Ground state of a symmetric quantum system

Special case of the oscillation theorem

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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

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

where we assumed that the wave function is normalized. Since

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

the energy becomes

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

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.

We conclude that the wave function of a nondegenerate ground state of the Schrödinger equation is an even function when the system conserves parity (spatial inversion). This holds for any number of spatial dimensions with $V(-\boldsymbol{r}) = V(\boldsymbol{r})$.