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# The quantum behavior of a particle in a square well of finite, unidimensional potential. The entangled fate of Schrödinger's cat

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# Abstract

An in depth look to the quantum behavior of a particle in a unidimensional finite, square box of potential energy is presented. Wave function normalization constants are fully determined and are used to establish an expression to calculate the particle allowed energy eigenstates based in the confinement condition for each of the two possible wave function symmetries. These eigenstates turn out to be degenerate and it becomes possible to configure confined systems so that the particle confinement/near free duality condition, also known as entanglement is present. This condition, obtained by using the particle mean presence probability density function of the two wave function symmetries of the system degenerate states, is illustrated with a couple of calculation examples.

Keywords: Quantum system, degenerate eigenvalues, entanglement, Rydberg unit of energy.

# System definition

Let's consider a potential well which has a width of 2a (m) and a height of  $U_0$  (eV) for  $|x| \ge a$  while for |x| < a is equal to 0, see Figure 1. The particle under study is an electron of charge q (C), rest mass  $m_0$  (kg) and an energy E (eV) such that  $0 < E < U_0$ . The system's mathematical description is the following

 $U(x) = U_0$  (eV)for  $x \le -a$  (region I)U(x) = 0for |x| < a (regionII) $U(x) = U_0$  (eV)for  $x \ge a$  (regionIII)



Figure 1. System definition.

The time independent one dimensional Schrödinger equation in terms of the Rydberg unit of energy, Ry (eV), is - see Appendix A -

$$\frac{d^2\varphi(x)}{dx^2} = \frac{U(x) - E}{r_H^2 Ry} \varphi(x) \quad (1/m^{5/2})$$
(4)

where  $r_H$  (m) is the H atom Bohr radius. Ry is given by

$$Ry = \frac{1}{2qm_0} \left(\frac{\hbar}{r_H}\right)^2 = 13.6056931\ 230445 \quad (eV)$$
(5)

where  $\hbar$  is the Planck constant h (J-s) divided by  $2\pi$ .

The equation system to solve

$$\frac{d^2 \varphi_I(x)}{dx^2} = \frac{U_0 - E}{r_H^2 R y} \varphi_I(x) = \alpha_1^2 \varphi_I(x) \quad (1/m^{5/2}), \ x \le -a$$
(6)

$$\frac{d^2 \varphi_{II}(x)}{dx^2} = -\frac{E}{r_H^2 R y} \varphi_{II}(x) = -\alpha_2^2 \varphi_{II}(x) \quad (1/m^{5/2}), |x| < a$$
(7)

$$\frac{d^2 \varphi_{III}(x)}{dx^2} = \frac{U_0 - E}{r_H^2 R y} \varphi_{III}(x) = \alpha_1^2 \varphi_{III}(x) \quad (1/m^{5/2}), x \ge a$$
(8)

where  $\varphi_{I}$ ,  $\varphi_{II}$  and  $\varphi_{III}$  (m<sup>1/2</sup>) stand for the particle wave function for regions I, II and III, respectively. Also, the following definitions have been made

$$\alpha_1 \equiv F_{\sqrt{U_0 - E}} \; ; \; \alpha_2 \equiv F_{\sqrt{E}} \qquad (1/m) \tag{9}$$

$$F = \frac{1}{r_H} \frac{1}{\sqrt{R_y}} = 5.123167 \text{ x } 10^9 (1/\text{m/eV}^{1/2})$$
(10)

#### **General solution**

There are numerous alternatives to solve this system. Examples are given in references [1,2,3,4]. The system (6) to (8) has the following general solution

$$\varphi_I(x) = A e^{\alpha_1 x} + B e^{-\alpha_1 x} \quad (1/m^{1/2}) \quad x \le -a$$
(11)

$$\varphi_{II}(x) = C\cos(\alpha_2 x) + D\sin(\alpha_2 x) \quad (1/m^{1/2}) \quad |x| < a$$
(12)

$$\varphi_{III}(x) = Ee^{\alpha_1 x} + Ge^{-\alpha_1 x} \quad (1/m^{1/2}) \quad x \ge a$$
(13)

where A, B, C, D, E and G are normalization constants to be evaluated shortly.

#### **Even solution case**

Considering  $x \rightarrow \infty$  and the quantum mechanics postulate which states that all valid wave functions for any quantum system must vanish at infinite coordinate limits, it follows from (11) an (13) that

$$B = 0$$
,  $E = 0$  and  $A = F$  (14)

Now, from (12), for this symmetry case we have

$$D = 0 \tag{15}$$

With these expressions, (11), (12) and (13) become

$$\varphi_{I,ev}(x) = A e^{\alpha_{1,ev} x} \quad (1/m^{1/2}) \quad x \le -a \tag{16}$$

$$\varphi_{II,ev}(x) = C\cos(\alpha_{2,ev}x) \quad (1/m^{1/2}) \quad |x| < a$$
(17)

$$\varphi_{III,ev}(x) = Ae^{-\alpha_{1,ev}x} \quad (1/m^{1/2}) \quad x \ge a \tag{18}$$

These functions, evaluated at  $x = \pm a$  and considering that one of the quantum mechanics postulates states that all valid wave functions and their first derivative have to be continuous and single-valued along the whole system, give the following expressions

$$\varphi_{I,ev}(-a) = \varphi_{II,ev}(-a) = Ae^{-\alpha_{1,ev}a} = C\cos(-\alpha_{2,ev}a)$$
(19)

$$\varphi_{II,ev}(a) = \varphi_{III,ev}(a) = C\cos(\alpha_{2,ev}a) = Fe^{-\alpha_{1,ev}a}$$
(20)

$$\frac{d\varphi_{I,ev}(-a)}{dx} = \frac{d\varphi_{II,ev}(-a)}{dx} = A\alpha_{1,ev}e^{-\alpha_{1,ev}a} = -C\alpha_{2,ev}\sin(-\alpha_{2,ev}a)$$
(21)

$$\frac{d\varphi_{II,ev}(a)}{dx} = \frac{d\varphi_{III,ev}(a)}{dx} = -C\alpha_{2,ev}\sin(\alpha_{2,ev}a) = -F\alpha_{1,ev}e^{-\alpha_{1,ev}a}$$
(22)

Then, we obtain

$$A = F = C\cos(\alpha_{2,ev}a)e^{\alpha_{1,ev}a} \quad (1/\text{cm}^{1/2})$$
(23)

$$A = F = C \frac{\alpha_{2,ev}}{\alpha_{1,ev}} \sin(\alpha_{2,ev}a) e^{\alpha_{1,ev}a} \quad (1/\text{cm}^{1/2})$$
(24)

(23) converts (16), (17) and (18) into

$$\varphi_{I,ev}(x) = C\cos(\alpha_{2,ev}a)e^{\alpha_{1,ev}(x+a)} \quad (1/m^{1/2}) \quad x \le -a$$
(25)

$$\varphi_{II,ev}(x) = C\cos(\alpha_{2,ev}x) \quad (1/m^{1/2}) \quad |x| < a$$
(26)

$$\varphi_{III,ev}(x) = C\cos(\alpha_{2,ev}a)e^{-\alpha_{1,ev}(x-a)} \quad (1/m^{1/2}) \quad x \ge a$$
(27)

#### C is determined in Appendix B and is given by

$$C = \frac{1}{\sqrt{a + \frac{\sin(2\alpha_{2,ev}a)}{2\alpha_{2,ev}} + \frac{\cos^2(\alpha_{2,ev}a)}{\alpha_{1,ev}}}} \quad (1/m^{1/2})$$
(28)

Now, dividing (23) by (24)

$$\alpha_{2,ev}\tan(\alpha_{2,ev}a) - \alpha_{1,ev} = 0 \tag{29}$$

which, using (9) and (10), gives

$$\sqrt{E_{ev}}\tan(aF\sqrt{E_{ev}}) - \sqrt{U_0 - E_{ev}} = 0$$
(30)

Resolving (30), either numerically or graphically, provides the particle allowed energy levels for the even wave functions describing its behavior.

## Odd solution case.

Following a similar derivation as above, the solution for this symmetry case is found to be

$$\varphi_{I,od}(x) = -D\sin(\alpha_{2,od}a)e^{\alpha_{1,od}(x+a)} \quad (1/m^{1/2}) \quad x \le -a$$
(31)

$$\varphi_{II,od}(x) = D\sin(\alpha_{2,od}x) \quad (1/m^{1/2}) \quad |x| < a$$
(32)

$$\varphi_{III,od}(x) = D\sin(\alpha_{2,od}a)e^{-\alpha_{1,od}(x-a)} \quad (1/m^{1/2}) \quad x \ge a$$
(33)

D is determined in Appendix C and is given by

$$D = \frac{1}{\sqrt{a - \frac{\sin(2\alpha_{2,od}a)}{2\alpha_{2,od}} + \frac{\sin^2(\alpha_{2,od}a)}{\alpha_{1,od}}}}$$
(34)

The continuity conditions for this case give

$$\alpha_{2,ev}\cot(\alpha_{2,ev}a) + \alpha_{1,ev} = 0 \tag{35}$$

then, the expression to determine the particle allowed energy values for odd wave functions is

$$\sqrt{E_{od}} \cot(aF \sqrt{E_{od}}) + \sqrt{U_0 - E_{od}} = 0$$
(36)

Now, rearranging (35) this way

$$\alpha_{2,ev}\sin(\alpha_{2,ev}a) = \alpha_{1,ev}\cos(\alpha_{2,ev}a) \tag{37}$$

multiplying both sides by the cosine term,

$$\alpha_{2,ev}\sin(\alpha_{2,ev}a)\cos(\alpha_{2,ev}a) = \alpha_{1,ev}\cos^2(\alpha_{2,ev}a)$$
(38)

using the double-angle trigonometric identity sin(2z) = 2sin(z)cos(z), (38) gives

$$\frac{\sin(2\alpha_{2,ev}a)}{2\alpha_{1,ev}} = \frac{\cos^2(\alpha_{2,ev}a)}{\alpha_{2,ev}}$$
(39)

Let's now consider (35) and write it as

$$\alpha_{2,od}\cos(\alpha_{2,od}a) = -\alpha_{1,od}\sin(\alpha_{2,od}a) \tag{40}$$

multiplying both sides by the sine term,

$$\alpha_{2,od} \sin(\alpha_{2,od} a) \cos(\alpha_{2,od} a) = -\alpha_{1,od} \sin^2(\alpha_{2,od} a)$$
(41)

again, using sin(2z) = 2sin(z)cos(z) in (41), gives

$$\frac{\sin(2\alpha_{2,od}a)}{2\alpha_{1,od}} = -\frac{\sin^2(\alpha_{2,od}a)}{\alpha_{2,od}}$$
(42)

Interestingly, both terms in (39) and in (42) appear in *C* and *D* expressions, (28) and (34), respectively. Then, using (39) in (30), the following is derived

$$0.5\sqrt{E_{ev}}\sin(2aF\sqrt{E_{ev}}) = \sqrt{U_0 - E_{ev}}\cos^2(aF\sqrt{E_{ev}})$$
(43)

Also, with (42), (36) becomes

$$0.5\sqrt{E_{od}}\sin(2aF\sqrt{E_{od}}) = -\sqrt{U_0 - E_{od}}\sin^2(aF\sqrt{E_{od}})$$
(44)

#### Analytical energy eigenvalues for particle confinement cases.

Even waveform confinement.

This case is obtained when (25) and (27) vanish. This is obtained for

$$\cos(\alpha_{2,ev,C}a) = 0 \tag{45}$$

which is true for

$$\alpha_{2,ev,n,C}a = \frac{\pi}{2}n \quad , n = 1,3,5,\dots$$
(46)

This, using (9) and (10), gives

$$E_{ev,n,C} = Ry \left( \pi \frac{r_H}{2a} n \right)^2 \quad (eV), n = 1,3,5,\dots$$
(47)

Odd waveform confinement.

Now, the vanishing condition for (31) and (33) implies

$$\sin(\alpha_{2,ev,C}a) = 0 \tag{48}$$

Which is met for

$$\alpha_{2,odd,m,C}a = \pi \frac{m}{2}$$
,  $m = 2,4,6,...$  (49)

Again, with (9) and (10), we get

$$E_{od,m,C} = Ry \left( \pi \frac{r_H}{2a} m \right)^2$$
 (eV),  $m = 2,4,6,...$  (50)

Note that if we use for the vanishing condition the left side of either (43) or (44), we can write

$$\sin(2\alpha_{2,ev/od,C}a) = 0 \tag{51}$$

Which is met for

$$2\alpha_{2,ev/odd,s,C}a = \pi s$$
,  $s = 1,2,3,...$  (52)

Now, with (9) and (10), we derive

$$E_{ev/od,s,C} = Ry \left( \pi \frac{r_H}{2a} s \right)^2$$
 (eV),  $s = 1,2,3,...$  (53)

This expression merges (47) and (50) values, odd *s* values provide confined even wave functions and also non-confined odd wave functions which have a certain tunneling level involved; for *s* even values, the confined/tunneling roles are interchanged between the two wave symmetries. This condition of a given allowed energy level corresponding to two different waveforms is known as eigenstate degeneracy and is the fundamental explanation for the Schrödinger's cat in a box paradox and the eerie phenomenon of entanglement he introduced.

#### Mean of the two probability density functions for degenerated eigenstates.

For any *s* value, let's use the particle presence probability density function for each of the two symmetry wave functions,  $\varphi_{ev,s}^2$  and  $\varphi_{od,s}^2$ , to define their mean probability density function as follows

$$\varphi_{mpd,s}(x) = \frac{\varphi_{ev,s}^2(x) + \varphi_{od,s}^2(x)}{2} \quad (1/m)$$
(54)

This parameter has physical sense if, for example, we consider a certain multiplicity of identical systems such that the particle energy is the same in all of them and is supposed that both particle wave function symmetries in the degenerated states have equal likelihood of being present.

#### **Calculation examples.**

#### System A. $a = 16r_H$ (m). $U_0 = 4.72089$ (eV).

Graphical and analytical calculation of the particle allowed energies  $E_s$  for this system are shown in Figure 2. As can be seen there are six energy levels for this case, the highest of which was established by fine tuning  $U_0$  to the value given above such that  $U_0 - E_6 \sim 10 \mu eV$ .



Figure 2. Determination of allowed particle energies for system A.

The particle wave functions  $\varphi_{ev/odd,s}$  for s = 1 to 4 are plotted is Figure 3.



Figure 3. System A particle wave functions for first four quantum numbers showing the confinement/non confinement alternating nature described above.

The system A wave functions for s = 5 and 6 are plotted in Figure 4. For s = 5, the wave functions behave as described in Fig. 3. For s = 6, confinement is again present for the odd symmetry wave function, however, for the even symmetry case the particle becomes loose, that is, behaves like a near free particle. Then, this allowed energy level can have a particle in either a fully localized condition or in an almost fully spread one. This configuration is known as entanglement.



Figure 4. *s* = 5 and 6 particle wave functions in system A. For *s* = 5, the confinement/non confinement behavior is similar as in Fig. 3. For s = 6, the non-confined case (even WF) becomes extreme such that the particle becomes nearly free while the confined case (odd WF) remains like all *s* values.

The system A particle presence probability functions and their corresponding cumulative probability functions are depicted in Figures 5 and 6, respectively. Note that all the zero crossings of the wave functions in Figures 3 and 4 become particle exclusion points inside the well, that is, its presence probability vanishes at these locations.



Figure 5. Particle presence probability density functions for *x* <= 0. System A.



Figure 6. Cumulative particle presence probability functions for *x* <= 0. System A.

Let's now consider the mean particle presence probability densities defined in (54) and shown in Figure 7. *a*) with their cumulative traces given in Figure 7. *b*). As compared with the previous two Figures we notice that the particle exclusion points inside the well are now not present and that the cumulative particle presence probability functions are nearly linear for s = 1 to 5, two aspects somehow reminiscent of Classical Mechanics predictions inside the well.

The  $\varphi_{mpd,6}$  case illustrates the archetype of Quantum Mechanics phenomenon of particle entanglement whose cumulative presence probabilities inside and outside the well are both nearly 50 %. In terms of Schrödinger's cat in a box fate, rather than alive or dead, we can say that the pet, when searched for, can be found 50 % of the times at home inside the box and the other 50 % observed to be wandering around out of the box. The quite striking thing is that the cat can interchange presence sites instantly, without any energy transfer involved, a phenomenon known as teleportation.



Figure 7. *a*) System A mean probability density functions and *b*) their corresponding particle presence cumulative probability.

## Case B. $a = (\pi/2)r_H$ (m). $U_{\theta} = Ry + 1.88E^{-6}$ (eV).

Graphical and analytical calculation of the only particle allowed energy for this system are shown in Figure 8-*a*). This time, the fine tuning of  $U_0$  to reach the value given above was such that  $E_1 = Ry$ . Figure 8-*b*) depicts the particle wave functions, now with the even case being confined and the odd case being near free.



Figure 8. *a*) Allowed single particle energy level for system B determination. b) Corresponding confined, even, and near-free, odd wave functions.

System B particle presence probability functions and their mean are plotted in Figure 9-a) while their corresponding cumulative traces are presented in Figure 9-b). As above, a particle 50 % inside-50 % outside the well presence probability is obtained for this single allowed energy level system.



Figure 9. *a*) Particle presence probability density functions and of their mean. b) Corresponding cumulative traces.

#### Conclusions.

An analysis of the quantum behavior of a particle interacting with a unidimensional, square and finite box of potential energy system was presented. By solving the system's timeindependent Schrödinger equation - written in terms of the Rydberg unit of energy Ry -, the particle allowed energy levels for confined conditions were determined graphically and analytically. The mean particle presence probability function concept was introduced and used to illustrate the occurrence of the particle entanglement phenomenon in a couple of calculation examples.

### Appendix A. The Rydberg unit of energy derived from the Schrödinger equation.

The time-independent unidimensional Schrödinger equation for a particle of rest mass  $m_0$  (kg) having an energy E (J) in a given system of potential energy U(x) (J) is written as

$$\frac{d^2\varphi(x)}{dx^2} - \frac{2m_0}{\hbar^2} (U(x) - E) \,\varphi(x) = 0 \quad (1/m^{5/2}) \tag{A1}$$

where  $\varphi(x)$  (1/m<sup>1/2</sup>) is the particle wave function,  $\hbar$  (J-s) is the Planck's constant h divided by  $2\pi$ . If we consider that the particle is an electron with charge q (C) and make use of the atom Bohr radius  $r_H$  (m), we can transform the above expression as follows

$$\frac{d^2\varphi(x)}{dx^2} - \frac{2m_0}{\hbar^2} (U(x) - E) \varphi(x) (\frac{q}{q} \frac{r_H^2}{r_H^2}) = 0 \quad (1/m^{5/2})$$
(A2)

with this, U and E are converted into eV units.

Then, (A2) can be rearranged as

$$\frac{d^2\varphi(x)}{dx^2} = \frac{U(x) - E}{r_H^2 \hbar^2 / (2r_H^2 q m_0)} \varphi(x) \quad (1/m^{5/2})$$
(A3)

which becomes

$$\frac{d^2\varphi(x)}{dx^2} = \frac{U(x) - E}{r_H^2 Ry} \varphi(x) \quad (1/m^{5/2})$$
(A4)

where the constant Ry (eV), the Rydberg unit of energy - which corresponds to the highest energy photon that can be emitted/absorbed by an atom -, is written as

$$Ry = \frac{1}{2qm_0} \left(\frac{\hbar}{r_H}\right)^2 = 13.605 \ 693 \ 123 \ 0445 \ (eV)$$
(A5)

This number was calculated using CODATA internationally recommended 2018 values of the NIST Fundamental Physical Constants site [1]. It has a relative standard uncertainty (rsu) of  $6.54 \times 10^{-12}$  with respect to NIST provided definition which is as follows

$$Ry_{NIST} = \frac{m_0}{2q} (\alpha c)^2 = \frac{m_0}{2q} v_1^2 = 13.605 \ 693 \ 122 \ 994 \ (eV) \ (rsu \ 1.9 \ x \ 10^{-12})$$
(A6)

where  $\alpha$  is the Sommerfeld's or finite-structure constant, c (m/s) is the speed of light in vacuum and  $v_1$  is the electron orbit exit speed.

#### Appendix B. Constant C evaluation.

To determine the normalization constant C in (25) to (27), it is necessary to apply the quantum mechanics postulate which stablishes that the particle probability presence density must integrate to 1 through all the system. Then, we have to evaluate

$$1 = \int_{-\infty}^{-a} (\varphi_{I,ev}(x))^2 dx + \int_{-a}^{a} (\varphi_{II,ev}(x))^2 dx + \int_{a}^{\infty} (\varphi_{II,ev}(x))^2 dx$$
(I1)

$$1 = C^{2} \left( \cos^{2}(\alpha_{1,ev}a) \int_{-\infty}^{-a} e^{2\alpha_{1,ev}(x+a)} dx + \int_{-a}^{a} \cos^{2}(\alpha_{2,ev}x) dx + \cos^{2}(\alpha_{1,ev}a) \int_{a}^{\infty} e^{-2\alpha_{1,ev}(x-a)} dx \right)$$
(I2)

$$1 = C^{2} \left( \frac{\cos^{2}(\alpha_{2,ev}a)}{2\alpha_{1,ev}} e^{2\alpha_{1,ev}(x+a)} \Big|_{-\infty}^{-a} + \left(\frac{x}{2} + \frac{\sin(2\alpha_{2,ev}x)}{4\alpha_{2,ev}}\right) \Big|_{-a}^{a} - \frac{\cos^{2}(\alpha_{2,ev}a)}{2\alpha_{1,ev}} e^{-2\alpha_{1,ev}(x-a)} \Big|_{a}^{\infty} \right)$$
(I3)

$$1 = C^{2} \left\{ \frac{\cos^{2}(\alpha_{2,ev}a)}{2\alpha_{1,ev}} + a + \frac{\sin(2\alpha_{2,ev}a)}{2\alpha_{2,ev}} + \frac{\cos^{2}(\alpha_{2,ev}a)}{2\alpha_{1,ev}} \right\}$$
(I4)

$$C = \frac{1}{\sqrt{a + \frac{\sin(2\alpha_{2,ev}a)}{2\alpha_{2,ev}} + \frac{\cos^2(\alpha_{2,ev}a)}{\alpha_{1,ev}}}} \quad (1/m^{1/2})$$
(I5)

#### Appendix C. Constant D determination.

D in (31) to (33) is determined as follows

$$1 = \int_{-\infty}^{-a} (\varphi_{I,od}(x))^2 dx + \int_{-a}^{a} (\varphi_{II,od}(x))^2 dx + \int_{a}^{\infty} (\varphi_{II,od}(x))^2 dx$$
(II1)

$$1 = D^{2} \left( \sin^{2}(\alpha_{1,od}a) \int_{-\infty}^{-a} e^{2\alpha_{1,od}(x+a)} dx + \int_{-a}^{a} \sin^{2}(\alpha_{2,od}x) dx + \sin^{2}(\alpha_{1,od}a) \int_{a}^{\infty} e^{-2\alpha_{1,od}(x-a)} dx \right)$$
(II2)

$$1 = D^{2} \left( \frac{\sin^{2}(\alpha_{2,od}a)}{2\alpha_{1,od}} e^{2\alpha_{1,od}(x+a)} \bigg|_{-\infty}^{-a} + \left(\frac{x}{2} - \frac{\sin(2\alpha_{2,od}x)}{4\alpha_{2,od}}\right) \bigg|_{-a}^{a} - \frac{\sin^{2}(\alpha_{2,od}a)}{2\alpha_{1,od}} e^{-2\alpha_{1,od}(x-a)} \bigg|_{a}^{\infty} \right)$$
(II3)

$$1 = D^2 \left\{ \frac{\sin^2(\alpha_{2,od} a)}{2\alpha_{1,od}} + a - \frac{\sin(2\alpha_{2,od} a)}{2\alpha_{2,od}} + \frac{\sin^2(\alpha_{2,od} a)}{2\alpha_{1,od}} \right\}$$
(II4)

$$D = \frac{1}{\sqrt{a - \frac{\sin(2\alpha_{2,od}a)}{2\alpha_{2,od}} + \frac{\sin^2(\alpha_{2,od}a)}{\alpha_{1,od}}}}$$
(II5)

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