PROJECT#1 **Particle in a box –Finite Potential well**

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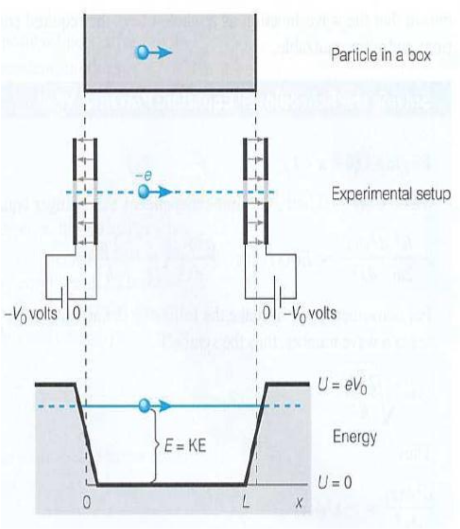
1. Purpose

By solving the Schrödinger equation for interacting particles, we try to get the wave function.

2. Introduction

By solving the equation, we get the equation below.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x)=E\psi(x)$$



Region 1 (0<x<L, U=0)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}=E\psi(x)$$

$$\psi(x)=A\sin kx+B\cos kx$$

$$k=\sqrt{\frac{2mE}{\hbar^2}}$$

Region 2 and 3 (x<0 and x>L, U=U_0)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+U_0\psi(x)=E\psi(x)$$

$$\psi(x)=\begin{cases}Ce^{\alpha x}+De^{-\alpha x} & \text{where } x<0\\ Fe^{\alpha x}+Ge^{-\alpha x} & \text{where } x>L \text{ and}\end{cases}\qquad \alpha\equiv\sqrt{\frac{2m(U_0-E)}{\hbar^2}}$$

Then by using the smoothness and normalization of $\psi(x)$

$$\psi(x)=\begin{cases}Ce^{\alpha x} & \text{where } x<0\\ A\sin kx+B\cos kx & \text{where } 0<x<L\\ Ge^{-\alpha x} & \text{where } x>L\end{cases}\qquad (1)$$

$$\text{where } k\equiv\sqrt{\frac{2mE}{\hbar^2}} \text{ and } \alpha\equiv\sqrt{\frac{2m(U_0-E)}{\hbar^2}}$$

Then consider the continuity of $\psi(x)$ and d$\psi(x)$/dx at x=0 and L. We get the equation below.

$$2\cot kL=\frac{k}{\alpha}-\frac{\alpha}{k}\Rightarrow\text{put}\quad f(k)=2\cos Lk-\left(\frac{k}{\sqrt{a-k^2}}-\frac{\sqrt{a-k^2}}{k}\right)\sin Lk$$

$$\text{where}\quad a=\sqrt{\frac{2mU_0}{\hbar^2}}$$

By numerical method, we try to get k and E.

4. Result

(i) U0=0.1 [eV]

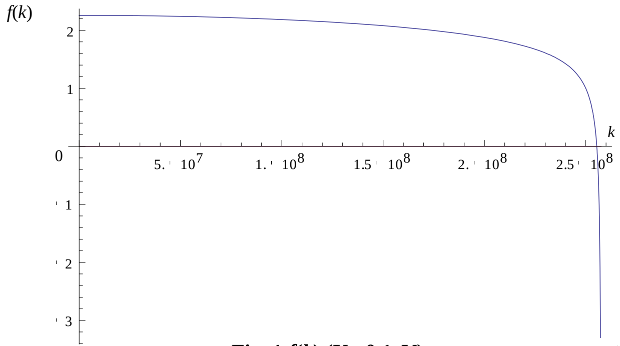


Fig. 1 *f*(*k*) (U_0=0.1eV)

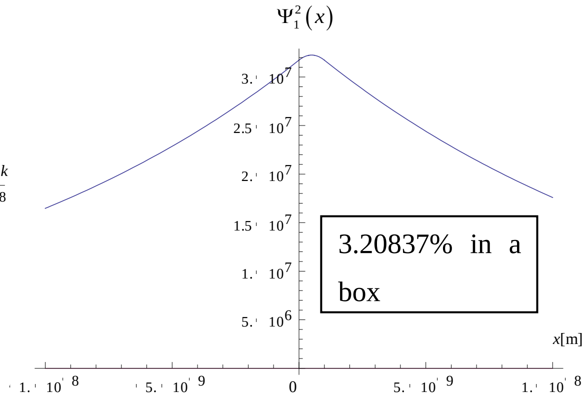


Fig. 2 Probability Ψ_1(x)^2 of Eq. (1) (U_0=0.1eV)

E1=0.098378eV (k= 2.55e8)

P*dL=1.69e-34

(ii)U_0=0.03[eV]

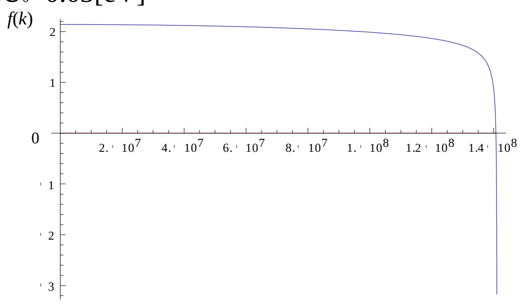


Fig. 3 f(k) (U_0=0.03eV)

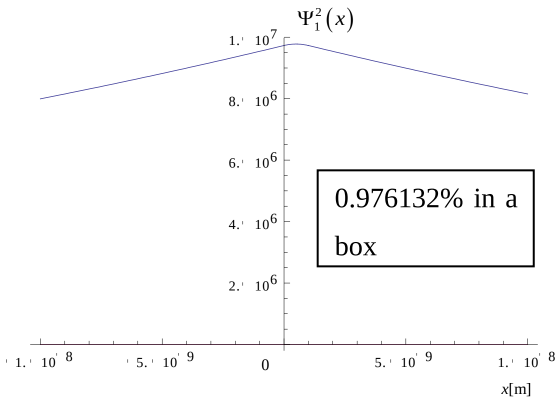


Fig. 4 Probability Ψ_1(x)^2 (U_0=0.03eV)

E1=0.029852eV (k= 1.41e8)

P*dL=9.33e-35

(iii)U0=30000[eV] (When U0 is huge number.)

Table 1 Numerical and analytic energy

n	En[eV]	
	analytic	U0=30000[eV]
1	14.88190223	14.5
2	59.5276089	57.874358
3	133.93712	130.215625
4	238.1104356	231.490707
5	372.0475557	361.69699
6	535.7484801	520.830551
7	729.2132091	708.886998
8	952.4417425	925.861196
9	1205.43408	1171.747259
10	1488.190223	1446.536688

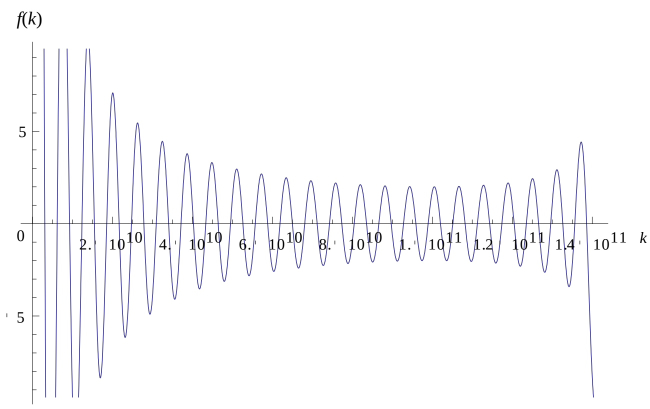


Fig. 5 f(k) (U_0=30000eV)

11	1800.710169	1750.222573
12	2142.993921	2082.795388
13	2515.041476	2444.244487
14	2916.852836	2834.559413
15	3348.428001	3253.72476
16	3809.76697	3701.727737
17	4300.869743	4178.553223
18	4821.736321	4684.181613
19	5372.366704	5218.594991
20	5952.76089	5781.77245
21	6562.918882	6373.687677
22	7202.840677	6994.314174
23	7872.526278	7643.62573
24	8571.975682	8321.585686
25	9301.188891	9028.159069
26	10060.1659	9763.306253
27	10848.90672	10526.97997
28	11667.41135	11319.12699
29	12515.67977	12139.68767
30	13393.712	12988.59548
31	14301.50804	13865.77078
32	15239.06788	14771.12237
33	16206.39152	15704.54662
34	17203.47897	16665.91385
35	18230.33023	17655.07208
36	19286.94529	18671.8351
37	20373.32415	19715.97243
38	21489.46681	20787.19096
39	22635.37329	21885.10356
40	23811.04356	23009.17904
41	25016.47764	24158.68208
42	26251.67553	25332.46624
43	27516.63722	26528.62864
44	28811.36271	27743.4656
45	30135.85201	28967.17167

The particle exists 99.9993% in a box.

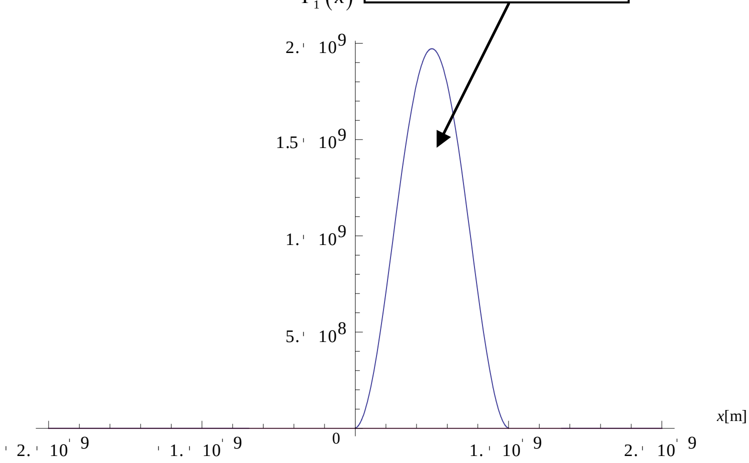


Fig. 6 Probability $\Psi_1(x)$^2 (U_0=30000eV)

We get almost same values(2.9% error for n=27), so my program is right for U_0=30000eV.

Cf. Normalization

B=C, A= $\frac{\alpha}{k}$ C, and G= $Ce^{\alpha L}$ because of the smoothness and normalization of $\psi_n(x)$ and the symmetry of a box.

I integrated $\left|\psi_n(x)\right|^2$ for entire x by Monte Carlo's method and got $C=\sqrt{\ }$ 1/the value of the integral.

5. Question

(i)As $U_0 \to 0$, but it is still not 0, does *f*(*k*)=0 have solution (*k* or *E*) ?

As $E \to U_0$, $\alpha \to 0$, $\frac{k}{\alpha} \to \infty$, and $f(k) \to -\infty < 0$.

$f(k) \xrightarrow[k\to 0]{} 2 + L\sqrt{a} > 0$ because $L\frac{\sqrt{a-k^2}}{Lk}\sin Lk \xrightarrow[k\to 0]{} L\sqrt{a}$ .Then *f*(*k*) is a continuous function for [0, $\sqrt{a}$] function because it consists of sink, cosk, k, and 1/ $\sqrt{a-k^2}$, so this function must have at least one solution for [0, $\sqrt{a}$].

But if $U_0 = 0$, there is no well, so a particle keeps moving and we can't specify the position of the particle.