Quantum Mechanics formula

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1 Time-independent perturbation theory

1.1 non-degenerate

$\hat{H} = \hat{H}_0 + \hat{V}$, where $\hat{V}$ is the perturbation.
At $\hat{V} = 0$, the problem is exactly solved below.
$\hat{H}_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$
$\hat{H} = \hat{H}_0 + \lambda\hat{V}$
$(\hat{H}_0 + \lambda\hat{V})|n(\lambda)\rangle = E_n(\lambda)|n(\lambda)\rangle$
wave function:
$|n^{(1)}\rangle = \sum\limits_{m\neq n} \frac{\langle m^{(0)}|\hat{V}|n^0\rangle}{E_n^{(0)}-E_m^{(0)}}|m^{(0)}\rangle$
$|n^{(2)}\rangle = \sum\limits_{m\neq n}\sum\limits_{m'\neq n} \frac{V_{mm'}V_{m'n}}{(E_n^{(0)}-E_m^{(0)})(E_n^{(0)}-E_{m'}^{(0)})}|m^{(0)}\rangle$
$where\, V_{mn} \equiv \langle m^{(0)}|V|n^{(0)}\rangle \neq \langle m|V|n\rangle$
$-\sum\limits_{m\neq n} \frac{V_{mn}V_{nn}}{(E_n^{(0)}-E_m^{(0)})^2}|m^{(0)}\rangle$
$|n(\lambda)\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots$
energy shift:
$\Delta_n \equiv E_n - E_n^{(0)} = \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots,$

$E_n^{(1)} = \langle n^{(0)}|\hat{V}|n^{(0)}\rangle = V_{nn}$
$E_n^{(2)} = \sum\limits_{m\neq n} \frac{|V_{nm}|^2}{E_n^{(0)}-E_m^{(0)}} = \sum\limits_{m\neq n} \frac{V_{nm}V_{mn}}{E_n^{(0)}-E_m^{(0)}}$

1.2 quadratic Stark effect

The polarizability α of an atom is defined in terms of the energy shift of the atomic state as follow: $\Delta = -\frac{1}{2}\alpha|E|^2$
$H_0 = \frac{\mathbf{p}^2}{2m} + V_0(r)$ and $V = -e|\mathbf{E}|z$ ($e < 0$ for the electron)
The ground state of hydrogen atom is non-degenerate.
$\Delta_k = -e|\mathbf{E}|z_{kk} + e^2|\mathbf{E}|^2 \sum_{j\neq k} \frac{|z_{kj}|^2}{E_k^{(0)}-E_j^{(0)}} + \cdots$ $z_{kk} = 0$, $\alpha = -2e^2 \sum\limits_{k\neq 0}^{\infty} \frac{|\langle k^{(0)}|z|1,0,0\rangle|^2}{\left[E_0^{(0)}-E_k^{(0)}\right]}$

1.3 degenerate spectrum

$H_0|m^{(0)}\rangle = E_D^{(0)}|m^{(0)}\rangle$
$V_{mm'} = \langle m^{(0)}|\hat{V}|m'^{(0)}\rangle$
1. Identify degenerate unperturbed eigenkets and construct the perturbation matrix $[V_{mn}]$, a g $\times$ g matrix if the degeneracy is g-fold.
2. Diagonalize the perturbation matrix by solving, as usual, the appropriate secular equation.

$$\det\left[V - \left(E - E_D^{(0)}\right)\right] = 0$$

3. Identify the roots of the secular equation with the **first-order energy shifts**; the base kets that diagonalize the V matrix are the correct **zeroth-order kets** that the perturbed kets approach in the limit $\lambda \to 0$.
4. For higher orders, use the formulas of the corresponding non-degenerate perturbation theory except in the summations, where we exclude all contri- butions from the unperturbed kets in the degenerate subspace D.
Second order correction:

2 Time-dependent perturbation theory

Interaction picture:
$|\alpha, t_0; t\rangle_I = e^{iH_0t/\hbar}|\alpha, t_0; t\rangle_S$, $A_I \equiv e^{iH_0t/\hbar}A_S e^{-iH_0t/\hbar}$.
$i\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle_I = V_I|\alpha, t_0; t\rangle_I$, $|\alpha, t_0; t\rangle_I = \sum_n c_n(t)|n\rangle$.
$\omega_{nm} \equiv \frac{(E_n - E_m)}{\hbar} = -\omega_{mn}$
$c_n^{(0)}(t) = \delta_{ni}$ (independent of t)

$$c_n^{(1)}(t) = \frac{-i}{\hbar}\int_{t_0}^t \langle n|V_I(t')|i\rangle dt'$$
$$= \frac{-i}{\hbar}\int_{t_0}^t e^{i\omega_{ni}t'}V_{ni}(t')\,dt'$$
$$c_n^{(2)}(t) = \left(\frac{-i}{\hbar}\right)^2 \sum_m \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' e^{i\omega_{nm}t'}V_{nm}(t')\,e^{i\omega_{mi}t''}V_{mi}(t'')$$
$$P(i\to n) = \left|c_n^{(1)}(t) + c_n^{(2)}(t) + \cdots\right|^2$$

3 Spherical harmonics and angular momentum

3.1 normalization

The normalization of spherical harmonics varies and here we adopt the convention in QM: $\int Y_{l'}^{m'^*}(\theta,\phi)Y_l^m(\theta,\phi)d\Omega = \delta_{ll'}\delta_{mm'}$
$\int f d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} f sin(\theta)d\theta$
$\int f dx^3 = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \int_0^{\infty} f sin(\theta) r^2 dr$

3.2 angular momentum operator

$J_+ = J_x + iJ_y, J_- = J_x - iJ_y \iff J_x = \frac{J_+ + J_-}{2}, J_y = \frac{J_+ - J_-}{2i}$
$Eigenstate\, of\, L\, and\, L_z: \langle\hat{\mathbf{n}}|l,m\rangle = Y_l^m(\theta,\phi) = Y_l^m(\hat{\mathbf{n}})$
$J_\pm|j,m\rangle = \sqrt{(j\mp m)(j\pm m+1)}\hbar|j,m\pm 1\rangle$
$J^2|j,m\pm 1\rangle = j(j+1)\hbar^2|j,m\pm 1\rangle, J_z|j,m\pm 1\rangle = m\hbar|j,m\pm 1\rangle$

3.3 parity and conjugate

$\hat{\pi}\{\theta,\phi\} \to \{\pi-\theta, \pi+\phi\}$,
$\hat{\pi}Y_l^m(\theta,\phi) \to Y_l^m(\pi-\theta,\pi+\phi) = (-1)^l Y_l^m(\theta,\phi)$
$Y_l^{m*}(\theta,\phi) = (-1)^m Y_l^{-m}(\theta,\phi)$

3.4 list of spherical harmonics of low order

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}, \quad Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$
$$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}(\sin\theta)e^{\pm i\phi}, Y_2^0 = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right)$$
$$Y_2^{\pm 1} = \mp\sqrt{\frac{15}{8\pi}}(\sin\theta\cos\theta)e^{\pm i\phi}$$
$$Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}}\left(\sin^2\theta\right)e^{\pm 2i\phi}$$

4 Spherical operator, Wigner-Eckart Theorem and selection rule

4.1 tensor operators

$T_q^{(k)} = Y_{l=k}^{m=q}(\mathbf{V})$

4.2 selection rule

$\left\langle \alpha', j'm' \middle| T_q^{(k)} \middle| \alpha, jm \right\rangle = 0,$

unless $m' = q + m$ and $|j - k| \leq j' \leq |j + k|$