

1. A system of two identical spin $\frac{1}{2}$ particles are in a 1-dimensional simple harmonic oscillator potential with Hamiltonian

$$H = \frac{p_1^2 + p_2^2}{2m} + \frac{1}{2}m\omega^2(x_1^2 + x_2^2) \quad (1)$$

- a. What is the energy of the ground state? What is the total spin of the ground state? Why not the other possible total spin?

Each particle is in the SHO ground state with energy $\frac{1}{2}\hbar\omega$, so the total energy is $\hbar\omega$. The space wave function is $\psi_0(x_1)\psi_0(x_2)$, so the spin state must be antisymmetric, singlet, spin 0. Spin 1 would be interchange-symmetric, and with a symmetric space state this is forbidden by the exclusion principle.

- b. What is the energy of the first excited state? How much degeneracy does this state have? Describe the space and the spin wave functions of the degenerate states.

For the first excited state one of the particles is in the SHO first excited state, and the other one is in the ground state. The energy is $\frac{1}{2}\hbar\omega + \frac{3}{2}\hbar\omega = 2\hbar\omega$. The space wave function can be symmetric, $\psi_0(x_1)\psi_1(x_2) + \psi_0(x_2)\psi_1(x_1)$ or antisymmetric, $\psi_0(x_1)\psi_1(x_2) - \psi_0(x_2)\psi_1(x_1)$. The former goes with singlet spin, the latter with triplet spin, a total of four possibilities.

2. To the Hamiltonian (1) we now add the spin-dependent perturbation

$$H' = \lambda\delta(x_1 - x_2)\mathbf{S}_1 \cdot \mathbf{S}_2$$

- a. How large is the change of the energies of the ground and first excited states, to first order in λ ? Does the perturbation remove the degeneracy?

We have

$$\langle H' \rangle = \lambda \langle \delta \rangle \langle S_1 \cdot S_2 \rangle = \lambda \langle \delta \rangle \left\langle \frac{1}{2}(S^2 - S_1^2 - S_2^2) \right\rangle = \frac{\lambda}{2} \langle \delta \rangle \left\langle S^2 - \frac{3}{2} \right\rangle,$$

so the spin factor is $-\frac{3}{2}$ for singlet and $+\frac{1}{2}$ for triplet. However, in the space factor $\langle \delta \rangle$ the δ -function makes $x_1 = x_2$ and annuls any antisymmetric wave function. Hence the energy change vanishes for all triplet states, $\Delta E_{1,\text{triplet}} = 0$. For the ground state we have

$$\begin{aligned} \langle \delta \rangle &= \int \int \psi_0^*(x_1)\psi_0^*(x_2)\delta(x_1 - x_2)\psi_0(x_1)\psi_0(x_2)dx_1dx_2 = \int (\psi_0^*(x_1)\psi_0(x_1))^2 dx_1 \\ &= \frac{1}{\pi} \int e^{-2x^2} dx_1 = 1/\sqrt{2\pi}, \end{aligned}$$

and $\Delta E_0 = -3\lambda/\sqrt{8\pi}$. Similarly $\Delta E_{1,\text{singlet}} = -3\lambda/4\sqrt{2\pi}$.

- b. Show that, to first order, the system does not make a transition to the first excited states if it is initially in the unperturbed ground state, and the perturbation is then turned on. To which second excited states can it make a transition? Specify them by the spin quantum number.

We need $\langle 0|H'|1\rangle$. Since $S_1 \cdot S_2$ is diagonal in the singlet-triplet basis, the spin factor is non-vanishing only for the transition to the singlet state. The space factor could then be non-zero on symmetry grounds – the two particles of a singlet *can* be at the same location. But in this case the integrand is odd in x (three single-particle ground states and one first excited state, all at the same x) and therefore the integral vanishes. The lowest possible transition would be to the singlet second excited states (where there are zero or two odd factors in the integral).

3. For a certain perturbed Hamiltonian,

$$H = H_0 + H'$$

it is known that H' commutes with H_0 ,

$$[H_0, H'] = 0, \quad (2)$$

and that H_0 has non-degenerate energy eigenvalues.

a Show that, in the unperturbed basis, all matrix elements $\langle m|H'|n\rangle$ for $m \neq n$ vanish.

Since H_0 and H' commute, they can be simultaneously diagonalized. Since H_0 has distinct eigenvalues, there is only one basis in which it is diagonal, so that must also be the basis in which H' is diagonal. More formally, evaluate the matrix elements of the commutator (2) in the unperturbed basis:

$$\langle m|[H_0, H']|n\rangle = E_m \langle m|H'|n\rangle - \langle m|H'|n\rangle E_n = (E_m - E_n) \langle m|H'|n\rangle = 0.$$

Since $E_m \neq E_n$ if $m \neq n$, then $\langle m|H'|n\rangle = 0$.

b Show that the first order correction to the energy levels is exact.

Because of the above, the eigenfunctions $|n_0\rangle$ of H_0 are also eigenfunctions $|n\rangle$ of H :

$$E_n = \langle n|H|n\rangle = \langle n_0|H_0|n_0\rangle + \langle n_0|H'|n_0\rangle = E_{0n} + \langle n_0|H'|n_0\rangle.$$

Alternatively: the second (and higher) energy corrections involve only off-diagonal matrix elements of H' , so these corrections all vanish.

c Suppose H' is time-dependent: it is turned on for some time T and then turned off again. Can it induce any transitions between unperturbed levels? If not, why not? If yes, give an example!

No. The expression for the transition rate involves only off-diagonal elements of H' . (If H_0 had degenerate energies, and H' would split them, there would be transitions between those.)

4. For an attractive δ -function potential there is only one bound state. Consider the 1D Hamiltonian with a double δ -function potential,

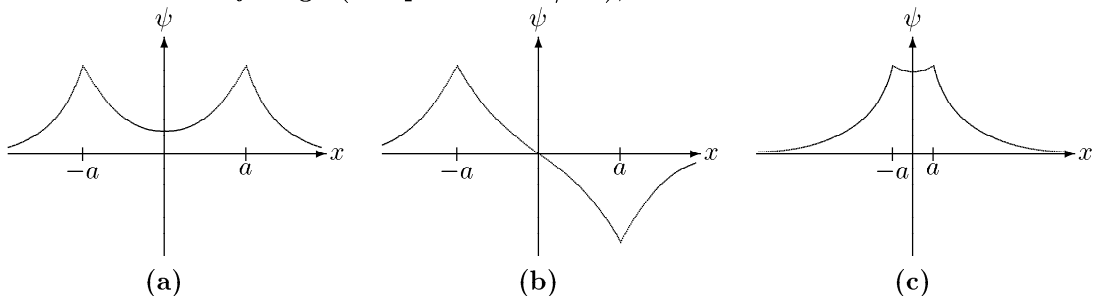
$$H = \frac{p^2}{2m} - \lambda[\delta(x+a) + \delta(x-a)] \quad (\lambda > 0)$$

a What does the symmetry $H(x) = H(-x)$ of this Hamiltonian imply about its eigenfunctions?

In general it means that if $\psi(x)$ is an eigenfunction, so is $\psi(-x)$; hence eigenfunctions can be chosen to be symmetric or antisymmetric under the reflection $x \rightarrow -x$. In this case of one-dimensional bound states, there is no degeneracy, hence eigenfunctions are either symmetric or antisymmetric.

b How many bound states are there in this potential? Sketch it/them!

If λa is sufficiently large (compared to $\hbar^2/2m$), there are two bound states:



(a) ground state (b) excited state (c) only ground state for small a .

For small λa the situation is the same as for $a = 0$, that is the single δ -function potential: only one bound state.

c For simplicity take $\lambda = 1, \hbar = 1, m = \frac{1}{2}$. Then for $a = 0$ (single well, $V(x) = -2\delta(x)$) the solution to the time-independent Schrödinger equation

$$-\psi'' + V(x)\psi = E\psi \quad \text{is} \quad E = -1, \quad \psi = e^{-|x|}. \quad (3)$$

This same ψ can be a trial function for the variational principle, which may not be too bad for small a . Use it to find an upper bound for the double-delta-function potential. How do you

deal with the discontinuous slope at $x = 0$?

The given ψ is normalized, so we get the variational principle E from (3) by multiplying by ψ^* and integrating,

$$E = \int_{-\infty}^{\infty} (-\psi^* \psi'' + V \psi^* \psi) dx. \quad (4)$$

Because ψ and V are symmetric one is tempted to re-write this integral as $2 \int_{0+}^{\infty} (-\psi^* \psi'' + V \psi^* \psi) dx$, but this would neglect the δ -function in ψ'' at $x = 0$. The easiest way to account for that is first to integrate (3) by parts and then use the symmetry:

$$\begin{aligned} E &= \int_{-\infty}^{\infty} (\psi^{*'} \psi' + V \psi^* \psi) dx = 2 \int_0^{\infty} (\psi^{*'} \psi' + V \psi^* \psi) dx \\ &= 2 \int_0^{\infty} [e^{-2x} - \lambda \delta(x-a) e^{-2x}] dx = 2(\frac{1}{2} - \lambda e^{-2a}). \end{aligned}$$

For $\lambda = 1$ and $a = 0$ this becomes $E = -1$ as in (3). Note that for large a the result is $E = +1$, which is of course a very bad approximation since bound states have $E < 0$ (the correct result for $a \rightarrow \infty$ is the same as for a single δ -function well, $E = -\frac{1}{4}$).

Alternatively you can evaluate the δ -function in ψ'' , obtaining $\psi''(x) = \psi(x) + 2\delta(x)$, and use (4).

Useful formulas ($m = \omega = \hbar = 1$):

$$\text{SHO ground state : } \left(\frac{1}{\pi}\right)^{1/4} e^{-\frac{1}{2}x^2} \quad \text{SHO 1st excited state : } \left(\frac{4}{\pi}\right)^{1/4} x e^{-\frac{1}{2}x^2}$$

$$\int_{-\infty}^{\infty} e^{-x^2/a^2} dx = \sqrt{\pi}a \quad \int_{-\infty}^{\infty} x^2 e^{-x^2/a^2} dx = \sqrt{\pi}a^3/2$$