Exact integrability of the two-level system: Berry's phase and nonadiabatic corrections

Nilanjana Datta and Gautam Ghosh
Saha Institute of Nuclear Physics, 92, Acharya Prafulla Chandra Road, Calcutta 700 009, India

M. H. Engineer
Physics Department, Bose Institute, 93/1 Acharya Prafulla Chandra Road, Calcutta 700 009, India
(Received 25 August 1988)

The general time-dependent quantum two-level system is shown to admit an exact invariant. This leads to a classical formulation of the problem, which is then solved by standard techniques of Hamiltonian mechanics. Berry's phase and nonadiabatic corrections to it emerge as an asymptotic limit of the exact dynamics. A novel connection between Berry's phase and Hannay's angle is shown to exist in this case.

I. INTRODUCTION

Holonomy effects in nonrelativistic physics as exemplified by Berry's phase[1–3] in quantum mechanics and its classical counterpart, Hannay's angle,[4,5] are now well understood theoretically. Such effects manifest themselves in important modifications of the classical[6] and quantum[7] adiabatic theorems. Quantally, an eigenfunction corresponding to a simple eigenvalue of a multiparameter Hamiltonian, when continued adiabatically in a closed circuit Γ in the parameter space, picks up a phase which is in addition to the dynamical phase and depends solely on the geometry of Γ. In a similar way, an integrable classical system undergoing such adiabatic excursion suffers an additional shift of a geometric nature in its angle variables conjugate to the adiabatically conserved actions. The original assumptions of Berry regarding the instantaneous eigenstates being nondegenerate and the adiabatic theorem remaining valid during the transport in parameter space were subsequently dropped in two important generalizations. Wilczek and Zee[8] solved for the evolution of a degenerate subspace under closed adiabatic cycling and Aharonov and Anandan[9] allowed the evolution to be nonadiabatic provided the system returns exactly to its initial state (apart from a phase, of course).

For nonadiabatic transports corrections to the geometric phase have been calculated by Berry[10] in an iterative scheme. The method proposed consists in applying a succession of unitary transformations to define a sequence of representations of the evolving state and a corresponding sequence of Hamiltonians responsible for their time development. Thus at each step one could make the adiabatic approximation and define a geometric phase. The total phase acquired by the wave function over and above the phase calculated on the basis of instantaneous dynamics comes out to be a sum of the above-mentioned geometric phases and a residual dynamical part. Since each term of the series, thus defined, contains the adiabatic parameter (characterizing the rate at which the Hamiltonian is cycled) to infinitely high order, the expansion is nonperturbative. Rather Berry regards the iterations as successive superadiabatic transformations to moving frames (in Hilbert space) attempting to cling ever more closely to the evolving state. It is further shown that since the departure from adiabaticity causes transitions, the wave function cannot continue to change in its phase part only and this fact is reflected in the ultimate divergence of the sequence of approximants obtained through the iterative procedure. As an example, Berry calculated the first few corrections to the geometric phase for a spin-$\frac{1}{2}$ system coupled to a magnetic field varying along a parallel of latitude on the unit sphere.

In this paper we have defined for the two-level spin system a single transformation to a frame where the evolution is entirely dynamical. This is facilitated by the fact that this system, although explicitly time dependent, admits an exact invariant and the quantal equations of motion appear formally to have an underlying classical Hamiltonian structure similar to the one that has recently been studied by us.[11] We exploit this particular feature to construct a "canonical transformation" to "action-angle" variables, the "action" variable being chosen to be the above-mentioned invariant. As early as 1960, Dykhne[12] noticed that the replacement $x \rightarrow \psi$ and $t \rightarrow x$ reduces Newton's equation with a time-dependent linear restoring force to the time-independent Schrödinger equation, which he then analyzed. This procedure could be inverted and Hannay[4,5,8] suggested that the Berry phase for one degree of freedom systems could be calculated by reducing the Schrödinger equation to one corresponding to a "classical" quadratic Hamiltonian. An unexpected relationship between Hannay's angle for the associated classical system and Berry's phase for the two-level system emerges. This is somewhat different from the connection that is known to exist at the semiclassical level[5] and that becomes exact for Hamiltonians which are linear in the action variables.[13] For the spin-$\frac{1}{2}$ system Berry's phase is exactly related to Hannay's angle for a Hamiltonian in Grassmann variables.[14,15] Ours is a new result in that Berry's phase for the spin-$\frac{1}{2}$ system emerges from Hannay's angle for a complex, albeit formal, oscillator Hamiltonian. Furthermore, we could look upon the single transformation proposed by us as the product of all the transformations in the iterative scheme discussed earlier and we display, for a latitude variation of the parameters, an expression of the geometric phase which is identical to the one obtained by Berry.

Section II contains the main body of our result: "Hamiltonian formulation," reduction to action-angle variables, exact solution for the phase and its adiabatic limit, i.e., Berry's phase. We then present an expansion of the phase in the adiabaticity parameter and derive a few nonadiabatic corrections. In the concluding section we discuss the nature of the invariant and construct it explicitly for the Rabi problem of spin resonance.

II. TWO-LEVEL SPIN SYSTEM

Consider then the Hermitian Hamiltonian defined in a two-dimensional Hilbert space spanned by the basis states $|1\rangle$ and $|2\rangle$. Without loss of generality we can write

$$H=\varepsilon|1\rangle\langle 1|-\varepsilon|2\rangle\langle 2|+\gamma|1\rangle\langle 2|+\gamma^*|2\rangle\langle 1| \; , \tag{1}$$

where ε and γ are, for the moment, arbitrary functions of time. Later we will require their derivatives to vanish as $|t|\rightarrow\infty$ and for that it would be sufficient to require $H(t)$ analytic in a strip including the real t axis. At any time t, the instantaneous normalized eigenstates of the Hamiltonian defined in (1) are

$$|\pm\rangle=\frac{\gamma}{[|\gamma|^2+(\varepsilon\mp\hbar\omega)^2]^{1/2}}|1\rangle - \frac{\varepsilon\mp\hbar\omega}{[|\gamma|^2+(\varepsilon\mp\hbar\omega)^2]^{1/2}}|2\rangle \tag{2}$$

belonging, respectively, to the eigenvalues $\pm\hbar\omega$ where $\hbar\omega=(\varepsilon^2+|\gamma|^2)^{1/2}$.

An arbitrary normalized state $|\psi\rangle$ $(=C_1|1\rangle+C_2|2\rangle)$ will develop in time according to the Schrödinger equation which in terms of the coefficients C_1 and C_2 will yield first-order equations that can be uncoupled in the usual way. The equation for C_2, for example, is given by

$$\ddot{C}_2-\frac{\dot{\gamma}^*}{\gamma^*}\dot{C}_2+[\omega^2-(i/\hbar)(\dot{\varepsilon}-\varepsilon\dot{\gamma}^*/\gamma^*)]C_2=0 \; , \tag{3}$$

where an overdot indicates time differentiation. The corresponding equation for C_1 is obtained by the replacement $\gamma^*\rightarrow\gamma$, $\varepsilon\rightarrow-\varepsilon$.

These equations have the formal appearance of the classical Newton's equations of motion of an oscillator with a time-dependent frequency and a velocity-dependent interaction term. We have to look for complex solutions of these equations if they are to exhibit Berry's phase. If the coefficients of these equations were real we could have applied the usual techniques of classical mechanics to solve them. We will show that the solutions thus arrived at can be explicitly checked to be valid even when the coefficients are complex.

Thus treating C_2 as a coordinate one can write down a formal "Lagrangian," define a "canonical momentum" and thereby a "Hamiltonian" from which the equations of motion of C_1 and C_2 are obtainable as "Hamilton's equations." Thus, for example, with C_2 treated as a coordinate we have the expressions

$$L=(1/2\gamma^*)(\dot{C}_2-i\varepsilon C_2/\hbar)^2-\gamma C_2^2/(2\hbar^2) \; , \tag{4}$$

$$p\equiv\frac{\partial L}{\partial \dot{C}_2}=(1/\gamma^*)(\dot{C}_2-i\varepsilon_2 C_2/\hbar) \; , \tag{5}$$

$$H=(1/2)(\gamma^*p^2+2i\varepsilon pC_2/\hbar+\gamma C_2^2/\hbar^2) \; . \tag{6}$$

The Hamiltonian, as deduced above, describes a complex extension of the generalized harmonic oscillator (GHO) which may be obtained from the usual oscillator Hamiltonian through a time-dependent scaling and rotation in phase space. Now it is known that the GHO admits an exact invariant which is a generalization of the Lewis invariant[16] for the usual oscillator with time-dependent frequency. This holds true even in the complex extension and we have for the invariant

$$I=\tfrac{1}{2}(C_2^2/r^2+\{r[p+i\varepsilon C_2/(\hbar\gamma^*)]-\dot{r}C_2/\gamma^*\}^2) \; . \tag{7}$$

The constancy of I [easily checked by direct differentiation and use of the following equation, viz., Eq.(8)] thus expresses a relationship between the wave function and its first derivative. The auxiliary function $\gamma(t)$ can be chosen to be any particular solution of the differential equation

$$\frac{d}{dt}(\dot{r}/\gamma^*)-(ir/\hbar)\frac{d}{dt}(\varepsilon/\gamma^*)+\varepsilon^2r/(\hbar^2\gamma^*)-\gamma^*/r^3 +\gamma r/\hbar^2=0 \; . \tag{8}$$

The existence of the invariant I implies that, in principle, through a time-dependent canonical transformation we can choose I to be the new "momentum" variable P. This, in fact, is achieved with the help of a "generating function" $F_2(C_2,P)$ (the subscript indicating its position in the standard Goldstein classification) in the following way:

$$(C_2,p)\xrightarrow{F_2(C_2,P)}(Q,P) \; ,$$

$$p=\frac{\partial F_2}{\partial C_2}, \quad Q=\frac{\partial F_2}{\partial P} \; .$$

In our case, a generating function given by

$$F_2(C_2,P)=-(n+1/2)\pi P\pm P\sin^{-1}C_2/(2Pr^2)^{1/2} \pm(C_2/2r)(2P-C_2^2/r^2)^{1/2} +[C_2^2/(2\gamma^*)][(\dot{r}/r)-i\varepsilon/\hbar] \tag{9}$$

yields the desired "canonically conjugate" variables

$$P=I \; , \quad Q=-\tan^{-1}\{(r^2/C_2)[p+i\varepsilon C_2/(\hbar\gamma^*)]-r\dot{r}/\gamma^*\} \; , \tag{10}$$

and the new "Hamiltonian"

$$K\equiv H+\frac{\partial F_2}{\partial t}=\gamma^*P/r^2 \; . \tag{11}$$

K being a function of P only, the pair (P,Q) may be regarded as action-angle variables and the dynamical problem considered as essentially solved.

The solution $Q(t)$ as obtained from Hamilton's equation $\dot{Q}=\partial K/\partial P$ is

$$Q(t)=\int_{-\infty}^{t}(\gamma^*/r^2)dt+\delta \tag{12}$$

(where δ is an arbitrary constant of integration) and involves the auxiliary variable $r(t)$. Treating ε and γ as slowly changing functions of time one can obtain solutions for r in adiabatic perturbation theory. The first two terms of this expansion when inserted in Eq. (12) yield

$$Q(\infty)=\int_{-\infty}^{\infty}\omega(t)dt-(i/2\hbar)\times\int_{-\infty}^{\infty}(\gamma^*/\omega)\frac{d}{dt}(\varepsilon/\gamma^*)dt+\delta\ . \tag{13}$$

The second term is to be regarded as Hannay's angle for the Hamiltonian (6) since it represents the "angle" change occurring in addition to the time integral of the instantaneous "frequency." When converted to a surface integral in the parameter space spanned by ε, $\mathrm{Re}\gamma$ and $\mathrm{Im}\gamma$, this term can be easily shown to equal $(\Omega/2-\pi)$ where Ω is the solid angle subtended by a surface spanning the circuit at the origin.

The exact solution for C_2 as obtained from Eqs. (10), (12), and (7) is

$$C_2=(2P)^{1/2}r\cos\left[\int_{-\infty}^{t}(\gamma^*/r^2)dt+\delta\right]\ .$$

By direct differentiation one obtains expressions for $\dot{C}_2$ and $\ddot{C}_2$ which upon substitution reduce the left-hand side of Eq. (3) to zero, when use is made of the auxiliary equation (8).

The desired adiabatic solution for C_2 is now obtained by substituting Eq. (12) in Eq. (10) and then approximating γ^*/r^2:

$$C_2=\left[\frac{2P\gamma^*}{\omega-[i\gamma^*/(2\hbar\omega)](d/dt)(\varepsilon/\gamma^*)}\right]^{1/2}\sin\left[\int_{-\infty}^{t}\left[\omega-[i\gamma^*/(2\hbar\omega)]\frac{d}{dt}(\varepsilon/\gamma^*)\right]dt\right]\ , \tag{14}$$

where the boundary condition $C_2\ (t=-\infty)=0$ has been imposed. Under closed adiabatic cycling, the factor $\gamma^{*1/2}$ undergoes a phase change of π and hence the two instantaneous components that make up Eq. (14) acquire geometric phases:

$$\gamma_{\pm}=\pi\mp(\Omega/2-\pi)=\mp\Omega/2\ .$$

Higher-order corrections in the adiabaticity parameter (λ) can be systematically obtained by writing $d/dt=\lambda d/d\tau$ and the solution of Eq. (8) as $r(t)=r_0(t)+\lambda r_1(t)+\lambda^2 r_2(t)\ \cdots$. Up to order λ^3, the expansion for γ^*/r^2 reads

$$\gamma^*/r^2=\gamma^*/r_0^2-2\lambda\gamma^* r_1/r_0^3-\lambda^2(2\gamma^* r_2/r_0^3-3\gamma^* r_1^2/r_0^4)-\lambda^3(2\gamma^* r_3/r_0^3-6\gamma^* r_1 r_2/r_0^4+4\gamma^* r_1^3/r_0^5)\ , \tag{15}$$

where

$$r_0=(\gamma^*/\omega)^{1/2}\ , \tag{16}$$

$$r_1=[i\gamma^* r_0/(4\omega^2\hbar)]\frac{d}{d\tau}(\varepsilon/\gamma^*)\ , \tag{17}$$

$$r_2=-[5r_0^5/(32\hbar^2\omega^2)]\left[\frac{d}{d\tau}(\varepsilon/\gamma^*)\right]^2-[r_0^2/(4\omega)]\frac{d}{d\tau}\left[(1/\gamma^*)\frac{dr_0}{d\tau}\right]\ , \tag{18}$$

$$r_3=-[15i\gamma^* r_0^5/(128\hbar^3\omega^4)]\left[\frac{d}{d\tau}(\varepsilon/\gamma^*)\right]^3-[\gamma^*/(4\omega^2)]\frac{d}{d\tau}\left[(1/\gamma^*)\left[\frac{dr_1}{d\tau}\right]\right]-[i\gamma^{*2}/(4\omega^4\hbar)\left[\frac{d}{d\tau}(\varepsilon/\gamma^*)\right]\frac{d}{d\tau}\left[(1/\gamma^*)\frac{dr_0}{d\tau}\right]\ . \tag{19}$$

Thus

$$\gamma^*/r^2=\omega-[i\gamma^*/(2\omega\hbar)]\frac{d}{dt}(\varepsilon/\gamma^*)+(r_0/2)\frac{d}{dt}\left[(1/\gamma^*)\left[\frac{dr_0}{dt}\right]\right]+[\gamma^{*2}/(8\omega^3\hbar^2)]\left[\frac{d}{dt}(\varepsilon/\gamma^*)\right]^2+[i\gamma^{*3}/(16\omega^5\hbar^3)]\left[\frac{d}{dt}(\varepsilon/\gamma^*)\right]^3+[i\gamma^* r_0/(8\hbar\omega^2)]\left[\frac{d}{dt}(\varepsilon/\gamma^*)\right]\frac{d}{dt}\left[(1/\gamma^*)\frac{dr_0}{dt}\right]+(r_0/2)\frac{d}{dt}\left[(1/\gamma^*)\frac{dr_1}{dt}\right]\ . \tag{20}$$

For a latitude variation of the parameters

$$\varepsilon = B\cos\vartheta,\quad \gamma = B\sin\vartheta\exp[-i\phi(t)]\ ,$$

one obtains, keeping terms up to order λ^3, for the geometric phase

$$\Delta\phi = \mp[\pi(1-\cos\vartheta)+[\hbar\sin^2\vartheta/(8B)]\int_{-\infty}^{\infty}\dot{\phi}^2 dt + [\hbar^2\sin^2\vartheta\cos\vartheta/(16B^2)]\int_{-\infty}^{\infty}\dot{\phi}^3 dt\ , \qquad (21)$$

where we have imposed the analyticity requirements mentioned at the beginning. The corrections obtained in this way are, of course, the same (but for numerical factors) as that obtained by Berry in his iterative scheme. The difference arises because the Hamiltonian considered by us may be written as $\mathbf{B}\cdot\boldsymbol{\sigma}$ (the components of $\boldsymbol{\sigma}$ being the Pauli spin matrices) which is twice the one considered by Berry.

III. DISCUSSION

Before concluding let us make a few remarks about the nature of the invariant. In the adiabatic limit, it reduces to H/ω, that is, the action $(1/2\pi)\oint p\, dC_2$. Thus the invariant I may be considered to grow out of the adiabatic invariant action when the time dependence becomes arbtirary. Also, closed-form expressions for I may be obtained in certain special cases. An example that comes to mind is the Rabi problem of spin resonance[17] where $\varepsilon=\text{const}$ and $\gamma=|\gamma|\exp(i\omega_0 t)$. Here the equation for $r(t)$ can be explicitly solved to yield

$$r^2/\gamma^* = (\omega_0^2/4-\omega_0\varepsilon/\hbar+\omega^2)^{-1/2} \equiv \beta^{-1/2} \qquad (22)$$

and therefore

$$I = [\beta^{1/2}/(2\gamma^*)][C_2^2+(1/\beta)(\dot{C}_2+i\omega_0 C_2/2)^2]\ .$$

The adiabatic expansion in this case reduces to a power-series expansion of the exact solution in the small parameter ω_0/ω, as can be easily checked.

Our analysis has worked so nicely because the underlying classical Hamiltonian turned out to be quadratic. We may observe that the Heisenberg equation of motion $\dot{\boldsymbol{\sigma}} \propto \boldsymbol{\sigma}\times\mathbf{B}$ provides a set of coupled time-dependent oscillator equations for the components of the spin operator, and therefore a similar analysis can, in principle, be carried out in the Heisenberg picture as well.

ACKNOWLEDGMENTS

We thank Professor M. V. Berry for an enlightening discussion of his iterative procedure for calculating adiabatic phases.

[1]M. V. Berry, Proc. R. Soc. London, Ser. A **392**, 45 (1985).
[2]B. Simon, Phys. Rev. Lett. **51**, 2167 (1983).
[3]J. Anandan and L. Stodolsky, Phys. Rev. D **35**, 2597 (1987).
[4]J. H. Hannay, J. Phys. A **18**, 221 (1985).
[5]M. V. Berry, J. Phys. A **18**, 15 (1985).
[6]V. I. Arnold, *Mathematical Methods of Classical Mechanics* (Springer, New York, 1978).
[7]A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1962), Vol. 2; see also T. Kato, J. Phys. Soc. Jpn. **5**, 435 (1950).
[8]F. Wilczek and A. Zee, Phys. Rev. Lett. **52**, 2111 (1984).
[9]Y. Aharanov and J. Anandan, Phys. Rev. Lett. **58**, 1593 (1987). The phase discovered by these authors, although differently defined, agrees with that of Berry in some situations.
[10]M. V. Berry, Proc. R. Soc. London, Ser. A **414**, 31 (1987).
[11]M. H. Engineer and G. Ghosh, J. Phys. A **21**, L95 (1988).
[12]A. M. Dykhne, Zh. Eksp. Teor. Fiz. **38**, 570 (1960) [Sov. Phys.—JETP **11**, 411 (1960)].
[13]G. Ghosh and B. Dutta-Roy, Phys. Rev. D **37**, 1709 (1988). A wave-packet argument is used to extract Hannay's angle in the classical limit.
[14]E. Gozzi and W. D. Thacker, Phys. Rev. D **35**, 2388 (1987).
[15]N. Datta and G. Ghosh (unpublished).
[16]H. R. Lewis, Phys. Rev. Lett. **18**, 510 (1967). The invariant discovered by Lewis follows from the asymptotic theory of Kruskal; see M. Kruskal, J. Math. Phys. **3**, 806 (1962).
[17]See, e.g., J. J. Sakurai, *Modern Quantum Mechanics* (Benjamin, New York, 1985).