Boundary conditions for the wave functions and Gamow vectors

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Abstract

We introduce a new kind of boundary conditions for the wave functions, which admit solutions in the form of Gamow vectors for a wide class of potentials. We discuss in detail an example of an unstable quantum oscillator.

1 Introduction

The main equation of the non-relativistic quantum mechanics is the Schrödinger equation\textsuperscript{1}

\[ H\psi = -\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi = E\psi. \] (1)

Eq. (1) is not sufficient for the construction of the physically meaningful solutions. For bound states one uses the Hilbert space condition

\[ \int |\psi(x)|^2 dx < \infty, \] (2)

which leads to the real eigenvalues of the Hamiltonian. Gamow solutions on the other hand are obtained if one assumes that the asymptotic behavior of the wave function \( \psi(x) \) is a purely outgoing wave. Such a boundary condition

\textsuperscript{1}From now on I will use the units, where \( \hbar = 1 \).
leads to complex eigenvalues [1] of the Hamiltonian and the corresponding
discrete solutions are interpreted as wave functions of unstable states.

The other kind of the continuity conditions for the wave function $\psi(x)$
is related to the form of the potential $V(x)$. The wave function and its first
derivative are assumed to be continuous at finite jumps of the potential. The
only notable exception is when the potential becomes infinite and at such a
point the wave function is assumed to vanish and its first derivative is not
assumed to be continuous.

In this paper we consider the potential wall in the form of the Dirac delta
function $\Omega \delta(x)$ (3)
in the presence of an infinite oscillator wall. We then present explicit solutions
for such a system with the boundary condition in the form of the outgoing
wave. This leads to the Gamow wave functions with complex eigenvalues of
the Hamiltonian. From the explicit solution we can study the behavior of
the wave function $\psi(x)$ at the point $x = 0$, where the Dirac delta potential
wall is present. We find that at this point the wave function is continuous
and the first derivative has a finite jump. We generalize these results to an
arbitrary form of the potential.

The plan of the paper is the following. In Section 2 we present the case of
the quantum unstable oscillator. In Section 3 we discuss the wave function
of the quantum unstable oscillator and analyze its properties. In Section 4 we
generalize the results obtained in Section 3 and discuss the new boundary
conditions for the wave function and draw conclusions from our results.

2 Unstable quantum oscillator – general discussion

Harmonic oscillator is one of the best known physical systems. It is charac-
terized by the equidistant energy levels. We consider here the system which
is the superposition of two potentials: on the left hand side the motion is
bounded by the “oscillator wall”

$$V_o = \begin{cases} 
\frac{m_0^2}{2} x^2 & \text{for } x \leq 0 \\
0 & \text{for } x > 0.
\end{cases} \quad (4)$$
At the origin we insert the semi-transparent potential wall in the form of the Dirac delta function
\[ V_\delta(x) = \Omega \delta(x). \] (5)

The total Hamiltonian is thus equal
\[ H = \frac{p^2}{2m} + V_0(x) + V_\delta(x). \] (6)

It turns out that the system described by the Hamiltonian (6) is exactly soluble [4] and one can find the energy levels and eigenfunctions. We seek the solution by the method of the Green’s function [5, 3] for the Hamiltonian (6).

For the determination of \( G(x, x'; E) \) we must impose boundary conditions and we choose
\[ G(x, x'; E) \to \begin{cases} \text{is bounded} & \text{for } x \to -\infty \\ \sim e^{ikx} & \text{for } x \to +\infty \end{cases}. \] (7)

It turns out that one can treat the admixture of the potential \( V_\delta(x) \) in the Hamiltonian (6) as a perturbation. It means that first we find the Green’s function \( G_0(x, x'; E) \) of the potential \( H_0 \)
\[ H_0 = \frac{p^2}{2m} + V_0(x) \] (8)
and then the full Green’s function \( G(x, x'; E) \) of (6) is determined from the formula
\[ G(x, x'; E) = G_0(x, x'; E) + \frac{G_0(x, 0; E)G_0(0, x'; E)}{\frac{1}{\Omega} - G_0(0, 0; E)}. \] (9)

The function \( G(x, x'; E) \) given in Eq. (9) is an exact result, i.e., we have the explicit expression for the Green’s function of the Hamiltonian (6).

From Eq. (6) one can also find the eigenvalues \( E_n \) of the Hamiltonian from the poles of the Green’s function in the complex plane of energy. In our case it means that we must find zeros of the denominator in Eq. (9)
\[ \frac{1}{\Omega} - G_0(0, 0; E) = 0. \] (10)

The eigenfunctions \( \psi_n(x) \) for the \( n \)-th pole are obtained from the residue of the pole of the Green’s function at \( E = E_n \)
\[ G(x, x'; E) \sim \frac{\psi_n(x)\psi_n(x')}{E - E_n}. \] (11)
In our case we find from Eq. (9) that the eigenfunction $\psi_n(x)$ is equal
\begin{equation}
\psi_n(x) = \frac{G_0(x, 0; E)}{N_n},
\end{equation}
where $E_n$ is the position of the $n$-th pole and the normalization factor $N_n$ is equal
\begin{equation}
N_n^2 = -\frac{\partial}{\partial E} G_0(0, 0; E).
\end{equation}

3 Energy eigenfunctions of the quantum unstable oscillator

We will now apply the formalism sketched in Section 2 to the Hamiltonian (6). The Green’s function $G_0(x, x'; E)$ is obtained from the solutions $\psi^{\pm\infty}(x)$ of the Schrödinger equation for the Hamiltonian $H_0$ in Eq. (8)
\begin{equation}
\left(\frac{p^2}{2m} + V_0(x)\right) \psi^{\pm\infty}(x) = E\psi^{\pm\infty}(x),
\end{equation}
which fulfill the boundary conditions
\begin{equation}
\psi^{-\infty}(x) \quad \text{is bounded for } x \to -\infty
\end{equation}
\begin{equation}
\psi^{+\infty}(x) \sim e^{ikx} \quad \text{for } x \to +\infty.
\end{equation}
Such boundary conditions are sufficient for the determination of the function $\psi^{+\infty}(x)$ uniquely and of the function $\psi^{-\infty}(x)$ up to a multiplicative constant$^2$. The functions $\psi^{\pm\infty}(x)$ are equal
\begin{equation}
\psi^{-\infty}(x) = \begin{cases} 
  e^{-\frac{1}{2}\xi^2} \left( 1 \right. & 1 F_1 \left( \frac{3-2\epsilon}{2} \frac{1}{2} ; \xi \right) - 2\xi \left( \frac{1}{2} \right) \left. \Gamma \left( \frac{3-2\epsilon}{2} \frac{1}{2} ; \xi \right) \right) F_1 \left( \frac{3-2\epsilon}{2} \frac{1}{2} ; \xi \right) \quad \text{for } x \leq 0 \\
  \frac{1}{2} \left( 1 - \frac{2\xi}{k} \sqrt{\frac{\hbar}{m\omega}} \right) F_1 \left( \frac{\hbar\omega}{m\omega} \frac{1}{2} \right) e^{ikx} + \text{c.c.} \quad \text{for } x \geq 0
\end{cases}
\end{equation}
and
\begin{equation}
\psi^{+\infty}(x) = \begin{cases} 
  e^{-\frac{1}{2}\xi^2} \left( 1 \right. & 1 F_1 \left( \frac{3-2\epsilon}{2} \frac{1}{2} ; \xi \right) - 2\xi \left( \frac{1}{2} \right) \left. \Gamma \left( \frac{3-2\epsilon}{2} \frac{1}{2} ; \xi \right) \right) F_1 \left( \frac{3-2\epsilon}{2} \frac{1}{2} ; \xi \right) \quad \text{for } x \leq 0 \\
  e^{ikx} \quad \text{for } x \geq 0
\end{cases}
\end{equation}

$^2$This constant is determined from the condition $\psi^{-\infty}(0) = 1$
where $F_1(\alpha, \beta; z)$ is the confluent hypergeometric function, $\Gamma(z)$ is the Euler’s gamma function and $\xi, \epsilon$ and $k$ are equal

$$\xi = \sqrt{\frac{m\omega}{\hbar}}, \quad \epsilon = \frac{E}{\hbar\omega}, \quad k = \frac{\sqrt{2mE}}{\hbar} = \sqrt{\frac{m\omega}{\hbar}}\sqrt{2\epsilon}. \quad (17)$$

The Green’s function $G_0(x, x'; E)$ is obtained from the functions $\psi^{\pm\infty}(x)$:

$$G_0(x, x'; E) = C_0 \begin{cases} \psi^{-\infty}(x)\psi^{+\infty}(x') & \text{for } x \leq x' \\ \psi^{+\infty}(x)\psi^{-\infty}(x') & \text{for } x \leq x' \end{cases} \quad (18)$$

and the normalization constant $C_0$ is determined from the Wronskian of two solutions $\psi^{\pm\infty}(x)$ and is equal

$$C_0 = i\frac{2m}{\hbar^2} \frac{1}{k + 2i\sqrt{\frac{m\omega}{\hbar}\Gamma\left(\frac{3-2\epsilon}{4}\right)}}. \quad (19)$$

From (12) and (13) we see that the $n$-th eigenfunction of the Hamiltonian (6) with the purely outgoing wave boundary conditions at infinity is equal:

$$\psi_n(x) = \frac{G_0(x, 0; E_n)}{N_n} = \frac{C_0}{N_n} \begin{cases} \psi^{-\infty}(x)\psi^{+\infty}(0) & \text{for } x \leq 0 \\ \psi^{+\infty}(x)\psi^{-\infty}(0) & \text{for } x \geq 0 \end{cases}. \quad (20)$$

The point $x = 0$ is where the semi-transparent Dirac delta potential is inserted and now we will study the properties of the wave function at this point. The function $\psi_n(x)$ is continuous at the point $x = 0$ since

$$\lim_{\varepsilon \to 0}(\psi_n(\varepsilon) - \psi_n(-\varepsilon)) = \lim_{\varepsilon \to 0}(\psi^{+\infty}(\varepsilon)\psi^{-\infty}(0) - \psi^{+\infty}(0)\psi^{-\infty}(-\varepsilon)) = 0. \quad (21)$$

The derivative of the function $\psi'_n(x)$ is not continuous since differentiating the function $\psi_n(x)$ from the left one obtains

$$\lim_{\varepsilon \to 0}\psi'_n(\varepsilon) = \lim_{\varepsilon \to 0}\frac{C_0}{N_n}\psi^{+\infty}(\varepsilon)\psi^{-\infty}(0) = \frac{C_0}{N_n}\psi^{+\infty}(0)\psi^{-\infty}(0) \quad (22a)$$

and for the derivative from the right we get

$$\lim_{\varepsilon \to 0}\psi'_n(-\varepsilon) = \lim_{\varepsilon \to 0}\frac{C_0}{N_n}\psi^{+\infty}(0)\psi^{-\infty}(-\varepsilon) = \frac{C_0}{N_n}\psi^{+\infty}(0)\psi^{-\infty}(0). \quad (22b)$$
The discontinuity of the derivative of the wave function $\psi_n(x)$ at the point $x = 0$ is thus equal
\[
\lim_{\epsilon \to 0} (\psi_n'(\epsilon) - \psi_n'(-\epsilon)) = C_0 \left. \frac{N_n}{N_n} W(\psi^{-\infty}(x), \psi^{+\infty}(x)) \right|_{x=0},
\]
where $W(\psi^{-\infty}(x), \psi^{+\infty}(x))$ is the Wronskian of the wave functions $\psi^{-\infty}(x)$, $\psi^{+\infty}(x)$ and it is equal to $1/C_0$ from the condition on the Green’s function. Thus finally we obtain
\[
\lim_{\epsilon \to 0} (\psi_n'(\epsilon) - \psi_n'(-\epsilon)) = \frac{1}{N_n}.
\]  

4 Generalization and discussion of the results

Eq. (24) contains our main result and it demonstrates that for the potential of the Dirac delta type (3) the wave function is continuous and its first derivative has a finite jump. This discontinuity can be identified with the presence of the semi-transparent wall and such a potential can be used in the construction of models of unstable system that decay in time.

Eq. (24) was obtained for a special case of of the potential in the shape of the Dirac delta function, but Eq. (24) can serve as the starting point for a generalization to an arbitrary potential to produce decaying systems. Let us suppose that we have a potential $V(x)$. We can make the walls of such a potential to be semi-transparent if we solve the corresponding Schrödinger equation with the following boundary conditions for the wave function $\psi(x)$:

1. The wave function $\psi(x)$ is continuous.

2. The first derivative of the wave function $\psi'(x)$ is discontinuous at the point $x_0$, where $V(x_0) = E$ and the jump of the derivative is given by the formula
\[
\lim_{\epsilon \to 0} (\psi'(x_0 + \epsilon) + \psi'(x_0 - \epsilon)) = g(E),
\]
where $g(E)$ is a given function.

3. $\psi(x) \sim e^{\pm ikx}$ for $x \to \pm \infty$.

The wave function obtained from these boundary conditions will describe an unstable system with complex energy eigenvalues.
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