IF/UFRJ
Graduate Quantum Mechanics I
2023/1 – Raimundo

Problem Set #14

14/11/2023 - due by 27/11/2023 at 12:00 noon

1. In the study of degenerate perturbation theory, we separated the perturbation $\mathcal{H}_1$ into $\mathcal{H}_D \equiv \sum_K P_K \mathcal{H}_1 P_K$ and $\mathcal{H}' \equiv \sum_{K \neq K'} P_K \mathcal{H}_1 P_{K'}$, where the K's denote groups of states forming (quasi-degenerate or degenerate) subspaces, and the P_K's are the projectors onto these subspaces. Let $\{|E^{(0)}_{K,n}\rangle\}$ and $\{|E_{K,n}\rangle\}$ be eigenstates of $\mathcal{H}_0$ and $\mathcal{H}_0 + \mathcal{H}_1$, respectively, with the n labelling the states within group K; the indices a_n and b_n, corresponding to the other quantum numbers, have been omitted, for simplicity. We assume that when $\mathcal{H}_1 \to 0$, the subspace spanned by $|E^{(0)}_{K,n}\rangle$ belonging to a value of K coincides with the subspace selected by the projector P_K. Let us suppose now that the perturbation is such that it does not connect states within a given subspace, i.e., that
$$\langle E^{(0)}_{K,n}|\mathcal{H}_1|E^{(0)}_{K,n'}\rangle = 0,\ \forall n, n' \in K,$$
for one or more K. Therefore, the perturbative treatment for states in this subspace must be adapted. To this end, we first derive an eigenvalue equation more suitable to this case.

   (a) (i) Show that the time-independent Schrödinger equation may be written as
   $$[\mathcal{H}_0 - E^{(0)}_{K,n}]|E_{K,n}\rangle = Q_K[\Delta_{Kn} - \mathcal{H}_1]|E_{K,n}\rangle, \tag{1}$$
   where $Q_K \equiv \mathbb{1} - P_K$ projects onto the subspace orthogonal to K. That is, $[\mathcal{H}_0 - E^{(0)}_{K,n}]|E_{K,n}\rangle$ belongs to a subspace orthogonal to K; this generalises the corresponding result for non-degenerate states.

   (ii) With this, here we may also act with $[\mathcal{H}_0 - E^{(0)}_{K,n}]^{-1}$ onto Eq. (1), to obtain a particular solution. Show that the solution of (1) may be written as
   $$|E_{K,n}\rangle = P_K|E_{K,n}\rangle + \frac{Q_K}{\mathcal{H}_0 - E^{(0)}_{K,n}}[\Delta_{Kn} - \mathcal{H}_1]|E_{K,n}\rangle, \tag{2}$$

where the solution to the homogeneous equation (i.e. without perturbation) of the non-degenerate case, $|E_n^{(0)}\rangle$, is now replaced by the projection of $|E_{K,n}\rangle$ onto the corresponding unperturbed *subspace*, $P_K|E_{K,n}\rangle$.

(iii) Show, finally, that the eigenvalue equation for $|E_{K,n}\rangle$ may be written as

$$P_K\mathcal{H}_1\left(1+\frac{Q_K}{E_{K,n}^{(0)}-\mathcal{H}_0}(\Delta_{K,n}-\mathcal{H}_1)\right)^{-1}P_K|E_{K,n}\rangle = \Delta_{K,n}P_K|E_{K,n}\rangle. \quad (3)$$

(b) Consider the case of a degenerate two-dimensional subspace (that is, $E_{K,i}^{(0)} = E_K^{(0)}$, with $i = 1,\ 2$), and suppose all matrix elements of $\mathcal{H}_1$ between unperturbed states belonging to this subspace are zero. Show that, to second order in $\mathcal{H}_1$, the energy shifts are given by the roots of the quadratic equation,

$$(\Delta - M_{11})(\Delta - M_{22}) = |M_{12}|^2\ , \quad (4)$$

where

$$M_{ij} = \sum_{K',n'}\frac{\langle E_{K,i}^{(0)}|\mathcal{H}_1|E_{K',n'}^{(0)}\rangle\langle E_{K',n'}^{(0)}|\mathcal{H}_1|E_{K,j}^{(0)}\rangle}{E_K^{(0)}-E_{K',n'}^{(0)}}. \quad (5)$$

2. To an isotropic two-dimensional harmonic oscillator, whose Hamiltonian is given by

$$\mathcal{H}_0 = \frac{1}{2m}\left(P_x^2+P_y^2\right)+\frac{1}{2}m\omega^2\left(X^2+Y^2\right),$$

we apply a perturbation

$$V = \delta m\omega^2 XY,$$

where $\delta \ll 1$. Obtain the first non-vanishing corrections to the three smallest eigenvalues of $\mathcal{H}_0$.

3. A hydrogen atom is in the presence of a uniform external electric field, $\boldsymbol{\mathcal{E}} = \mathcal{E}\hat{\mathbf{z}}$, whose magnitude is much smaller than the Coulomb field of the proton. Consider the electron's reduced mass the same as its rest mass, and denote by $|n\ell m\rangle$ the electron states in the absence of $\boldsymbol{\mathcal{E}}$. *[N.B.: In what follows, the arguments used to set the matrix elements to zero must be carefully justified, while the non-vanishing matrix elements may be considered as known.]*

(a) Determine the selection rules for the following matrix elements:

(i) $\langle n10|x|100\rangle$

(ii) $\langle n10|y|100\rangle$

(iii) $\langle n10|z|100\rangle$

(iv) $\langle n\,\ell\,m_\ell|z|n'\,\ell'\,m'_\ell\rangle$

(b) Obtain, to first order in $\mathcal{E} \equiv |\boldsymbol{\mathcal{E}}|$, the corrections to the energy of the first excited state of the atom.

(c) Obtain an expression for the expectation value of the electric dipole in the ground state, to lowest order in $\mathcal{E}$. Comment.

4. Consider four spins fixed in position on the vertices of a square, with interactions between spins on nearest neighbours and with a transverse magnetic field. The Hamiltonian is given by

$$\mathcal{H} = -\Gamma\left(\sigma_1^x + \sigma_2^x + \sigma_3^x + \sigma_4^x\right) - J\left(\sigma_1^z\sigma_2^z + \sigma_2^z\sigma_3^z + \sigma_3^z\sigma_4^z + \sigma_4^z\sigma_1^z\right),$$

where J and Γ are two positive constants with dimensions of energy, and the σ's are the Pauli matrices.

(a) Discuss physically the ground state in the limiting cases $\Gamma \ll J$ and $\Gamma \gg J$.

(b) Show that the system in invariant when each spin undergoes a rotation by π around the x-axis, carried out by

$$\Pi \equiv \sigma_1^x\sigma_2^x\sigma_3^x\sigma_4^x.$$

(c) Obtain, to lowest order in perturbation theory, the corrections (energy and eigenstate) to the ground state of this system, considering both $\Gamma \ll J$ and $\Gamma \gg J$. [*Hints: (1) Use different unperturbed basis sets in these two regimes; (2) Exploit the* Π*-symmetry in both cases when constructing the unperturbed basis sets; (3) You only need to consider the* $k = 0$ *sector of the translation eigenvectors; explain why.*]