Double Spiral Energy Surface
in One-dimensional Quantum Mechanics of Generalized Pointlike Potentials

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We analyze the eigenvalue problem of a quantum particle on the line with the generalized pointlike potential of three parameter family. It is shown that the energy surface in the parameter space has a set of singularities, around which different eigenstates are connected in the form of paired spiral stairway. An exemplar wave-function aholonomy is displayed where the ground state is adiabatically turned into the second excited state after cyclic rotation in the parameter space.

KEYWORDS: one-dimensional system, δ′ potential, non-trivial topology in quantum mechanics, exotic wave-function aholonomy

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The evolution of physical states under the cyclical variation of environmental variables has been one of the key concepts of thermodynamics and its engineering applications. That concept has entered into the quantum mechanics with the discovery of Berry phase [1,2] and its subsequent non-Abelian generalization [3]. A quantum eigenstate of parametric Hamiltonian can be adiabatically turned into a different state belonging to the same energy multiplet after the cyclic change of the parameters. The discovery has had profound impacts in the various fields of theoretical physics. Most notable among them is its implication on the origin of the gauge field.

Underlying the phenomena of Berry phase is the structure of the energy surface in the parameter space in the form of two cones, one upside-down which touch each other at the apices. If there can be other non-trivial structure than the double cones, that could lead to the exotic wave-function aholonomy and gauge field structure which are more exotic than the Berry phase phenomena.

In this paper, we report the finding of just such non-trivial energy surface in parameter space in one of the simplest conceivable quantum system, that of a one-dimensional particle subject to a potential which is zero except at a single point. The energy surface of the system is characterized by a singularity which acts as a branch point that connects different energy levels in the form of double spiral. By the cyclical variation of the parameters around the singularity, one can adiabatically transform, for example, the ground state into the second excited state.

Let us start by introducing our model system. The most general pointlike potential in one dimension with time-reversal symmetry is of three parameter family δx δy δz. It has been something of a mystery until its explicit construction in terms of self-adjoint local operator has been devised [3,4]. Here, we outline the procedure. We define a function consisting of three Dirac’s deltas placed next to each other in one dimension;

\[ \xi(x; v_-, u, v_+; a) = v_- \delta(x + a) + u \delta(x) + v_+ \delta(x - a). \]  

We let the strengths \( v_- \), \( v_+ \) and \( u \) to vary with the distance \( a \) in the form

\[ v_-(a) = -\frac{1}{2a} + \frac{\gamma - 1}{2\delta}, \] 
\[ v_+(a) = -\frac{1}{2a} + \frac{\alpha - 1}{2\delta}, \] 
\[ u(a) = -\frac{1}{2a} \frac{\alpha \gamma - 1}{2\beta a^2}. \]

where \( \alpha, \beta, \gamma \) and \( \delta \) are the real numbers which satisfy the constraint

\[ \alpha \gamma - \beta \delta = 1. \]

The zero distance limit of the function \( \xi(x) \) defines the generalized pointlike potential

\[ \chi(x; \alpha, \beta, \gamma, \delta) \equiv \lim_{a \to 0} \xi(x; v_-(a), u_0(a), v_+(a); a), \]

which, when used in the Schrödinger equation

\[ \left[ -\frac{1}{2} \frac{d^2}{dx^2} + \chi(x; \alpha, \beta, \gamma, \delta) \right] \psi(x) = E(\alpha, \beta, \gamma, \delta) \psi(x), \]

yields the eigenfunction \( \psi(x) \) that has discontinuity at \( x = 0 \) both in \( \psi(x) \) itself and in its derivative \( \psi'(x) \), whose amount is specified by

\[ \psi'(0+) + \alpha \psi'(0-) = -\beta \psi(0-) \] 
\[ \psi(0+) + \gamma \psi(0-) = -\delta \psi'(0-). \]

The constraint, Eq. (3) guarantees the self-adjointness of the Hamiltonian operator of Eq. (4), which is equivalent, in physical term, to the requirement of the continuity of the probability flux at \( x = 0 \).

In order to make the quantum spectra discrete, we place the system in a finite region on the line (“one-dimensional billiard”) of the length \( L \), depicted in Fig. 1, by imposing the wave functions to disappear at \( x = -rL \) and \( x = (1 - r)L \).
where \( k = \gamma \) is out of our usual intuition, we look at the eigenvalues explicitly calculable. We opt for an elementary derivation.

The positive energy solution of Eq. (5) is written in the form

\[
\psi(x) = A_+ \sin k(x - L + rL) \quad (x > 0),
\]

\[
\psi(x) = A_- \sin k(x + rL) \quad (x < 0),
\]

where \( k = \sqrt{2E} \) is the linear momentum. For the negative energy case \( E < 0 \), one makes the replacement

\[
\sin \rightarrow \sinh, \quad \cos \rightarrow \cosh, \quad k \rightarrow \kappa.
\]

where \( \kappa = \sqrt{-2E} \). From Eqs. (6) and (7), one obtains the eigenvalue equation for the case of \( E > 0 \) in the form

\[
F(k) = 0
\]

where

\[
F(k) = \alpha \sin k(1 - r)L \cos krL + \gamma \cos k(1 - r)L \sin krL + \beta \frac{1}{k} \sin k(1 - r)L \sin krL + \delta k \cos k(1 - r)L \cos krL.
\]

The corresponding eigenfunction is obtained from the relation

\[
A_+ \frac{\alpha}{A_-} = \alpha \cos k(1 - r)L \cos krL - \gamma \sin k(1 - r)L \sin krL + \beta \frac{1}{k} \cos k(1 - r)L \sin krL - \delta k \sin k(1 - r)L \cos krL.
\]

The negative eigenvalue (when it exists) can be obtained in a parallel manner with the replacement Eq. (8).

Since visualizing the four-dimensional energy surface is out of our usual intuition, we look at the eigenvalues as functions of two parameters \((\alpha, \beta)\) with a fixed value \( \gamma = \gamma_0 \), namely,

\[
E(\alpha, \beta) \equiv E(\alpha, \beta, \gamma = \gamma_0, \delta = \frac{\alpha \gamma_0 - 1}{\beta}).
\]

A curious feature of the energy surface Eq. (12) is that the value of \( \delta \) becomes indefinite for a special point in the parameter space \((\alpha^*, \beta^*) = (1/\gamma_0, 0)\). Since the function \( F(k) \), Eq. (10) is a smooth function of all parameters \((\alpha, \beta, \gamma, \delta)\), this implies that the energy eigenvalue is also indefinite at this point, namely

\[
E(\alpha^*, \beta^*) \text{ indefinite for } (\alpha^*, \beta^*) = (\frac{1}{\gamma_0}, 0).
\]

We look at the neighbourhood of the singularity by defining the polar coordinate \((\rho, \theta)\) around the singularity;

\[
\alpha = \frac{1}{\gamma_0} - \rho \sin(\theta)
\]

\[
\beta = \rho \cos(\theta).
\]

The equation Eq. (10) takes the form

\[
F(k) = \frac{1}{\gamma_0} \sin k(1 - r)L \cos krL + \gamma_0 \cos k(1 - r)L \sin krL - \gamma_0 k \cos k(1 - r)L \cos krL \tan \theta + O(\rho).
\]

Neglecting the term of \( O(\rho) \), we can express the solution of Eq. (10) analytically as

\[
\theta(k) = \arctan \left( \frac{1}{k \gamma_0^2} \tan k(1 - r)L + \frac{1}{k} \tan krL \right).
\]

This function is multivalued. But at each branch \( \theta_n(k) \), it satisfies \( d\theta_n/dk > 0 \), therefore can be inverted to obtain an increasing function \( k_n(\theta) \). On the other hand, \( k(\theta) \) as a whole is periodic with the period \( \pi \), reflecting the periodicity of \( F(k) \). These two facts can be made compatible only when each branch \( k_n(\theta) \) is connected to the next branch after moving up for the period \( \pi \). Same hold for the function \( \kappa(\theta) \) below zero energy. A notable fact is that one has \( \kappa \to \infty \) when \( \theta \to 0_+ \), which means that a bound state emerge from negative infinite energy.

FIG. 2. The solution Eq. (13) of the Schrödinger equation around the singularity at \((\alpha, \beta) = (1/\gamma_0, 0)\). The \( \gamma_0 \) is chosen to be \(-1\). Other parameters are \( L = 1 \) and \( r = 0.618034 \).
at \( \theta = 0, \pi, 2\pi, \ldots \). The situation can be best understood by inspecting the Fig. II where the function \( k(\theta) \) is drawn for the case of \( L = 1, r = (\sqrt{5} - 1)/2 \approx 0.618034 \) and \( \gamma_0 = -1 \). We now easily see the remarkable property of the energy eigenvalue around the singularity, which can be expressed as

\[
E_n(\theta + \pi) = E_{n+1}(\theta),
\]
and therefore

\[
E_n(\theta + 2\pi) = E_{n+2}(\theta).
\]

Note the fact that while Eq. (17) is an approximation based on the expansion Eq. (15), the relation Eq. (18) is an exact one.

![Energy surface](image)

**FIG. 3.** Energy surface \( E(\alpha, \beta) \) with a fixed value for \( \gamma = \gamma_0 = -1 \). Other parameters are \( L = 1 \) and \( r = 0.618034 \).

Although essential features of the energy surface around the singularity is expressed in Eq. (18) and Fig. II, it is helpful to look at the full energy surface \( E(\alpha, \beta) \) around the singularity, Eq. (14), which is depicted in Fig. III. The values for \( r \) and \( \gamma_0 \) are the same as in Fig. II. But here, the energy is calculated directly from Eqs. (9), (10) without any approximation. The spiral structure is clearly discernible from this figure. Because of the approximate periodicity of \( E(\alpha, \beta) \) by the period \( \pi \) as expressed in Eq. (14), the structure is approximately axis-symmetric with respect to the singular axis. The resulting structure is a double spiral stairway, somewhat reminiscent of the celebrated double helix of DNA in its appearance.

Next, we take a brief look at the gauge field structure behind the scene. In the manner of Wilczek and Zee, adopting the vector notation \( \vec{\lambda} = (\alpha, \beta) \), we consider the evolution of the eigenstate \( \phi_n(\vec{\lambda}) \) with the adiabatic variation of the parameter \( \vec{\lambda} \) that start from \( \vec{\lambda}_0 \), at which point we set \( \phi_n(\vec{\lambda}_0) = \psi_n(\vec{\lambda}_0) \). We then have

\[
\phi_n(\vec{\lambda}) = \sum_m U_{n,m}(\vec{\lambda}, \vec{\lambda}_0) \psi_m(\vec{\lambda}_0)
\]

with the evolution matrix \( U \) given by the path-ordered integral

\[
U(\vec{\lambda}, \vec{\lambda}_0) = P \exp \left( \int_{\vec{\lambda}_0}^{\vec{\lambda}} \vec{A}(\vec{x}) \cdot d\vec{x} \right)
\]

where \( \vec{A} \) is the Berry-Mead connection defined by

\[
\vec{A}_{n,m}(\vec{\lambda}) = \left\langle \psi_n(\vec{\lambda}) \left| \frac{\partial}{\partial \lambda} \psi_m(\vec{\lambda}) \right. \right\rangle.
\]

The non-trivial nature of the connection \( \vec{A}(\vec{\lambda}) \) is evident in the evolution integral over a closed-loop \( C \)

\[
U_{n,m}(C) = \delta_{n,m+2} \quad \text{if} \quad C \text{ encircles } \vec{\lambda}^* = (\alpha^*, \beta^*)
\]

\[
= \delta_{n,m} \quad \text{otherwise},
\]

which is just another expression of the spiral structure, Eq. (15).

It is instructive to look at the way an eigenfunction at a given parameter value \( (\alpha, \beta) \) is turned into the second-nest higher state after the rotation around the singularity. In Fig. IV, an example of such wave-function morphology is displayed. One essential feature is the node change which occurs at the crossing of \( \beta = 0 \) line. On this line, the system is separated into the non-communicating two subsystems at \( x = 0 \) because of the infinite value of \( \delta \). The reason of nodal change is that the approach to \( \beta = 0 \) line from the \( \beta > 0 \) side and \( \beta < 0 \) side are physically distinct because they each correspond to \( \delta = \mp \infty \) and \( \delta = \mp \infty \) respectively. (The composite signs are for the case of \( \alpha \gamma_0 > 1 \) and \( \alpha \gamma_0 < 1 \) respectively, in turn.) Yet, at \( \beta = 0 \) line, two cases get connected smoothly.

It is easy to see that the energy surface has a similar structure after interchanging the role of \( \beta \) and \( \delta \). One therefore has the singularity in \( (\alpha, \delta) \) space at the point \( (1/\gamma_0, 0) \). Also one can interchange the parameter set \( (\alpha, \gamma) \) and \( (\beta, \gamma) \) to get the singularity in \( (\gamma, \delta) \) space, etc. It would be very interesting if one could represent the full four-dimensional energy surface in intuitive fashion, although doing so would require a real ingenuity.

We now place our findings in broader context. Looking at the spiral structure of Fig. IV, one is inevitably reminded with the Bender-Wu singularity which is found in the energy surface of a complex parameter of the quartic quantum oscillator. Although we do not find any direct link between our problem and the quartic oscillator, the similarity is still intriguing.
It is natural to search for other quantum systems whose parametric energy surface has similar structure. Whether the new type of aboholonomy found in our example is as ubiquitous as the Berry phase aboholonomy is an important question. It is known that the contact interactions on one-dimensional line have immediate generalization as the contact interactions on the graph. That could be one place where one might find more examples of interesting wave-function morphology. Also, a recent work on “homeopathic” quantum system seems to have certain relevance to the aboholonomy discussed here.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{The ground state is turned into the second higher state when the parameters (\(\alpha, \beta\)) trace an adiabatic cycle around the singularity (\(\alpha^*, \beta^*\)) and come back to the original value.}
\end{figure}

It is obvious that the structure of the parameter space expressed by Eqs. (3) and (6) is the crucial element in bringing the double spiral structure in energy surface and resulting wave-function aboholonomy. In mathematical term, the parameters (\(\alpha, \beta, \gamma, \delta\)) span a \(SL(2, \mathbb{R})\) manifold, which is isomorphic to the hyper-cylindrical manifold \(S^1 \times \mathbb{R}^2\). The non-trivial structure of this manifold as expressed in the non-zero homotopy group is a basis for the spiral aboholonomy found in the current model. The mathematical classification and generalization along this line should open up a new vista for the search of other systems with aboholonomy. It is worth pointing out, in this context, that certain gauge field theories possess the characteristics called chiral anomaly which can be understood in terms of the structure similar to Eq. (22).

Finally, we would like to stress the potential utility of our findings in the fast-developing nano-device technology. In the coming age of quantum information processing and “quantum mechanical engineering”, we might even contemplate the actual applications of the current scheme of wave-function morphology in manipulating the wave functions to obtain the quantum states of desired shapes and energies. This might be achieved either in quantum dot settings as the potential problem of Eqs. (a) - (f), or in the heterojunction settings as discussed in Ref. [15].

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