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GEOMETRIC PHASES AND EXACTLY SOLVABLE TIME-DEPENDENT POTENTIALS

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A method of constructing periodic time-dependent Hamiltonians admitting exact solutions is used to study the geometric phase. The approach is based on the transformation of soluble time-independent equations into time-dependent ones by employing a set of special time-dependent transformation operators. A class of periodic time-dependent Hamiltonians with cyclic solutions is constructed in a closed analytic form and the nonadiabatic geometric phase is determined in terms of the obtained solutions.

Для изучения геометрических фаз используется метод конструирования периодических зависящих от времени гамильтонианов, допускающих точные решения уравнения Шредингера. Подход основан на преобразовании точно решаемых стационарных уравнений в нестационарные с использованием набора специальных зависящих от времени операторов преобразования. Класс периодических зависящих от времени гамильтонианов вместе с циклическими решениями конструируется в замкнутом аналитическом виде. В терминах полученных решений определяются неадиабатические геометрические фазы.

1. CONSTRUCTION OF A TIME-DEPENDENT HAMILTONIAN

A great deal of investigations in quantum computers refresh interest towards the Berry phase effect [1] in quantum mechanics. The idea of using unitary evolution operators produced by non-Abelian Berry phase as quantum calculations was proposed by Zanardi, Pachos, Rasetti [2, 3] and realized by Pachos and Chountasis [4] in a concrete model of holonomic quantum computer. In our view, the time-dependent and time-independent exactly solvable models in quantum theory make it possible to simulate these processes.

Suppose that the state $|\Psi(t)\rangle$ of a dynamical system evolves according to the matrix Schrödinger equation

$$i\frac{d|\Psi(r,t)\rangle}{\partial t} = H(r,t)|\Psi(r,t)\rangle, \quad H(r,t) = p_r^2 + V(r,t), \tag{1}$$

with $\hbar = 1$ and T periodic time-dependent Hamiltonian, $H(t) = H(t+T)$, the potential matrix $V(r,t) = \{V_{ij}(r,t)\}$ is Hermitian and p_r is the momentum operator. Our goal is to

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give the procedure for obtaining a wide class of time-dependent Hamiltonians $H(t)$ for which exact solutions of (1) can be found. To this end, we use the time-independent Hamiltonian

$$\widetilde{H}(r) = p_r^2 + V(r) \tag{2}$$

with a real symmetric potential matrix $V(r)$ and $\hbar^2/2m = 1$, and a unitary time-dependent transformation $\mathcal{S}(t)$

$$|\Psi(r,t)\rangle = \mathcal{S}(t)|\Phi(r,t)\rangle, \tag{3}$$

by means of which the known time-independent Hamiltonian (2) is changed to the time-dependent one

$$H(t) = \mathcal{S}(t)\widetilde{H}\mathcal{S}^{\dagger}(t) + i\dot{\mathcal{S}}(t)\mathcal{S}^{\dagger}(t). \tag{4}$$

Here $|\Phi(r,t)\rangle$ satisfies the equation of motion (1) with the time-independent Hamiltonian $\widetilde{H}(r)$ and it is taken in the form

$$|\Phi(r,t)\rangle = \exp\left(-i\widetilde{H}(r)t\right)|\Phi(r,0)\rangle. \tag{5}$$

Clearly, the solutions $|\Psi(r,t)\rangle$ and $|\Phi(r,t)\rangle$ can be properly defined by solutions of the time-independent problem

$$\widetilde{H}|\Phi(\widetilde{\mathcal{E}})\rangle = \widetilde{\mathcal{E}}|\Phi(\widetilde{\mathcal{E}})\rangle. \tag{6}$$

Note, if the system of Schrödinger equations (6) with some known time-independent Hamiltonian $\widetilde{H}(r)$ is exactly soluble, the system of Eq. (1) with the time-dependent Hamiltonian (4) admits exact solutions too. The result depends on transformation operators $\mathcal{S}(t)$ and the choice of initial states.

Now consider reconstruction of the 2×2 periodic time-dependent Hamiltonian taken in the form (1). We start with the time-independent Hamiltonian (2) with the 2×2 real symmetric potential matrix $V(r)$, $V_{12}(r) = V_{21}(r)$. By means of a unitary time-dependent transformation taken in the form

$$\mathcal{S}(t) = \exp\left(-i\mathbf{s}\cdot\mathbf{h}(t)\right) = \exp\left(-i\sum_{i=1}^{3} s_i h_i(t)\right) \tag{7}$$

the time-independent Hamiltonian (2) with regard to Eqs. (1) and (4) turns to the time-dependent Hamiltonian

$$H(r,t) = p_r^2 + \exp\left(-i\mathbf{s}\cdot\mathbf{h}(t)\right)V(r)\exp\left(i\mathbf{s}\cdot\mathbf{h}(t)\right) + (\mathbf{s}\cdot\dot{\mathbf{h}}(t)). \tag{8}$$

Here $\mathbf{s} = (1/2)\boldsymbol{\sigma}$ is the spin operator; $\boldsymbol{\sigma} = (\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3)$ and $\hat{\sigma}_i$ are the Pauli matrices and a dot means a time-derivative. The solutions of (1) with Hamiltonian (8), according to (3) and (5), are represented as

$$|\Psi(r,t)\rangle = \exp\left(-i\mathbf{s}\cdot\mathbf{h}(t)\exp\left(-i\widetilde{H}(r)t\right)|\Phi(r,t=0)\rangle\right). \tag{9}$$

It is convenient to present the 2×2 intrinsic time-independent Hamiltonian (2) by the sum of diagonal and zero trace matrices:

$$\widetilde{H}(r) = \left(p_r^2 + \frac{V_{11}(r) + V_{22}(r)}{2}\right)\hat{I} + \begin{pmatrix} \dfrac{V_{11}(r) - V_{22}(r)}{2} & V_{12}(r) \\ V_{21}(r) & -\dfrac{V_{11}(r) - V_{22}(r)}{2} \end{pmatrix} \tag{10}$$

$$= \left(p_r^2 + q(r)\right)\hat{I} + 2(\mathbf{s}\cdot\mathbf{B}(r)), \tag{11}$$

with the evident notations: $q(r) = (V_{11}(r) + V_{22}(r))/2$, $B_1(r) = V_{12}(r)$, $B_2(r) = 0$, $B_3(r) = (V_{11}(r) - V_{22}(r))/2$ and $\hat{I}$ is the identity matrix. It is evident that the Hamiltonian for the two-coupled system of equations corresponds to the three- or two-dimensional problem with coordinates B_i dependent on the extra parameter r. Then the time-dependent Hamiltonian (8) can be represented as

$$H(r,t) = \Big(p_r^2 + q(r)\Big)\hat{I} + 2\exp(-i\mathbf{s}\cdot\mathbf{h}(t))(\mathbf{s}\cdot\mathbf{B}(r))\exp(i\mathbf{s}\cdot\mathbf{h}(t)) + (\mathbf{s}\cdot\dot{\mathbf{h}}(t) = \\ = \Big(p_r^2 + q(r)\Big)\hat{I} + 2(\mathbf{s}\cdot\mathbf{B}(r,t)). \quad (12)$$

Obviously, the transformation (7) does not change the first term of (11) (or (10)) and transforms the second term. The Hamiltonians in the forms (12) and (8) can be used for describing the motion of a spin $1/2$-particle in the space-nonuniform and time-dependent magnetic field or can be applied for investigating multi-level atoms and nuclei.

In terms of the evolution operator $\mathcal{U}(t) = \mathcal{U}(t,0)$, the solution $|\Psi(r,t)\rangle$ is

$$|\Psi(r,t)\rangle = \mathcal{U}(t)|\Psi(r,0)\rangle, \quad \mathcal{U}(0) = 1. \quad (13)$$

It is easy to find from (9) and (13) a very important relationship between the operators $\mathcal{U}(t)$ and $\mathcal{S}(t)$. In the case when $|\Psi(r,0)\rangle = |\Phi(r,0)\rangle$ it is

$$\mathcal{U}(t) = \mathcal{S}(t))\exp(-i\widetilde{H}t) = \exp(-i\mathbf{s}\cdot\mathbf{h}(t))\exp(-i\widetilde{H}t). \quad (14)$$

The evolution operator in one period is written as $\mathcal{U}(T) = \exp(-i\mathbf{s}\cdot\mathbf{h}(T))\exp(-i\widetilde{H}T)$. Now let us consider cyclic solutions that after one period T ($T = 2\pi/\omega$) are recovered up to the phase, i.e. initial states $|\Psi_\nu(0)\rangle$ are eigenvectors of $\mathcal{U}(T)$

$$|\Psi_\nu(r,T)\rangle = \mathcal{U}(T)|\Psi_\nu(r,0)\rangle = \exp(-i\beta_\nu)|\Psi_\nu(r,0)\rangle, \quad (15)$$

where $\exp(-i\beta_\nu)$ are eigenvalues of $\mathcal{U}(T)$ and β_ν is the total phase. Let us demand that initial states are eigenvectors of the time-independent Hamiltonian $\widetilde{H}$, $|\Psi_\nu(r,0)\rangle = |\Phi_\nu(r)\rangle$. It is possible if $\mathcal{U}(T)$ and $\widetilde{H}$ commute $[\mathcal{U}(T),\widetilde{H}] = 0$. Then, we immediately obtain that $\mathcal{S}(T)$ and $\widetilde{H}$ commute: $\mathcal{U}^\dagger(T)\widetilde{H}\mathcal{U}(T) = \mathcal{S}^\dagger(T)\exp(-i\widetilde{H}T)\widetilde{H}\exp(i\widetilde{H}T)\mathcal{S}(T) = \mathcal{S}^\dagger(T)\widetilde{H}\mathcal{S}(T) = \widetilde{H}$, i.e. $[\mathcal{S}(T),\widetilde{H}] = 0$. It is one of the conditions on the choice of transformations $\mathcal{S}(t)$. Other properties of $\mathcal{S}(t)$ are evident: they have to be unitary and possess the same matrix dimension as $\widetilde{H}$. With allowance for (9) the recurrent solutions at any time are written as

$$|\Psi_\nu(r,t)\rangle = \exp(-i\mathbf{s}\cdot\mathbf{h}(t))\exp(-i\widetilde{E}_\nu t)|\Phi_\nu(r)\rangle. \quad (16)$$

It is evident now that in order to determine the cyclic solutions, we need time-independent solutions. Thus, whenever $\widetilde{H}(r)$ is an exactly soluble time-independent Hamiltonian, the properly generated time-dependent system of equations has cyclic exact solutions. The same is valid if the stationary equation with the known $\widetilde{H}(r)$ is solved numerically, then we construct corresponding time-dependent Hamiltonians in an explicit form in terms of numerical solutions $|\Phi_\nu(r)\rangle$ of time-independent problem (6). The evolution of an arbitrary initial state $|\Psi(r,0)\rangle = \sum_\nu \alpha_\nu|\Psi_\nu(r,0)\rangle$ can be represented as a superposition of a basis set of recurrent linearly independent vector solutions, $|\Psi(r,t)\rangle = \sum_\nu \alpha_\nu|\Psi_\nu(r,t)\rangle$.

2. GEOMETRIC PHASES

Now we can proceed to calculations of physical quantities, such as a geometric phase, associated with the evolution of cyclic solutions [1], a dynamical phase and an expectation value of Hamiltonian $H(t)$. To find the dynamical phase δ_ν, we need the expectation value $\epsilon_\nu(t)$

$$\delta_\nu = \int_0^T \epsilon_\nu(t)dt, \tag{17}$$

$$\epsilon_\nu(t) = \langle\Psi_\nu(r,t)|H(t)|\Psi_\nu(r,t)\rangle = \langle\Psi_\nu(r,0)|\mathcal{U}^\dagger(t)H(t)\mathcal{U}(t)|\Psi_\nu(r,0)\rangle. \tag{18}$$

By using (14) and (4) we have $\mathcal{U}^\dagger(t)H(t)\mathcal{U}(t) = \mathrm{e}^{i\widetilde{H}(r)t}\Big(\widetilde{H}(r) - i\mathcal{S}^\dagger(t)\dot{\mathcal{S}}(t)\Big)\mathrm{e}^{-i\widetilde{H}(r)t}$. Since for cyclic solutions $|\Psi_\nu(r,0)\rangle = |\Phi_\nu(r)\rangle$ and $|\Phi_\nu(r)\rangle$ is an eigenstate vector of $\widetilde{H}(r)$ with eigenvalue $\widetilde{\mathcal{E}}_\nu$, we express the expectation value $\epsilon_\nu(t)$ and the dynamical phase δ_ν as

$$\epsilon_\nu(t) = \widetilde{\mathcal{E}}_\nu - \langle\Phi_\nu(r)|i\mathcal{S}^\dagger(t)\dot{\mathcal{S}}(t)|\Phi_\nu(r)\rangle, \tag{19}$$

$$\delta_\nu = \widetilde{\mathcal{E}}_\nu T - \int_0^T \langle\Phi_\nu(r)|i\mathcal{S}^\dagger(t)\dot{\mathcal{S}}(t)|\Phi_\nu(r)\rangle dt. \tag{20}$$

The geometric phase φ_ν, given by removing the dynamical phase from the total phase β_ν, is

$$\varphi_\nu = \beta_\nu - \delta_\nu = \beta_\nu - \widetilde{\mathcal{E}}_\nu T + \int_0^T \langle\Phi_\nu(r)|i\mathcal{S}^\dagger(t)\dot{\mathcal{S}}(t)|\Phi_\nu(r)\rangle dt. \tag{21}$$

In the cases when the components of $\mathbf{h}(t)$ are linear functions of time, $h_i(t) = \omega_i t$, the expectation values of $H(t)$ and spin-expectation values for corresponding cyclic solutions are time-independent. Indeed, the relation (19), with account of $\mathcal{S}_i(t) = \exp(-i\sigma_i\omega_i t)$ gives the expectation values of $H(t)$

$$\epsilon^i_\nu = \langle\Phi_\nu(r)|\widetilde{H}(r)|\Phi_\nu(r)\rangle + \frac{\omega_i}{2}\langle\Phi_\nu(r)|\hat{\sigma}_i|\Phi_\nu(r)\rangle = \widetilde{\mathcal{E}}_\nu + \frac{\omega_i}{2}\bar{\hat{\sigma}}^i_\nu, \tag{22}$$

where the quantities $\bar{\hat{\sigma}}^i_\nu$ are the spin-expectation values

$$\bar{\hat{\sigma}}^i_\nu = \langle\Psi_\nu(r,t)|\hat{\sigma}_i|\Psi_\nu(r,t)\rangle = \langle\Phi_\nu(r)|\hat{\sigma}_i|\Phi_\nu(r)\rangle \tag{23}$$

and do not depend on time. Therefore, and ϵ^i_ν in (22) does not depend on time, too.

It is known that the classical periodic system returns to its initial state after a period, while the quantum system multiplies by an additional Berry phase. For the dynamical phase δ_ν from (20) with (22) we get

$$\delta^i_\nu = \int_0^T \epsilon^i_\nu(t)dt = \widetilde{\mathcal{E}}_\nu T + \pi\bar{\hat{\sigma}}^i_\nu. \tag{24}$$

Removing the dynamical phase (24) from the total phase $\beta_\nu = \pi + \widetilde{\mathcal{E}}_\nu T$, we get the geometric phase φ_ν^i

$$\varphi_\nu^i = (\beta_\nu - \delta_\nu^i) = \pi(1 - \bar{\tilde{\sigma}}_\nu^i). \tag{25}$$

Obviously, the geometric phase is determined by the spin-expectation value $\bar{\tilde{\sigma}}_\nu^i$ along the rotating axis. The so-called spin alignment occurs. If $\bar{\tilde{\sigma}}_\nu^i = 0$, changing the dynamic phase angle in a period is determined as $\beta_\nu = \widetilde{\mathcal{E}}_\nu T$; respectively, the geometric phase is $\varphi_\nu^i = \pi$. In other words, changing of the geometric phase in n periods is equal to $n\pi$. It means that for an even number of periods $n = 2, 4, 6, \ldots$, φ_ν^i is a multiple of 2π and the geometric Berry phase has no effect on time-dependent periodic solutions. It is a property of stationary solutions. As evident from (25), for an odd number of periods, the wave function's sign changes. So, quantization of Berry phase is related to the spin-alignment quantization and it is important for nuclear high-spin physics (see [6,7]). If within one period $\bar{\tilde{\sigma}}_\nu^i = 1/2$, then for the odd number of periods $n = 1, 3, 5, \ldots$, φ_ν^i is a multiple of $\pi/2$, i.e. $\varphi_\nu^i = n\pi/2$; for an even number of periods $n = 2, 4, 6, \ldots$, $\varphi_\nu^i = n\pi$ is a multiple of π and for $n = 4, 8, 12, \ldots$ the geometric phase again has no effect on periodic solutions.

Note also that the position probability density in a given point of space-time

$$P(r,t) = ||\Psi_\nu(r,t)\rangle|^2 = ||\Phi_\nu(r)\rangle|^2 \tag{26}$$

does not depend on time. From (22)–(26) it follows that Eq. (1) for the obtained family of the time-dependent potential matrices possesses solutions and properties like time-independent ones. So, one of the applications of this approach is modelling quantum systems such as wells and wires with the properties of dynamic localization. In our mind, the presented method is effective for generating time-dependent periodic Hamiltonians with corresponding geometric phase, which can be useful for investigation of quantum computing.

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