Physical Aspects of Singularities in Quantum Mechanics

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Quantum singularities on a line furnish a rich variety of exotic phenomena in physics, such as spectral duality, Berry phase, scale anomaly, supersymmetry, or even quantum copy through tunneling, which are normally found in more complex systems. How these can appear out of the simple setup of a line system with just a point singularity will be sketched, starting from the basics of how to treat singularities in quantum mechanics.

KEYWORDS: singularity, duality, Berry phase, scale anomaly, supersymmetry, quantum tunneling

1. Introduction

Singularities in quantum mechanics arise in various situations, for instance, as defects in a homogeneous material or divergent points in the potential describing a system. On a line (*i.e.*, in one dimension), quantum mechanics is known to admit physically distinct singularities which form a four parameter family[1,2] given by the unitary group $U(2)$. The diversity of the quantum singularities leads to several exotic phenomena, including duality in spectrum, Berry phase, scale anomaly and supersymmetry.[3–5] Below, some of these will be discussed briefly after presenting how the $U(2)$ family arises for the description of a singularity. Further, we argue that *quantum copy* (copy of the profile of an arbitrary state) may be possible when combined with caustics realized under a singular potential.

2. $U(2)$ Family of Singularities

Given a system of a line $-\infty < x < \infty$ with a point singularity, say at $x = 0$, the first question one has to address is how to specify the physical nature of the singularity in quantum mechanics. On the most general basis, the answer is given from the requirement of unitarity (probability conservation), or equivalently the self-adjointness of the Hamiltonian,

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}, \tag{1}$$

defined on the line with the singularity removed, namely on $x \neq 0$. This implies that the probability current $j(x) = -\frac{i\hbar}{2m}\left((\psi^*)'\psi - \psi^*\psi'\right)(x)$ be continuous at the singular point $x = 0$, and the most general solution for this is expressed by the connection condition,[6,7]

$$(U - I)\Psi + iL_0(U + I)\Psi' = 0. \tag{2}$$

Here U is a matrix, called *characteristic matrix* belonging to $U(2)$, $L_0 \neq 0$ is a real constant and

$$\Psi = \begin{pmatrix} \psi(+0) \\ \psi(-0) \end{pmatrix}, \quad \Psi' = \begin{pmatrix} \psi'(+0) \\ -\psi'(-0) \end{pmatrix}, \tag{3}$$

are vectors defined from the boundary values of the wave function $\psi(\pm 0) = \lim_{x\to\pm 0}\psi(x)$ and their derivatives. The $U(2)$ arbitrariness for the solution suggests that there exist the $U(2)$ family of singularities allowed quantum mechanically, characterized by the connection condition (2). For instance, for $U = \sigma_1$ (where σ_i are Pauli matrices) the connection condition (2) reduces to $\psi(+0) = \psi(-0)$, $\psi'(+0) = \psi'(-0)$, that is, it represents the 'free system' where there is no singularity. On the other hand, the choice $U = -I$ leads to the Dirichlet condition $\psi(+0) = \psi(-0) = 0$ while $U = I$ gives the Neumann condition $\psi'(+0) = \psi'(-0) = 0$.

We also mention that, if the system has impenetrable boundaries such as the infinite potential wall, we need an additional $U(1)$ parameter to each of the boundaries to specify the boundary condition there.

When the singularity arises as a divergent point of a potential, on the other hand, it may be possible that the wave function (and/or its derivative) also diverges there. If this happens, then the above prescription to specify the singularity becomes ill-defined. However, even in such cases the Wronskian $W[\phi, \psi](x) = \phi(x)\psi'(x) - \psi(x)\phi'(x)$ evaluated for two arbitrary states ϕ and ψ remains well-defined, and this suggests that we may furnish the connection condition (2) in terms of the generalized boundary vectors[8]

$$\Psi = \begin{pmatrix} W[\psi, \varphi_1]_{+0} \\ W[\psi, \varphi_1]_{-0} \end{pmatrix}, \quad \Psi' = \begin{pmatrix} W[\psi, \varphi_2]_{+0} \\ -W[\psi, \varphi_2]_{-0} \end{pmatrix} \tag{4}$$

using some states φ_1, φ_2 for 'reference' to provide the Wronskians. In fact, for a suitable choice of the reference states the generalized boundary vectors (4) reduce to (3) if the states ψ are well-defined at the singularity. In this sense, the boundary vectors (4) furnish a generalization of (3) to cases where the latter is ill-defined.

3. Spectral Space

To discuss the physical content of the singularities on a line, it is convenient to introduce the following decomposition of the characteristic matrix,[3,4]

$$U = V^{-1}DV, \tag{5}$$

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with the parametrization,

$$D = \begin{pmatrix} e^{i\theta_+} & 0 \\ 0 & e^{i\theta_-} \end{pmatrix}, \qquad V = e^{i\frac{\mu}{2}\sigma_2} e^{i\frac{\nu}{2}\sigma_3} \tag{6}$$

where $\theta_\pm \in [0, 2\pi)$ and $\mu \in [0, \pi]$, $\nu \in [0, 2\pi)$. Our motivation behind this decomposition comes from the fact that the parity $\mathcal{P}$ and the half-reflection $\mathcal{R}$,

$$\mathcal{P}: \quad \psi(x) \to (\mathcal{P}\psi)(x) := \psi(-x), \tag{7}$$

$$\mathcal{R}: \quad \psi(x) \to (\mathcal{R}\psi)(x) := [\Theta(x) - \Theta(-x)]\psi(x), \tag{8}$$

induce the change in the boundary condition as

$$U \xrightarrow{\mathcal{P}} \sigma_1 U \sigma_1, \qquad U \xrightarrow{\mathcal{R}} \sigma_3 U \sigma_3, \tag{9}$$

and yet the energy eigenstates remain to be the eigenstates under the new boundary conditions*. This implies that one can actually change V in (6) in the decomposed U without changing the spectrum. In other words, the energy spectrum of the system is determined solely by the two angle parameters (θ_+, θ_-) in D in the characteristic matrix U. From these spectral parameters, we we may define the more convenient scale parameters,

$$L(\theta_\pm) = L_0 \cot \frac{\theta_\pm}{2}. \tag{10}$$

These appear, for instance, in the bound states $\psi_\pm(x) \propto e^{-|x|/L(\theta_\pm)}$ which exist if $L(\theta_+) > 0$ and/or $L(\theta_-) > 0$.

From the foregoing argument we realize that the parameter space $U(2)$ can be regarded as the product of the spectral space, given by the torus† $T^2 \simeq U(1) \times U(1) = \{(\theta_+, \theta_-)\}$ in D, and the remaining non-spectral space, given by the sphere S^2 parametrized by μ and ν in V. These two parameters represent the phase shift at the singularity and the degree of mixture of the limiting values of the state at $x = \pm 0$. This characterization of the parameters remain to be true even if there exists an symmetric potentials $V(-x) = V(x)$ on top of the singularity.

4. Duality, Berry Phase, Supersymmetry

We now discuss some of the physically interesting phenomena occurring under the family of singularities mentioned in the Introduction.

4.1 Duality

To discuss the spectral duality, for definiteness let us restrict ourselves to parity invariant singularities. Since the parity transformation $\mathcal{P}$ induces the change (9), parity invariant singularities are characterized by those U satisfying $\sigma_1 U \sigma_1 = U$. The general solution is given by

$$U = U(\theta_+, \theta_-) = e^{i(\theta_+ P_1^+ + \theta_- P_1^-)}, \tag{11}$$

where we have used $P_1^\pm = \frac{1 \pm \sigma_1}{2}$, which is obtained by setting the isospectral parameters $(\mu, \nu) = (\pi/2, 0)$ in (6). Then we notice that the free system $U = \sigma_1$ is realized in this parity invariant subfamily of singularities at $(\theta_+, \theta_-) = (0, \pi)$. This suggests that, in order to measure the strength of the interaction at the singularity, one may define the 'coupling constants' by

$$g_+(\theta_+) := \tan \frac{\theta_+}{2}, \qquad g_-(\theta_-) := \cot \frac{\theta_-}{2}, \tag{12}$$

so that $g_+(0) = g_-(\pi) = 0$ at the free point. Now consider the half reflection $\mathcal{R}$ in (8), which induces the exchange $\theta_+ \leftrightarrow \theta_-$ through (9). But since $\mathcal{R}$ preserves the spectrum, spectral duality must hold in the system, that is, the spectrum is unchanged even if we exchange the parameters (θ_+, θ_-) which causes the corresponding transformation of the coupling constants. In particular, if the parameters fulfill $\theta_+ = \theta_- \pm \pi$, then we find the reciprocal behaviour

$$(g_+(\theta_+), g_-(\theta_-)) \xrightarrow{\mathcal{R}} (-1/g_+(\theta_+), -1/g_-(\theta_-)). \tag{13}$$

This shows that the system has the spectral duality between the strong versus weak couplings.

4.2 Berry phase

Nest, we consider the opposite situation, that is, the case where the spectral parameters are fixed to the free point $(\theta_+, \theta_-) = (0, \pi)$ whereas the isospectral parameters (μ, ν) are free to vary. The resultant subfamily is the scale invariant subfamily consisting of singularities invariant under the Weyl scale transformation,

$$\mathcal{W}_\lambda: \quad \psi(x) \longrightarrow (\mathcal{W}_\lambda \psi)(x) := \lambda^{\frac{1}{2}} \psi(\lambda x), \tag{14}$$

for real λ. For the sake of discussion, we shall make the entire spectrum discrete by placing infinite potential walls at $x = \pm l$ and impose the Dirichlet boundary conditions there (*i.e.*, we put the particle in the box $[-l, l]$). The energy eigenstates are

$$\psi_n(x) = c_+(\mu)\, \xi_n^+(x) + c_-(\mu) e^{i\nu}\, \xi_n^-(x), \tag{15}$$

where we have used $c_\pm(\mu) = \cos\frac{\mu}{2} \mp \sin\frac{\mu}{2}$ and

$$\xi_n^\pm(x) = \sqrt{\frac{1}{l}} \sin k_n(x \mp l)\Theta(\pm x), \tag{16}$$

with $k_n = \left(n - \frac{1}{2}\right)\frac{\pi}{2l}$ for $n = 1, 2, 3, \ldots$. Let us now vary the isospectral parameters (μ, ν) along a loop C on the isospectral sphere S^2. After completing one cycle of the variation, each eigenstate must return to the initial one up to an phase pertinent to the state, $\psi_n \to e^{i\gamma(C)}\psi_n$. This phase $\gamma(C)$ is the Berry phase, which in this case can be evaluated by $\gamma(C) = \oint_C A$ with the Berry connection,

$$A = i\langle \psi_n | d\psi_n \rangle = -\frac{1}{2}(1 + \sin\mu)\, d\nu, \tag{17}$$

where d is the exterior derivative in the parameter space. Note that the curvature $F = dA$ is just the magnetic field of the Dirac monopole, $F = -\frac{1}{2}\cos\mu\, d\mu d\nu$.

A similar observation of states under a cyclic change can be made on the spectral torus, rather than the isospectral sphere. There, one finds non-Abelian an-

* Together with the product $\mathcal{Q} = i\mathcal{P}\mathcal{R}$, the three discrete transformations $\{\mathcal{P}, \mathcal{Q}, \mathcal{R}\}$ form an $su(2)$ ispospectral algebra.[4)]

† In fact, one can show that the spectrum is unchanged under the interchange of the parameters, and hence the actual parameter space is given by a Möbius strip with boundary.[9)]

holonomy (Abelian anholonomy is the Berry phase) where now each level do not return to the initial one after completing one cycle, even though the entire spectrum returns to the initial one.

4.3 Supersymmetry

The spectral duality under the exchange $\theta_+ \leftrightarrow \theta_-$ implies that, when $\theta_+ = \theta_-$, there will be degeneracy in the energy levels, and this in turn suggests that the system may accommodate supersymmetry (SUSY). In fact, there exists a class of systems with a point singularity possessing SUSY. To see this, it is convenient to regard the line system as a set of two half lines, and use, instead of the wave function $\psi(x)$ and the Hamiltonian H in (1), those expressed in the two-component vector space,

$$\Psi(x) = \begin{pmatrix} \psi_+(x) \\ \psi_-(x) \end{pmatrix}, \qquad H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \otimes I, \tag{18}$$

where we have defined $\psi_+(x) = \psi(x)$ for $x > 0$ and $\psi_-(-x) = \psi(x)$ for $x > 0$ and I is the 2×2 identity matrix. Upon this reformulation, we consider the supercharge,

$$Q = -i\lambda \frac{d}{dx} \otimes \sigma_{\vec{a}} + \mathbf{1} \otimes \sigma_{\vec{b}} \tag{19}$$

with $\lambda = \hbar/2\sqrt{m}$ and

$$\sigma_{\vec{a}} = \sum_{i=1}^{3} a_i \sigma_i, \quad \sigma_{\vec{b}} = \sum_{i=1}^{3} b_i \sigma_i, \quad |\vec{a}| = 1, \quad \vec{a}\cdot\vec{b} = 0, \tag{20}$$

with real vectors $\vec{a}$, $\vec{b}$. The conditions (20) assure the relation $2Q^2 = H + |\vec{b}|^2$ and, hence, if we absorb the constant $|\vec{b}|^2$ into the Hamiltonian (which causes just the corresponding constant energy shift), we obtain, for properly chosen set of supercharges Q_i for $i = 1, \ldots, N$ (in case the system admits more than one supercharges), the standard SUSY algebra,

$$\{Q_i, Q_j\} = H\,\delta_{ij}. \tag{21}$$

An important point, however, is that for the system to be supersymmetric the supercharge Q must leave the connection conditions invariant, at least for energy eigenstates. This is seen to be the case if one of the two spectral parameter is π and the other non-zero, *e.g.*, $\theta_+ = \theta \neq 0$ and $\theta_- = \pi$, and further if the supercharge takes the form $Q = V^{-1} q(\alpha, c; \theta) V$ with

$$\begin{aligned} q(\alpha, c; \theta) = &-i\lambda \frac{d}{dx} \otimes e^{-i\frac{\alpha}{2}\sigma_3} \sigma_1 e^{i\frac{\alpha}{2}\sigma_3} \\ &+ \mathbf{1} \otimes \left[-\frac{\lambda}{L(\theta)} e^{-i\frac{\alpha}{2}\sigma_3} \sigma_2 e^{i\frac{\alpha}{2}\sigma_3} + c\,\sigma_3 \right], \end{aligned} \tag{22}$$

where $L(\theta)$ is the scale parameter defined in (10). Since α is arbitrary, we find that there are two independent supercharges, *i.e.*, the system has an $N = 2$ SUSY.

For extension, one may consider systems with two infinite walls as we did in discussing the Berry phase, or double the number of lines. One then observes by a similar argument that there do arise various types of systems admitting $N = 1$, 2 or 4 SUSY, some are broken (the ground state is not annihilated by the SUSY transformation) and some are not, and some have a number of bound states while some have none.[10)]

5. Quantum Tunneling and Copy

If the singularity occurs as a divergent point of a potential $V(x)$, and if the potential is a special type allowing for caustics,[11)] then we can find interesting phenomena as a result of the combination of quantum singularity and caustics. As an example, let us consider the potential,

$$V(x) = \frac{m\omega^2}{2} x^2 + g\frac{1}{x^2}. \tag{23}$$

which is known to admit classical caustics. In quantum mechanics, the general solution for the Schrödinger equation $H\psi_n(x) = E_n\psi_n(x)$ is given by a linear combination of the two independent solutions,

$$\phi_n^{(1)}(x) := y^{c_1 - 1/2} e^{-y^2/2} F\left(\frac{c_1 - \lambda_n}{2}, c_1; y^2\right), \tag{24}$$

$$\phi_n^{(2)}(x) := y^{c_2 - 1/2} e^{-y^2/2} F\left(\frac{c_2 - \lambda_n}{2}, c_2; y^2\right), \tag{25}$$

where $F(\alpha, \gamma; z)$ is the confluent hypergeometric function, $\lambda_n = E_n/\hbar\omega$ and we have used $c_1 = 1+a$, $c_2 = 1-a$ and

$$a = \frac{1}{2}\sqrt{1 + \frac{8mg}{\hbar^2}}, \qquad y = \sqrt{\frac{m\omega}{\hbar}}\,x. \tag{26}$$

We then observe that, if the coupling constant g is in the range,

$$0 < g < \frac{3\hbar^2}{8m}, \tag{27}$$

then we have $\frac{1}{2} < a < 1$, and therefore both of the two solutions (30) are square integrable, even though $\phi_n^{(2)}$ may diverge at $x = 0$. Demanding that the general solution fulfill the connection condition (2) specified by U, one obtains the spectral condition,

$$\frac{1}{c_2 - c_1}\sqrt{\frac{m\omega}{\hbar}} \frac{\Gamma\left((c_1 - \lambda_n)/2\right)}{\Gamma\left((c_2 - \lambda_n)/2\right)} \frac{\Gamma(c_2)}{\Gamma(c_1)} = -\frac{1}{L(\theta_\pm)}. \tag{28}$$

This shows that, in general, there exist two series of energy levels, one specified by $L(\theta_+)$ and the other by $L(\theta_-)$. For instance, if the singularity is free, $U = \sigma_1$, then we have the two series of eigenstates,

$$\psi_n^{(1)}(x) = N^{(1)}\,\phi_n^{(1)}(|x|)\left[\Theta(x) - \Theta(-x)\right], \tag{29}$$

$$\psi_n^{(2)}(x) = N^{(2)}\,\phi_n^{(2)}(|x|), \tag{30}$$

with the eigenvalues,

$$E_n^{(1)} = (2n + 1 + a)\hbar\omega, \quad E_n^{(2)} = (2n + 1 - a)\hbar\omega, \tag{31}$$

for $n = 0, 1, \ldots$. Note that in the limit $g \to 0$ ($a \to 1/2$) these states reduce to the familiar eigenstates of the harmonic oscillator as expected. Such a smooth limit does not exist for other singularities. For example, at the

Dirichlet point $U = -I$, one obtains the doubly degenerate energy levels $E_n = (2n + c_1)\hbar\omega$ which do not reduce to those of the harmonic oscillator. In passing, we point out that this case $U = -I$ is in fact the one adopted conventionally to provide the connection condition when we analyse the Calogero model.[12)]

Having solved the quantum system, we now examine if the singularity, or physically speaking, the infinite potential wall at $x = 0$, allows quantum tunneling. The answer is yes: for the free point case $U = \sigma_1$, for instance, the generic state

$$\psi(x) = \sum_n (c_n^{(1)}\psi_n^{(1)}(x) + c_n^{(2)}\psi_n^{(2)}(x)) \qquad (32)$$

has the probability current at the singularity,

$$j(\pm 0) = \frac{ia\hbar}{m}\sum_{n,l}\left\{(c_n^{(1)})^* c_l^{(2)} - (c_n^{(2)})^* c_l^{(1)}\right\}, \qquad (33)$$

which is non-vanishing[‡] in general. More direct evidence may be gained from the transition amplitude,

$$K(x_f, t_f; x_i, t_i) = \langle x_f | e^{-\frac{i}{\hbar}H(t_f - t_i)} | x_i \rangle, \qquad (34)$$

which can be evaluated exactly in this case. We then find that, for the transition time $T := t_f - t_i \neq k\pi/\omega$ ($k = 0, 1, 2, \dots$), the amplitude is expressed in terms of the modified Bessel function, and from it we learn that the transition across the singularity is indeed allowed.

The remarkable point is that, at the periods $T = k\pi/\omega$, the amplitude turns out to be

$$\begin{aligned} K(x_f, t_f; x_i, t_i) = (-1)^k \cos(ak\pi)\delta(x_f - x_i) \\ + i(-1)^k \sin(ak\pi)\delta(x_f + x_i). \end{aligned} \qquad (35)$$

The first term on the r.h.s. represents the classical caustics corresponding to the return of the particle to its initial position, while the second term implies that the particle can reach the mirror point, too, thanks to the quantum tunneling. Thus, the classical caustics phenomenon has been modified at the quantum level, producing the mirror image of the original profile prepared at the initial time $t = t_i$, with the weight factors being the functions of the parameter a determined from the coupling constant g (and the characteristic matrix U for the general case). This implies that one may 'copy' an original profile prepared on the $x > 0$ side, for instance, to the other $x < 0$ side after the periods, and that this can be done with desirable weight factors, if one can control the relevant parameters of the factors freely.[13)] This copying process in not in conflict with the no-go theorem[14)] of quantum cloning, because the process takes place in one Hilbert space rather than two as presumed in the theorem.

6. Discussions

We have outlined above some of the interesting physical phenomena that can arise in systems with a point singularity. It is remarkable that putting just a singular point on a line enables us to realize those phenomena which are usually discussed or found in more involved systems, such as gauge field theory or string theory. It is perhaps safe to say that the key element for those quantum phenomena is not in the complexity of the system nor in the infinity of the physical degrees of freedoms of the system. Rather, it seems that the essence lies in the part of the definition of the system required only for quantum theory. Indeed, the $U(2)$ variety of the singularities derives from the demand of the self-adjointness of the Hamiltonian operator and hence this cannot occur in classical theory. Needless to say, the variety is meaningful only in quantum theory.

Finally, we wish to mention three possible extensions of this work. The first is the obvious one, that is, we may study less trivial systems — with more singular points, non-trivial topology (quantum networks) *etc.* — by the same procedure. In view of the recent rapid progress of nano-technology, this may lead to some application in the near future. The second is to seek novel quantum phenomena — such as the anomalous caustics — under singular potentials, and thereby find their possible use. Further, one may also consider situations where the system has a part that can be regarded as a black box, such as one having an infinite potential finite area or a black hole. There, normalizability of states may no longer be required on account of the physical absence of the area in the system, and hence our procedure to treat singularities and, possibly the physical outcomes as well, may be relevant. We expect that these will be materialized in parallel with the advance of experiments which hopefully confirm the theoretical predictions made in this article.

[‡] There are, of course, exceptional cases where the tunneling is prohibited, such as those defined at the Dirichlet or Neumann point. These form the subfamily called 'separated subfamily'.

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