A new approach to bound states in potential wells

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A method for calculating the energies of the bound states of a particle in a potential well is presented. A generalization of the Bohr–Sommerfeld quantization rule is obtained.
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I. INTRODUCTION

In this paper we present a simple method for calculating the energies of the bound states of a nonrelativistic particle in a potential well[1] (see also Refs. 2–5). To demonstrate the method, we first consider the one-dimensional rectangular potential well, $V(x)$, (Fig. 1),

$$V(x)=\begin{cases}0 & \text{for } |x|>L/2\\ -V_0 & \text{for } |x|\leqslant L/2,\end{cases} \tag{1}$$

where V_0 is the potential depth, and L is its width.

In the usual approach, in order to find bound states, we need to find the solutions of the Schrödinger equation, which vanish at $|x|\to\infty$. For the potential (1) this wave function is

$$\Psi(x)=\begin{cases}A\exp(k_U'x) & \text{at } x<-L/2\\ B\exp(ikx)+C\exp(ikx) & \text{at } -L/2\leqslant x\leqslant L/2\\ D\exp(-k_U'x) & \text{at } x>L/2,\end{cases} \tag{2}$$

where $k=\sqrt{2mE}/\hbar, E$ is the particle energy with respect to the bottom of the well, m is the particle mass, $k_U'=\sqrt{U-k^2}$, and $U=2mV_0/\hbar^2$. In the following we shall omit the constant $\hbar^2/2m$. It means that all the energies are measured in a system of units in which $\hbar^2/2m=1$.

Matching this wave function and its derivatives at two points $(x=\pm L/2)$ gives a homogeneous system of four equations for coefficients A, B, C, and D, and the condition of compatibility for this system gives an equation for the eigenenergy E_n, or the wave number k_n defined as $k_n=\sqrt{2mE_n}/\hbar$. Of course, in our simple case of the symmetrical potential (1) the number of equations can be reduced to two,[1] because one can consider separately symmetrical and antisymmetrical wave functions, for which $A=\pm D$ and $B=\pm C$. However, for potential wells of general form that is not possible, and we need to solve the system of four or more equations.

We want to show a different way to derive the equation for the eigenenergies E_n (or for the wave numbers k_n), which may be generalized to potentials of arbitrary form. It is based on the requirement of self-consistency of reflections from both walls of the potential well, which gives a physical insight into the nature of bound states and leads to generalization of the Bohr quantization rule.

The method is described in the following section. It is demonstrated there with the help of the potential well (1), which from a pedagogical point of view seems to be the most appropriate.

In Sec. III we generalize our method for the nonsymmetrical potential well, and in Sec. IV we show how the well-known Bohr–Sommerfeld quantization rule can be modified.

II. SELF-CONSISTENT REFLECTIONS IN THE POTENTIAL WELL (1)

Let us consider a particle in the well which starts to propagate from the left wall $(x=-L/2)$ toward the right one at $x=L/2$. This propagation is described by the wave function

$$\exp(ik[x+L/2]). \tag{3}$$

The amplitude of this starting wave is taken to be unity because its magnitude is irrelevant.

After reaching the right wall at $(x=L/2)$, the particle acquires the phase factor $\exp(ikL)$, is reflected from the right wall with reflection amplitude $\rho(k)$, and starts propagating toward the left wall, which is described by the wave function

$$\rho(k)\exp(ikL)\exp(-ik[x-L/2]). \tag{4}$$

After reaching the left wall, the particle acquires an additional phase factor $\exp(ikL)$, and after being reflected from the left wall with the reflection amplitude $\rho(k)$, which is here identical to that of the right wall, the particle starts to move again from the left wall to the right, which is described by the following wave function:

$$\rho^2(k)\exp(2ikL)\exp(ik[x+L/2]), \tag{5}$$

which is identical to (3) except for the amplitude.

However, and this is the main point, if the particle is in an eigenstate, the wave function should be stationary. Therefore, (5) should be identical to (3). This is possible only for those k for which

$$\rho^2(k)\exp(2ikL)=1. \tag{6}$$

The solution of this equation gives all the eigenvalues k_n and therefore $E_n=k_n^2$.

The next step is to find $\rho(k)$ and to substitute it into (6). Reflection of a particle with wave number k from a potential step of height $U>k^2$ is total and is representable in the form of a phase factor (see Appendix A):

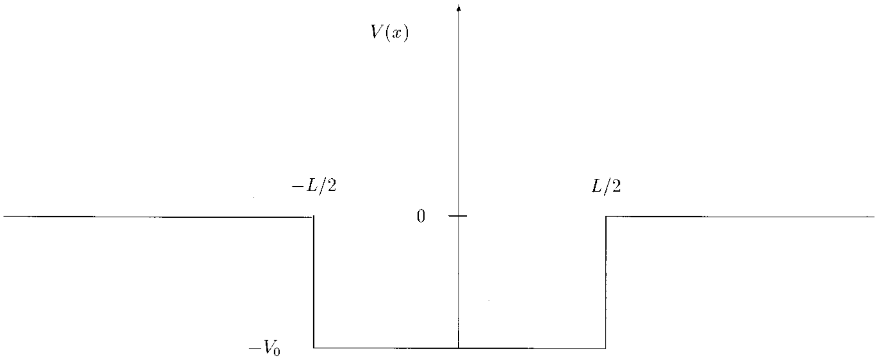

Fig. 1. Square potential well of width L and depth V_0.

$$\rho(k)\equiv\rho(k,U)=\frac{k-ik_U'}{k+ik_U'}=\exp(-2i\phi(k,U)), \tag{7}$$

where $k_U'=\sqrt{U-k^2}$, and the phase $\phi(k,U)$ is

$$\phi(k,U)=\arctan\left(\frac{k_U'}{k}\right)=\arccos\left(\frac{k}{\sqrt{U}}\right). \tag{8}$$

For clarity the step height U of the potential is explicitly pointed out everywhere.

Substitution of (7) into (6) gives

$$\exp(2ikL-4i\phi(k,U))=1\to kL-2\arccos\left(\frac{k}{\sqrt{U}}\right)=n\pi, \tag{9}$$

where n is an integer, which can be also -1 and 0. The value $n=-1$ corresponds to $k=0$, which means a constant wave function for a particle on the bottom of the well; however this constant should be 0, because the wave function should vanish at $|x|=\infty$. Thus the lowest acceptable eigenvalue is $n=0$.

The highest level is near the edge of the well: $k\approx\sqrt{U}$. It means that the highest level in the well corresponds to

$$n_{\max}=\text{integer}(\sqrt{U}L),$$

where integer (x) means greatest integer, contained in x.

III. GENERALIZATION TO THE NONSYMMETRICAL WELL

Equation (6) can be easily generalized to more complicated potentials. For instance, if the two walls are somehow different, then Eq. (6) becomes

$$\rho_l(k)\rho_r(k)\exp(2ikL)=1, \tag{10}$$

where $\rho_{l,r}(k)=\exp(-2i\phi_{l,r}(k))$ are the reflection amplitudes and $\phi_{l,r}(k)$ are their phases for reflection from the left and right walls of the well, respectively. Thus relation (9) is generalized to

$$kL-\phi_r(k)-\phi_l(k)=n\pi. \tag{11}$$

For instance, let us consider the well shown in Fig. 2. The reflection amplitude at the left wall is now

$$\rho_l(k)=\rho(k,W)=\frac{k-ik_W'}{k+ik_W'}=\exp(-2i\phi(k,W)), \tag{12}$$

where $k_W'=\sqrt{W-k^2}$, and

$$\phi(k,W)=\arctan\left(\frac{k_W'}{k}\right)=\arccos\left(\frac{k}{\sqrt{W}}\right). \tag{13}$$

Thus, Eq. (11) for eigenlevels is:

$$kL-\arccos\left(\frac{k}{\sqrt{U}}\right)-\arccos\left(\frac{k}{\sqrt{W}}\right)=n\pi, \tag{14}$$

or

$$kL-\arccos\left(\frac{k^2-k_U'k_W'}{\sqrt{UW}}\right)=n\pi. \tag{15}$$

A more complicated nonsymmetrical potential well with the same level to the right and left is shown in Fig. 3. The reflection amplitude from the right wall is the same $\rho_r(k)=\rho(k,U)$, as above, but $\rho_l(k)$ requires some calculation. It can be easily performed by splitting the potential with an infinitesimal gap (see Refs. 6–12), as shown in Appendix B:

$$\rho_l(k)=\rho(k,W,d)+\frac{\tau^2(k,W,d)\rho(k,U)}{1-\rho(k,U)\rho(k,W,d)}$$
$$=\frac{\rho(k,W,d)+\rho(k,U)[\tau^2(k,W,d)-\rho^2(k,W,d)]}{1-\rho(k,U)\rho(k,W,d)}, \tag{16}$$

where we have introduced notations for reflection $\rho(k,W,d)$ and transmission $\tau(k,W,d)$ amplitudes of the rectangular potential barrier of height W and width d. These amplitudes, using the same technique (see Appendix C), can be represented in the form

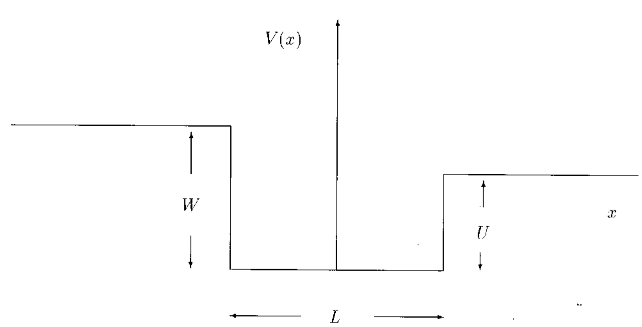

Fig. 2. The square potential well of width L with two different levels: W at the left and U at the right walls, respectively.

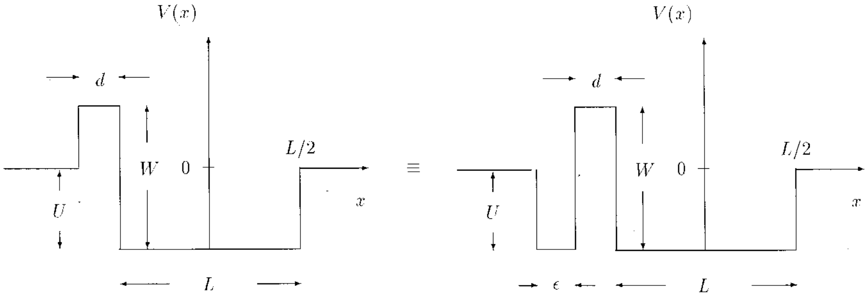

Fig. 3. The square potential well of width L and depth U (in units $\hbar^2/2m=1$) with a barrier $W-U$ of width d at the left wall. The potential on the left is equivalent to the potential at the right with the barrier separated from the well by an infinitesimal gap ϵ.

$$\rho(k,W,d)=\rho(k,W)\,\frac{1-\exp(-2k'_W d)}{1-\rho^2(k,W)\exp(-2k'_W d)}, \tag{17}$$

$$\tau(k,W,d)=\exp(-k'_W d)\,\frac{1-\rho^2(k,W)}{1-\rho^2(k,W)\exp(-2k'_W d)}, \tag{18}$$

where $\rho(k,W)$ is defined in (12) and (13).

It is seen that for $d\to 0$, we have $\rho(k,W,d)\propto -id\to 0, \tau(k,W,d)\to 1$, and from (16) it follows that $\rho_l(k)\to\rho(k,U)$. For $d\to\infty$ we have $\rho(k,W,d)\to\rho(k,W)$, $\tau(k,W,d)\propto i\exp(-k'_W d)\to 0$, and from (16) it follows that $\rho_l(k)\to\rho(k,W)$, because in that case the potential of Fig. 3 becomes transformed to that of Fig. 2.

Taking into account these considerations, we can represent (17) and (18) in the form

$$\begin{aligned}\rho(k,W,d)&=-i|\rho(k,W,d)|\exp(i\phi(k,W,d)),\\ \tau(k,W,d)&=|\tau(k,W,d)|\exp(i\phi(k,W,d)),\end{aligned} \tag{19}$$

where $|\rho(k,W,d)|^2+|\tau(k,W,d)|^2=1$, and

$$\phi(k,W,d)=\arctan\{\cot[2\phi(k,W)]\tanh(k'_W d)\}. \tag{20}$$

This phase has the following asymptotic behavior:

$$\phi(k,W,d)\to\begin{cases}0 & \text{for } d\to 0\\ \pi/2-2\phi(k,W) & \text{for } d\to\infty.\end{cases} \tag{21}$$

Substitution of (19) into (16) gives $\rho_l(k)=\exp(-2i\phi_l(k))$, where

$$\phi_l(k)=\phi(k,U)-\phi(k,W,d)+\arctan\left(\frac{|\rho(k,W,d)|\cos(2\phi(k,U)-\phi(k,W,d))}{1+|\rho(k,W,d)|\sin(2\phi(k,U)-\phi(k,W,d))}\right). \tag{22}$$

Substitution of (22) into (11) gives the following equation for eigenvalues k_n of k:

$$\begin{aligned}&kL+2\phi(k,U)-\phi(k,W,d)\\ &\quad+\arctan\left(\frac{|\rho(k,W,d)|\cos(2\phi(k,U)-\phi(k,W,d))}{1+|\rho(k,W,d)|\sin(2\phi(k,U)-\phi(k,W,d))}\right)\\ &\quad=n\pi.\end{aligned} \tag{23}$$

IV. GENERALIZATION OF THE BOHR–SOMMERFELD QUANTIZATION RULES

The Bohr–Sommerfeld quantization rule is:[13]

$$\int_a^b k(x)\,dx-\pi/2=n\pi. \tag{24}$$

Let us see how well this rule is satisfied in the potential well

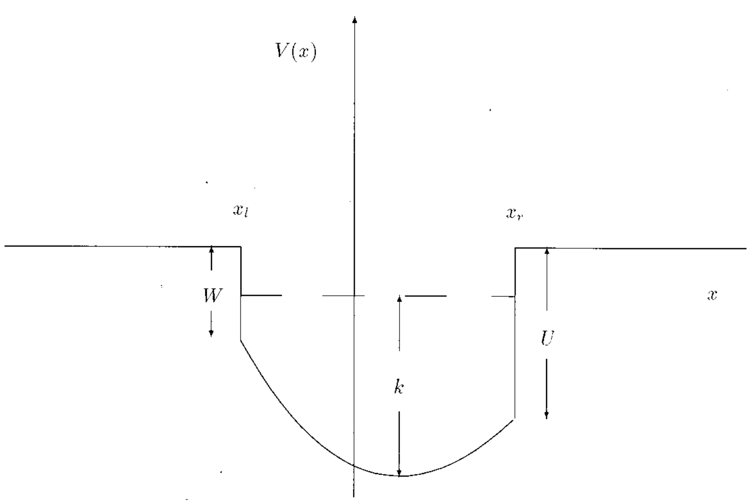

Fig. 4. The potential well with variable potential and steps at two end points $x_{l,r}$ of height W at the left and U at the right edge. For the particle with sufficiently high energy k^2 with respect to the well bottom the quasiclassical approximation is valid everywhere inside the well.

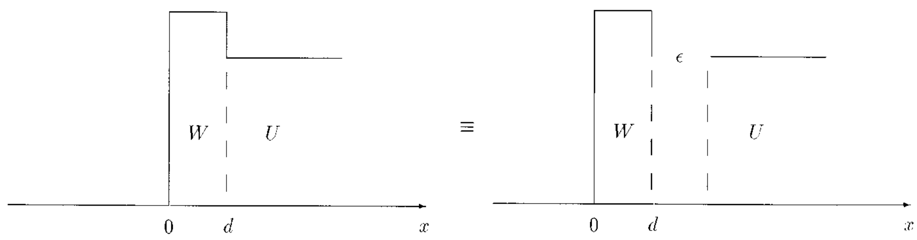

Fig. 5. Reflection from the potential of the left wall in Fig. 3. This potential can be split by an infinitesimal gap ϵ.

(1). Because in this case $k(x)=k$ does not depend on x, we obtain

$$\int_{-L/2}^{L/2} k\,dx = kL,$$

and the precise quantization rule becomes (9). This means that $\pi/2$ must be replaced by $2\arccos(k/\sqrt{U})$. The last quantity becomes π if $U\to\infty$; thus the quantization rule for infinite U becomes $kL-\pi=n\pi$ with integer $n\geqslant 0$. Thus the precise quantization rule (9) deviates from (24). This shows that the quantization rule (24) should be modified to

$$\int_a^b k(x)dx-\phi_l(k)-\phi_r(k)=n\pi, \tag{25}$$

where $\phi_{l,r}(k)$ are the reflection phases at the turning points $x_{l,r}$, where $k(x_{l,r})=0$. It is complicated in general to define such a reflection. Here we consider a simple case of a potential, shown in Fig. 4. The reflection phases for such a potential are

$$\phi_l=\arccos\sqrt{\frac{k^2-V(x_l)}{W}},\quad \phi_r=\arccos\sqrt{\frac{k^2-V(x_r)}{U}}, \tag{26}$$

and the quantization rule (25) is as follows:

$$\int_a^b k(x)dx-\arccos\sqrt{\frac{k^2-V(x_l)}{W}}-\arccos\sqrt{\frac{k^2-V(x_r)}{U}}$$
$$=\pi. \tag{27}$$

It is possible to find the phases even in more general cases, and we shall consider this in other publications.

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APPENDIX A: REFLECTION FROM A STEP POTENTIAL

We recall here how to find the amplitude $\rho(k,U)$ for reflection of a particle with wave number k from the potential step of height U. Let suppose that the step is at $x\geqslant 0$. The wave function of the particle is

$$\Psi(x)=\begin{cases}\exp(ikx)+\rho(k,U)\exp(-ikx)NN & \text{at } x<0\\ \tau(k,U)\exp(-k'_U x) & \text{at } x>0,\end{cases} \tag{28}$$

where $\tau(k,U)$ is the transmission amplitude inside the potential.

Matching the wave function and its derivative at the point $x=0$ gives two equations:

$$1+\rho(k,U)=\tau(k,U),\quad ik[1-\rho(k,U)]=-k'_U\tau(k,U). \tag{29}$$

Solution of these equations gives

$$\rho(k,U)=\frac{k-ik'_U}{k+ik'_U},\quad \tau(k,U)=\frac{2k}{k+ik'_U}, \tag{30}$$

which gives the result (7).

APPENDIX B: REFLECTION FROM THE LEFT SIDE OF THE WELL IN FIG. 3

Let us split the potential as shown in Fig. 5. Denote reflection and transmission amplitudes of the first rectangular barrier as ρ_1 and τ_1, and reflection amplitude of the second step as ρ_2. Then, taking into account multiple reflections inside the gap of infinitesimal width ϵ, where the phase acquired between the walls can be neglected, we obtain for the reflection ρ_{12} of the whole system the infinite sum

$$\rho_{12}=\rho_1+\sum_{n=0}^{\infty}\tau_1\rho_2(\rho_1\rho_2)^n\tau_1=\rho_1+\frac{\tau_1^2\rho_2}{1-\rho_1\rho_2}, \tag{31}$$

from which formula (16) is directly obtained.

APPENDIX C: REFLECTION AND TRANSMISSION OF A RECTANGULAR BARRIER

Let us look at the rectangular barrier of height W and width d in Fig. 5, and denote reflection and transmission amplitudes from vacuum into the barrier as ρ_1,τ_1, and reflection and transmission amplitudes from inside the barrier into vacuum as ρ_2,τ_2. It is easy to show in the same way as in Appendix A, that

$$\tau_1=\frac{2k}{k+ik'_W},\quad \tau_2=\frac{2ik'_W}{k+ik'_W},\quad \rho_1=-\rho_2=\frac{k-ik'_W}{k+ik'_W},$$

and that $\tau_1\tau_2=1-\rho_1^2$. In the same way as in Eq. (31), we can obtain formulas for reflection, ρ, and transmission, τ, of the whole barrier. Indeed, taking into account multiple reflections at the two edges at $x=0$, and $x=d$, and also extinction $e=\exp(-k_W d)$ for propagation between the edges, we get ρ and τ as sums of infinite geometrical progressions:

$$\rho=\rho_1+\sum_{n=0}^{\infty}\tau_2\rho_2(\rho_2 e)^{2n}\tau_1$$
$$=\rho_1+\frac{\tau_1\tau_2\rho_2}{1-\rho_2^2e^2}=\rho_1\frac{1-e^2}{1-\rho_1^2e^2},$$
$$\tau=e\sum_{n=0}^{\infty}\tau_2(\rho_2 e)^{2n}\tau_1=e\,\frac{\tau_1\tau_2}{1-\rho_1^2e^2}=e\,\frac{1-\rho_1^2}{1-\rho_1^2e^2},$$

which leads directly to (17) and (18).

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