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Schrödinger Equation Via Laplace-Beltrami Operator

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Abstract: *In this work firstly we consider Schrödinger differential equation which satisfies to find wave functions that are important for microscopic systems. Then we generalize these equations by using Laplace-Beltrami operator and compare results we obtained with solutions of Schrödinger differential equations.*
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I. Introduction

As we know, in the quantum mechanics microscopic systems are analyzed by means of wave function $\Psi(t,r) \neq 0 \in \Omega$ will be defined which is obtained by solving Schrödinger

$$i\hbar \frac{\partial \Psi(t,r)}{\partial t} = -\frac{h^2}{2m}\nabla^2 \Psi(t,r) + V(r)\Psi(t,r) \tag{1}$$

for some potential $V(r)$ where $m, \hbar$ and i are mass, Planck constant and the square root of (-1) respectively [2]. In fact, differential equations which satisfy conditions of the foundation of quantum mechanics may be found. But we will consider Schrödinger equation because of the fact that this equation is compatible with experiments.

Schrödinger equation can be expressed as follows:

$$i\hbar \frac{\partial \Psi(t,r)}{\partial t} = H\Psi(t,r)$$

Where

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

is called Hamiltonian operator [2]. Note that we look for wave functions such that member of

$$\Omega = \{\Psi(t,r) \neq 0 \in L^2 : D\Psi \text{ is continous}\}.$$

Now we define a new Hamiltonian

$$\tilde{H} = -\frac{\hbar^2}{2m}\nabla\lambda\nabla + V(r)$$

by means of Laplace-Beltrami operator $L = \nabla\lambda\nabla$. Here $\lambda = 1 + \varepsilon p(r)$ where $p(r)$ is a nonnegative function [1]. In this case for modified Schrödinger equation we have

$$i\hbar \frac{\partial \Psi(t,r)}{\partial t} = \tilde{H}\tilde{\Psi}(t,r).$$

By using separation of variables we obtain time-dependent term $\tilde{T}$ as $\tilde{T} = e^{-\frac{i\gamma t}{h}}$
like Schrödinger equation. Here values γ which will be determined later is not energy values as we will see in the last part of the paper and it will be used to find eigenfunction from below

$$\tilde{H}\tilde{\varphi}(r) = \gamma\tilde{\varphi}(r). \tag{2}$$

Equation (2) is independent of time modified Schrödinger equation. When considering equation (2), it is easy to see that operator $\tilde{H}$ is a Hermitian operator. So if we obtain real eigenvalues, then we can say that eigenfunctions corresponding to different γ from an orthonormal set with in addition to using normalization.

Here we first try to determine eigenvalues of (2). To do this one may be expected to solve modified Schrödinger equation, but because of the fact that to obtain both solutions of modified Schrödinger equation and eigenvalues from these solutions is not easy always. Therefore we use a different treatment. This includes the following equivalent

$$H\varphi(r)=E\varphi(r) \tag{3}$$

in modified Schrödinger equation where E is energy value. In this case,

$$\tilde{H}\tilde{\varphi}=-\frac{\hbar^2}{2m}\nabla.(\lambda\nabla\tilde{\varphi})+V\tilde{\varphi}$$
$$=-\frac{\hbar^2}{2m}(\nabla\lambda).(\nabla\tilde{\varphi})-\frac{h^2}{2m}\lambda\nabla^2\tilde{\varphi}+V\tilde{\varphi}$$
$$=-\frac{h^2}{2m}(\nabla\lambda).(\nabla\tilde{\varphi})+\lambda\left[-\frac{h^2}{2m}\nabla^2\tilde{\varphi}+\frac{V}{\lambda}\tilde{\varphi}\right].$$

In the second term above coefficient of λ is like the right side of (3).
Our aim is to solve (2) by using (3). Generally, we may need to use perturbation theory but even some physical case like the infinity square well may not need. In cases like Coulomb potential or Newtonian potential we obtain a new potential like inverse square potential by using $\lambda = r$. This potential have considered in [3,4,5].So we can approach eigenvalues of (2) by using results we obtained.
Consequently, we can find eigenfunctions corresponding eigenvalues we obtain and compare these functions with functions found from (3).
Here in order to avoid to use perturbation theory, we consider the infinite square well.

1.1The Infinity Square Well

$$V(x)=\begin{cases}0 & ,\ 0\le x\le a\\ \infty & ,\ other\,cases\end{cases}$$

potential and $p(x)=x$ in one dimension. So solution of (3) is

$$\varphi(x)=A\sin(kx) \tag{4}$$

where $A=\sqrt{\frac{2}{a}}$ and $k=\frac{\sqrt{2mE}}{\hbar}=\pm\frac{n\pi}{a}$, so $E=\frac{n^2\pi^2\hbar^2}{2ma^2}$. Consider Modified Schrödinger equation is as follows:

$$-\frac{h^2}{2m}\frac{d\lambda}{dx}\frac{d\tilde{\varphi}}{dx}+\lambda\left(H\tilde{\varphi}\right).$$

By using (3) and (4) the equation becomes

$$\frac{d\tilde{\varphi}}{dx}+\frac{dx}{d\lambda}\varsigma^2\tilde{\varphi}=A\lambda\frac{dx}{d\lambda}k^2\sin(kx)$$

where $\varsigma^2=\frac{2m\gamma}{h^2}$ and we have

$$\tilde{\varphi}=k^2e^{-\frac{\varsigma^2}{a}x}\left[\int e^{-\frac{\varsigma^2}{a}x}(1+\varepsilon x)\frac{A}{\varepsilon}\sin(kx)\,dx\right]$$
$$=\frac{Ak^2}{\left(\varsigma^4+\varepsilon^2k^2\right)^2}\left\{\sin(kx)\left[\varepsilon x\varsigma^6+\varsigma^6-\varepsilon^2\varsigma^4+\varsigma^2\varepsilon^3k^2x+\varepsilon^2\varsigma^2k^2+\varepsilon^4k^2\right]\right.$$
$$\left.-\cos(kx)\left[k\varsigma^4\varepsilon^2x+\varepsilon\varsigma^4k-2k\varsigma^2\varepsilon^3+\varepsilon^4k^3x+\varepsilon^3k^3\right]\right\}$$

as solutions. Now for both to show the consistency of operation and to determine eigenvalues, we look for a $\varepsilon \to 0$ case. When ε goes to 0, $\tilde{\varphi} \to \frac{Ak^2}{\varsigma^3}\left[\varsigma^6 \sin(kx)\right] = A\left(\frac{k}{\varsigma}\right)^2 \sin(kx).$

Hence $k = \varsigma$ or $\gamma = E = \frac{n^2\pi^2\hbar^2}{2ma}$. These values of γ absolutely an approach, we can see that from both graphics and condition of continuous.

Now by using treatment $\gamma \cong E$ if we consider modified Schrödinger equation

$$-(1+\varepsilon x)\frac{h^2}{2m}\frac{d^2\tilde{\varphi}}{dx^2} - \frac{\varepsilon\hbar^2}{2m}\frac{d\varphi^2}{dx} = \gamma\tilde{\varphi},$$

we have solutions with the index as

$$\tilde{\varphi}_n(x) = \frac{1}{\sqrt{\varepsilon}}\left\{BesselI\left[0, \frac{2\sqrt{2}}{\hbar\varepsilon} i\sqrt{m\gamma_n(1+\varepsilon x)}\right]C_{n1} + BesselK\left[0, \frac{2\sqrt{2}}{\hbar\varepsilon} i\sqrt{m\gamma_n(1+\varepsilon x)}\right]C_{n2}\right\}.$$

where $BesselI[n,z]$ and $BesselK[n,z]$ give the modified Bessel function of first kind $I_n(z)$ and second kind $K_n(z)$ respectively. But the second term described above approach infinity as x goes to 0 for big ε Therefore we take $C_{n2} = 0.$

Consequently, we obtain

$$\tilde{\varphi}_n(x) = \tilde{C}_n I_0\left(\frac{2\sqrt{2}}{\hbar\varepsilon} i\sqrt{m\gamma_n(1+\varepsilon x)}\right), \qquad \tilde{C}_n = \frac{C_{n1}}{\sqrt{\varepsilon}}$$

In fact, we know that Bessel function I_0 has oscillation on the x-axes so have infinity roots. If we can find these roots easily we can determine truth values of γ from $\tilde{\varphi}(a) = 0$ or more explicitly from

$$I_0\left(\frac{2\sqrt{2}}{\hbar\varepsilon} i\sqrt{m\gamma_n(1+\varepsilon a)}\right) = 0.$$

In order to determine $\tilde{C}_n$ we can use normalization, such follows: From

$$1 = \int_{-\infty}^{\infty} |\varphi|^2 dx = \int_0^a |\varphi|^2 dx$$

$$= \left|\tilde{C}_n\right|^2 \int_0^a \left|I_O\left(\frac{2\sqrt{2}}{\hbar\varepsilon} i\sqrt{m\gamma_n(1+\varepsilon a)}\right)\right|^2 dx$$

as

$$\tilde{C}_n = \left[\int_0^a |I_0|^2 dx\right]^{-\frac{1}{2}}.$$

Finally, we have

$$\tilde{\varphi}_n(x) = \left[\int_0^a |I_0|^2 dx\right]^{-\frac{1}{2}} I_0\left(\frac{2n\pi i}{a\varepsilon}\sqrt{1+\varepsilon x}\right)$$

and compare these solutions with for some values of n, ε and a.

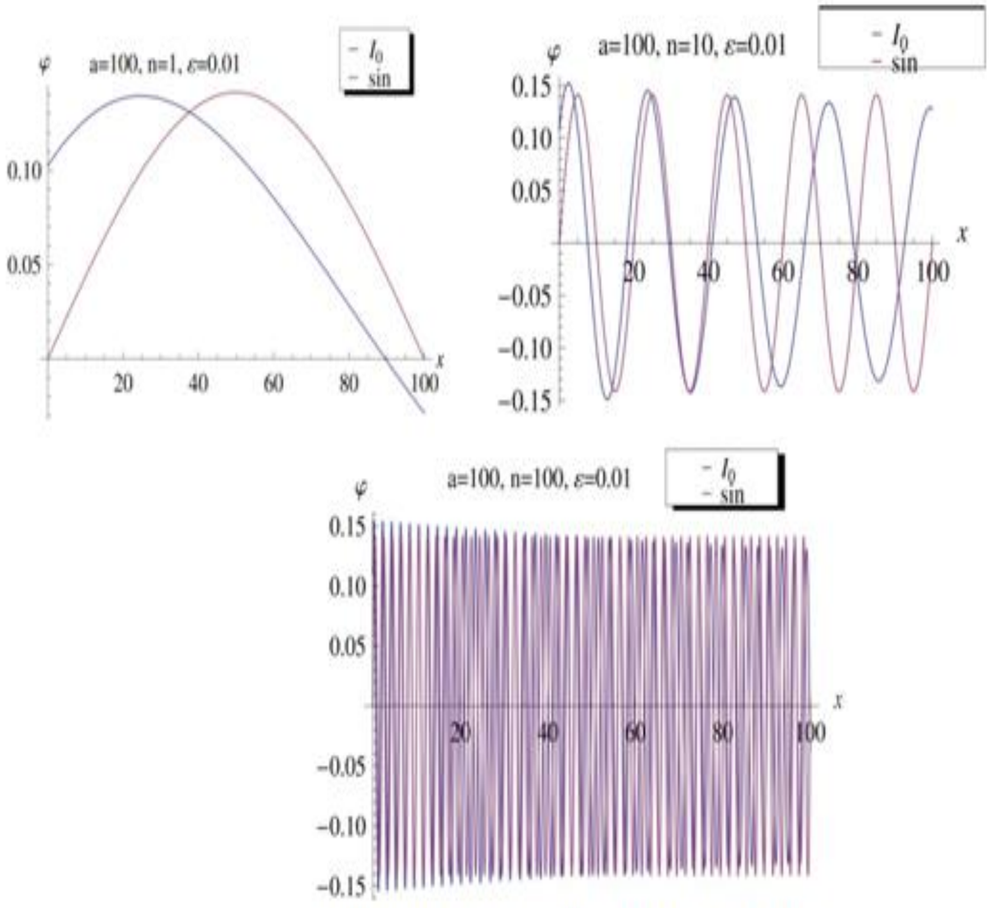

Figure1. Graphics for some values of n, ε and a.

As we see when n increases, curves approach each other more and more. Therefore the expectation values and other will be computed for $n=1$. In fact, even though we need general wave function $\Phi(t,x)$ for computation, we can do this by using the function $\tilde{\varphi}_n$ for small n. So for $a=100,\ n=1,\ \varepsilon=0,01$

$$\langle x\rangle_{\tilde{\varphi}}=\int_0^a \tilde{\varphi}_1 x \tilde{\varphi}_1^* dx \cong 31.4 \quad , \quad \langle x\rangle_{\varphi}=\int_0^a \varphi_1 x \varphi^*{}_1 dx = 50$$

We can see that there is a big difference between $\tilde{\varphi}_1$ and φ_1. Actually, our aim is not to obtain close values. If so we can take ε as more small. And standard deviations are as follows:

$$\sigma_{x\tilde{\varphi}_1} \cong 18.6 \quad and \quad \sigma_{x\varphi_1} \cong 18.1$$

From here we can say that functions have nearly same dispersion as we will see from figure 1. It is clear that values found above are more close each other for larger n .We see also that from the following table

n	1	5	10	100
$<x>_{\tilde{\varphi}}$	31.4	44.2	46.5	47
$<x>_{\varphi}$	50	50	50	50
$\sigma_{x\tilde{\varphi}}$	18.52	29.13	29.54	28.89
$\sigma_{x\varphi}$	18.08	28.5	28.77	28.86

References

[1]. Charles Z. Martin, Variational formulas for the Green function. Anal. Math. Phys.2:89103,2012
[2]. David J. Griffiths, Introduction to quantum mechanics(second edition), Pearson Education Inc.,2005
[3]. E. A. Guggenheim, The inverse square potential field, Proc.Phys.Soc.;1966, Vol.89
[4]. Elise Guillaumin-Espana et al., Classical and quantum dynamics in an inverse square potential. Journal of mathematical physics 55,103509, 2014
[5]. Wolfgang Bietenholz et al ., Comment on " the two-dimensional motion of a particle in an inverse square potential: classical and quantum aspect", Journal of mathematical physics 56, 104101,2015

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