Quantum Mechanics 2
Spring 2019

Homework 2 Problems

1. Two identical spin-zero bosons are placed in an infinite square well of width a. They interact weakly with one another, via the potential

$$V(x_1, x_2) = -aV_0\delta(x_1 - x_2)$$

(a) First, ignoring the interaction between the particles, find the ground state and the first excited state- both the wave functions and the associated energies.

Solution: Let us first remind ourselves of the solution to the infinite square well for a single particle. The potential of the well is:

$$V(x) = \{ \begin{array}{cc} 0 & 0 < x < a \\ \infty & x \notin (0, a) \end{array}$$

The eigenfunctions and eigenvalues are:

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$$
$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

For two particles in a well not interacting, the wave functions are just linear combinations of products of 1D wavefunctions and energies are just sums of the energies of the two particles. For bosons, the two particle wavefunctions must furthermore be symmetric under interchange of the particles. The lowest two energies are simply $E_{11} = 2E_1$ and $E_{12} = E_1 + E_2$. The corresponding wavefunctions are simply:

$$\psi_{11}(x_1, x_2) = \frac{2}{a}\sin(\frac{\pi x_1}{a})\sin(\frac{\pi x_2}{a})$$
$$\psi_{12}(x_1, x_2) = \frac{\sqrt{2}}{a}\Big(\sin(\frac{\pi x_1}{a})\sin(\frac{2\pi x_2}{a}) + \sin(\frac{2\pi x_1}{a})\sin(\frac{\pi x_2}{a}))\Big)$$

(b) Use first-order perturbation theory to estimate the effect of the particle-particle interaction on the energies of the ground state and the first excited state.

Solution: First the ground state. The first order correction to the energy is:

$$\begin{aligned} E_{11}^{(1)} &= \int_0^a dx_1 \int_0^a dx_2 \psi_{11}(x_1, x_2) * (-aV_0 \delta(x_1 - x_2))\psi_{11}(x_1, x_2) \\ &= \frac{-4V_0}{a} \int_0^a dx_1 \int_0^a dx_2 \sin(\frac{\pi x_1}{a})\sin(\frac{\pi x_2}{a})\delta(x_1 - x_2)\sin(\frac{\pi x_1}{a})\sin(\frac{\pi x_2}{a}) \\ &= \frac{-4V_0}{a}\frac{a}{\pi} \int_0^\pi du \sin(u)^4 \\ &= -\frac{3}{2}V_0 \end{aligned}$$

A similar calculation for the first excited state results in a first order correction to the energy $E_{12}^{(0)} = -2V_0$. In both cases, the interaction lowers the energy of the particles.

2. Consider a particle of mass m in an infinite square well of width $2a$ centered at $x = 0$. Now add a small perturbation to the potential

$$V'(x) = \{ \begin{array}{cc} -\lambda v & -a < x \leq 0 \\ \lambda v & 0 < x < a \end{array}$$

where λ is a small number. Treating $V'(x)$ as a small perturbation, use perturbation theory to find (a) the eigenvalues to second order in λ and (b) the eigenstates to first order in λ.

(a) Eigenvalues

Solution: First let us write down the unperturbed eigenfunctions and eigenvalues for the infinite square well situated in this particular problem:

$$\psi_n(x) = \sqrt{\frac{1}{a}}\sin(\frac{n\pi(x+a)}{2a})$$
$$E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}$$

Using these wave functions, one can see that the first order corrections to the energies must be zero since the potential is odd. To calculate the second order corrections, we must compute the following:

$$\langle m|V'|n\rangle = \lambda v\Big[\int_0^a dx\psi_n(x)\psi_m(x) - \int_{-a}^0 dx\psi_n(x)\psi_m(x)\Big]$$

ψ_n is an even funcion for n odd and an odd function for n even. Therefore, $\langle m|V'|n\rangle \neq 0$ only if $n+m$ is odd. Let us then consider this case and proceed with the calculation.

$$\begin{aligned}
\langle m|V'|n\rangle &= 2\lambda v \int_0^a dx\psi_n(x)\psi_m(x) \\
&= \frac{2\lambda v}{a}\frac{2a}{\pi}\int_{\frac{\pi}{2}}^{\pi} du \ \sin(nu)\ \sin(mu) \\
&= \frac{2\lambda v}{\pi}\int_{\frac{\pi}{2}}^{\pi} du \ \cos((m-n)u) - \ \cos((m+n)u) \\
&= \frac{2\lambda v}{\pi}\Big(\frac{1}{m+n}\ \sin((m+n)\frac{\pi}{2}) - \frac{1}{m-n}\ \sin((m-n)\frac{\pi}{2})\Big)
\end{aligned}$$

Let us denote $f_k \equiv \ \sin(\frac{k\pi}{2})$ for integer k. Then we can write:

$$\langle m|V'|n\rangle = \frac{2\lambda v}{\pi}\Big(\frac{f_{m+n}}{m+n} - \frac{f_{m-n}}{m-n}\Big)$$

Next, what is relevant to the second order energy corrections is this quantity squared. Again, since we are only considering when $m \pm n$ is odd, if follows for this case that $f^2_{m\pm n} = 1$, and $f_{m+n}f_{m-n} = 1$ if n is even and it equals -1 if n is odd. Therefore, we have:

$$|\langle m|V'|n\rangle|^2 = \frac{4\lambda^2 v^2}{\pi^2}\Big(\frac{1}{(m+n)} \pm \frac{1}{m-n}\Big)^2$$
$$= \frac{4\lambda^2 v^2}{\pi^2} \left\{ \begin{array}{ll} \frac{4n^2}{(n^2-m^2)^2} & n \text{ is even} \\ \frac{4m^2}{(n^2-m^2)^2} & n \text{ is odd} \end{array} \right.$$

The second order energy corrections are therefore:

$$E_n^{(2)} = \frac{32ma^2\lambda^2 v^2}{\pi^4 \hbar^2} \left\{ \begin{array}{ll} \sum_{m \text{ odd}} \frac{4n^2}{(n^2-m^2)^3} & n \text{ is even} \\ \sum_{m \text{ even}} \frac{4m^2}{(n^2-m^2)^3} & n \text{ is odd} \end{array} \right.$$

We will leave the answer here though these sums can be explicitly computed.

(b) Eigenstates

Solution: All the brunt work is done since we computed $\langle m|V'|n\rangle$ explicitly so the answer can be written as a formal Fourier sum (Fourier because the eigenstates are trigonometric functions) with coefficients explicitly known.

3. Consider a simple harmonic oscillator potential $H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$. We ass a small perturbation in the system $H' = \lambda x^3$. Use perturbation theory to find (a) the eigenvalues to second order in λ and (b) the eigenstates to first order in λ.

   (a) Eigenvalues

   Solution: Let us remind ourselves of some useful facts and notation about the simple harmonic oscillator. The eigenstates are labeled as $|n\rangle$ for $n = 0, 1, 2, \ldots$ with eigenvalues $E_n = \hbar\omega(n + \frac{1}{2})$ normalized such that $\langle m|n\rangle = \delta_{mn}$. We can define 'raising' and 'lowering' operators $a^\dagger$ and a such that $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$ and these act upon the eigenstates with the following effect: $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, a|n\rangle = \sqrt{n}|n-1\rangle$.

Using these facts, we immediately see that the first order corrections to the eigenvalues must be zero since $\langle n|(a+a^\dagger)^k|n\rangle = 0$ for any odd integer k. Next, we move on to second order perturbation theory for which we first need to compute $\langle m|(a+a^\dagger)^3|n\rangle$:

$$\begin{aligned}\langle m|(a+a^\dagger)^3|n\rangle &= \langle m|(a^3 + a^2a^\dagger + aa^\dagger a + a^\dagger a^2 + a(a^\dagger)^2 + a^\dagger a a^\dagger + (a^\dagger)^2 a + (a^\dagger)^3|n\rangle \\ &= \sqrt{n(n-1)(n-2)}\langle m|n-3\rangle + 3n\sqrt{n}\langle m|n-1\rangle \\ &+ 3(n+1)\sqrt{n+1}\langle m|n+1\rangle + \sqrt{(n+3)(n+2)(n+1)}\langle m|n+3\rangle\end{aligned}$$

Therefore,

$$\begin{aligned}|\langle m|\lambda\Big(\frac{\hbar}{2m\omega}\Big)^{\frac{3}{2}}(a+a^\dagger)^3|n\rangle|^2 = \lambda^2\Big(\frac{\hbar}{2m\omega}\Big)^3\Big(&n(n-1)(n-2)\delta_{m(n-3)} + 9n^3\delta_{m(n-1)} \\ &+ 9(n+1)^3\delta_{m(n+1)} + (n+3)(n+2)(n+1)\delta_{m(n+3)}\Big)\end{aligned}$$

We ignore cross terms in the above computation as they will not contribute the the second order energy corrections when we sum over m. The correction is thus:

$$
\begin{aligned}
E_n^{(2)} &= \sum_m \frac{|\langle m|\lambda x^3|n\rangle|^2}{E_n - E_m} \\
&= \frac{\lambda^2\hbar^2}{8m^3\omega^4} \sum_m \Big(\frac{n(n-1)(n-2)}{n-m}\delta_{m(n-3)} + \frac{9n^3}{n-m}\delta_{m(n-1)} \\
&+ \frac{9(n+1)^3}{n-m}\delta_{m(n+1)} + \frac{(n+3)(n+2)(n+1)}{n-m}\delta_{m(n+3)}\Big) \\
&= \frac{\lambda^2\hbar^2}{8m^3\omega^4}\Big(\frac{n(n-1)(n-2)}{3} + 9n^3 \\
&- 9(n+1)^3 - \frac{(n+3)(n+2)(n+1)}{3}\Big) \\
&= \frac{\lambda^2\hbar^2}{8m^3\omega^4}\Big(\frac{n(n-1)(n-2)}{3} + 9n^3 \\
&- 9(n+1)^3 - \frac{(n+3)(n+2)(n+1)}{3}\Big) \\
&= -\frac{\lambda^2\hbar^2}{24m^3\omega^4}(86n^2 + 95n + 31)
\end{aligned}
$$

(b) Eigenstates to first order in λ.

Solution: This is a straightforward application of first order perturbation theory. With the heavy lifting already done, we will write down the answer:

$$
\begin{aligned}
|n\rangle^{(1)} &= \frac{\lambda}{\hbar\omega}\Big(\frac{\hbar}{2m\omega}\Big)^{\frac{3}{2}}\Big(\frac{\sqrt{n(n-1)(n-2)}}{3}|n-3\rangle + 3n\sqrt{n}|n-1\rangle \\
&- 3(n+1)\sqrt{n+1}|n+1\rangle - \frac{\sqrt{(n+3)(n+2)(n+1)}}{3}|n+3\rangle\Big)
\end{aligned}
$$

4. Consider the following matrix:

$$
\hat{H} = \begin{pmatrix} a_1 & 0 & b \\ 0 & a_2 & c \\ b & c & a_3 \end{pmatrix}.
$$

Treat the diagonals as the 'unperturbed' system and

(a) Comute the eigenvalues and eigenstates to second order and first order, respectively.

Solution: The unperturbed eigenvalues are a_1, a_2, a_3 corresponding to eigenvectors which are the unit column vectors which we will call ψ_1, ψ_2, ψ_3. To first order, all correction are zero. This is clear since the diagonal elements of the matrix $\hat{H}$ have no corrections. To second order, we have:

$$a_1^{(2)} = \sum_{m \neq 1} \frac{H_{1m} H_{m1}}{a_1 - a_m} = \frac{b^2}{a_1 - a_3}$$
$$a_2^{(2)} = \sum_{m \neq 2} \frac{H_{2m} H_{m2}}{a_2 - a_m} = \frac{c^2}{a_2 - a_3}$$
$$a_3^{(2)} = \sum_{m \neq 3} \frac{H_{3m} H_{m3}}{a_1 - a_m} = \frac{b^2}{a_3 - a_1} + \frac{c^2}{a_3 - a_2}$$

The corrections to the wave functions are:

$$\psi_1^{(2)} = \sum_{m \neq 1} \frac{H_{m1}}{a_1 - a_m} \psi_m = \frac{b}{a_1 - a_3} \psi_3$$
$$\psi_2^{(2)} = \sum_{m \neq 2} \frac{H_{2m} H_{m2}}{a_2 - a_m} = \frac{c}{a_2 - a_3} \psi_3$$
$$\psi_3^{(2)} = \sum_{m \neq 3} \frac{H_{3m} H_{m3}}{a_1 - a_m} = \frac{b}{a_3 - a_1} \psi_1 + \frac{c}{a_3 - a_2} \psi_2$$

(b) Consider the special case of $c = 0$. Find the exact eigenvalues and eigenstates. Compare these with the results from using perturbation theory.

Solution: In this case, the eigenvalue problem can be solved exactly. The results are:

$$\lambda = \frac{a_1 + a_3 \pm (a_1 - a_3)\sqrt{1 + \frac{4b^2}{(a_1 - a_3)^2}}}{2} \tag{1}$$

To second order in b, these eigrenvalues agree with those for a_1 and a_3. The eigenvalue of a_2 is exact in the $c \to 0$ limit. Similarly, the eigenvectors are: $\bar{\psi}_1 = \psi_1 + \frac{b}{\lambda_1 - a_3}\psi_3$ and $\bar{\psi}_3 = \psi_3 + \frac{b}{\lambda_3 - a_1}\psi_1$. When $\lambda_{1,3} = a_{1,3}$ to lowest order in b, we see that the exact eigenvectors reduce to the first order perturbed eigenvectors.

5. Suppose we perturb the infinite square well by putting a delta function ("bump") at the point $(\frac{a}{4}, \frac{a}{2}, \frac{3a}{4}) : H' = a^3 V_0 \delta(x - \frac{a}{4})\delta(y - \frac{a}{2})\delta(z - \frac{3a}{4})$. Find the first order corrections to the energy of the ground state and the (triply) degenerate first excited states.

   Solution: This problem is in essence no different than 1 but instead of having two particles in a 1D box, we have one particle in a 3d box. All the same techniques/arguments that apply in one case tend to apply in the other. The results we get are that to first order, only one of the three degenerate excited states are lifted in energy by $8V_0$ while the ground state lifts by $2V_0$.

6. Bonus Question: If first order perturbation theory is viewed as a linear transformation on Hilbert space, what property does that transformation have.

   Solution: It is anti-Hermitian.