2.6: Exercises

Exercises

Exercise 2.6.1

Use the variational theorem to prove that a 1D potential well has at least one bound state. Assume that the potential $V(x)$ satisfies (i) $V(x) < 0$ for all x, and (ii) $V(x) \rightarrow 0$ for $x \rightarrow \pm\infty$. The Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x). \tag{2.6.1}$$

Consider a (real) trial wavefunction

$$\psi(x;\gamma) = \left(\frac{2\gamma}{\pi}\right)^{1/4} e^{-\gamma x^2}. \tag{2.6.2}$$

Note that this can be shown to be normalized to unity, using Gauss' integral

$$\int_{-\infty}^{\infty} dx\; e^{-2\gamma x^2} = \sqrt{\frac{\pi}{2\gamma}}. \tag{2.6.3}$$

Now prove that

$$\begin{aligned}\langle E\rangle &= \int_{-\infty}^{\infty} dx\; \psi(x)\,\hat{H}\,\psi(x) \\ &= \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\,\left(\frac{d\psi}{dx}\right)^2 + \int_{-\infty}^{\infty} dx\; V(x)\,\psi^2(x) \\ &= A\sqrt{\gamma}\left[\sqrt{\gamma} + B\int_{-\infty}^{\infty} dx\; V(x)\, e^{-\gamma x^2}\right],\end{aligned} \tag{2.6.4}$$

where A and B are positive real constants to be determined. By looking at the quantity in square brackets in the limit $\gamma \rightarrow 0$, argue that $\langle E\rangle < 0$ in this limit. Hence, explain why this implies the existence of a bound state.

Finally, try generalizing this approach to the case of a 2D radially-symmetric potential well $V(x,y) = V(r)$, where $r = \sqrt{x^2+y^2}$. Identify which part of the argument fails in 2D. [For a discussion of certain 2D potential wells that *do* always support bounds states, similar to 1D potential wells, see Simon (1976).]

Exercise 2.6.2

In this problem, you will investigate the existence of bound states in a 3D potential well that is finite, uniform, and spherically-symmetric. The potential function is

$$V(r,\theta,\phi) = -U\Theta(a-r), \tag{2.6.5}$$

where a is the radius of the spherical well, U is the depth, and (r,θ,ϕ) are spherical coordinates defined in the usual way.

The solution involves a variant of the partial wave analysis discussed in Appendix A. For $E < 0$, the Schrödinger equation reduces to

$$\begin{cases}\left(\nabla^2 + q^2\right)\psi(r,\theta,\phi) = 0 \;\text{ where }\; q = \sqrt{2m(E+U)/\hbar^2}, & \text{for } r \leq a \\ \left(\nabla^2 - \gamma^2\right)\psi(r,\theta,\phi) = 0 \;\text{ where }\; \gamma = \sqrt{-2mE/\hbar^2}, & \text{for } r \geq a.\end{cases} \tag{2.6.6}$$

For the first equation (called the Helmholtz equation), we seek solutions of the form

$$\psi(r,\theta,\phi) = f(r)\,Y_{\ell m}(\theta,\phi), \tag{2.6.7}$$

where $Y_{\ell m}(\theta,\phi)$ are spherical harmonics, and the integers l and m are angular momentum quantum numbers satisfying $l \geq 0$ and $-l \leq m \leq l$. Substituting into the Helmholtz equation yields

$$r^2 \frac{d^2 f}{dr^2} + 2r \frac{df}{dr} + \left[q^2 r^2 - l(l+1)\right] f(r) = 0, \tag{2.6.8}$$

which is the **spherical Bessel equation**. The solutions to this equation that are non-divergent at $r=0$ are $f(r) = j_\ell(qr)$, where j_ℓ is called a **spherical Bessel function of the first kind**. Most numerical packages provide functions to calculate these (e.g., `scipy.special.spherical_jn` in Scientific Python).

Similarly, solutions for the second equation can be written as $\psi(r,\theta,\phi) = g(r)\, Y_{\ell m}(\theta,\phi)$, yielding an equation for $g(r)$ called the **modified spherical Bessel equation**. The solutions which do not diverge as $r \to \infty$ are $g(r) = k_\ell(\gamma r)$, where k_ℓ is called a **modified spherical Bessel function of the second kind**. Again, this can be computed numerically (e.g., using `scipy.special.spherical_kn` in Scientific Python).

Using the above facts, show that the condition for a bound state to exist is

$$\frac{q j_\ell'(qa)}{j_\ell(qa)} = \frac{\gamma k_\ell'(\gamma a)}{k_\ell(\gamma a)}, \tag{2.6.9}$$

where j_ℓ' and k_ℓ' denote the derivatives of the relevant special functions, and q and γ depend on E and U as described above. Write a program to search for the bound state energies at any given a and U, and hence determine the conditions under which the potential does not support bound states.

Further Reading

[1] Bransden & Joachain, §4.4, 9.2–9.3, 13.4

[2] Sakurai, §5.6, 7.7–7.8

[3] R. Courant and D. Hilbert, *Methods of Mathematical Physics* vol. 1, Interscience (1953).

[4] B. Simon, *The bound state of weakly coupled Schrödinger operators in one and two dimensions*, Annals of Physics **97**, 279 (1976).