Exercise 4. Quantum dots

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1 Statement

Consider a quantum dot modeled as a sphere of radius R within which an electron is confined. Outside this sphere, the potential is infinite, implying that the wave function of the electron must be zero at $r = R$. Show that the energy levels of such a quantum dot have the same expression as those of a particle in a box.

2 Solving the Schrödinger equation

In order to get the wave function of an electron trapped inside a radial box, we have to solve the time-independent Schrödinger equation. For this system, we assume a free particle:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

Since the system has spherical symmetry, the wave function only depends on the radius, and we can neglect the angular part. As a consequence, the only non-null part of the Laplacian operator is the radius derivatives.

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\right)\psi(r) = E\psi(r)$$
$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\left(2r\frac{\partial\psi}{\partial r} + r^2\frac{\partial^2\psi}{\partial r^2}\right)\right) = E\psi(r)$$

Now we can make a change of variable $\psi(r) = \frac{u(r)}{r}$ and calculate the derivatives:

$$\partial_r\psi = -\frac{1}{r^2}u(r) + \frac{1}{r}\partial_r u(r)$$
$$\partial_r^2\psi = \frac{2}{r^3}u(r) - \frac{2}{r^2}\partial_r u(r) + \frac{1}{r}\partial_r^2 u(r)$$

So we can substitute them in the differential equation and simplify it:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\left(-\frac{2}{r}u(r)+2\partial_r u(r)+\frac{2}{r}u(r)-2\partial_r u(r)+r\partial_r^2 u(r)\right)\right)=E\frac{u(r)}{r}$$
$$-\frac{\hbar^2}{2m}\partial_r^2 u(r)=Eu(r)$$

We can see that the function $u(r)$ must be an exponential $u(r)=e^{kr}$ being $k=\pm\frac{i}{\hbar}\sqrt{2mE}=\pm\frac{i}{\hbar}p$:

$$u(r)=Ae^{\frac{i}{\hbar}pr}+Be^{-\frac{i}{\hbar}pr}$$

If we apply the boundary condition $u(R)=0$ it can be simplified:

$$u(R)=Ae^{\frac{i}{\hbar}pR}+Be^{-\frac{i}{\hbar}pR}=0$$
$$B=-Ae^{2\frac{i}{\hbar}pR}$$

When using the result obtained in $u(r)$ we can extract the common factor and apply the property $2i\sin(x)=e^{ix}-e^{-ix}$

$$\begin{aligned}u(r)&=Ae^{\frac{i}{\hbar}pr}-Ae^{2\frac{i}{\hbar}pR}\cdot e^{-\frac{i}{\hbar}pr}\\&=Ae^{\frac{i}{\hbar}pR}(e^{\frac{i}{\hbar}(r-R)}-e^{-\frac{i}{\hbar}(r-R)})\\&=2Ae^{\frac{i}{\hbar}pR}\sin(\frac{p}{\hbar}(r-R))\end{aligned}$$

Now we see that if $r=0$ the function $\psi(r)=\frac{u(r)}{r}$ has a singularity. It can be saved if $u(0)=0$:

$$u(0)=2Ae^{\frac{i}{\hbar}pR}\sin(-\frac{p}{\hbar}R)=-2Ae^{\frac{i}{\hbar}pR}\sin(\frac{p}{\hbar}R)$$

The sine function vanishes only when:

$$\frac{p}{\hbar}R=\pi n$$

And we can conclude that the wave function is quantified with the integer number $n\in N$:

$$u(r)=2Ae^{\frac{i}{\hbar}pR}\sin(\frac{\pi n}{R}(r-R))$$

Finally, when substituting $p=\sqrt{2mE}$ in the equation of before we get the quantified energy levels:

$$\sqrt{2mE}=\frac{\hbar\pi n}{R}$$
$$E=\frac{\hbar\pi^2 n^2}{2mR^2}$$