Hidden scale in quantum mechanics

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We show that the intriguing localization of a free particle wave-packet is possible due to a hidden scale present in the system. Self-adjoint extensions (SAE) is responsible for introducing this scale in quantum mechanical models through the nontrivial boundary conditions. We discuss a couple of classically scale invariant free particle systems to illustrate the issue. In this context it has been shown that a free quantum particle moving on a full line may have localized wave-packet around the origin. As a generalization, it has also been shown that particles moving on a portion of a plane or on a portion of a three dimensional space can have unusual localized wave-packet.

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I. INTRODUCTION

In quantum mechanics usually the bound state system described by a Hamiltonian must have a scale in the Hamiltonian in order to localize it in a region of space. This is the reason a particle with only kinetic term is a free particle with wave-function spreading throughout the space with equal probability. Even a particle with a potential [1, 2, 3, 4], which transforms the same way the kinetic part transforms under scale transformation \( r \rightarrow \alpha r, t \rightarrow \alpha^2 t \), does not usually possess any bound state [5].

Despite this scale invariance in some problems [6] one can still expects bound state solution when quantization of the classical system is preformed. Because the process of quantization may introduce a scale into the system. SAE [7] is one way of introducing a scale in the system, thus leading to a quantum mechanical anomaly [1, 2, 3, 4, 6]. Thus although we don’t see the scale in the Hamiltonian, it is actually hidden in the boundary condition. SAE has been a rigorous method to find the most general boundary conditions for a quantum mechanical model so that the operator, for example the Hamiltonian, becomes self-adjoint. For the Hamiltonian it is necessary to be self-adjoint, because otherwise the time evolution of the quantum states generated by \( \mathcal{U} = \exp(-iHt) \) [2] will not be unitary. Unitarity is essential to keep the norm of the states unchanged through out the transformation. The other importance of the self-adjointness is that the eigen-values are guaranteed to be real.

Hidden scale problem, quantum anomaly and the implications of self-adjoint extensions, all these three can be found in the case of a free particle dynamics. Note that we call a particle free in the sense that the potential for the particle \( V = 0 \), i.e., it has only kinetic part in the Hamiltonian, \( H = p^2/2M \). Although the form of the Hamiltonian is the simplest of all, it raises lot of intriguing facts when viewed as a Hamiltonian of a localized wave packet. For example, the localization of a free particle on a half line [8, 9] is such an interesting problem, where SAE gives rise to bound state solutions by introducing a length scale into the system. Similarly for a particle confined on a whole plane can have bound state solution, once inequivalent quantization is made [10, 11]. The largest possible space dimensions in which a free particle can have bound state due to inequivalent quantization is \( N = 3 \). Beyond three dimensions the quantum centrifugal inverse square potential arising from pure kinetic term does not allow the localization of the wave-packet.

In this letter, in Sec. II we will discuss the problem of binding a free particle on a whole line by generalizing the problem of a particle on a half line. In Sec. III we discuss about a particle moving on a portion of a plane (see FIG. 2) and also discuss the problem of a free particle on a plane (see FIG. 1) in the context of hidden scale problem. Finally a free particle moving in some region of a three dimensional space has been shown to possess a bound state in Sec. IV. All these three problems are scale invariant due to the absence of any potential in the Hamiltonian. However the fact that very unusual bound state does exists in all these three cases was not known in the literature as far as our knowledge is concerned. We conclude in Sec. V.
II. PARTICLE ON A FULL LINE

Before discussing the problem of a free particle moving on a full line let us first review the problem on a half line [8, 9]. Because then particle on a full line is just a generalization. It is known that the free particle on a half line can be made self-adjoint and there exist a bound state of the particle. The 1-dimensional Hamiltonian for the particle in the interval \( x \in [0, \infty) \) is of the simple form \( (\hbar^2 = 2M = 1) \)

\[
H_{1D} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}.
\]  

We are interested in the bound state problem for the particle. The Hamiltonian is manifestly scale covariant under the transformation \( x \rightarrow \alpha x, t \rightarrow \alpha^2 t \). So there is no scale in the problem and it suggests that the particle does not have any bound state [9]. But the inequivalent quantization of the system with the self-adjoint domain

\[
D_{1D}^L = \{ \psi(x) \in \mathcal{L}^2(dx), \psi'(0) = L^{-1} \psi(0) \},
\]  

(2)

allows us to get a bound state solution with energy eigenvalue and eigenfunction respectively given by

\[
E_{1D} = -L^{-2}, \quad \psi(x)_{1D} = \sqrt{2L^{-1}} \exp(-L^{-1}x).
\]  

(3)

where \( L \) has to be positive and finite in order to make the solution \( \psi(x) \) square-integrable. The hidden scale \( L \), called the self-adjoint extension parameter, breaks the scale invariance of the system. This is a simple quantum mechanical example of scaling anomaly. The probability density for the wave-packet confined on a half line has been shown in FIG. 3.

We now generalize the same problem by considering it on a full line, \( x \in (-\infty, \infty) \) instead on a half line. The Hamiltonian now possesses reflection symmetry in addition to its scale invariance contrary to the half line case, which had only scale invariance. We can exploit the reflection symmetry of the problem to reduce it on the form [10] by using the transformation \( z = |x| \). So the analysis will be same, but the normalization constant of the bound state wave-function will now change due to reflection symmetry in the problem. The bound state solutions are

\[
E_{1D} = -L^{-2}, \quad \psi(|x|)_{1D} = \sqrt{L^{-1}} \exp(-L^{-1}|x|).
\]  

(4)

Note the simplicity of the result [10], but despite its simplicity it has remained unnoticed so far. It is however know for a long time that particle on a line with \( \delta \)-function potential has bound state solution [10, 12]. In fact the result is same as what we have obtained without any potential but using SAE. The probability density has a pick at the origin, which has been shown in FIG. 5.

III. PARTICLE ON A PLANE

To show the ring shaped localization of a free particle wave-function around the origin of a plane [10, 11, 13] due to the hidden scale, we consider a particle of mass \( M \) on \( x-y \) plane. The Hamiltonian of the system can be written in term of a 2-dimensional Laplacian \( H_{2D} = -\nabla^2 \). In polar co-ordinates \((\rho, \phi)\) the radial eigenvalue equation with eigen-value \( E \) can easily be separated with the radial Hamiltonian

\[
H_{2D}^\rho = -\partial_\rho^2 - 1/\rho \partial_\rho + m^2/\rho^2,
\]  

(5)

where \( \partial_\rho \) and \( \partial_\rho^2 \) is the 1-st and 2-nd order derivative w.r.t \( \rho \) respectively and \( m = 0, \pm 1, \pm 2, \ldots \) is the angular momentum quantum number. Usual practice is to define a very restricted symmetric domain for this system so that it can be extended to a self-adjoint domain. One of the possible domains over which the Hamiltonian is symmetric is of the form

\[
D_{2D} = \{ \psi(\rho) \in \mathcal{L}^2(\rho d\rho), \psi(0) = \psi'(0) = 0 \}.
\]  

(6)

The domain \( D_{2D} \) is so restricted that it fails to make \( H_{2D}^\rho \) self-adjoint. Then one seeks for a SAE. Using von Neumann’s method it can be shown that the domain over which the Hamiltonian \( H_{2D}^\rho \) is self-adjoint is of the following form

\[
D_{2D}^\Sigma(L^{-2}) = \{ D_{2D} + \psi(\rho, L^{-2}, \Sigma) | \psi(\rho, L^{-2}, \Sigma) \in D_A \},
\]  

(7)
where \( D_A \) is the domain of the operator \( H^*_L \), which is adjoint to \( H^L \). The dimensionless parameter \( \Sigma \in \mathbb{R} \) (mod \( 2\pi \)) is called the SAE parameter. Note that the dimension-full constant \( L \in \mathbb{R}^+ \) is incorporated into the domain \( D^L_{2D}(L^{-2}) \) through the elements \( \psi(r, L^{-2}, \Sigma) \) of the deficiency space, which is spanned by the solutions of the equation

\[
(H^*_{2D} + iL^{-2})\psi_{\pm}(\rho, L^{-2}) = 0.
\] (8)

The element \( \psi(\rho, L^{-2}, \Sigma) \) is explicitly written as \( \psi(\rho, L^{-2}, \Sigma) = \psi_{\pm}(\rho, L^{-2}) + \exp(i\Sigma)\psi_{-}(\rho, L^{-2}) \). Now the system defined by \( H_{2D} \) and \( D^L_{2D} \) has a length scale \( L \), hidden in the boundary condition. The bound state for the system is now exists for \( m = 0 \) wave and it will now depend on two independent parameters \( \Sigma \) and \( L \). The bound state energy \( E(L^{-2}, \Sigma) \) has certain interesting features, for example it is periodic in \( \Sigma \),

\[
E(L^{-2}, \Sigma) = E(L^{-2}, \Sigma + 2\pi).
\] (9)

So the bound state energy \( E(L^{-2}, \Sigma) \) can be written in terms of a periodic function \( F(\Sigma) \in \mathbb{R}^+ \) as

\[
E(L^{-2}, \Sigma) = -L^{-2}F(\Sigma).
\] (10)

The exact form of the function \( F(\Sigma) \) can be found from the domain \( D^L_{2D}(L^{-2}) \). The bound state eigenfunction for \( F(\Sigma) = 1 \) is of the form [1]

\[
\psi(\rho) = \frac{1}{\sqrt{\pi}}L^{-1}K_0(L^{-1}\rho), \tag{11}
\]

where \( K_0 \) is the modified Bessel function [14], which has logarithmic divergence at the origin but the probability density obtained from it goes to zero at origin, which has been shown in FIG. 1.

We now consider the situation, where the particle is moving on a part of the plane not on a whole plane and ask the question whether the method of SAE is still capable of binding the particle on the restricted region of the plane, for example in the region specified by \( \rho \in [0, \infty), \phi \in [0, 2\pi] \), where \( 0 \leq \beta \leq 1 \). This problem can be easily solved once the eigen-value equation for the angular operator \( L^2 = -\partial^2/\partial\phi^2 \) is solved. But we don’t need to explicitly solve the angular part for our discussion. What we need to know is that whether there exists any eigenvalue within the interval \( 0 \leq \tilde{m}^2 < 1 \), because then only we can expect bound state solutions. One can easily convince oneself that \( \chi(\phi) = \frac{1}{2\pi} \) is one of the eigen-functions of the operator \( L^2 \) with eigen-value \( \tilde{m} = 0 \). Note that \( \chi(\phi) \) has the time reversal symmetry [11]. Thus the radial Hamiltonian for \( \tilde{m} = 0 \) wave will be \( H^*_{2D} = -\partial^2/\partial\rho^2 - 1/\rho \partial\rho \), which has been shown in \([10]\) and \([11]\) to possess bound state solution. The probability density for the radial eigen-function has been plotted in FIG. 2. for \( \beta = 1/4 \).

\[
\text{FIG. 4: (color online)} \text{ A particle with } V = 0 \text{ is confined in a part of the 3-dimensional space specified by } r \in [0, 3], \theta \in [0, \pi/12], \phi \in [0, 2\pi]. \text{ The probability distribution } |\psi(r)|^2 \text{ of the particle as a function of the radial coordinate will look like FIG. 3, where probability density for a particle moving on a half line has been plotted. The reason for this similarity is obvious from the fact that for } \theta = 0, \text{ the solid angle reduces to a half line.}
\]

\[
\text{FIG. 5: (color online)} \text{ Bound state probability density } |\psi(x)|^2 \text{ of a particle on a full line } (x \in (-\infty, \infty)) \text{ with length scale } L = 1 \text{ has been plotted as a function of } x. \text{ The probability density is maximum at the origin.}
\]

IV. PARTICLE IN N-DIMENSIONS

We consider a free particle moving in \( N \) dimensional flat space. The Hamiltonian for the system is then written in the following form

\[
H_{ND} = -\nabla^2. \tag{12}
\]

Since \([12]\) has only kinetic term, it gives classically scale invariant action under the scale transformation \( r \rightarrow \alpha r, t \rightarrow \alpha^2 t \). Thus, usually it does not have any bound state solutions and only has free particle solutions \( \psi(\alpha r) = \exp(\pm i\mathbf{k} \cdot \mathbf{r}) \), where \( \mathbf{k} \) is the wave vector of the particle. The energy for the free particle eigen-function, \( E = k^2 \),
is continuous. We now seek for a nontrivial solution of the Schrödinger eigenvalue equation for the Hamiltonian $H_{ND}$. In spherical polar co-ordinates $(r, \phi, \theta)$ the radial Hamiltonian can be separated in the following form

$$H_{ND}^r = -\frac{1}{r^{N-1}} \frac{d}{dr} \left( r^{N-1} \frac{d}{dr} \right) + \frac{l(l + N - 2)}{r^2}$$

(13)

We can now use the transformation $R(r) = r^{-(N-1)/2} \chi(r)$ on the Schrödinger eigenvalue equation $H_{ND}^r \chi(r) = E_{ND} \chi(r)$. The Hamiltonian of the transformed eigenvalue equation $H_{ND}^r \chi(r) = E_{ND} \chi(r)$ has the very familiar form $H_{ND}^r = -\partial_r^2 + g/r^2$, with $g = l(l + N - 2) + 3 - N(N - 4)$. It can be shown that $H_{ND}^r$ have only one bound state for $-1/4 \leq g < 3/4$ [1]. One can check that for $l = 0$ and $2 \leq N < 4$ the effective coupling constant $g$ lies in the specified interval. Thus only s-waves for $N = 2$ and 3 support bound state [10]. The bound state solutions can be found from the self-adjoint domain

$$D_{ND}^s(L^2) = \{ D_{ND} + \psi(r, L^{-2}, \Sigma) \psi(r, L^{-2}, \Sigma) \in D_{NA} \},$$

(14)

where $D_{ND} = \{ \psi(r) \in L^2(r^{N-1} dr), \psi(0) = \psi'(0) = 0 \}$ and $D_{NA}$ is the domain of the adjoint Hamiltonian $H_{ND}^s$. Note that the scale $L$ is within the domain $D_{ND}^s(L^{-2})$, which has been introduced at the time of SAE. The bound state solution will now depend on the value of $g$ in the interval.

The bound state problem on a plane ($N = 2$) has been discussed in the previous section. Therefore we now concentrate the three dimensional ($N = 3$) problem. The Hamiltonian simply becomes $H_{3D}^s = -\partial_r^2$, because the dimensionless coupling $g = 0$, for $l = 0$ and $N = 3$. It is now a one dimensional problem on a half line, which has been discussed in Sec. II. The probability density for the wave-packet will be like FIG. 3.

One can also consider the situation where a particle is moving only in a portion of a 3-dimensional space, for example in the region $r \in [0, \infty)$, $\theta \in [0, \gamma \pi)$, $\phi \in [0, 2\pi)$, where $0 \leq \gamma \leq 1$. To solve this problem we need to solve the angular part. In fact in our purpose it is enough to know the coupling constant of the inverse square centrifugal term. One can convince oneself that $Y_{l}(\theta, \phi) = C$ (complex valued constant) is the trivial eige-function of $L^2$ with eigenvalue 0. Once again it reduces to a problem on a half line, discussed in Sec. II. In FIG. 4 particle confinement in a solid angle has been considered, where the probability density looks like FIG. 3.

V. CONCLUSION

Free particle Hamiltonian usually does not possess any bound state solution due to the absence of any scale in the problem. But we have discussed that the scale, hidden in the boundary condition, may be responsible to localize the wave packet. As an example we have discussed the known problem of particle on a half line and particle on a plane to show that the scale hidden within the boundary condition is responsible for localizing the wave-packet. We have also discussed that the free particle on a full line does have bound state if inequivalent quantization is considered. It is however known that a $\delta$-function potential can bind a particle on a full line. So one may think that the SAE induces a $\delta$-function potential in the system. Similar confinement of the wave packet has been shown to hold for the case of a particle moving on a portion of a plane and in a portion of a 3-dimensional space. These types of very unusual localized wave-packet in some portions of a two and three dimensional spaces does not seem to have appeared in literature.

VI. ACKNOWLEDGMENT

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