can also be obtained from (7.21) if we take into account that, for a force-free oscillator, $\beta_0 = 0$ and $\alpha_n(0) = 0$.

In conclusion let us discuss localized states of an electron in the crystal:

$$a_N(\mathbf{r} - \mathbf{r}_p, t) = P^{-1/2} \sum_K \exp(-i\mathbf{K} \cdot \mathbf{r}_p) \exp\left(-\frac{i}{\hbar} E_N(\mathbf{K})t\right) \Psi_{KN}(\mathbf{r}) \quad (8.5)$$

where N is a band index, \mathbf{K} is a wavevector, P is the number of cells, \mathbf{r}_p is a lattice point, $\Psi_{KN}(\mathbf{r})$ is a Bloch function. The functions $a_N(\mathbf{r} - \mathbf{r}_p, t)$ possess some useful properties. Firstly, they are solutions of the Schrödinger equation. Secondly, they have the Wannier functions as the initial conditions, hence we will call them the Wannier states. Thirdly, they form a complete orthonormal set at any moment of time, $\langle a_N(\mathbf{r} - \mathbf{r}_p, t) | a_{N'}(\mathbf{r} - \mathbf{r}_{p'}, t) \rangle_r = \delta_{N'N} \delta_{p'p}$. Fourthly, Wannier states of the parabolic band of a cubic crystal are quasi-energy states. For simplicity we will demonstrate the last property in the one-dimensional case. The energies in this case are given by

$$E_N(K) = E_N(0) + \frac{\hbar^2 K^2}{2m_N} \quad K = \frac{2\pi n}{Pa} \quad -\frac{1}{2}P < n \leq \frac{1}{2}P \quad (8.6)$$

where m_N is an effective mass, a is the size of a cell, n is an integer. The energy levels (8.6) satisfy the condition (8.1) with the parameters

$$E_0 = E_N(0) \quad \omega_0 = \frac{2\hbar\pi^2}{P^2 a^2 m_N} \quad k_n = n^2.$$

Therefore, the Wannier states (8.5) of the band N are cyclic states, corresponding to the degenerate eigenvalue of the Schrödinger operator $E_N(0)$. They all have the same mean energy and the same Berry phases:

$$\beta_N = \frac{\pi}{12} (2P^2 + 1 + 3(-1)^P).$$

9. Summary

The results of this paper lead to the conclusion that an adequate description of cyclic states of a quantum-mechanical system can be provided in terms of eigenvalues and

eigenvectors of the Schrödinger operator S_q rather than of the Hamiltonian. The fact that even in the adiabatic case there exists a non-trivial Berry phase which does not depend on the timescale of the perturbation is a strong argument for this conclusion. All the cyclic states of a system, including stationary states, are determined by the eigenvalues and associated eigenvectors of S_q . The notion of a quasi-energy state was introduced as an extension of the notion of a stationary state for the case of systems under periodic perturbations, where stationary states do not exist. However, even in the case of a system with a time-independent Hamiltonian, there exist quasi-energy states that are not eigenstates of the Hamiltonian. The Berry phases of such states are, in general, non-trivial.

There are two types of quasi-energy states related to the discrete spectrum of S_q . The wavefunctions of the states of the first type are single-valued functions of the frequency of the external perturbation ω in some intervals. These states have non-trivial Berry phases only for systems with time-dependent Hamiltonians. The wavefunctions of the states of the second type are cyclic only for some isolated values of the parameter ω , related to the resonance frequencies of the system. These states have non-trivial Berry phases both time-independent and time-dependent Hamiltonians. A 'classical' example of such a state is a coherent state of an harmonic oscillator.

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