Application of Geometric Phase in Quantum Computations

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This article is dedicated to memory of our dear friend, colleague and co-author Dr. Artur Tregubovich, (1961–2007)

Abstract

Geometric phase that manifests itself in number of optic and nuclear experiments is shown to be a useful tool for realization of quantum computations in so called holonomic quantum computer model (HQCM). This model is considered as an externally driven quantum system with adiabatic evolution law and finite number of the energy levels. The corresponding evolution operators represent quantum gates of HQCM. The explicit expression for the gates is derived both for one-qubit and for multi-qubit quantum gates as Abelian and non-Abelian geometric phases provided the energy levels to be time-independent or in other words for rotational adiabatic evolution of the system. Application of non-adiabatic geometric-like phases in quantum computations is also discussed for a Caldeira-Legett-type model (one-qubit gates) and for the spin 3/2 quadrupole NMR model (two-qubit gates). Generic quantum gates for these two models are derived. The possibility of construction of the universal quantum gates in both cases is shown.

Keywords: Quantum computer, Berry phase, Non-adiabatic geometric phase, Two-qubit gates

1 Introduction

The conceptions of quantum computer (QC) and quantum computation developed in 80-th [1], [2] were found to be fruitful both for computer science and mathematics as well as for physics [3]. Although a device being able to perform quantum computations is now far away from practical realization, there is a great number
of theoretical proposals of such a construct (see e.g. [6]–[18]). Intensive investigations on quantum information theory (see e.g. [4], [5], for a reference source on this subject) refreshed some interest on Berry phase [56]. The idea of using unitary transformations produced by Berry phase as quantum computations is proposed in [19], [20] and first realized in [21], [47] in a concrete model of holonomic quantum computer where the degenerate states of laser beams in non-linear Kerr cell are interpreted as qubits. For other references where Abelian Berry phase is considered in the context of quantum computer see e.g. [22]–[25]. If the corresponding energy level is degenerate non-Abelian phase takes place [57] that is actually a matrix mixing the states with the same energy. For further references on quantum computation based on non-Abelian geometric phase see e.g. [47]–[53].

On the other hand non-adiabatic analogue of Berry phase can exist and be measured if transitions in a given statistical ensemble do not lead to loose of coherence [71]. For loose of coherence in quantum computations related to geometric phase see [71]–[76]. Thus it is also possible to use the corresponding unitary operators to realize quantum gates. This fact has been noticed in [26], [27]. After that a lot of papers was published where the non-adiabatic phase is applied to realize the basic gates in different models of QC such as different NMR schemes [28]–[35], ion traps [36], [37], quantum dots [38], [39], and superconducting nanocircuits [40].

To analyze a concrete scheme for quantum computation based on geometric phase it is desirable to be aware of analytical expression for the evolution operator of the system at least at the moment when the measurement is performed. This article is concentrated on the computational aspect of geometric phase for the models which are relevant to QC. It should be emphasized that the form of the expression for the phase and the possibility of the derivation of such a formula itself thoroughly depend on the group-theoretic structure of the corresponding Hamiltonian. Therefore a method of the geometric phase calculation which would be more or less universal at least in the adiabatic case can appear to be useful. The material is divided in two parts. In section 2 the adiabatic geometric phase is considered. In subsection 2.1 we analyze the difficulties appearing in calculation of the Abelian adiabatic geometric phase (Berry’s phase) and propose a method of its explicit derivation for the case of the symmetric time-dependent Hamiltonian with constant non-degenerate energy levels. The symmetry of the Hamiltonian is supposed to reduce the Hamiltonian to that of a system with finite number of energy levels. In subsection 2.2 this method is generalized for the case when degeneration is present. In section 3 we consider non-adiabatic phase which can only conditionally be called ”geometric” for its dependence on concrete details of the dynamics. For this reason it is not possible to work out more or less general approach to the calculation of the non-adiabatic phase. Therefore two concrete cases are considered. In subsection 3.1 application of the Abelian non-adiabatic phase to one-qubit computation in a Caldeira-Legett-type model is considered. In subsection 3.2 we present an example of both non-Abelian and non-adiabatic phase computation in spin-3/2 quadrupole NMR resonance model.
2 Adiabatic Geometric Phase

2.1 Abelian Berry’s Phase

Here we consider a possible method of the adiabatic phase computation that seems to be effective in a broad range of practically relevant cases. Berry phase is a consequence of the adiabatic (or Born–Fock) theorem [55] which states that a parametric quantum system depending on a set of slowly (adiabatically) evolving parameters \( R_i(t), \quad i = 1, \ldots, N \) behaves in a quasi-stationary manner

\[
\hat{H}(R)|n(R)\rangle = E_n(R)|n(R)\rangle, \quad R = (R_1, \ldots, R_N)
\]

(1)

where \( \hat{H}(R) \) is the corresponding Hamiltonian and no energy level degeneration is assumed. The adiabaticity condition means that the frequencies \( \omega_n(R) = E_n(R)/\hbar \) are much greater than the characteristic Fourier frequencies of \( R_i(t) \). Thus the eigenvectors \( |n(R)\rangle \) evolve like

\[
|n(R)\rangle = \hat{S}(R)|n_0\rangle, \quad |n_0\rangle = |n(R(0))\rangle, \quad \hat{S}\hat{S}^\dagger = 1
\]

(2)

with unitary rotation \( \hat{S} \) describing the natural variation of \( |n(R)\rangle \) due to that of \( R(t) \). It corresponds to the following evolution law of the Hamiltonian

\[
\hat{H}(t) = \hat{S}(R(t))\hat{H}_0(t)\hat{S}^\dagger(R)
\]

(3)

where \( H_0(t) \) is diagonal in the basis \( \{|n_0\rangle\} \). What is the solution of the non-stationary Schrödinger equation

\[
\frac{i\hbar}{\partial t}\hat{U}(t)|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle
\]

(4)

for this case? A natural hypothesis would be that the evolution operator for \( |\psi\rangle \) has the form

\[
|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle
\]

where \( \hat{S} \) is defined by (2) and \( \hat{\Phi} \) simply produces the dynamic phase

\[
\hat{\Phi}(t)|n(R(t))\rangle = \exp\left(-i/\hbar \int_{0}^{t} E_n(\tau) d\tau\right)|n(R(t))\rangle.
\]

(5)

It is based on the analogue with the stationary case where evolution is simply represented by the dynamical phase factor \( \exp(-i/\hbar E_n t) \). Berry first observed [56] that the hypothesis is wrong. To see this it is sufficient to represent \( \hat{U} \) in the form

\[
\hat{U}(t) = \hat{S}(R(t))\hat{V}(t)
\]

and substitute it into the Schrödinger equation

\[
\frac{i\hbar}{\partial t}\hat{U}(t) = \hat{H}(t)\hat{U}(t).
\]

(6)
It gives
\[ i\hbar (\hat{V}\hat{V}^\dagger + \hat{S}^\dagger \nabla R \hat{S} \hat{R}) = \hat{H}_0(t). \]  
(7)

Now one can see that \( \hat{V} \) cannot be simply \( \hat{\Phi} \) because it has to cancel the second term in the right hand side of (7) besides of \( \hat{H}_0 \). It follows from (7) that
\[ \hat{V}(t) = \hat{\Gamma}(t)\hat{\Phi}(t) \]
where \( \hat{\Phi}(t) \) is determined by (5) and the following equation is valid for \( \hat{\Gamma}(t) \):
\[ \hat{\Gamma} \hat{\Gamma}^\dagger |n_0> = -(\hat{S}^\dagger \nabla R \hat{S}) |n_0>. \]  
(8)

It results in the evolution law for the state vector corresponding to the \( n \)-th energy level
\[ |\psi_n(t)> = e^{-i/\hbar \Phi_n(t)} e^{i\gamma_n(t)} |n(R(t))> \]  
where \( \Phi_n(t) \) is the phase factor in the right-hand side of (5) and \( \gamma_n(t) \) is given by
\[ \gamma_n(t) = \int_0^t A_n(R(\tau)) \dot{R}(\tau) d\tau, \quad A(R) = i <n|\nabla n(R)> = i \sum_{m \neq n} (\nabla R \hat{H}(R))_{mn} \left( E_n(R) - (E_m(R))^2 \right). \]  
(10)

Phase \( \gamma_n(t) \) becomes purely geometric while \( R(t) \) evolves cyclically: \( R(T) = R(0) \)
\[ \gamma_n(T) \equiv \gamma_n(\mathcal{C}) = \oint_{\mathcal{C}} A_n(R) dR. \]  
(11)

Here the integration contour \( \mathcal{C} \) is a closed curve in the parameter space described by \( R(t) \) as a radius-vector. It is easily seen from (11) that \( \gamma_n(\mathcal{C}) \) does not depend on the concrete details of the system’s dynamic if the adiabatic condition is held.

In this article we are interested in computing of \( \gamma_n(\mathcal{C}) \) in the most general case. The problem of derivation of \( \gamma_n(\mathcal{C}) \) was solved in various particular cases in large number of articles some years ago. First we would like to note that the straightforward formula
\[ B_n = \nabla R \times A_n = \sum_{m \neq n} \frac{(\nabla R \hat{H}(R))_{mn} \times (\nabla R \hat{H}(R))_{nm}}{(E_n(R) - (E_m(R))^2)} \]  
(12)
derived by Berry [56] by making use of the identity
\[ <m|\nabla n> = \frac{<m|\nabla \hat{H}|n>}{(E_n - E_m)}, \quad m \neq n \]
has not (despite of it’s beauty) much practical use because to apply it one should establish the analytical dependence of all \( E_n \) on \( R \) that is not a realistic task excluding some special cases. To see this one should attempt to apply formula (12) to the
case of a 3-level system substituting a generic solution $E_n(R)$ of the corresponding cubic equation therein.

It was first noticed in [61] that symmetries of the Hamiltonian $\hat{H}(R)$ play an important role in computing of $\gamma_n$. Indeed if one represents the result of the periodic motion $\hat{H}(0) = \hat{H}(T)$ as

$$|\psi(T) > = \hat{U}(T)|\psi(0) >$$

where as it follows from (11) $\hat{U}(T)$ must commute with $\hat{H}(0)$ so it can be represented as an exponent containing a linear combination of operators $\hat{X}_k$ which must commute with $\hat{H}(0)$ as well. Thus the operators $\hat{X}_k$ are integrals of motion and describe certain symmetries of the given system. Therefore in what follows we restrict ourselves with such systems whose Hamiltonian is an element of a finite Lie algebra. This assumption immediately gives the group-theoretic structure of $\hat{U}(T)$:

$$\hat{U}(T) = \exp \left( i \sum_i a_i H_i \right)$$

where $H_i$ are all linearly independent elements of the Cartan subalgebra and $a_i$ are some coefficients. Thus the problem reduces to computing of the coefficients $a_i$. In the simplest case of Lie algebras consisting of three elements this problem can be easily solved [62], [64], [65] for physically relevant cases of Heisenberg-Weyl algebra, $su(2)$ and $su(1,1)$. In each of them the evolution operator has the form

$$\hat{U}(t) = \exp \left( \zeta(t)\hat{X}_+ - \zeta^*(t)\hat{X}_- \right) \exp \left( i \phi(t) \hat{X}_3 \right)$$

provided the initial Hamiltonian is proportional to $\hat{X}_3$ where $\hat{X}_\pm$ and $\hat{X}_3$ are the corresponding generators of the algebras above. Their expressions for each concrete case are given in table 1. The Hamiltonian for $su(2)$ case describes an arbitrary spin in the magnetic field so all $J$’s are the angular momentum operators: $\hat{J}_\pm = 1/2(\hat{J}_1 \pm \hat{J}_2)$. $su(1,1)$ case corresponds to the evolution of squeezed states [66] of light in non-linear optics. Here $\hat{K}_+ = \hat{a}^{+2}/2$, $\hat{K}_- = \hat{a}^2/2$ and $\hat{K}_3 = \hat{a}^{+}\hat{a} + 1/2$ where $\hat{a}, \hat{a}^+$ are usual bosonic annihilation and creation operators. The last case represents a harmonic oscillator interacting with the time-dependent electric field. The simple commutation relations in these three algebras admit direct computation of Berry’s phase [62], [64], [65].

$$\gamma_m = m \oint_C \omega(\xi) = \int_S d \wedge \omega(\xi)$$

where $m$ is an eigenvalue of the corresponding $\hat{X}_3$, $S$ is the surface in the parameter space bounded by the closed curve $C$ and the expressions for $\omega(\xi)$ and its external derivative $d \wedge \omega(\xi)$ are given for each case in table 2. The geometric sense of the derived phase factor is the integral curvature over the surface bounded by the contour $C$ on the manifold the evolution operator belongs to. This manifold can
Table 1: Expressions for the operators $\hat{X}_\pm$, $\hat{X}_3$.

| Algebra | $X_+$ | $X_-$ | $X_3$ | Commutators |
|---------|-------|-------|-------|-------------|
| $su(2)$ | $\hat{J}_+$ | $\hat{J}_-$ | $\hat{J}_3$ | $[\hat{J}_3, \hat{J}_\pm] = \pm \hat{J}_\pm$ |
|         |       |       |       | $[\hat{J}_+, \hat{J}_-] = 2\hat{J}_3$ |
| $su(1.1)$ | $\hat{K}_+$ | $\hat{K}_-$ | $\hat{K}_3$ | $[\hat{K}_3, \hat{K}_\pm] = \pm \hat{K}_\pm$ |
|         |       |       |       | $[\hat{K}_+, \hat{K}_-] = -2\hat{K}_3$ |
| $H - W$  | $\hat{a}^+$ | $\hat{a}$ | $\hat{1}$ | $[\hat{1}, \hat{a}^+] = [\hat{1}, \hat{a}] = 0$ |
|          |        |       |       | $[\hat{a}, \hat{a}^+] = \hat{1}$ |

be generally expressed in the form $G/H$ where $G$ is the group manifold and $H$ is that of the stationary subgroup, i.e. the group whose Lie algebra consists of all operators commuting with $H(0)$ (in these three cases it is always $U(1)$). It is sphere in the case of $su(2)$, two-sheet hyperboloid in the case of $su(1.1)$ and plane in the case of Heisenberg-Weyl group. To complete the computation one has to establish correspondence between the complex parameter $\xi$ and physical parameters of the Hamiltonian. Let us do that for $SU(2)$. It is worth to notice that the result is completely determined by the geometric properties of the group and does not depend on the concrete representation. For this reason one can chose the fundamental representation of $SU(2)$ to simplify the derivation. Thus we take $H(0) = \omega_B \sigma_3$ which corresponds to the initial eigenvectors $|\pm> = (1(0), 0(1))^T$ ($T$ denotes transposition). The evolution operator generally parametrized by the spherical as

$$
\begin{pmatrix}
\cos\frac{\varphi}{2} & -\sin\frac{\varphi}{2} e^{-i\varphi} \\
\sin\frac{\varphi}{2} e^{i\varphi} & \cos\frac{\varphi}{2}
\end{pmatrix}
$$

(17)

rotates $H(0)$ into $H(t) = \omega_B n\sigma$ where $n = (\cos \varphi \sin \vartheta/2, \sin \varphi \sin \vartheta/2, \cos \vartheta/2)$ determines the direction of the magnetic field. On the other hand the direct computation of $exp(\zeta \hat{J}_+ - \zeta^* \hat{J}_-)$ gives for this representation $|\zeta| = \vartheta/2$, arg $\zeta = \varphi + \pi$. It leads to the well known expressions for the fictitious "strength field"

$$
B_\pm = \mp \frac{1}{2} \frac{R}{R^3}
$$

(18)

where $R$ denotes the true magnetic field vector in order not to confuse it with the
Table 2: Expressions for the forms $\omega$ and $d \wedge \omega$.

| Algebra | $\omega(\xi)$ | $d \wedge \omega(\xi)$ | Relation to $\zeta$ |
|---------|---------------|------------------------|---------------------|
| su(2)   | $\xi d\xi^* - \xi^* d\xi$ | $\frac{2 d\xi \wedge d\xi^*}{1 + |\xi|^2}$ | $|\xi| = \tan(|\zeta|)$, arg $\xi = \text{arg} \zeta$ |
| su(1.1) | $\xi d\xi^* - \xi^* d\xi$ | $\frac{2 d\xi \wedge d\xi^*}{1 - |\xi|^2}$ | $|\xi| = \tanh(|\zeta|)$, arg $\xi = \text{arg} \zeta$ |
| H-W     | $\xi d\xi^* - \xi^* d\xi$ | $2 d\xi \wedge d\xi^*$ | $\xi = \zeta$ |

fictitious one which determines the resulting Berry’s phase. It should be noted that the correspondence $\mathbf{R} \rightarrow \xi$ realizes the stereographic projection of the sphere with the coordinates $\vartheta, \varphi$ on the plane that points are labeled by $\xi$. The other two cases of $SU(1.1)$ and Heisenberg-Weyl groups can be considered in a similar manner.

Re-derivation of these simplest results has the intention to extract a universal idea of computing the geometric phase in more or less general case. For the sake of certainty let us assume the symmetry algebra of the Hamiltonian to be semisimple. It means that the generic evolution operator can be represented in the form

$$\hat{U}(t) = \prod_{\alpha \in \Delta_+} \hat{U}_\alpha(t)$$

(19)

where $\Delta_+$ denotes the set of the positive roots $\alpha$ and each $U_\alpha$ is analogous to (15) (see also table 1 for $su(2)$ and $su(1.1)$ cases):

$$\hat{U}_\alpha(t) = \exp \left( \zeta_\alpha(t) \hat{E}_\alpha - \zeta_\alpha^*(t) \hat{E}_{-\alpha} \right)$$

(20)

where the standard notations for the Cartan basis [67]

$$[H_\beta, \hat{E}_{\pm\alpha}] = \pm \alpha(H_\beta) \hat{E}_{\pm\alpha} \quad [\hat{E}_{\alpha}, \hat{E}_{-\alpha}] = H_\alpha, \quad [\hat{E}_\alpha, \hat{E}_\beta] = N_{\alpha\beta} \hat{E}_{\alpha+\beta}$$

(21)

are used. The pairs of generators $\hat{E}_{\pm\alpha}$ are analogous for $\hat{J}_\pm$ in $su(2)$ and $H_\alpha$’s are that of $\hat{J}_3$. Here $\alpha(H_\beta)$ and $N_{\alpha\beta}$ are constants that can be chosen rational and integer correspondingly. Taking account of the consideration above leads to some more detailed form for one-cycle evolution operator $\hat{U}(T)$ (14)

$$\hat{U}(\mathcal{C}) = \exp \left( i \sum_{\alpha \in \Delta_+} a^\alpha(\mathcal{C}) H_\alpha \right).$$

(22)
Each pair \((\hat{E}_\alpha, \hat{E}_{-\alpha})\) makes besides of the trivial group-theoretic contribution \(H_\alpha\) which produces the corresponding quantum number also a non-trivial one reflecting adiabatic dynamics of the system

\[
a^\alpha(C) = \oint_C \theta^\alpha(\zeta)
\]

(23)

where \(\theta_\alpha\) generally depends on all \(\zeta_\alpha(t)\). Thus to solve the problem one has to find this dependence making use of commutation relations (21) and then establish the connection between the parameters \(\zeta_\alpha(t)\) and the natural set of parameters \(R\) of the Hamiltonian. Unfortunately the hope to obtain a solution of even one of these two tasks that would be a non-trivial generalization of the above examples is not realistic. Neither the first part of the problem nor the second one could be solved in a way resulting in physically relevant explicit formulas having practical use. First the 1-forms \(\theta_\alpha\) fulfill Maurer-Cartan equations that express the quantity \(\hat{U}^\dagger d\hat{U}\) in terms of the 1-forms \(\omega_\alpha\) and \(\theta_i\)

\[
\hat{U}^\dagger(\zeta) d\hat{U}(\zeta) = i(\omega_\alpha(\zeta) \hat{E}_\alpha + \theta_i(\zeta) H_i)
\]

(24)

where the index \(i\) labels all linearly independent generators of the Cartan subalgebra (not all \(H_\alpha\) are so). For commutation relations (21) these equations take the form

\[
d \wedge \omega_\alpha = C_{\beta k}^\alpha \omega_\beta \wedge \theta_k + 1/2 C_{\beta \lambda}^\alpha \omega_\beta \wedge \omega_\lambda
\]

(25)

\[
d \wedge \theta_i = 1/2 C_i^\lambda \omega_\beta \wedge \omega_\lambda
\]

(26)

Equations (25), (26) describe the parallel transport on the coset manifold \(G/H\). The possibility to solve them depends on the manifold’s symmetry and of course is entirely determined by the structure constants \(C_\cdot\cdot\cdot\) that are built from the root vectors \(\alpha(\beta)\) and the constants \(N_{\alpha \beta}\). The general solution of this system can be constructed for very high symmetry of symmetric spaces [68] where the whole algebra can be split in two subsets \(X\) and \(Y\) such that

\[
[Y, Y] \subset Y, \quad [Y, X] \subset X, \quad [X, X] \subset Y.
\]

It is seen from (21) that the last condition is generally speaking not valid for our case because not all \(N_{\alpha \beta}\) are zeroes. Its geometric sense is that the considered coset spaces \(G/H\) are of more general symmetry type than symmetric spaces. Thus for \(G = SU(n)\) the space

\[
SU(n) / \underbrace{U(1) \times U(1) \ldots \times U(1)}_{n-1 \text{ times}}
\]

(27)

belongs to the more general class of Kählerian spaces. The general solution of (25), (26) for the types of spaces we are interested in is not obtained so far. Therefore the practical use of these equations is not high. Moreover the solution of the second part of the problem discussed is not possible for the same reason.
A simple and effective method of practical computation of geometric phase where it is not necessary to find the forms $\omega^\alpha, \theta^i$ is proposed in [75]. For this purpose we have to make some assumptions. First we regard the Hamiltonian to belong to a finite irreducible representation of a semisimple Lie algebra therefore $\hat{H}_0$ in (3) can always be represented as a finite matrix $\hat{H}_0 = R_i(t) H_i$ where the set $\{H_i\}$ is a basis of the Cartan subalgebra and $R_i(t)$ are parameters. Then we suppose the energy levels $E_m$ to be constants. It corresponds to a rotation-type evolution (3) where $\hat{H}_0$ does not depend on $t$. Such a situation takes place practically in all experiments on the geometric phase measurement. This makes it possible to regard $E_m$ as additional secondary parameters to be found just once (may be numerically).

The third assumption is that the spectrum remains always non-degenerate i.e., no crossing of energy levels occurs. As the spectrum of the Hamiltonian is finite, the state vector $|\varphi_m\rangle$ is a unit vector $m$ in $\mathbb{C}^n$, so $A_m$ is

$$A_m = \frac{i}{2} (m^* dm - m dm^*). \quad (28)$$

As the evolution is adiabatic, the spectrum of $H(t)$ remains always non-degenerate if it was so at the initial time. Then there is always a nonzero main minor of $H - E_m$ which we assume to consist always of the first $n - 1$ lines and columns of $H - E_m$.

Denoting the matrix consisting of the first $n - 1$ lines and columns of $H$ by $H_\perp$ we come to the condition

$$\det(H_\perp - E_m) \neq 0 \quad (29)$$

Making use of this condition one can represent $n$ in the uniform coordinates

$$m = \frac{(\xi_m, 1)}{\sqrt{1 + |\xi_m|^2}}$$

and express $\xi_m$ in terms of $H_{ij}$ for $1 \leq i, j \leq n - 1$ and $E_m$:

$$\xi_m = (H_\perp - E_m)^{-1} h, \quad h_i = -H_{in}, \quad (30)$$

where $h$ is a vector in $\mathbb{C}^{n-1}$ but not in $\mathbb{C}^n$. Thus we have for $A_m$

$$A_m = \frac{i}{2} (\xi_m^* d\xi_m - \xi_m d\xi_m^*). \quad (31)$$

where $\xi_m$ is completely determined by (30). Note that the result obtained is purely geometrical because it can be expressed of the Kählerian potential

$$F = \log(1 + |z|^2)$$

where $z$ is a vector in $\mathbb{C}^N$ consisting of $n(n - 1)/2$ independent components of all $\xi_m$. The function $F(z, z^*)$ determines all the geometrical properties of the state space (27). Particularly its metric tensor is

$$g_{ij} = \frac{\partial^2 F(z, z^*)}{\partial z_i \partial z_j^*}.$$
It should be emphasized that the simplification of the problem reached here is based on the fact that \( \dot{E}_m = 0 \) so one can include it in new parameters and use them rather than \( R_i \). Therefore the dependence of \( E_m \) on \( R \) is not required. One can calculate \( E_m \) numerically and substitute it into the formulas regarding this quantity as one more external parameter. Moreover to find \( \gamma_m \) one needs only the energy \( E_m \) but not the whole spectrum as in (12). It can become an important issue if one considers partially solvable models. The requirement \( \dot{E}_m = 0 \) is sufficient because otherwise one has to solve the secular equation at each moment \( t \) that is equivalent to the numerical solution of the non-stationary Schrödinger equation itself and therefore it makes the discussed method useless.

Let us now consider some simple applications of the proposed method. First let us see how it works for the trivial case \( n = 2 \). (1) reduces then to two linearly dependent equations

\[
(B_3 \mp B)\xi + (B_1 - iB_2) = 0
\]
\[
(B_1 + iB_2)\xi + (-B_3 \mp B) = 0
\]

Here we returned to the usual notations of the magnetic field components \( B_i \) and \( \pm B = \pm |B| \) is the energy of the state \( |\pm> \). Choosing one of the equations and taking the spherical coordinates we come to one of the relations

\[
\xi = -\tan \vartheta/2 \ e^{-i\varphi}, \quad \xi = \cot \vartheta/2 \ e^{-i\varphi}.
\]

for the upper and lower sign correspondingly. Thus these are the coordinates of stereographic projection made from the north (south) pole of the sphere. Substituting it into the formula for \( \omega_{\pm}(\xi) \) (see Table 2) and integrating over a contour \( C \) we get the well known result \[56\]

\[
\gamma_{\pm} = \pm \frac{1}{2} \oint_C \frac{\xi^* d\xi - \xi d\xi^*}{1 + |\xi|^2} = \pm \frac{1}{2} \Omega(C),
\]

where \( \Omega(C) \) is the solid angle corresponding to the closed contour \( C \) on the sphere.

One more example which is less trivial is a generic three-level system. The \( k \)-th eigenvector \( \xi_k \) is then two-dimensional and some trivial algebra gives for its components

\[
\xi_1 = \Delta_1/\Delta_0, \quad \xi_2 = \Delta_2/\Delta_0,
\]
\[
\Delta_0 = (H_{11} - E_k)(H_{22} - E_k) - |H_{12}|^2
\]
\[
\Delta_1 = H_{23}H_{12} - H_{13}(H_{22} - E_k)
\]
\[
\Delta_2 = H_{13}H^*_12 - H_{23}(H_{11} - E_k)
\]

Here we have omitted where possible the index \( k \). Substitution of these expressions into (31) gives the final formula for this case. Note that the use of formula (12)
here would lead to sufficient computational difficulties even after making further
simplifying assumptions [69]. The proposed approach makes concrete calculations
visibly easier and more compact although the final formulas are not of esthetic value.
For the illustrative purpose we take here the case when all \( H_{ij}, i \leq j \) but \( H_{12} \) do
not depend on \( t \). Then substitution of (32) into (31) gives

\[
\omega_k(\xi) = i C_k \left[ A - D_k \sin(\phi_{12} + \phi_{23} - \phi_{13}) \right] d\phi_{12},
\]

\[
C_k = \frac{|H_{13}| |H_{23}| |H_{12}|}{\Delta_0^2(E_k) + |\Delta_1(E_k)|^2 + |\Delta_2(E_k)|^2},
\]

\[
A = \frac{1}{|H_{13}|^2} - \frac{1}{|H_{23}|^2},
\]

\[
D_k = H_{11} + H_{22} - 2E_k
\]

where \( \phi_{ij} \) are arguments of the complex numbers \( H_{ij} \). As it was discussed above
the condition \( \Delta_0(t) \neq 0 \) is supposed to be held everywhere on \( C \). For other cases of
the geometric phase in the 3-level system see [63].

### 2.2 Non-Abelian Wilczek–Zee phase

Now we proceed with a more general case of degenerate spectrum. Quantum com-
putation for this case generated by an adiabatic loop in the control manifold is de-
termined by the same quasi-stationary Schrödinger equation (1) where each energy
level \( E_m \) corresponds to a set of eigenstates \( |m_a> \), \( a = 1, \ldots d_m \). Cyclic evolution
of the parameters results in

\[
|m_a(T)> = U_{ab}(T) |m_b(0)>
\]

where the matrix \( U \) is presented by a \( P \)-ordered exponent

\[
U(C) = P \exp \left( \oint_C A_m \right), \quad (A_m)_{ab} = i <m_b | dm_a > .
\]

In this section we generalize the proposed approach to the geometric phase compu-
tation for the generic case of degenerate energy levels [75].

The set of eigenvectors \( \xi_{ma}, a = 1, \ldots d_m \) must obey the equation

\[
(H_{\perp}^{(d_m)} - E_m) \xi_{ma} = h c_a.
\]

Here the matrix \( H_{\perp}^{(d_m)} \) is constructed from the first \( n - d_m \) lines and columns of \( H \),
\( c_a \) are arbitrary \( d_m \)-dimensional vectors and \( h \) is the following \( (n - d_m) \times d_m \)-matrix:

\[
\begin{pmatrix}
H_{1,n-d_m+1} & \cdots & H_{1,n} \\
\vdots & \ddots & \vdots \\
H_{n-d_m,n-d_m+1} & \cdots & H_{n-d_m,n}
\end{pmatrix}
\]
Of course it has sense only if the condition
\[ \det(H_{\perp}^{(d_m)}(t) - E_m) \neq 0 \] (40)
is valid along the evolution process. The set of vectors $\xi_{ma}$ must be orthogonalized by the standard Gram algorithm and after that we get the orthonormal set of the eigenvectors $z_a$ (here and below we has omitted the index $m$) in the form
\[ z_a = \frac{1}{\det \Gamma_{a-1}} \begin{pmatrix} x_1 \\ \vdots \\ \langle \xi_a \mid \xi_1 \rangle \end{pmatrix}, \] (41)
where $x_b = (\xi_b, c_b)$ and $c_a$ is chosen to be the standard orthogonal set $c_a = (0 \ldots 1 \ldots 0)$. The matrices $\Gamma_a$ are determined by
\[ \Gamma_a = \begin{pmatrix} 1 + \langle \xi_1 \mid \xi_1 \rangle & \cdots & \langle \xi_1 \mid \xi_a \rangle \\ \vdots & \ddots & \vdots \\ \langle \xi_a \mid \xi_1 \rangle & \cdots & 1 + \langle \xi_a \mid \xi_a \rangle \end{pmatrix} = 1 + Z_a^\dagger Z_a, \] (42)
where the $(n - d_m) \times a$-matrix $Z_a$ consists of $a$ first lines of the $(n - d_m) \times d_m$-matrix $Z = (H_{\perp}^{(d_m)} - E_m)^{-1} h$. Using (42) and (41) we come to the final expression for the matrix-valued 1-form $A$:
\[ A = \frac{i}{2} \frac{g_{ij} \xi_j^d \xi_i - d \xi_j^* \xi_i + 2 \omega_{ab}}{\det(1 + Z_{a-1}^\dagger Z_{a-1}) \det(1 + Z_{b-1}^\dagger Z_{b-1})}, \] (43)
where
\[ g_{ij} = \Gamma_i^a \Gamma_j^b, \quad \omega_{ab} = \langle \xi_j \mid d \text{Im}(g_{ab}) \mid \xi_i \rangle + \sum_{i=1}^{\min(a,b)} d \text{Im}(g_{ai}^i), \]
and $\Gamma_i^a$ is the cofactor of $\xi_i$ in $\Gamma_a$. Note that the change of our basis $c_a$ by $c'_a = U_{ab}(\Lambda) c_b$ leads to a standard gauge transformation of $A$
\[ A' = UAU^\dagger + i(dU)U^\dagger. \]
The formula (43) is the desired expression of $A$ in terms of the matrix elements of the Hamiltonian. It is correct if condition (40) is valid. It is not nevertheless a principal restriction because $d_m$ does not depend on time due to adiabaticity of the evolution and there is always at least one nonzero $n - d_m$-order minor of $H$. Then, if the minor we choose vanishes somewhere on the loop $C$ one can always take local coordinates such that the techniques considered is applicable on each segment of $C$. It should also be noted at the end of this section that the idea of physical realization of the quantum gates based on the concrete system driven by
external electromagnetic fields appears if one takes into account that for $A_n$, $E_\alpha$ can be realized by means of ordinary bosonic creation and annihilation operators, namely $E_\alpha = a_i^\dagger a_j$ for some $1 \leq i, j \leq n$. Then $E_\alpha$ represents nothing but two-mode squeezing operator. Thus the model considered can be applied to optical HQC with $n$ laser beams (the case $n=2$ is considered in [21]) and the logical gates $U_\alpha$ are just two-qubit transformations realized by transformation of two laser beams.

The method presented here enables one to build in principal any computation for HQC described by a Hamiltonian with a stationary spectrum in terms of experimentally measured values exactly the matrix elements of the Hamiltonian. The method depends weakly on the dimension of the qubit space which other models based on various parameterizations of the system’s evolution operator are very sensitive to. Application of this method to a concrete physical model will be discussed elsewhere.

3 Non-Adiabatic Geometric Phase

3.1 Abelian Non-Adiabatic Phase

The adiabatic condition of quantum system’s evolution is strong enough to restrict sufficiently the scope of the search for realistic candidates for practical realization of quantum computations despite of some attractive features of the adiabatic case such as fault tolerance due to independence of the evolution law on the details of the parameters’ dynamics etc. Therefore it is desirable to find physically relevant cases for which on the one hand this condition would be not necessary but on the other hand the coherency in such a system would be not yet violated so that the notion of the phase shift itself could have physical sense. As the adiabatic theorem is no longer valid the property of universality of the system’s dynamics (independence of the concrete form of the functions $R_i(t)$) is no more preserved and the evolution law is sufficiently more complicated. Then one cannot hope to carry out a general approach to derivation of the corresponding phase shift because in each case it depends on the fine details of the parameters variation. For the same reason the phase can be called ”geometric” only conditionally because geometric intuition is no more helpful for this case e.g. the result can be represented as an integral over $t$ rather than over a contour that expresses mathematically the thesis above. On the other hand non-adiabatic conditional geometric phase that was theoretically predicted in [60] can be measured if transitions taking place in the system do not lead to decoherence [71]. Therefore it is also possible to use the corresponding unitary operators to perform quantum calculations. This fact has been noticed in [26, 27] (see also [28–35] for further references).

Let us consider a parametric quantum system described by the Hamiltonian $H(R)$, where $R(t)$ is a set of arbitrarily evolving parameters. We suppose that evolution of the Hamiltonian is determined by unitary rotation [40] Looking for
particular solutions of the Schrödinger equation (4) (here we supposed $\hbar = 1$) we take a rotating frame by assigning $\tilde{\psi}(t) = U(t)\psi(t)$ and get in such a way

$$i\frac{\partial \tilde{\psi}}{\partial t} = (H_0(t) - i U^\dagger(t) \dot{U}(t)) \tilde{\psi}(t).$$

(44)

Of course, this transformation generally does not help to solve equation (4) due to the fact that the algebraic structure of the coupling term $-i U^\dagger \dot{U}$ can appear to be rather complicated and the last generally does not commute with $H_0$. However if a receipt is known how to evaluate the last term in (44), further solution of this equation is straightforward:

$$\psi(t) = e^{-i \phi_n(t)} T \exp \left( -i \int_0^t U^\dagger(\tau) \dot{U}(\tau) \, d\tau \right) \psi(0),$$

(45)

where $\phi_n(t) = \int_0^t E_n(\tau) \, d\tau$ is so called dynamic phase, $T$ denotes time-ordering and $E_n$ are elements of $H_0$ that is by definition diagonal. Of course if there is no way to find $U^\dagger(\tau) \dot{U}(\tau)$, expression (45) is useless.

Let us illustrate it for the simplest case of spin 1/2 in the non-adiabatically rotating magnetic field [72]. Uniform rotation in the plane $\vartheta = \text{const}$ is represented by

$$H(t) = e^{\pm i \omega_R t} \hat{J}_3 e^{-i \vartheta} \hat{J}_2 \left( \Omega \hat{J}_3 \right) e^{-i \vartheta} \hat{J}_2 e^{\mp i \omega_R t} \hat{J}_3$$

(46)

where the sign $+$ ($-$) corresponds to the left (right) polarization. Application of (44) to (46) gives for the Hamiltonian in the rotating frame

$$H_1(t) = e^{-i \vartheta} \hat{J}_2 \left( \Omega \hat{J}_3 \right) e^{-i \vartheta} \hat{J}_2 \pm \omega_R \hat{J}_3.$$  

(47)

To diagonalize Hamiltonian (47) one has to apply one more rotation to it

$$H_2(t) = V H_1(t) V^\dagger, \quad V = e^{i \vartheta^*} \hat{J}_2$$

where the angle $\vartheta^*$ does not coincide with $\vartheta$ due to the second non-adiabatic term. It should rather fulfill the condition

$$\tan \vartheta^* = \frac{\sin \vartheta}{\cos \vartheta \pm \omega_R/\Omega}. $$

(48)

The second term in the denominator of (48) is the measure of non-adiabaticity of the motion. It is clear that the angle $\vartheta^*$ replaces the usual azimuthal angle $\vartheta$ in the formula for the geometric-like phase:

$$\gamma_\pm = \mp m_3 2\pi \left( 1 - \cos \vartheta^* \right)$$

(49)

where $m_3$ is the third spin projection. Formula (49) is a natural generalization of the usual Berry’s formula for the adiabatic case and coincides with it in the limit
\( \omega_R/\Omega \to 0 \). Note that the dependence of the result on \( \omega_R \) reflects the fact the phase is no longer truly geometric because \( \omega_R \) characterizes the rotation velocity and thus the velocity of the motion along the contour in the parameter space.

As an example of the application of the non-adiabatic formula above we propose a realization of quantum gates for a concrete 4-level quantum system driven by external magnetic field \([77]\). Let us consider a system of two qubits in a bosonic environment described by the Hamiltonian

\[
H = H_S + H_B + H_{SB},
\]

where \( H_S \) is the Hamiltonian of two coupled spins

\[
H_S = H_S^{(0)} + H_S^{\text{int}} = \frac{\omega_{01}}{2} \sigma_{z1} \otimes 1_2 + \frac{\omega_{02}}{2} 1_2 \otimes \sigma_{z2} + \frac{J}{4} \sigma_{z1} \otimes \sigma_{z2},
\]

where \( J \) is the coupling constant, \( H_B \) is the Hamiltonian of the bosonic environment

\[
H_B = \sum_k \omega_{bk} (\hat{b}_k^+ \hat{b}_k + 1/2),
\]

and \( H_{SB} \) is the Hamiltonian of the spin-environment interaction.

\[
H_{SB} = H_{SB}^{(1)} + H_{SB}^{(2)},
\]

\[
H_{SB}^{(a)} = S_z^{(a)} \sum_k (g_{ak} \hat{b}_k^+ + g_{ak}^* \hat{b}_k) \quad a = 1, 2.
\]

Here

\[
S_z^{(1)} = \sigma_{z1} \otimes 1_2, \quad S_z^{(2)} = 1_2 \otimes \sigma_{z2},
\]

\( \sigma_z \) is the third Pauli matrix, \( 1_2 \) is 2 \( \times \) 2 unit matrix, \( \hat{b}_k^+, \hat{b}_k \) are bosonic creation and annihilation operators and \( g_{ak} \) are complex constants. We assume that the two spins under consideration are not identical so that \( \omega_{01} \neq \omega_{02} \). The Hamiltonian determined by \([50] - [51]\) is a natural generalization of Caldeira-Legett Hamiltonian \([74]\) for the case of two non-interacting spins. Let such a system be placed in the magnetic field affecting the spins but not the phonon modes. The only change to be made in the spin part \([51]\) is the substitution

\[
\omega_{s}\sigma_z \to B\sigma_z,
\]

Three components of \( B \) represent a control set for the qubits under consideration. Evolution of \( B(t) \) generates evolution of the reduced density matrix \( \rho_s(t) \) that describes the spin dynamics

\[
i \frac{\partial \rho_s(t)}{\partial t} = H_S \rho_s(t), \quad \rho_s(t) = U(t)\rho(0)U^+(t).
\]
Thus given curve in the control space corresponds to a quantum calculation in which each qubit is to be processed independently. To obtain such a calculation as a function of control parameters we first recall some common issues of spin dynamics. We consider the external magnetic field as a superposition of a constant component and a circular polarized wave:

\[ B = B_0 + B_1 e^{i\omega_R t}, \]  

(56)

where \( B_0 \) is perpendicular to \( B_1 \). It is well known that the case of the circular polarization is exactly solvable. The evolution of an individual spin corresponding to the Hamiltonian

\[ H = -\mu B \]  

(57)

is determined by \([15]\) where \( \hat{X}_\pm, \hat{X}_3 \) are replaced by \( S_\pm = S_x \pm iS_y, S_z \) correspondingly and

\[ \zeta(t) = |\zeta(t)| \exp(i\Delta\omega t + i\alpha(t) + i\pi/2), \]  

(58)

\[ |\zeta(t)| = \frac{\omega_\perp \sin(\Omega t/2)}{\sqrt{(\Delta\omega)^2 + \omega_\perp^2}}, \]

\[ \alpha(t) = \arctan \left( \frac{\Delta\omega}{\Omega} \tan(\Omega t/2) \right), \]

\[ \phi(t) = -\omega_\perp (\xi_1n_2 + \xi_2n_1), \]  

(59)

where \( \Delta\omega = \omega_\parallel - \omega_R, \Omega^2 = (\Delta\omega)^2 + \omega_\perp^2, \omega_\perp \) and \( \omega_\parallel \) are Rabi frequencies corresponding to \( B_0 \) and \( B_1 \) respectively and finally \( n \) is the unit vector along \( B_1 \).

It is known \([71]\) that the pure states acquire within the rotating wave approximation a phase factor that after one complete cycle \( T = 2\pi/\omega_R \) is:

\[ |m(T) > = \exp(-i\phi_D + i\gamma) |m(0) >, \]  

(60)

where \( m \) is the azimuthal quantum number and the phase is split in two parts: dynamic

\[ \phi_D = 2\pi m \frac{\Omega}{\omega_R} \cos(\theta - \theta^*) \]

and geometrical

\[ \gamma = -2\pi m \cos \theta^*, \]  

(61)

where \( \cos \theta = B_0/B \) (\( B = B_0 + B_1 \)) and \( \theta^* \) is determined by formula \((49)\). The phase shift between the states \( |\pm 1/2 > \) results then in

\[ \Delta\phi_g = -2\pi \cos \theta^* \]  

(62)
that is nothing but the solid angle enclosed by the closed curve $\mathbf{B}(0) = \mathbf{B}(T)$ on the Bloch sphere. If the rotation is slow such that $\omega_R/\Omega \to 0$ then $\theta^* \to \theta$ and phase shift\(^{(62)}\) coincides with the usual Berry phase.

Thus the adiabaticity condition is not really necessary for obtaining of the geometrical phase in an ensemble of spins if the decoherence time is much greater than $T$. Therefore one can attempt to use this phase to get quantum gates such as CNOT. Calculation of the corresponding phase factors is rather straightforward because the free and the coupling parts of the spin Hamiltonian commute with each other

$$\left[ H_{S}^{(0)}, H_{S}^{\text{int}} \right] = 0.$$ 

Therefore the coupling part can be diagonalized simultaneously with the free part by applying of the transformation $U = U_1 \otimes U_2$ where $U_{1,2}$ are the diagonalizing matrices for each single-spin Hamiltonian respectively. This simple fact together with the following obvious identity

$$U^\dagger \dot{U} = U_1^\dagger \dot{U}_1 \otimes 1_2 + 1_2 \otimes U_2^\dagger \dot{U}_2$$

the final formula for the part of the evolution operator that stands for the non-adiabatic geometric phase

$$U_g = \exp(-2\pi i \cos \theta_1^* S_{1z}) \otimes \exp(-2\pi i \cos \theta_2^* S_{2z}), \quad \text{(63)}$$

where

$$\tan \theta_1^* = \frac{\sin \theta_1}{\cos \theta_1 + \omega_R/\Omega_1}, \quad \tan \theta_2^* = \frac{\sin \theta_2}{\cos \theta_2 + \omega_R/\Omega_2}$$

and

$$\cos \theta_1 = \omega_{01}/\Omega_1, \quad \Omega_1^2 = \omega_{01}^2 + \omega_1^2,$$

$$\cos \theta_2 = \omega_{02}/\Omega_2, \quad \Omega_2^2 = \omega_{02}^2 + \omega_2^2.$$ 

Note that gate\(^{(63)}\) is symmetric with respect to the spin transposition as it should be and does not depend on $J$ that is typical for geometrical phase in spin systems where the phase depends only on the position drawn by the vector $\mathbf{B}$ on the Bloch sphere. As $J$ does not affect this position, it is absent in the final result. We do not consider here the dynamic phase determining by the factor

$$U_d = \exp \left(-\frac{i}{\hbar} \tilde{H}_S T \right).$$

It is so because one can eliminate it by making use of the net effect of the compound transformation proposed in \(^{[22]}\). After this transformation that is generated by two different specifically chosen contours the dynamic phase acquired by the different
spin states becomes the same and the geometric phase of each state is counted twice. After that we get (up to a global phase) the following quantum gate

\[
U_g = \begin{pmatrix}
  e^{i(\gamma_1 + \gamma_2)} & 0 & 0 & 0 \\
  0 & e^{i(\gamma_1 - \gamma_2)} & 0 & 0 \\
  0 & 0 & e^{i(-\gamma_1 + \gamma_2)} & 0 \\
  0 & 0 & 0 & e^{-i(\gamma_1 + \gamma_2)}
\end{pmatrix}.
\] (64)

Thus we have constructed the quantum gate, which possess the advantage to be fault tolerant with respect to some kinds of errors such as the error of the amplitude control of \(B\). On the other hand this approach makes it possible to get rid of the adiabaticity condition that strongly restricts the applicability of the gate. Instead of this condition one needs some more weak one: \(\tau \gg \omega^{-1}_R\), where \(\tau\) is the decoherence time.

### 3.2 Non-Abelian and Non-adiabatic Phase

In this section we give an example of both non-Abelian and non-adiabatic phase for a concrete 4-level quantum system driven by external magnetic field \([76]\). Let us consider a spin-3/2 system with quadrupole interaction. Physically it can be thought of as a single spin-3/2 nucleus. A coherent ensemble of such nuclei manifest geometric phase when placed in rotating magnetic field. This phase is non-Abelian due to degenerate energy levels with respect to the sign of the spin projection. Depending on the experiment setup the phase can be both adiabatic as in Rb experiment by Tycko \([70]\) and non-adiabatic as in Xe experiment by Appelt et al \([71]\). This non-Abelian phase results in mixing of \(\pm 1/2\) states in one subspace and \(\pm 3/2\) in another one and thus can be regarded as a 2-qubit gate. The gate is generated by a non-Abelian effective gauge potential \(A\) that is the subject of computation in this section.

We assume the condition of the \(^{131}\)Xe NMR experiment to be held so one does not need to trouble about the coherency in the system. The last is described by the following Hamiltonian in the frame where the magnetic field is parallel to the z-axis \((\hbar = 1)\)

\[
H_0 = \omega_0(J_3^2 - 1/3 j(j + 1)).
\] (65)

Here and in what follows we omitted the hat symbol over all \(J\)’s for the sake of simplicity. For a spin-3/2 system we choose the third projection of the angular momentum in the form

\[
J_3 = \begin{pmatrix}
  3/2 & 0 & 0 & 0 \\
  0 & -3/2 & 0 & 0 \\
  0 & 0 & 1/2 & 0 \\
  0 & 0 & 0 & -1/2
\end{pmatrix} = \begin{pmatrix}
  3/2\sigma_3 & 0 \\
  0 & 1/2\sigma_3
\end{pmatrix},
\] (66)
Then two other projection operators are

\[ J_1 = \begin{pmatrix} 0 & 0 & \sqrt{3}/2 & 0 \\ 0 & 0 & 0 & \sqrt{3}/2 \\ \sqrt{3}/2 & 0 & 0 & 1 \\ 0 & \sqrt{3}/2 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} \sigma_1 \end{pmatrix}, \]  

(67)

\[ J_2 = \begin{pmatrix} 0 & 0 & 0 & -\sqrt{3}/2 \\ 0 & 0 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & 0 & i & 0 \\ -\sqrt{3}/2 & 0 & i & 0 \end{pmatrix} = \begin{pmatrix} 0 & -i \frac{\sqrt{3}}{2} \\ i \frac{\sqrt{3}}{2} \sigma_3 \sigma_2 \end{pmatrix}. \]  

(68)

In the laboratory frame the Hamiltonian takes the form

\[ H = \omega_0((Jn)^2 - 1/3j(j + 1)) = e^{-i\varphi J_z} e^{-i\theta J_y} H_0 e^{i\varphi J_z} e^{i\theta J_y}. \]  

(69)

Rotation around the z-axis means that \( \varphi = \omega_1 t \) and one should perform the unitary transformation

\[ |\psi> = U_1 |\tilde{\psi}>, \quad U_1 = e^{-i\omega_1 t J_z}. \]  

(70)

In the rotating frame we get

\[ H_1 = e^{-i\theta J_y} (\omega_0 J_y^2 - \omega_1 \tilde{J}_3) e^{i\theta J_y} - \frac{5\omega_0}{4}, \]  

(71)

where

\[ \tilde{J}_3 = e^{i\theta J_y} J_z e^{-i\theta J_y}. \]

Expression (71) is equivalent to

\[ H_1 = \begin{pmatrix} \omega_0 - \frac{3}{2} \omega_1 \cos \theta \sigma_3 & \omega_1 \sqrt{3}/2 \\ \omega_1 \sqrt{3}/2 & -\omega_0 - \frac{1}{2} \omega_1 \cos \theta \sigma_3 + \omega_1 \sin \theta \sigma_1 \end{pmatrix}. \]  

(72)

It is convenient to diagonalize this matrix in two steps. First we get rid of \( \sigma_1 \) in the last matrix element by performing of the block-diagonal transformation

\[ U_2 = \text{diag}(1, e^{-i\alpha \sigma_3}), \]  

(73)

where \( \tan \alpha = 2 \tan \theta \). Thereafter the Hamiltonian \( H_1 \) reads

\[ H_1 = \begin{pmatrix} \omega_0 - \frac{3}{2} \omega_1 \cos \theta \sigma_3 & \omega_1 \sqrt{3}/2 \\ \omega_1 \sqrt{3}/2 & -\omega_0 - \frac{1}{2} \omega_1 \cos \theta \cos \alpha \sigma_3 \end{pmatrix}. \]  

(74)

At the second step we apply the transformation

\[ \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}, \]  

(75)
where \( \beta_1, \beta_2 \) are diagonal \( 2 \times 2 \) matrices that must obey the unitarity condition

\[
|\beta_1|^2 + |\beta_2|^2 = 1. \tag{76}
\]

Supposing \( \beta_1, \beta_2 \) to be real and performing transformation \([75]\) we come to the diagonalization condition in the form

\[
\xi (\beta_1^2 - \beta_2^2) + (\lambda_1 - \lambda_2) \beta_1 \beta_2 = 0, \tag{77}
\]

where \( \lambda_1, \lambda_2 \) are \( 2 \times 2 \) diagonal matrices and \( \xi \) is a parameter

\[
\lambda_1 = \omega_0 - 3/2 \omega_1 \cos \theta \sigma_3, \tag{78}
\]
\[
\lambda_2 = -\omega_0 - 1/2 \omega_1 \cos \theta \cos \alpha \sigma_3, \tag{79}
\]
\[
\xi = \omega_1 \sqrt{3/2} \sin \theta \tag{80}
\]

Assuming \( \beta_2 = \mu \beta_1 \) where \( \mu \) is a diagonal \( 2 \times 2 \) matrix as well we come to the following expressions for the matrix elements of \( \mu \)

\[
\mu_i = k_i + \sqrt{1 + k_i^2}, \tag{81}
\]

where

\[
k_i = \frac{\Delta \lambda_i}{2\xi}, \quad \Delta \lambda_i = \lambda_{1i} - \lambda_{2i}.
\]

Finally we get for the matrix elements of \( \beta_{1,2} \)

\[
\beta_{1i}^2 = 1/2 (1 + k_i^3)^{-1/2} \left( k_i + \sqrt{1 + k_i^2} \right)^{-1}, \tag{82}
\]
\[
\beta_{2i}^2 = 1/2 \left( 1 + \frac{k_i}{\sqrt{1 + k_i^2}} \right), \tag{83}
\]

Now one can evaluate the connection 1-form. It is convenient to represent it as follows:

\[
A = iU^+ dU = A d\phi = \begin{pmatrix} A_{3/2} & A^{tr} \\ A^{tr} & A_{1/2} \end{pmatrix} d\phi, \tag{84}
\]

where all matrix elements of \( A \) denote \( 2 \times 2 \) matrix-valued blocks, \( U = U_1 U_2 U_3 \) and \( U_i \) are determined by \([70],[73],[75]\) correspondingly. Here tilde denotes a
transposed matrix. After some algebra we get for the matrix elements of (84)

\[ A^{tr} = \frac{1}{2} \beta_1 \beta_2 (3 - \cos \alpha) \sigma_3 + \frac{1}{2} \sin \alpha \beta_2 \sigma_1 \beta_1, \] (85)

\[ A_{3/2} = (a_{3/2} + b_{3/2} \sigma_3 + c_{3/2} \sigma_1) d\phi, \] (86)

\[ a_{3/2} = \frac{1}{4} (3\beta_{11} - 3\beta_{12} + \beta_{21}^2 \cos \alpha - \beta_{22}^2 \cos \alpha), \] (87)

\[ b_{3/2} = \frac{1}{4} (3\beta_{11} + 3\beta_{12} + \beta_{21}^2 \cos \alpha + \beta_{22}^2 \cos \alpha), \] (88)

\[ c_{3/2} = -\frac{1}{2} \sin \alpha \beta_{21} \beta_{22}, \] (89)

\[ A_{1/2} = (a_{1/2} + b_{1/2} \sigma_3 + c_{1/2} \sigma_1) d\phi, \] (90)

\[ a_{1/2} = \frac{1}{4} (3\beta_{11}^2 - 3\beta_{12}^2 + \beta_{21}^2 \cos \alpha - \beta_{22}^2 \cos \alpha), \] (91)

\[ b_{1/2} = \frac{1}{4} (3\beta_{11}^2 + 3\beta_{12}^2 + \beta_{21}^2 \cos \alpha + \beta_{22}^2 \cos \alpha), \] (92)

\[ c_{1/2} = -\frac{1}{2} \sin \alpha \beta_{11} \beta_{12}, \] (93)

where \( d\phi = \omega_1 dt \). Note that as \( A \) does not depend on time, the final solution does not require \( T \)-ordering. It should be also emphasized here that in the non-adiabatic case we discuss the term \( A_{3/2} \) contains non-diagonal terms that is not the case when the adiabaticity condition is held \([58]\). Now the solution of the problem takes a particular form of (45):

\[ \psi(t) = e^{-i\phi_n(t)} e^{-i\omega_1 t A} \psi(0), \] (94)

Formula (94) solves the problem of the evolution control for the system under consideration. The resulting quantum gate is entirely determined by \( A \) and the evolution law of the magnetic field, i.e. by a contour in the parameter space. Of course it is always possible to choose the parameters so that \( A \) turns out to generate a 2-qubit transformation that produces a superposition of basis states. For this reason the gate can be thought of as a universal one \([14]\). Of course, a suitable speed of the parameters evolution can not be reached by rotation of the sample as it took place in the experiment by authors of \([71]\). Nevertheless it is clear that this manner of control is not principle and one could imagine a situation where the parameters evolution is provided by the controlling magnetic field by adding a non-stationary transverse component. It should be also noted here that general formulas \([85]\) do
not provide an apparent way to realize CNOT gate or another common 2-qubit gate. They just give the evolution law of the system provided that the external parameters vary as shown above. To knowledge of the authors other examples of computation of a conditional geometric phase that would be both non-Abelian and non-adiabatic are absent. To provide the gates of common interest one has to invent some special case of the parameters variation which makes the generic evolution operator more simple and transparent. This subject is out of the scope of this article.

4 Conclusion

The approach developed in [75]–[77] is to be applied in the models where it is not possible to reduce the computation of the geometric phase to the case of 2-level system. Among those relevant to QC one can point out e.g. the model with anisotropic Heisenberg ferromagnetism where the exchange term in (51) is determined by a matrix of constants $J_{ab}$ rather than by a single constant $J$. In this case the Zeeman terms $H_s^{(0)}$ no longer commute with the exchange term $J_{ab} S_a \otimes S_b$ and to derive the expression for the geometric phase it is necessary to consider a more general case of 4-level system. The problem becomes more complicated also if the superfine electron-nucleus spin interaction must be taken into account. It is the case for the Kane model of silicon QC [79]. The effective dimension of the system’s Hamiltonian is then 16. It is hopeless to attempt to obtain an exact analytic expression for the system’s dynamics which should be investigated numerically (see e.g. [78] ) but it is nevertheless possible to derive an exact formula at least for the adiabatic phase.

One more problem to be mentioned here is interaction with the environment. It can appear to be important not only for such issue as decoherence but it also can in principle contribute to the geometric phase. The simplest way to see it is to consider the model described by (50)–(51). If the external electromagnetic wave field can affect not only the qubits but the phonons as well. The phonon degrees of freedom can produce Heisenberg–Weyl-like geometric phase that can fill the sign of the spin projection due to electron-phonon term (53), (54). Some more complicated interaction between the qubits and the environment makes it necessary to compute the geometric phase for a system with the symmetry algebra which is larger than $su(2)$ and cannot be reduced to the last one (in the sense of the phase derivation).

Other field of application could be multi-beam optical schemes for quantum computations where several energy levels must be included in the scheme to provide two-qubit operations. Besides of some special cases [80] it can require more general methods for the geometric phase computation.

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