Exam Solutions, FY2045 03.12.2018

Problem 1: Time-Independent Perturbation Theory

Here, most answers can be figured out from a symmetry argument. Each term in the energy correction is a spatial integral from $-L/2$ to $L/2$ over the product of three functions. If this product is an odd function the term will be zero. The perturbation is antisymmetric so all first order corrections have to be zero. For the groundstate, since it has the cos form (even), only terms that involve the sine form (odd) will contribute to the second order correction. The infinite square well has an infinite number of eigenstates, thus the second order correction has an infinite number of terms. In perturbation theory, convergence is not assured in the power-series expansion.

- [ ] In time-independent perturbation theory, the power series expansion of the energy $E_n = E_n(\lambda) = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$ always converges
- [x] Only terms that involve states of the form $|m\rangle = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ will contribute to $E_0^{(2)}$ ✔
- [x] All first order energy corrections will be zero ✔
- [ ] All second order energy corrections will be zero
- [x] For $E_0^{(2)}$, the summation above will have an infinite number of terms ✔

Problem 2: Spin-Spin Coupling, Fermions

The names triplett and singlett come from the formula for multiplicity (2S+1), hence triplett refers to S=1 and singlett to S=0. The wavefunction of two identical fermions has to be antisymmetric with respect to exchanging their coordinates. The spin part of the triplett is symmetric and the singlett antisymmetric. Hence, the spatial wavefunction of the triplett has to be antisymmetric and the one of the singlett symmetric so that the total wavefunction is antisymmetric with respect to exchanging coordinates.

- [x] Measuring the total spin **S** of the system the possible results are **S** = 0 and **S** = 1 ✔
- [x] If the total spin of the system is **S**=1 then the spatial wavefunction has to be antisymmet[ric] with respect to exchanging the coordinates of the two particles ✔
- [ ] If the total spin of the system is **S**=3, then the spatial wavefunction has to be antisymmetric with respect to exchanging the coordinates of the two particles
- [ ] If the total spin of the system is **S**=1, then the spatial wavefunction has to be symmetric with respect to exchanging the coordinates of the two particles
- [ ] Measuring the total spin **S** of the system the possible results are **S** = 1 and **S** = 3
- [x] If the total spin of the system is **S**=0 then the spatial wavefunction has to be symmetric [wit]h respect to exchanging the coordinates of the two particles ✔

Problem 3: Commutator Relations - Ladder Operator

Assume $|\psi\rangle$ to be an eigenstate of $\widehat{O}$. Then writing out the commutator relation and applying to $|\psi\rangle$ we have:

$$\left[\widehat{O}, \widehat{A}\right] |\psi\rangle = c\widehat{A}\psi\rangle$$

$$\widehat{O}\widehat{A}|\psi\rangle - \widehat{A}\widehat{O}|\psi\rangle = c\widehat{A}\psi\rangle$$

$$\widehat{O}\widehat{A}|\psi\rangle - \widehat{A}\lambda_O|\psi\rangle = c\widehat{A}\psi\rangle$$

$$\widehat{O}\left(\widehat{A}|\psi\rangle\right) = (\lambda_O + c)\left(\widehat{A}\psi\rangle\right)$$

Thus, $\widehat{A}\psi\rangle$ is also an eigenfunction of $\widehat{O}$. In particular $\widehat{A}$ is a ladder operator incrementing the eigenvalues by c. (If there is a minimum or maximum eigenvalue then the generated ladder is unique and $\widehat{O}$ has a discrete spectrum of eigenvalues.) However, the number of eigenstates can be infinite. Eigenstates of $\widehat{O}$ are not eigenstates of $\widehat{A}$. There is no requirement that $\widehat{A}$ is hermitian and by definition they do not commute.

- [ ] $\hat{O}$ must have a finite number of eigenstates
- [ ] Eigenstates of $\hat{O}$ are also eigenstates of $\hat{A}$
- [ ] $\hat{O}$ and $\hat{A}$ are hermitian
- [x] If $|\psi\rangle$ is an eigenstate of $\hat{O}$, then $\hat{A}|\psi\rangle$ is also an eigenstate of $\hat{O}$ ✔
- [x] $\hat{O}$ and $\hat{A}$ do not commute ✔

Problem 4: Commutator Relations

Eigenstates of a hermitian operator with different eigenvalue are orthonormal so $\langle a|\widehat{H}|c\rangle$, $\langle a|\widehat{H}|d\rangle$, $\langle b|\widehat{H}|c\rangle$, and $\langle b|\widehat{H}|d\rangle$ must be 0. From the following argument, also $\langle a|\widehat{H}|b\rangle$ has to be 0. Let $|r\rangle$ and $|s\rangle$ be eigenstates of $\widehat{F}$:

$$\widehat{F}|r\rangle = \lambda_r|r\rangle, \quad \widehat{F}|s\rangle = \lambda_s|r\rangle, \quad \lambda_r \neq \lambda_s$$
$$\left[\widehat{F}, \widehat{H}\right] = 0 = \langle r|\left[\widehat{F}, \widehat{H}\right]|s\rangle = \langle r|\widehat{F}\widehat{H}|s\rangle - \langle r|\widehat{H}\widehat{F}|s\rangle$$
$$= \langle \widehat{F}r|\widehat{H}s\rangle - \langle r|\widehat{H}|\lambda_s s\rangle = (\lambda_r - \lambda_s)\langle r|\widehat{H}|s\rangle$$

Since $\lambda_r \neq \lambda_s$, $\langle s|\widehat{H}|r\rangle = 0$.

- [x] $\langle a|\hat{H}|b\rangle = 0$ ✔
- [ ] $\langle c|\hat{H}|d\rangle = 0$
- [x] $\langle a|\hat{H}|c\rangle = 0$ ✔
- [x] $\langle b|\hat{H}|d\rangle = 0$ ✔
- [x] $\langle b|\hat{H}|c\rangle = 0$ ✔
- [x] $\langle a|\hat{H}|d\rangle = 0$ ✔

Problem 5: Time-Dependent Perturbation Theory

a) Inserting the expansion

$$|\Psi(t)\rangle = \sum_n a_n(t)|\Psi_n^0(t)\rangle$$

into the time-dependent Schrödinger equation and using the product rule gives:

$$\sum_n \left(i\hbar\frac{da_n}{dt}|\Psi_n^0(t)\rangle + a_n \underbrace{i\hbar\frac{d}{dt}|\Psi_n^0(t)\rangle}_{E_n|\Psi_n^0(t)\rangle} \right) = \sum_n a_n \left(\underbrace{\widehat{H}_0|\Psi_n^0(t)\rangle}_{E_n|\Psi_n^0(t)\rangle} + \widehat{V}(t)|\Psi_n^0(t)\rangle \right)$$

The last term on the left hand side and the first term on the right hand side are equal and drop. Multiplying by the bra $\langle\Psi_k^0(t)|\cdot$ (and using orthogonality $\langle\Psi_k^0(t)|\Psi_n^0(t)\rangle = \delta_{kn}$) yields:

$$i\hbar\frac{da_k(t)}{dt} = \sum_n \left\langle \Psi_k^0(t)|\widehat{V}(t)|\Psi_n^0(t)\right\rangle a_n(t)$$

b) The essential approximations are that the system is initially ($t = 0$) in the eigenstates i of the unperturbed system so $a_n = \delta_{ni}$ and that the perturbation is weak (and/or we consider a sufficiently short time).

$$i\hbar\frac{da_k(t)}{dt} \approx \sum_n e^{i\omega_{kn}t}V_{kn}(t)\delta_{ni} = e^{i\omega_{ki}t}V_{ki}(t)$$

Integration for state number f leads to:

$$a_f(t) - a_f(0) = \frac{1}{i\hbar}\int_0^t e^{i\omega_i t'}V_{fi}(t')\,dt'$$

Since we are assuming $a_n = \delta_{ni}$ for $t = 0$ we have:

$$a_f(t) \approx \delta_{fi} + \frac{1}{i\hbar}\int_0^t e^{i\omega_{fi}t'}V_{fi}(t')\,dt'$$

c) Inserting the harmonic perturbation

$$\hat{V}(r,t) = \hat{\mathcal{V}}(r)e^{-i\omega t} + \hat{\mathcal{V}}^\dagger(r)e^{i\omega t}$$

into

$$a_f(t) \approx \delta_{fi} + \frac{1}{i\hbar}\int_0^t e^{i\omega_{fi}t'}V_{fi}(t')\,dt'$$

($V_{fi} = \langle\psi_f|\hat{V}|\psi_i\rangle = \langle\psi_f|\hat{\mathcal{V}}_{fi}|\psi_i\rangle e^{-i\omega t} + \langle\psi_f|\hat{\mathcal{V}}_{fi}^\dagger|\psi_i\rangle e^{i\omega t} = \mathcal{V}_{fi}e^{-i\omega t} + \mathcal{V}_{fi}^* e^{i\omega t}$) gives:

$$a_{i\to f}(t) = \frac{1}{i\hbar}\mathcal{V}_{fi}\int_0^t e^{i(\omega_{fi}-\omega)t'}dt' + \frac{1}{i\hbar}\mathcal{V}_{if}^*\int_0^t e^{i(\omega_{fi}+\omega)t'}dt'$$

($\mathcal{V}_{fi}$ is time independent and $\delta_{fi} = 0$). Integration leads to:

$$a_{i\to f}(t) = \mathcal{V}_{fi}\frac{1 - e^{i(\omega_{fi}-\omega)t}}{\hbar(\omega_{fi}-\omega)} + \mathcal{V}_{if}^*\frac{1 - e^{i(\omega_{fi}+\omega)t}}{\hbar(\omega_{fi}+\omega)}$$

Since $\mathcal{V}_{fi}$ is assumed to be small the transition amplitude will only be significant if the denominator is small, i.e. $\omega \approx \pm\omega_{fi}$.

Problem 6: Rectangular Box

$$\psi_{n_x n_y n_z}(r) = A\sin\frac{n_x\pi x}{L_x}\sin\frac{n_y\pi y}{L_y}\sin\frac{n_z\pi z}{L_z}$$

a) The energy eigenvalues can be found from the Schrödinger equation. The potential inside the box is $V = 0$. Thus:

$$\hat{H}\psi_{n_x n_y n_z}(r) = E\psi_{n_x n_y n_z}(r) = -\frac{\hbar^2}{2m}\nabla^2\psi_{n_x n_y n_z}(r)$$
$$E_{n_x n_y n_z} = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

b) Assuming that L$_x$=L$_z$, and L$_y$ = 2L.

$$E_{n_x n_y n_z} = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + \frac{n_y^2}{4} + n_z^2\right)$$
$$E_{111} = \frac{9}{4}\frac{\hbar^2\pi^2}{2mL^2}$$
$$E_{121} = 3\frac{\hbar^2\pi^2}{2mL^2}$$
$$E_{131} = \frac{17}{4}\frac{h^2\pi^2}{2mL^2}$$
$$E_{211} = E_{112} = \frac{21}{4}\frac{\hbar^2\pi^2}{2mL^2}$$

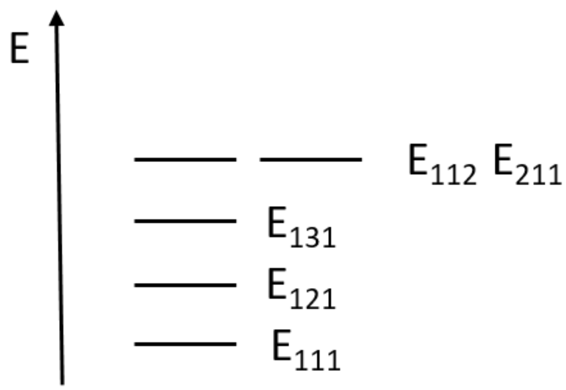

Figure 1: Qualtitative sketch.

c) Given seven identical spin 1/2 particles and assuming the system to be in the ground-state, levels with energies E_{111}, E_{121}, E_{131} will host two particles each. The remaining particle is in the degenerate levels with energies E_{112}, E_{211}. (Here one may choose to put the particle in either of the states) From:

$$dW = -dE = PdV$$
$$P = -\frac{dE}{dV},\ P_i = -\frac{dE}{AdL_i}$$

Assuming that the seventh particle is in state ψ_{112}, the total energy is:

$$E_{tot} = 2E_{111} + 2E_{121} + 2E_{131} + E_{112}$$
$$E_{tot} = \frac{\hbar^2\pi^2}{2m}\left(\frac{7}{L_x^2} + \frac{29}{L_y^2} + \frac{10}{L_z^2}\right)$$

The force and pressure in the x-direction are:

$$F_x = -\frac{dE}{dL_x} = 7\frac{\hbar^2\pi^2}{mL^3}$$
$$p_x = \frac{F_x}{A} = \frac{F_x}{2L\cdot L} = \frac{7}{2}\frac{\hbar^2\pi^2}{mL^5}$$

The pressures for the y- and z- directions are then:

$$p_y = \frac{29}{8}\frac{\hbar^2\pi^2}{mL^5},\ p_z = \frac{10}{2}\frac{\hbar^2\pi^2}{mL^5}$$

Problem 7: Spin - Matrix Representation

a) The matrix representation of the raising operator:

$$\hat{S}_+ = \hat{S}_x + i\hat{S}_y = \frac{1}{2}\hbar\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{1}{2}\hbar\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{1}{2}\hbar\begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}$$

Applying the raising operator once to find $\chi_{+,z}$ and once more to yield the zero vector:

$$\hat{S}_+\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\Rightarrow \quad \chi_{+,z} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\hat{S}_+\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

b) The eigenvalues are found from (see formula sheet):

$$\hat{S}_y = \frac{1}{2}\hbar\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$det\begin{pmatrix} -\lambda & -i\frac{\hbar}{2} \\ i\frac{\hbar}{2} & -\lambda \end{pmatrix} = \lambda^2 - \frac{1}{4}\hbar^2 i(-i)$$

$$\Rightarrow \quad \lambda = \pm\frac{1}{2}\hbar = S_{\pm,y}$$

And the eigenvectors:

$$\begin{pmatrix} -\frac{1}{2}\hbar & -\frac{1}{2}\hbar i \\ \frac{1}{2}\hbar i & -\frac{1}{2}\hbar \end{pmatrix}\chi_{+,y} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Rightarrow \chi_{+,y} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{2}\hbar & -\frac{1}{2}\hbar i \\ \frac{1}{2}\hbar i & \frac{1}{2}\hbar \end{pmatrix}\chi_{-,y} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\Rightarrow \quad \chi_{-,y} = \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix}$$

c) Solution Alternative 1 (As suggested in the problem description) The Hamiltonian can be written as:

$$\hat{H} = -\frac{\omega}{2}\hat{S}_i = -\frac{\hbar\omega}{4}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Inserting into the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = -\frac{\hbar\omega}{4}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$$

This gives us the two coupled equations:

$$\frac{\partial}{\partial t}a(t) = \frac{\omega}{4}b(t)$$
$$\frac{\partial}{\partial t}b(t) = -\frac{\omega}{4}a(t)$$

Differentiating the second equation with respect to time and setting into the first one (and vice versa) gives :

$$\frac{\partial^2}{\partial t^2}a(t) = -\frac{\omega^2}{4^2}a(t)$$
$$\frac{\partial^2}{\partial t^2}b(t) = -\frac{\omega^2}{4^2}b(t)$$

From the general solution of this differential equation (provided in the problem description):

$$a(t) = A_+ e^{i\frac{\omega}{4}t} + A_- e^{-i\frac{\omega}{4}t}$$
$$b(t) = \frac{4}{\omega}\frac{\partial a(t)}{\partial t} = iA_+ e^{i\frac{\omega}{4}t} - iA_- e^{-i\frac{\omega}{4}t}$$

So $\psi(t)$ is written as:

$$\psi(t) = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \begin{pmatrix} A_+ e^{i\frac{\omega}{4}t} + A_- e^{-i\frac{\omega}{4}t} \\ iA_+ e^{i\frac{\omega}{4}t} - iA_- e^{-i\frac{\omega}{4}t} \end{pmatrix}$$

Using the initial conditions (t=0) to determine the the coefficients A_+, A_-:

$$\psi(t=0) = \begin{pmatrix} A_+ + A_- \\ iA_+ - iA_- \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$\Rightarrow \quad A_+ = A_- = \frac{1}{2}$$
$$\psi(t) = \frac{1}{2}\begin{pmatrix} e^{i\frac{\omega}{4}t} + e^{-i\frac{\omega}{4}t} \\ ie^{i\frac{\omega}{4}t} - ie^{-i\frac{\omega}{4}t} \end{pmatrix} = \begin{pmatrix} \cos\left(\frac{\omega t}{4}\right) \\ -\sin\left(\frac{\omega t}{4}\right) \end{pmatrix}$$
$$\Rightarrow \quad \psi\left(\frac{\pi}{2\omega}\right) = \begin{pmatrix} \cos\left(\frac{\pi}{8}\right) \\ -\sin\left(\frac{\pi}{8}\right) \end{pmatrix}$$

Solution Alternative 2 (Expanding the state into eigenfunctions of the Hamiltonian) We can expand any state in terms of the stationary states (the two eigenstates represent a complete basis set), i.e.:

$$\psi(t) = a_+\chi_{+,y}e^{-i\frac{E_+}{\hbar}t} + a_-\chi_{-,y}e^{-i\frac{E_-}{\hbar}t}$$

The coefficients a_+,a_- are found as always by projecting $\psi(t)$ on the eigenstates:

$$a_+ = \langle\chi_{+,y}|\psi(t)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}$$
$$a_- = -\frac{1}{\sqrt{2}}$$

Hence $\psi(t)$ is written as:

$$\psi(t) = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}e^{\frac{i\omega t}{4}} - \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ i \end{pmatrix}e^{-\frac{i\omega t}{4}} =$$

$$= \frac{1}{2}\begin{pmatrix} e^{\frac{i\omega t}{4}} + e^{-\frac{i\omega t}{4}} \\ ie^{\frac{i\omega t}{4}} - ie^{-\frac{i\omega t}{4}} \end{pmatrix} =$$

$$\begin{pmatrix} \cos\left(\frac{\omega t}{4}\right) \\ -\sin\left(\frac{\omega t}{4}\right) \end{pmatrix}$$

$$\Rightarrow \quad \psi\left(\frac{\pi}{2\omega}\right) = \begin{pmatrix} \cos\left(\frac{\pi}{8}\right) \\ -\sin\left(\frac{\pi}{8}\right) \end{pmatrix}$$