Berry's phase for anharmonic oscillators

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We study classical and quantum anholonomy for nonlinear oscillators which support linear or quadratic spectra. The validity of the semiclassical relation between Berry's phase and Hannay's angle is investigated.

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I. INTRODUCTION

The purpose of this paper is twofold. First we want to calculate Berry's phase and Hannay's angle [1–4] for a number of analytically solvable potentials and, second, to explore the limits of validity of the semiclassical relation that exists between the phase and the angle. Although the semiclassical relation [2] was derived by Berry almost simultaneously with the discovery of the phase named after him, and was found to be exact for the generalized harmonic oscillator, there were no subsequent attempts to study its validity for other potentials. This is unfortunate, considering the fact that semiclassical relations in physics (e.g., the WKB quantization formula) have long been the subject of extensive investigation. It is common wisdom that semiclassical mechanics is exactly valid for quadratic Hamiltonians. Nevertheless there are other potentials for which exact quantization conditions [5–8] do exist. Here we choose this class of potentials for our investigation.

This paper is organized as follows. In Sec. II we give the formulas for the anharmonic phases and angles, which will be needed for our calculations. Section III is the main body of our paper, where we calculate these anholonomies for a class of potentials. We end with a discussion of the results obtained in Sec. IV.

II. BERRY'S PHASE AND HANNAY'S ANGLE

The geometric phase acquired by a quantal system whose Hamiltonian depends on a set of parameters which are adiabatically varied in a closed cycle ($\mathcal{C}$) is given by

$$\gamma_n(\mathcal{C}=\partial s)=-\int_s \mathbf{V}_n\cdot d\mathbf{s}\ . \tag{1}$$

The invariance of the quantum number n of the system is guaranteed by the quantum adiabatic theorem which holds for nondegenerate bound states. The vector field $\mathbf{V}_n$ is given by

$$\mathbf{V}_n=\mathrm{Im}\nabla_R\times\langle n|\nabla_R|n\rangle \tag{2}$$

with ∇_R being the gradient operator involving the parameter set $(\mathbf{R})$.

For an integrable parameter-dependent classical Hamiltonian with one degree of freedom, the anholonomy resulting from an adiabatic cyclic change of the parameters manifests itself as an extra shift

$$\Delta\theta(I,\mathcal{C}=\partial s)=-\frac{\partial}{\partial I}\int_s \mathbf{W}\cdot d\mathbf{s}\ , \tag{3}$$

in the angle variable θ, corresponding to the adiabatically conserved action I. This is referred to as Hannay's angle. The vector field $\mathbf{W}$ is given by,

$$\mathbf{W}(I,\mathbf{R})=(1/2\pi)\oint d\theta\,\nabla_R p(\theta,I;\mathbf{R})\times\nabla_R q(\theta,I;\mathbf{R})\ . \tag{4}$$

The functional forms displayed in Eq. (4) represent instantaneous transformations from coordinate and momentum to action-angle variables for frozen values of the parameters. The semiclassical relation connects the vector fields $\mathbf{V}_n$ and $\mathbf{W}$ in an amazingly simple way, viz.,

$$\mathbf{V}_n(\mathbf{R})=-(1/\hbar)\mathbf{W}(I,\mathbf{R})\ , \tag{5}$$

where the quantum number n and the action I are related by the semiclassical action quantization,

$$I=(n+1/2)\hbar\ . \tag{6}$$

Therefore for a quasicontinuous spectrum one can write

$$\Delta\theta=-\frac{\partial\gamma_n}{\partial n}\ . \tag{7}$$

The genesis of the above formula is a stationary phase evaluation of the matrix element in $\mathbf{V}_n$ from Eq. (2), in the coordinate representation, and use of the semiclassical approximation for the wave function associated with a torus with given action values.

III. QUANTUM AND CLASSICAL ANHOLONOMIES

A. Quantum anholonomy

We will consider quantum-mechanical Hamiltonians of the form

$$H=(\tfrac{1}{2})\{Ap^2+B[f(x)p+pf(x)]\}+V'(x)\ , \tag{8}$$

where A and B are time-dependent parameters and the potential $V'(x)$ also contains such parameters as its strength and range. The choice of the functions $f(x)$ and $V'(x)$ will be dictated by analytical solvability. The term containing B is essential for the existence of anholonomy, breaking as it does the time-reversal invariance of the system. The symmetrized form of this term ensures the Hermiticity of the Hamiltonian.

The wave function ψ, which is a solution of the Schrödinger equation, may be written as

$$\psi=\phi \exp\left[-(iB/A\hbar)\int f(x)dx\right] , \qquad (9)$$

with ϕ satisfying the equation

$$-\frac{A\hbar^2}{2}\frac{d^2\phi}{dx^2}+V(x)\phi=E\phi , \qquad (10)$$

the modified potential $V(x)$ being given by

$$V(x)=V'(x)-B^2f^2/2A . \qquad (11)$$

Example 1: Harmonic oscillator with centripetal barrier (HOCB). We make the choice $f(x)=x$; $V(x)=U_0[1/(cx)-cx]^2$. Hence the Hamiltonian [9] to be dealt with is

$$H=(A/2)[p+(B/A)x]^2+U_0[1/(cx)-cx]^2 , \qquad (12)$$

where A, B, and U_0 are considered to be adiabatically varying external parameters. In this case the wave function is

$$\psi=\phi \exp[-iBx^2/(2A\hbar)] , \qquad (13)$$

with ϕ satisfying the differential equation

$$\frac{d^2\phi}{dx^2}+\frac{2}{A\hbar^2}[(E+2U_0)-U_0c^2x^2-U_0/(c^2x^2)]\phi=0 . \qquad (14)$$

Stationary solutions of Eq. (14) can readily be obtained by the identification of this equation with the radial equation

$$\frac{d^2\chi}{dr^2}+(2m/\hbar^2) \times[E-mw^2r^2/2-\hbar^2l(l+1)/(2mr^2)]\chi=0 , \qquad (15)$$

for the modified radial wave function, $\chi(r)=rR(r)$, of the three-dimensional harmonic oscillator, under the mapping

$$x\to r,\ (2AU_0c^2)^{1/2}\to\omega,\ 1/A\to m ,$$
$$E+2U_0\to E,\ 2U_0/(Ac^2)\to l(l+1)\hbar^2 . \qquad (16)$$

The unnormalized solutions of Eq. (15) are given by

$$\chi(\rho)=\rho^{l+1}\exp(-\rho^2/2)L_n^{l+1/2}(\rho^2) , \qquad (17)$$

where $\rho=ra_0$, $a_0=(m\omega/\hbar)^{1/2}$, and $L_n^{l+1/2}$ are the generalized Laguerre polynomials.

The energy eigenvalues of the isotropic three-dimensional oscillator, in terms of the principal quantum number N $(=2n+l)$, are $E=(N+3/2)\hbar\omega$. The presence of the infinite barrier at the origin for the given potential $V(x)$ [Eq. (12)] ensures that we can treat the problem in the half space $x>0$. The boundary conditions for the radial problem therefore remain applicable to the present problem as well. Although the quantization still demands that the difference $n\,[=(N-l)/2]$ be an integer, the quantum numbers N and l need not individually be so.

The transformations (16) therefore enable us to directly obtain the energy eigenvalues of this Hamiltonian as

$$E=[(2n+\alpha+\tfrac{3}{2})(2AU_0\hbar^2c^2)^{1/2}]-2U_0 \qquad (18)$$

$(n=0,1,2,\dots)$ and the corresponding energy eigenfunctions (upon normalization) as

$$\phi_n(y)=\left[\frac{2U_0c^2}{A\hbar^2}\right]^{1/2}\left[\frac{\Gamma(n+1)}{\Gamma(\alpha+n+\frac{3}{2})}\right]^{1/2} \times\exp[-y^2/2]y^{\alpha+1}L_n^{\alpha+1/2}(y^2) , \qquad (19)$$

where we have introduced the dimensionless variable y $[=(2U_0c^2/A\hbar^2)^{1/2}x]$ and replaced the quantum number l by α to indicate that it need not be an integer. The complete normalized wave function is thus given by

$$\psi_n(x)=\phi_n(x)\exp[-iBx^2/(2A\hbar)] . \qquad (20)$$

Substituting for ψ_n in the expression for $\mathbf{V}_n$ (in the coordinate representation) yields

$$\mathbf{V}_n(\mathbf{R})=-[(n+\alpha/2+\tfrac{3}{4})/(\sqrt{2}c)] \times[\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)] . \qquad (21)$$

Berry's phase is hence obtained to be

$$\gamma_n(\mathcal{C})=[(n+\alpha/2+\tfrac{3}{4})/(\sqrt{2}c)] \times\int_s[\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)]\cdot d\mathbf{s} . \qquad (22)$$

Example 2: The Morse potential [10,11]. For the following choice of the gauge function and the potential:

$$f(x)=e^{-cx},\quad V(x)=U_0[e^{-2cx}-2e^{-cx}] , \qquad (23)$$

the wave function is $\psi=\phi\exp[iB\exp(-cx)/(Ac\hbar)]$ with ϕ satisfying the equation

$$\frac{d^2\phi}{dx^2}+\frac{2}{A\hbar^2}[E-U_0(e^{-2cx}-2e^{-cx})]\phi=0 . \qquad (24)$$

Energy eigenvalues and standard normalized solutions of Eq. (24), for $E<0$, are obtained in terms of the variables:

$$\xi=[8U_0/(Ac\hbar^2)]e^{-cx},\quad s=[-2E/(Ac^2\hbar^2)]^{1/2} ,$$

and

$$n=[2U_0/(Ac^2\hbar^2)]^{1/2}-(s+\tfrac{1}{2}) ,$$

as

$$E_n=U_0\left[1-\left[\frac{Ac^2\hbar^2}{2U_0}\right]^{1/2}(n+\tfrac{1}{2})\right] \qquad (25)$$

and

$$\phi_n(\xi)=[2sc\Gamma(n+1)/\Gamma(n+2s+1)]^{1/2} \times\exp[(-\xi/2)\xi^sL_n^{2s}(\xi) , \qquad (26)$$

respectively [$L_n^{2s}(\xi)$ being the generalized Laguerre polynomials.]

Choosing A, B, and U_0 as the parameters, we get Berry's phase to be

$$\gamma_n(\mathcal{C})=\frac{1}{\sqrt{2}}(n+\tfrac{1}{2})\int_s[\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)]\cdot d\mathbf{s}\ . \tag{27}$$

Example 3: The Poschl-Teller potential [11,12]. On choosing $f(x)=\tanh cx$ and $V(x)=-U_0\operatorname{sech}^2 cx$ we obtain the wave function

$$\psi=\phi_n\exp[(-iB/c\hbar A)\ln(\cosh cx)]\ , \tag{28}$$

ϕ_n being a solution of the Schrödinger equation corresponding to the Poschl-Teller potential. In terms of the variables $\xi=\tanh cx$ and $\gamma=b-n$, where

$$b=(\tfrac{1}{2})[1+8U_0/(Ac^2\hbar^2)]^{1/2},\quad n=0,1,2,\dots\ , \tag{29}$$

we obtain the normalized solutions

$$\phi_n=|N|(1-\xi^2)^{(\nu-1/2)}C_n^\nu(\xi)\ , \tag{30}$$

$$|N|^2=\left[\frac{n!\Gamma(\nu)\Gamma(2\nu)}{\sqrt{\pi}\Gamma(\nu-\frac{1}{2})\Gamma(2\nu+n)}\right]\ , \tag{31}$$

where $C_n^\nu(\xi)$ are the Gegenbauer polynomials. The energy eigenvalues are given by

$$E_n=-(Ac^2\hbar^2/8)\left[-(1+2n)+\left[1+\frac{8U_0}{Ac^2\hbar^2}\right]^{1/2}\right]^2 . \tag{32}$$

Hence the normalized wave function is

$$\psi_n(x)=|N|\phi_n(\tanh cx)\exp\{-[iB/(Ac\hbar)]\ln(\cosh cx)\} \tag{33}$$

and Berry's phase is obtained as

$$\gamma_n(\mathcal{C})=\left[\frac{1}{2c\hbar}\right]\int_s\nabla_R\left[\frac{(2b-n)(2n+1)-n}{4b^2}\right]\times\nabla_R(B/A)\cdot d\mathbf{s}\ . \tag{34}$$

B. Classical anholonomy

The classical analogue of the quantum-mechanical Hamiltonian given by Eq. (8) will be taken to be

$$H=(\tfrac{1}{2})[Ap^2+2Bf(x)p]+V'(x)$$

or

$$H=(A/2)[p+(B/A)f(x)]^2+V(x)\ , \tag{35}$$

where $V(x)=V'(x)-(B^2/2A)f^2(x)$.

With the choices of $f(x)$ and $V(x)$ given earlier we need to cast this Hamiltonian in action-angle form, in order to calculate the anholonomies in the classical case.

Example 1: HOCB potential. With the Hamiltonian given by

$$H=(A/2)[p+(B/A)x]^2+U_0[1/(cx)-cx]^2\ , \tag{36}$$

the canonical action I, defined as

$$I=(1/2\pi)\oint p\,dx\ , \tag{37}$$

is found to be

$$I=H/(8AU_0c^2)^{1/2} \tag{38}$$

upon substitution from Eq. (36) for p in Eq. (37) and integrating between the turning points [which are solutions of $H=V(x)$]. The conjugate angle variable θ is obtained from Hamilton's characteristic function $W(x,I)$ [13] through the transformation equation

$$\theta=\frac{\partial W(x,I)}{\partial I}\ , \tag{39}$$

where $W(x,I)$, which is the solution of the Hamilton-Jacobi equation, is given by the indefinite integral,

$$W=\int^x p(H(I),x)dx\ . \tag{40}$$

We therefore have in the case of the HOCB potential

$$\theta=\sin^{-1}\left[\frac{H+2U_0-2U_0c^2x^2}{(H^2+4U_0H)^{1/2}}\right]. \tag{41}$$

Expressing x and p in terms of these action and angle variables and evaluating the integral of Eq. (4) gives

$$\mathbf{W}(I,\mathbf{R})=[I/(\sqrt{2}c)][\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)]\ . \tag{42}$$

Hence from Eqs. (3) and (42) we obtain Hannay's angle for the HOCB potential as

$$\Delta\theta=-\frac{1}{\sqrt{2}c}\int_s[\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)]\cdot d\mathbf{s}\ . \tag{43}$$

Example 2: Morse potential. For the classical Hamiltonian,

$$H=(A/2)[p+(B/A)e^{-cx}]^2+U_0[e^{-2cx}-2e^{-cx}]\ , \tag{44}$$

the action and angle variables are, respectively, found to be

$$I=(1/c)[(-2H/A)^{1/2}+(2U_0/A)^{1/2}]\ , \tag{45}$$

$$\theta=\sin^{-1}\left[\frac{H\exp(cx)+U_0}{[U_0(U_0+H)]^{1/2}}\right]. \tag{46}$$

To simplify the subsequent evaluation of Hannay's angle, we make a canonical transformation from x and p to a new pair of variables x' and p': $x\to x'=\exp(-cx)$, $p\to p'=-(p/c)\exp(-cx)$. Expressing x' and p' in terms of the action and angle variables, (θ,I), we have

$$x'=-\frac{H(I)}{U_0+[U_0^2+U_0H(I)]^{1/2}}\ ,$$

$$p'=(B/cA)+\left[-\frac{2U_0[U_0+H(I)]}{Ac^2H(I)}\right]^{1/2}\cos\theta\ .$$

Substitution of x' and p' in Eq. (4) yields the vector field

$$\mathbf{W}(I,\mathbf{R})=\left[\frac{I}{\sqrt{2}}\right][\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)]\ , \tag{47}$$

and hence Hannay's angle

$$\Delta\theta=-(1/\sqrt{2})\int_s[\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)]\cdot d\mathbf{s}\ , \tag{48}$$

The semiclassical relation between the quantum and classical anholonomies is thus seen to hold exactly for both the HOCB potential and the Morse potential.

Example 3: Poschl-Teller potential. We consider the classical Hamiltonian

$$H=(A/2)[p+(B/A)\tanh(cx)]^2-U_0\operatorname{sech}^2(cx)\ . \qquad (49)$$

Rather than going through the straightforward, although tedious, action-angle formulation, we demonstrate for this potential a WKB-like procedure for solving the equation of motion. It may happen that for certain potentials, a point coordinate transformation together with a scaling of time casts the equation of motion into that of an oscillator, which can then be easily analyzed to extract the anholonomy. This seems to be the case for both the Poschl-Teller and the Morse potentials. It is obvious that Hannay's angle, being insensitive to the rate of time evolution of the parameters, will remain unaffected under such a time scaling. Transforming the coordinate x to the variable $\xi=\tanh(cx)$ and scaling the time such that $d\tau=\operatorname{sech}^2(cx)dt$ reduces Hamilton's canonical equations, in this case, to the pair

$$\xi'=Ac[p+(B/A)\xi],\quad p'=-(B/A)\xi'-2cU_0\xi\ , \qquad (50)$$

where prime denotes differentiation with respect to τ. The solution of the differential equation resulting from the decoupling of the above equations is $\xi=z/\sqrt{2}$, with z satisfying

$$z''+[-cA(B/A)'+2c^2AU_0-3A'^2/(4A^2)+A''/(2A)]z=0\ . \qquad (51)$$

The resemblance of this equation to that of simple harmonic motion allows us to interpret the coefficient of z as the square of the "frequency" ω. Now, since the parameters A, B, and U_0 vary adiabatically, only terms linear in their first-order derivatives are significant. Hence in the adiabatic case we have

$$\omega\approx(2AU_0c^2)^{1/2}\left[1-\frac{1}{4cU_0}(B/A)'\right]\ . \qquad (52)$$

It is to be noted that the second term in eq. (52) is a scaled time derivative. Hence its integral with respect to τ can evidently be expressed as a line integral over a closed circuit in parameter space. It is therefore a purely geometric angle shift which is to be identified as the Hannay's angle $\Delta\theta$. Thus

$$\Delta\theta=-(1/2\sqrt{2})\int(A/U_0)^{1/2}(B/A)'d\tau$$
$$=-(1/2\sqrt{2})\oint(A/U_0)^{1/2}\nabla_R(B/A)\cdot\mathbf{dR}$$

or by Stokes' theorem,

$$\Delta\theta=-(1/2\sqrt{2})\int_s[\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)]\cdot\mathbf{ds}\ . \qquad (53)$$

The canonical action variable for the Poschl-Teller potential is given by

$$I=(2/Ac^2)^{1/2}[(U_0)^{1/2}-\sqrt{-H}\,]\quad(H<0)\ . \qquad (54)$$

The semiclassical quantization condition for this action yields the energy eigenvalues

$$E_n=-(A\hbar^2c^2/8)[-(2n+1)+(8U_0/Ac^2\hbar^2)^{1/2}]^2\ . \qquad (55)$$

The above expression matches with the exact quantum-mechanical energy eigenvalue [Eq. (32)] only in the "deep well" limit for which $8U_0/(Ac^2\hbar^2)\gg1$. Hence in comparing the classical and quantum anholonomies for the Poschl-Teller potential, we confine ourselves to this limit. Moreover we consider small values of the quantum number n.

Now from Eq. (34) for Berry's phase we obtain, upon differentiation with respect to n,

$$\frac{\partial\gamma_n}{\partial n}=\frac{1}{2c\hbar}\int_s\left[\nabla_R\left[\frac{b-n+\frac{1}{2}}{b^2}\right]\times\nabla_R(B/A)\right]\cdot\mathbf{ds}\ , \qquad (56)$$

where $b=(\frac{1}{2})[1+8U_0/(Ac^2\hbar^2)]^{1/2}$. In the "deep well" limit, for small quantum numbers, $b\approx(\frac{1}{2})[8U_0/(Ac^2\hbar^2)]^{1/2}\gg n-\frac{1}{2}$. Therefore

$$\frac{\partial\gamma_n}{\partial n}=\frac{1}{2c\hbar}\int_s[\nabla_R(1/b)\times\nabla_R(B/A)]\cdot\mathbf{ds}$$
$$=\frac{1}{2\sqrt{2}}\int_s[\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)]\cdot\mathbf{ds}\ .$$

Thus it is seen that in the deep well limit the semiclassical relation is valid for the Poschl-Teller potential as well.

IV. DISCUSSIONS

We therefore observe that for all the potentials considered the vector field governing the phase has (apart from numerical factors) the form $\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)$. Moreover, the quantum number dependence is linear in all the cases, although the Hamiltonians considered were either linear or quadratic in the actions. To understand this fact let us cast the Hamiltonian of the generalized harmonic oscillator in the form

$$H=(A/2)[p+(B/A)x]^2+(U_0/2)x^2\ ,$$

for which the frequency is $(AU_0)^{1/2}$ and Hannay's angle turns out to be

$$\Delta\theta=-(\tfrac{1}{2})\int_s[\nabla_R(A/U_0)^{1/2}\times\nabla_R(B/A)]\cdot\mathbf{ds}\ .$$

We have seen that for the Poschl-Teller potential, the classical equation of motion can be cast into an oscillator form through a canonical transformation coupled with time dilation. This can also be seen to be true for the Morse potential. For the HOCB potential, the equation of motion is the same as the radial equation for the three-dimensional oscillator. Thus at the classical level the equations for all the three potentials have the same structure. We must reemphasize that time dilation has no effect on the angle anholonomy, which has a purely geometric nature. We also observe that for other choices of parameters for which the equations cannot be brought to the oscillator form, the semiclassical relation is violated. For example, for the Morse potential, if we choose the range (c) instead of the strength (U_0) of the potential, along with A and B, to be the relevant parameters, Berry's phase has an additional contribution, apart from the one satisfying the semiclassical relation. Time scaling, in this case, fails to transform the equation of motion to the oscillator form.

We are also aware of the role of symmetry in determining geometric phases. For the generalized oscillator, the Hamiltonian can be written as a linear combination of SU(1,1) group generators and the anholonomy can be calculated directly from symmetry considerations [14]. However, for other potentials, the generators do not possess such simple forms and one therefore does not know how to extract the anholonomy directly from symmetry. We have shown elsewhere [15] that whenever the Hamiltonian can be written in terms of the generators of a Lie group the geometric phase factorizes into a part which depends on the representation of the group and another part which is purely geometric and representation independent. This seems to be the case for the Hamiltonians considered above and moreover the fact that they provide identical geometrical parts must imply that the underlying symmetry is the same.

In conclusion, we want to make a few more observations. As remarked in the Introduction, the potentials considered are the ones for which exact quantization conditions are available. Another common feature is that the bound-state spectra of these potentials can be connected to the irreducible representations of SU(2) by a technique of embedding in a higher-dimensional space [16,17]. Furthermore these potentials share the property of "shape invariance" in that they can be constructed as supersymmetric partner potentials [18] which are related in a particular way. The other unifying feature which emerges from our work is that their anholonomies are governed by the same vector field and also that the semiclassical relation holds exactly. Thus the present work extends the class of problems that are illustrative of classical and quantum anholonomies and thereby presents several interesting interrelationships and generalizations.

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