Ground state of a symmetric quantum system

Special case of the oscillation theorem

Christophe De Beule (christophe.debeule@gmail.com)

For simplicity, we consider one spatial dimension. Generalizations to higher dimensions are straightforward. We start from the Hamiltonian

$$H = \frac{p^2}{2m} + V(x),$$

where the potential is symmetric: $V(-x) = V(x)$. In this case, the Hamiltonian commutes with the parity operator P. This means that if $|n\rangle$ is an eigenket of the Hamiltonian with energy E_n, then $P|n\rangle$ is also an eigenket with the same energy. If $|n\rangle$ is *nondegenerate*, we have

$$P|n\rangle = \alpha|n\rangle,$$

and since $P^2 = 1$, we find $\alpha = \pm 1$. Therefore the wave function of a nondegenerate eigenstate of H is either even or odd:

$$\psi_n(-x) = \langle -x|n\rangle = \langle x|P|n\rangle = \pm\psi_n(x).$$

Now assume that the ground state is nondegenerate so that it is also a parity eigenstate. In this case, the most general wave function can be written as

$$\psi_0(x) = f(x)e^{i\chi(x)},$$

with $f(x) \geq 0$ and $\chi(x)$ real functions, and

$$\begin{aligned} f(-x) &= f(x) \\ \chi(-x) &= \chi(x) + (1-\alpha)\frac{\pi}{2}, \end{aligned}$$

with $\alpha = \pm 1$, the parity eigenvalue of $\psi_0(x)$. Note that for an odd wave function, we require $f(0) = 0$. The ground-state energy is given by

$$\begin{aligned} E_0 &= \int dx\, \psi_0^*(x) H \psi_0(x) \\ &= -\frac{\hbar^2}{2m}\int dx\, \psi_0^*(x)\frac{d^2}{dx^2}\psi_0(x) + \int dx\, f(x)^2 V(x), \end{aligned}$$

where we assumed that the wave function is normalized. Since

$$\begin{aligned} \frac{d}{dx}\psi_0(x) &= \frac{df}{dx}e^{i\chi(x)} + i\frac{d\chi}{dx}f(x)e^{i\chi(x)} \\ \frac{d^2}{dx^2}\psi_0(x) &= \frac{d^2 f}{dx^2}e^{i\chi(x)} + 2i\frac{d\chi}{dx}\frac{df}{dx}e^{i\chi(x)} + i\frac{d^2\chi}{dx^2}f(x)e^{i\chi(x)} - \left(\frac{d\chi}{dx}\right)^2 f(x)e^{i\chi(x)}, \end{aligned}$$

the energy becomes

$$\begin{aligned} E_0 &= -\frac{\hbar^2}{2m}\int dx\left[f(x)\frac{d^2 f}{dx^2} - \left(f(x)\frac{d\chi}{dx}\right)^2\right] + \int dx\, f(x)^2 V(x) \\ &= \frac{\hbar^2}{2m}\int dx\left[\left(\frac{df}{dx}\right)^2 + \left(f(x)\frac{d\chi}{dx}\right)^2\right] + \int dx\, f(x)^2 V(x). \end{aligned}$$

Here we already left out the imaginary parts since they should vanish because E_0 is real for a normalizable wave function. Alternatively, you can see that these parts form a total differential. Since the ground state is by definition the lowest possible energy, we see that we should have $\chi(x) =$ constant to lower the kinetic energy. Since the wave function is only determined up to a constant phase, we can take $\chi = 0$. We find that the ground-state wave function should be an even function:

$$\psi_0(x) = f(x),$$

which can be chosen real with energy

$$E_0 = \int dx \left[\frac{\hbar^2}{2m} \left(\frac{df}{dx} \right)^2 + f(x)^2 V(x) \right].$$

Note that this is only true if the ground state is nondegenerate. Otherwise, we can make linear combinations that are not parity eigenstates.

So we find that the wave function of a nondegenerate ground state of the Schrödinger equation is an even function. This holds in any spatial dimensions with $V(-\boldsymbol{r}) = V(\boldsymbol{r})$.