The Berry's phase, nonlocal potentials and coupled channel problems

1995 J. Phys. A: Math. Gen. 28 2353

(http://iopscience.iop.org/0305-4470/28/8/025)

J. Phys. A: Math. Gen. 28 (1995) 2353–2358. Printed in the UK

The Berry's phase, non-local potentials and coupled channel problems

Tapas Mukherjee†, Manabendra Mukherjee†, Amit Kundu‡ and Binayak Dutta-Roy‡

† Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700032, India
‡ Saha Institute of Nuclear Physics 1/AF Bidhannagar, Calcutta 700064, India

Received 10 November 1994

Abstract. The Berry's phase for non-local potentials is studied, the salient differences vis-à-vis the case of local potentials is discussed and the generalization to the problem of coupled channels is presented.

Physical systems possessing two relatively disparate time scales often permit a natural analysis wherein the fast variables are first dealt with, taking the slow variables to adopt fixed (though arbitrary) values, and then the resulting effective equation of motion (for the nth eigenstate) governed by the slow variables are found to involve the curl of an 'external' vector potential V_n (induced by the fast variables). Berry's influential paper [1] has placed this feature in the general perspective of quantum mechanics. V_n is called the Berry's connection and $W_n = \nabla \times V_n$ the Berry's curvature, while the line integral of the connection in the space of slow variables or parameters, wherein the curl too was defined, is the Berry's phase, which for a closed path would be the 'magnetic-like' flux threaded by it.

A simple model in this context was provided by Berry [2] through what he terms a 'generalized harmonic oscillator', described by the Hamiltonian

$$H = \tfrac{1}{2}[\xi(t)x^2 + \eta(t)(xp + px) + \zeta(t)p^2] \tag{1}$$

where ξ, η, ζ are slowly varying parameters, while x and p are the position and momentum variables of the 'oscillator'. The Berry's curvature, for the state labelled by the quantum number n, is readily found to be

$$W_n = -\frac{(n+\frac{1}{2})}{2}\nabla\left[\frac{\zeta}{(\xi\zeta - \eta^2)^{1/2}}\right] \times \nabla\left(\frac{\eta}{\zeta}\right) \tag{2}$$

where ∇ represents the gradient operator in the space of parameters (ξ, η, ζ). Such a result, as we shall see, can readily be extended to yield analogous conclusions for several other local potentials [3]. Furthermore, we show that similar formulae can be arrived at for non-local potentials as well. Such interactions appear naturally through exchange terms in physically relevant situations such as, for example, in the time-dependent Hartree–Fock theory or in the case of state-dependent potentials. Lastly, we shall discuss the case of coupled-channel problems, for which non-local separable potentials provide an analytically soluble model, enabling us to discern a new feature for such a situation.

0305-4470/95/082353+06$19.50

The Berry's connection V_n is given by

$$V_n = \mathrm{Im}\langle n|\nabla|n\rangle. \tag{3}$$

To ensure the appearance of a phase in a tractable form the Hamiltonian should be chosen such that it is Hermitian (but not real Hermitian), and the simplest way to do so (for a spinless particle) is to choose the Hamiltonian appropriately generalized to

$$H = \frac{A}{2}\left[p + \frac{B}{A}f(x)\right]^2 + U(x) \tag{4}$$

where A, B and the strength of the potential $U(x)$ shall be taken to be the parameters which shall be varied, and $f(x)$ is a function which shall be suitably chosen for convenient display of results. Of course the anholonomy that arises thereby is 'trivial' in that the momentum operator $\hat{p}$, represented by $-\mathrm{i}\hbar\frac{\partial}{\partial x}$, could just as well be taken to be $-\mathrm{i}\hbar\frac{\partial}{\partial x} + g(x)$, where $g(x)$ is any real function, as it would keep intact [4] the canonical commutation relation $[\hat{x}, \hat{p}] = \mathrm{i}\hbar$ and would therefore be physically equivalent, as indeed the effect of this replacement merely results in a change of the state function by a multiplicative phase factor $\exp[-\frac{\mathrm{i}}{\hbar}\int^x \mathrm{d}y\, g(y)]$. Berry's curvature has already been worked out [3] for three local potentials:

(a) Harmonic oscillator with centripetal barrier on the semi-line ($x > 0$),

$$U(x) = \lambda\left[\frac{1}{cx} - cx\right]^2 \tag{5}$$

with

$$f(x) = x$$

and energy eigenvalues

$$E_n = [(2n + \alpha + \tfrac{3}{2})(2A\lambda\hbar^2c^2)^{1/2}] - 2\lambda.$$

The Berry's curvature is

$$W_n = -\left[\frac{(n + \frac{\alpha}{2} + \frac{3}{4})}{\sqrt{2}c}\right]\nabla\left(\frac{A}{\lambda}\right)^{1/2} \times \nabla\left(\frac{B}{A}\right). \tag{6}$$

(b) The Morse potential

$$U(x) = \lambda[\mathrm{e}^{-2cx} - 2\mathrm{e}^{-cx}] \tag{7}$$

with

$$f(x) = \mathrm{e}^{-cx}.$$

The Berry's curvature is

$$W_n = \frac{1}{\sqrt{2}}(n + \tfrac{1}{2})\nabla\left(\frac{A}{\lambda}\right)^{1/2} \times \nabla\left(\frac{B}{A}\right). \tag{8}$$

(c) The Pöschl–Teller potential

$$U(x) = -\lambda \operatorname{sech}^2 cx \tag{9}$$

with

$$f(x) = \tanh cx.$$

The Berry's curvature is

$$\boldsymbol{W}_n = \frac{1}{2c\hbar}\nabla\left[\frac{(2b-n)(2n+1)-n}{4b^2}\right] \times \nabla\left(\frac{B}{A}\right) \tag{10}$$

where

$$b = \frac{1}{2}\left[1 + \frac{8\lambda}{Ac^2\hbar^2}\right]^{1/2}.$$

To these examples we may append the cases:

(d) The rectangular-well potential on the semi-line

$$U(x) = -U_0\theta(x_0 - x) \tag{11}$$

where θ is the Heviside step function. Taking $f(x) = \alpha$, a constant say, the Berry's curvature is readily seen to be

$$\boldsymbol{W} = -\frac{\alpha}{2\hbar}\nabla\left(\frac{1}{\beta^2}\right) \times \nabla\left(\frac{B}{A}\right) \tag{12}$$

where β is related to the binding energy through $\beta^2 = |E|/A\hbar^2$.

(e) The delta function potential $U(x) = -U_0\delta(x)$ with $-\infty < x < +\infty$ and $f(x) = \alpha$ which yields

$$\boldsymbol{W} = -\frac{\alpha}{2\hbar}\nabla\left(\frac{1}{\beta^2}\right) \times \nabla\left(\frac{B}{A}\right) \tag{13}$$

β^2 being $|E|/A\hbar^2$, as before.

In all the cases involving the local potentials one notices the structure of the Berry's curvatures is comprised of the vector product of gradients in parameter space of a function of the binding energy (through β) and of the ratio B/A. To illustrate the nature of Berry's phase for non-local potentials in a tractable manner it is convenient to choose the example of a non-local but separable potential $U(x, x') = -\lambda h(x)h(x')$ on the semi-line so that the relevant Schrödinger equation becomes

$$\frac{A}{2}\left[-\mathrm{i}\hbar\frac{\partial}{\partial x} + \frac{B}{A}f(x)\right]^2 \Psi(x,t) - \lambda h(x)\int \mathrm{d}x'\, h(x')\Psi(x',t) = \mathrm{i}\hbar\frac{\partial\Psi}{\partial t}. \tag{14}$$

For the instantaneous eigenfunction $\Psi(x)$ of energy $E = |E|$ a substitution $\Psi(x) = \mathrm{e}^{-\mathrm{i}\chi(x)}\phi(x)$ yields the equation

$$\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2} + \tilde{\lambda}\mathrm{e}^{\mathrm{i}\chi(x)}h(x)\int_0^\infty \mathrm{d}x'\, h(x')\mathrm{e}^{-\mathrm{i}\chi(x')}\phi(x') = \beta^2\phi(x) \tag{15}$$

where $\tilde{\lambda} = 2\lambda/A\hbar^2$ and $\beta^2 = 2|E|/A\hbar^2$ and $\chi = \frac{1}{\hbar}\frac{B}{A}\int^x \mathrm{d}x'\, f(x')$. Taking $f(x) = \alpha$ and $h(x) = \mathrm{e}^{-\mu x}$, this equation is easily solved to give

$$\phi(x) = N(\mathrm{e}^{-\beta x} - \mathrm{e}^{-(\mu - \mathrm{i}a)x}) \tag{16}$$

where the normalization constant is given by

$$N = \left[\left\{\frac{2\mu\beta}{\mu+\beta}\right\}\frac{(\mu+\beta)^2 + a^2}{(\mu-\beta)^2 + a^2}\right]^{1/2}. \tag{17}$$

Here $a = B/A\hbar$, and the binding energy is obtainable from $\beta = -\mu + \sqrt{\frac{\tilde{\lambda}}{2\mu} - a^2}$ and a bound state exists only if $\lambda > 2\mu A\hbar^2(\mu^2 + a^2)$. The Berry's curvature can be evaluated from equation (3) and yields

$$W = \alpha\left[-\frac{1}{\hbar}\nabla\left(\frac{N^2}{4\beta^2}\right) \times \nabla\left(\frac{B}{A}\right) + \mu\hbar\nabla N^2 \times \nabla\left(\frac{B}{\lambda}\right)\right]. \tag{18}$$

While the first term is analogous to what is obtained for local potentials, we find an additional contribution to the Berry's curvature (with the appearance of the gradient in parameter space of the normalization constant) possessing a considerably more complicated structure. The source of the involved expression for the Berry's curvature in the case of non-local potentials may be ascribed to the fact that, as the parameters vary, the wavefunction undergoes a change which, because of its folding with the potential, induces a change in the effective potential which in turn inflicts an additional modification of wavefunction. One could indeed expect such features to appear in situations involving non-local potentials, such as for example the time-dependent Hartree–Fock approach.

The problem of coupled channels appears in various areas of the physics of atoms, molecules, nuclei and elementary particles. While actual situations are tractable only through complicated numerical procedures, we go on to employ non-local separable potentials to obtain a model for such coupled-channel problems which admit an analytical approach through which we may generate the notion of Berry's phase in this context. Considering channels (characterized by mass parameters A_i) where the interactions are given by non-local separable potential (taken to be exponential on the semi-line $0 \leqslant x < \infty$, as before) the set of coupled-channel Schrödinger equations are given by

$$\frac{A_i}{2}\left(p + \frac{B_i}{A_i}\right)^2 \psi_i(x) - \sum_j \lambda_{ij}\mathrm{e}^{-\mu x}\int_0^\infty \mathrm{d}x'\, \mathrm{e}^{-\mu x'}\psi_j(x') = -|E_i|\psi_i(x) \tag{19}$$

where B_i are introduced as before to make the Hamiltonian Hermitian but not real Hermitian.

Defining

$$\psi_i(x) = \mathrm{e}^{-\mathrm{i}a_i x}\phi_i(x) = c_i\mathrm{e}^{-\mathrm{i}a_i x}(\mathrm{e}^{-\beta_i x} - \mathrm{e}^{-(\mu - \mathrm{i}a_i)x}) \tag{20}$$

where $a_i = B_i/A_i\hbar$, $\beta_i^2 = 2|E_i|/A_i\hbar^2$ and c_i are constants fixing the normalization and the relative weight of different channels in the bound state, we arrive at the eigenvalue equations

$$2\mu|\mathcal{R}_i|^2 - \tilde{\lambda}_{ii} = \sum_{i \neq j}\tilde{\lambda}_{ij}\frac{\Delta_j}{\Delta_i} \tag{21}$$

where $\tilde{\lambda}_{ij} = 2\lambda_{ij}/A_i\hbar$ and $\Delta_i \equiv c_i\mathcal{P}_i/\mathcal{R}_i = c_i\frac{\mu-\beta_i-\mathrm{i}a_i}{\mu+\beta_i+\mathrm{i}a_i}$.

This set of coupled algebraic equations for the energy eigenvalues gives the condition for the existence of bound states. The condition that Δ_i/Δ_j is real determines the relative phase between the ith and jth channel weight factors

$$\theta_{ij} = \arctan\left[2\mu(a_i - a_j)\frac{\mu^2 + a_i a_j - \frac{a_i\beta_j^2 - a_j\beta_i^2}{a_i - a_j}}{(\mu^2 - \beta_i^2 - a_i^2)(\mu^2 - \beta_j^2 - a_j^2) + 4\mu^2 a_i a_j}\right]. \tag{22}$$

The normalization condition of the wavefunction

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}$$

gives

$$\sum_i \frac{\mu + \beta_i}{2\mu\beta_i}|\Delta_i|^2 = 1.$$

Using equation (3), the Berry's connection and curvature obtained for the eigenstate are

$$\boldsymbol{V} = \sum_i |c_i|^2\left[-\frac{\nabla a_i}{4\beta_i^2} + \nabla\left(\frac{a_i}{|\mu + \beta_i + ia_i|^2}\right) + \frac{\mu + \beta_i}{2\mu\beta_i}\left|\frac{\mu - \beta_i - ia_i}{\mu + \beta_i + ia_i}\right|^2 \nabla(\mathrm{Im}\ln c_i)\right] \tag{23}$$

$$\begin{aligned}\boldsymbol{W} = \sum_i \Bigg[&-\frac{1}{\hbar}\nabla\left(\frac{|c_i|^2}{4\beta_i^2}\right) \times \nabla\left(\frac{B_i}{A_i}\right) + \mu\hbar\nabla(|c_i|)^2 \times \nabla\left(\frac{B_i}{\lambda_{ii} + \sum_{j\neq i}\lambda_{ij}|\frac{\Delta_j}{\Delta_i}|}\right) \\ &+ \nabla\left(\frac{\mu + \beta_i}{2\mu\beta_i}\left|\frac{\mu - \beta_i - \mathrm{i}a_i}{\mu + \beta_i + \mathrm{i}a_i}\right|^2\right) \times \nabla(\mathrm{Im}\ln c_i)\Bigg]\end{aligned} \tag{24}$$

respectively.

In a simpler case of a two-channel problem we determine the Berry's curvature

$$\begin{aligned}\boldsymbol{W} = \Bigg[&-\frac{1}{\hbar}\nabla\left(\frac{c^2}{4\beta_1^2}\right) \times \nabla\left(\frac{B_1}{A_1}\right) + \mu\hbar\nabla(c^2) \times \nabla\left(\frac{B_1}{\lambda_{11} + m\lambda_{12}}\right) \\ &-\frac{1}{\hbar}\nabla\left(\frac{\rho^2c^2}{4\beta_2^2}\right) \times \nabla\left(\frac{B_2}{A_2}\right) + \mu\hbar\nabla(\rho^2c^2) \times \nabla\left(\frac{B_2}{\lambda_{22} + \lambda_{21}/m}\right) \\ &-\nabla\left(\frac{\mu + \beta_2}{2\mu\beta_2}\left|\frac{\mu - \beta_2 - \mathrm{i}a_2}{\mu + \beta_2 + \mathrm{i}a_2}\right|^2\right) \times \nabla\theta_{12}\Bigg]\end{aligned} \tag{25}$$

where

$$m = \rho\left[\left\{\frac{(\mu - \beta_2)^2 + a_2^2}{(\mu + \beta_2)^2 + a_2^2}\right\}\left\{\frac{(\mu + \beta_1)^2 + a_1^2}{(\mu - \beta_1)^2 + a_1^2}\right\}\right]^{1/2}$$

ρ being the amplitude of the relative weight factors; the energy-dependent parameters are related to the 'Q value' through $\beta_2^2 = \frac{A_1}{A_2}\beta_1^2 + \frac{2Q}{A_2\hbar^2}$.

Comparing the expression for the Berry's curvature for the two-channel case (viz equation (25)) with that for the single-channel situation (18) one may note the additional term involving $\nabla\theta_{12}$ which signifies the contribution from the change due to adiabatic variation of the underlying parameters emanating from the relative phase of the weight factors of the two channels.

In conclusion, the Berry's phase for non-local potentials has been discussed and this has provided us with a soluble model eminently suitable for exposing an additional feature that arises in the case of coupled-channel problems.

Acknowledgment

One of the authors (BD-R) is grateful to Professor Meher Engineer of the Bose Institute, for useful discussions and encouragement.

References

[1] Berry M V 1984 *Proc. R. Soc.* A **392** 45
[2] Berry M V 1985 *J. Phys. A: Math. Gen.* **18** 15
[3] Datta N and Ghosh G 1992 *Phys. Rev.* A **46** 5358
[4] Dirac P A M 1958 *The Principles of Quantum Mechanics* 4th edn (Oxford: Oxford University Press) pp 92–3