QUANTUM DOTS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.20.

An unusual problem involving the variational principle is as follows. Suppose a particle is constrained to move in two dimensions in a cross-shaped region. We can specify the cross shape by recognizing that it is symmetric in each octant of the xy plane. In the first octant (bounded by the x axis and the line $y=x$) the allowed region is bounded by the x axis, the line $y=x$ and the horizontal line $y=+a$. This region is then reflected about the line $y=x$ to get the allowed region in the second octant, and then the total region is the first quadrant is replicated in the other three quadrants to get the cross.

What kinds of energy levels are allowed in such a system? We can consider first the limiting case where the particle is far out along the arm of the cross extending towards $+x$. Out here, we have essentially an infinite square well of width $2a$ in the y direction, and a free particle in the x direction. That is, we can write the Schrödinger equation as

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right)\psi=E\psi \tag{1}$$

and use separation of variables so that $\psi=X(x)Y(y)$. The y equation is just that of the infinite square well, so its energy levels are given by

$$E_y=\frac{(n\pi\hbar)^2}{2m(2a)^2} \tag{2}$$

The energy due to the free particle contribution in the x direction must be positive, so any particle that can escape to infinity must have an energy greater than E_y; in other words, a particle cannot escape to infinity (that is, it's in a bound state) if its energy is lower than the ground state ($n=1$) of the square well:

$$E<\frac{(\pi\hbar)^2}{8ma^2} \tag{3}$$

Clearly, trying to calculate the exact energy levels for a potential with such an odd shape would be very difficult, but we can use the variational principle to get an upper bound on this energy. The trial function is

$$\psi = \begin{cases} A\left(1-\frac{|xy|}{a^2}\right)e^{-\alpha} & |x|\le a \text{ and } |y|\le a \\ A\left(1-\frac{|x|}{a}\right)e^{-\alpha|y|/a} & |x|\le a \text{ and } |y|> a \\ A\left(1-\frac{|y|}{a}\right)e^{-\alpha|x|/a} & |x|> a \text{ and } |y|\le a \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

The parameter α is the variational parameter. The first line is in the square of side $2a$ centred on the origin, the second line is in the top and bottom arms of the cross and the third line is in the left and right arms. The wave function is of course zero outside the cross, since the potential is infinite there and the particle cannot exist there.

First, we need to find A from normalization. We can use the symmetry of the problem and of ψ to simplify the integrals, since the problem is symmetric in all 8 octants. Thus we can integrate over the first octant and multiply the result by 8. Therefore

$$8\left[\int_0^a\int_y^a + \int_0^a\int_a^\infty\right]\psi^2 dx\,dy = 1 \tag{5}$$

$$\int_0^a\int_y^a\left(1-\frac{xy}{a^2}\right)^2 e^{-2\alpha}dx\,dy + \int_0^a\int_a^\infty\left(1-\frac{y}{a}\right)^2 e^{-2\alpha x/a}dx\,dy = \frac{1}{8A^2} \tag{6}$$

$$A = \frac{3e^\alpha}{2a}\sqrt{\frac{2\alpha}{11\alpha+6}} \tag{7}$$

Now to work out $\langle H\rangle$ we need the derivatives of ψ. We need to be careful at the boundaries between the regions, since although ψ is continuous there, its first derivative isn't, so the second derivative will contain delta functions. We get, again considering only the first octant:

$$\frac{1}{A}\frac{\partial\psi}{\partial x} = \begin{cases} -\frac{y}{\alpha^2}e^{-\alpha} & x<a \\ -\frac{\alpha}{a}\left(1-\frac{y}{a}\right)e^{-\alpha x/a} & x>a \end{cases} \tag{8}$$

$$\frac{1}{A}\frac{\partial^2\psi}{\partial x^2} = \begin{cases} 0 & x<a \\ \frac{\alpha^2}{a^2}\left(1-\frac{y}{a}\right)e^{-\alpha x/a} & x>a \end{cases} \tag{9}$$

The first derivative is discontinuous along the line $x = a$, so there we get

$$\frac{1}{A}\frac{\partial\psi}{\partial x}=\begin{cases}-\frac{y}{\alpha^2}e^{-\alpha} & x=a_-\\ -\frac{\alpha}{a}\left(1-\frac{y}{a}\right)e^{-\alpha} & x=a_+\end{cases} \tag{10}$$

so we get a step change at $x=a$ in the amount of

$$\left.\frac{\partial\psi}{\partial x}\right|_+-\left.\frac{\partial\psi}{\partial x}\right|_-=A\left[-\frac{\alpha}{a}\left(1-\frac{y}{a}\right)+\frac{y}{\alpha^2}\right]e^{-\alpha} \tag{11}$$

The derivative of a step function is a delta function, so at $x=a$ we have

$$\left.\frac{\partial^2\psi}{\partial x^2}\right|_{x=a}=A\left[-\frac{\alpha}{a}\left(1-\frac{y}{a}\right)+\frac{y}{\alpha^2}\right]e^{-\alpha}\delta(x-a)$$

and the complete derivative is then

$$\frac{1}{A}\frac{\partial^2\psi}{\partial x^2}=\begin{cases}\left[-\frac{\alpha}{a}\left(1-\frac{y}{a}\right)+\frac{y}{\alpha^2}\right]e^{-\alpha}\delta(x-a) & x\le a\\ \frac{\alpha^2}{a^2}\left(1-\frac{y}{a}\right)e^{-\alpha x/a} & x>a\end{cases} \tag{12}$$

In the y direction, we get, for $x<a$

$$\frac{1}{A}\frac{\partial\psi}{\partial y}=\begin{cases}-\frac{x}{a^2}e^{-\alpha} & y>0\\ \frac{x}{a^2}e^{-\alpha} & y<0\end{cases} \tag{13}$$

so for $y\neq 0$, we have

$$\frac{\partial^2\psi}{\partial y^2}=0 \tag{14}$$

Because of the discontinuity at $y=0$ we get another delta function, so the total second derivative is, for $x<a$

$$\frac{\partial^2\psi}{\partial y^2}=-\frac{2x}{a^2}e^{-\alpha}\delta(y) \tag{15}$$

For $x>a$

$$\frac{1}{A}\frac{\partial\psi}{\partial y}=\begin{cases}-\frac{1}{a^2}e^{-\alpha x/a} & y>0\\ \frac{1}{a^2}e^{-\alpha x/a} & y<0\end{cases} \tag{16}$$

Again, the second derivative is zero on both sides of the x axis, but there is a delta function on the axis:

$$\frac{\partial^2\psi}{\partial y^2} = -\frac{2A}{a^2}e^{-\alpha x/a}\delta(y) \tag{17}$$

We can now put all this together to calculate $\langle H\rangle$. First, the term excluding the delta functions. Since both second derivatives are zero for $x < a$, there is only the contribution from $x > a$:

$$H_1 = -\frac{A^2\hbar^2}{2m}\int_0^a\int_a^\infty \frac{\alpha^2}{a^2}\left(1-\frac{y}{a}\right)^2 e^{-2\alpha x/a}dx\,dy \tag{18}$$

Next, the term resulting from the delta function in the x derivative. We set $x = a$ and then integrate over y:

$$H_2 = -\frac{A^2\hbar^2}{2m}e^{-2\alpha}\int_0^a\left(1-\frac{y}{a}\right)\left[-\frac{\alpha}{a}\left(1-\frac{y}{a}\right)+\frac{y}{\alpha^2}\right]dy \tag{19}$$

Finally, the terms resulting from the delta functions in the y derivative. We set $y = 0$ and integrate over x:

$$H_3 = \frac{1}{2}\left[\frac{A^2\hbar^2}{ma^2}e^{-2\alpha}\int_0^a x\,dx - \frac{A^2\hbar^2}{ma}\int_a^\infty e^{-2\alpha x/a}dx\right] \tag{20}$$

The factor of $\frac{1}{2}$ in H_3 comes from the fact that the x axis is shared between two octants, so only half the integral over the delta function contributes to the first octant.

We can evaluate these integrals using Maple (or by hand; none of them is difficult, but there's a lot of calculation) to find, after simplifying:

$$\langle H\rangle = 8(H_1+H_2+H_3) \tag{21}$$

$$= \frac{3\hbar^2}{ma^2}\left(\frac{\alpha^2+2\alpha+3}{6+11\alpha}\right) \tag{22}$$

We can find the value of α that minimizes this by taking the derivative as usual, and we get

$$\alpha_{min} = \frac{1}{11}\left(-6\pm\sqrt{267}\right) \tag{23}$$

We require $\alpha > 0$ in order for the integrals above to converge, so we must take the positive root. Plugging this back into $\langle H\rangle$ we find

$$\langle H\rangle = \frac{1.058\hbar^2}{ma^2} < \frac{\pi^2\hbar^2}{8ma^2} = \frac{1.234\hbar^2}{ma^2} \tag{24}$$

The upper bound given by the variational principle is thus below the minimum energy at which a particle can escape, so there is at least one bound state in this system.