29:5742 Homework 6
Due 3/8

1. Use the definitions

$$\| |\psi\rangle \| = \langle\psi|\psi\rangle^{1/2}$$

and

$$|||O||| = \underbrace{\sup}_{\| |\psi\rangle \| \neq 0} \frac{\| O|\psi\rangle \|}{\| |\psi\rangle \|}$$

to show

a.

$$\| O|\psi\rangle \| \leq |||O||| \| |\psi\rangle \|$$

b.

$$|||O_1 + O_2||| \leq |||O_1||| + |||\,|||O_2|||$$

c.

$$|||O_1 O_2||| \leq |||O_1|||\;|||O_2|||$$

2. Consider a two state system with unperturbed Hamiltonian $H_0 := E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|$ with $E_2 > E_1$ and perturbing interaction for $t > 0$, $V(t) = \gamma e^{i\omega t}|1\rangle\langle 2| + \gamma e^{-i\omega t}|2\rangle\langle 1|$ where ω and γ are real positive constants.

   a. Assume that at time $t = 0$ the system is in the state $|1\rangle$. Find the exact probability for the system to found in each of these states at later times.

   b. Do the same calculation using first order time dependent perturbation theory.

   c. Both probabilities exhibit oscillations. Find the frequency that maximizes the amplitude of the oscillations of the probability to find the system in the second state.

   * Hint - the time dependence in the Hamiltonian can be eliminated by a rotation about the z axis.

3. A one dimensional harmonic oscillator is in its ground state for $t < 0$. For $t \geq 0$ is it subject to a time-dependent but spatially uniform force (not potential) in the x-direction

$$F(t) = F_0 e^{-i\omega t}$$

Use first order time-dependent perturbation theory to find the probability of finding the oscillator in its first excited state as a function of time.

4. Consider the Hamiltonian

$$H = \begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix} \qquad E_2 > E_1$$

Assume that a and b are small. Compare the exact eigenvalues of this matrix to the eigenvalues obtained using second order degenerate perturbation theory.

5. Consider the Hamiltonian

$$H = \begin{pmatrix} E_1 & \lambda \cos(\omega t) \\ \lambda \cos(\omega t) & E_2 \end{pmatrix} \qquad \lambda = \lambda^*$$

If λ is small and the system is initially in the state

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

find the probability as a function of time that is will be in the state

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

6. A one electron atom in its ground state is placed in a uniform electric field in the z direction. Obtain an approximate expression for the induced electric dipole moment of this atom by considering the expectation value of ez with respect to the perturbed ground state vector created in first order perturbation theory (assume that the ground state is non-degenerate).

* Hint - This problem involves an infinite sum - the trick to perfom the sum is to find an operator F with the property $[F, H_0] = z$. This cancels the denominator allowing one use use the completeness relation.

Homework 6

1a $$|||O||| = \sup_{\||\psi\rangle\| \neq 0} \|O|\psi\rangle\| / \||\psi\rangle\|$$

$$\geq \|O|\chi\rangle\| / \||\chi\rangle\| \quad \text{for any } |\chi\rangle \neq 0$$

$$\|O|\chi\rangle\| \leq |||O||| \cdot \||\chi\rangle\|$$

1b $$|||O_1 + O_2||| = \sup_{\||\psi\rangle\| \neq 0} \frac{\|(O_1 + O_2)|\psi\rangle\|}{\||\psi\rangle\|}$$

note for vectors $\||V_1\rangle + |V_2\rangle\| \leq \||V_1\rangle\| + \||V_2\rangle\|$

$$\leq \sup_{\||\psi\rangle\| \neq 0} \left(\frac{\|O_1|\psi\rangle\|}{\||\psi\rangle\|} + \frac{\|O_2|\psi\rangle\|}{\||\psi\rangle\|} \right) \leq$$

$$\sup_{\||\chi_1\rangle\| \neq 0} \frac{\|O_1|\chi_1\rangle\|}{\||\chi_1\rangle\|} + \sup_{\||\chi_2\rangle\| \neq 0} \frac{\|O_2|\chi_2\rangle\|}{\||\chi_2\rangle\|}$$

$$= |||O_1||| + |||O_2|||$$

1c $$|||O_1 O_2||| = \sup_{\||\psi\rangle\| \neq 0} \frac{\|O_1 O_2|\psi\rangle\|}{\||\psi\rangle\|} \leq |||O_1||| \sup_{\||\psi\rangle\| \neq 0} \frac{\|O_2|\psi\rangle\|}{\||\psi\rangle\|}$$

$$= |||O_1||| \cdot |||O_2|||$$

2 $$H = \begin{pmatrix} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_2 \end{pmatrix} \qquad |\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

a) exact solution – we begin by rotating the Hamiltonian using a time dependent rotation

$$\mathcal{U}(t) = \begin{pmatrix} e^{i\frac{\omega}{2}t} & 0 \\ 0 & e^{i\frac{\omega}{2}t} \end{pmatrix}$$

$$\mathcal{U}(t)\, H\, \mathcal{U}^{+}(t) = \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2} \end{pmatrix} \begin{pmatrix} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_2 \end{pmatrix} \begin{pmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix}$$

$$= \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2} \end{pmatrix} \begin{pmatrix} E_1 e^{i\omega t/2} & \gamma e^{i\omega t/2} \\ \gamma e^{-i\omega t/2} & E_2 e^{-i\omega t/2} \end{pmatrix}$$

$$= \begin{pmatrix} E_1 & \gamma \\ \gamma & E_2 \end{pmatrix} = H(0)$$

Define

$$|\psi'(t)\rangle = \mathcal{U}(t)\, |\psi_s(t)\rangle$$

$$|\psi_s(t)\rangle = \mathcal{U}^{+}(t)\, |\psi'(t)\rangle$$

$$\mathcal{U}(t)\, H(t)\, \mathcal{U}^{+}(t) = H(0)$$

$$i\hbar \frac{d|\psi'\rangle}{dt} = i\hbar \frac{d\mathcal{U}}{dt} \mathcal{U}^{+} \cdot |\psi'\rangle + \mathcal{U}(t)\, i\hbar \frac{d|\psi_s\rangle}{dt}$$

$$= i\hbar \frac{d\mathcal{U}}{dt} \mathcal{U}^{+} |\psi'\rangle + \mathcal{U}(t) H(t) \mathcal{U}^{+}(t) \mathcal{U}(t) |\psi_s(t)\rangle$$

$$= \left(i\hbar \frac{d\mathcal{U}}{dt} \cdot \mathcal{U}^{+}\right) |\psi'\rangle + H(0)\, |\psi'\rangle$$

Note that

$$\frac{d\mathcal{U}}{dt} \mathcal{U}^{+} = \begin{pmatrix} -i\frac{\omega}{2} & 0 \\ 0 & i\frac{\omega}{2} \end{pmatrix}$$

$$i\hbar \frac{d|\psi'\rangle}{dt} = \underbrace{\begin{pmatrix} E_1 - i\frac{\omega}{2} i\hbar & \gamma \\ \gamma & E_2 + i\frac{\omega}{2} i\hbar \end{pmatrix}}_{H'} |\psi'(t)\rangle$$

This is an ordinary time independent Schrodinger equation — we need to solve the eigenvalue problem for H'

$$\det\begin{pmatrix} \lambda - E_1 - \frac{\omega\hbar}{2} & -\gamma \\ -\gamma & \lambda - E_2 + \frac{\omega\hbar}{2} \end{pmatrix} = 0$$

$$\lambda^2 - \lambda(E_1+E_2) - (E_1+\tfrac{\omega\hbar}{2})(E_2-\tfrac{\omega\hbar}{2}) - \gamma^2 = 0$$

$$\lambda_\pm = \tfrac{1}{2}(E_1+E_2) \pm \tfrac{1}{2}\sqrt{(E_1+E_2)^2 - 4(E_1+\tfrac{\omega\hbar}{2})(E_2-\tfrac{\omega\hbar}{2}) + 4\gamma^2 + \omega^2\hbar^2}$$

$$= \tfrac{1}{2}(E_1+E_2) \pm \tfrac{1}{2}\sqrt{(E_1-E_2)^2 + 2\omega\hbar(E_1-E_2) + 4\gamma^2 + \omega^2\hbar^2}$$

The general solution for $|\psi'(t)\rangle$ has the form

$$|\psi'\rangle = C_+\begin{pmatrix} \gamma \\ \lambda_+ - E_1 - \frac{\hbar\omega}{2} \end{pmatrix} e^{-i\lambda_+ t/\hbar} + C_-\begin{pmatrix} \gamma \\ \lambda_- - E_1 - \frac{\hbar\omega}{2} \end{pmatrix} e^{-i\lambda_- t/\hbar}$$

where C_+ and C_- are determined by the initial condition

$$|\Psi'(0)\rangle = |\Psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

this requires

$$1 = (C_+ + C_-)\gamma$$

$$0 = C_+(\lambda_+ - E_1 - \tfrac{\hbar\omega}{2}) + C_-(\lambda_- - E_1 - \tfrac{\hbar\omega}{2})$$

the second equation gives

$$C_- = -C_+ \frac{\lambda_+ - E_1 - \frac{\hbar\omega}{2}}{\lambda_- - E_1 - \frac{\hbar\omega}{2}}$$

$$C_+\left(1 - \frac{\lambda_+ - E_1 - \frac{\hbar\omega}{2}}{\lambda_- - E_1 - \frac{\hbar\omega}{2}}\right) = C_+\left(\frac{\lambda_- - \lambda_+}{\lambda_- - E_- - \frac{\hbar\omega}{2}}\right) = \frac{1}{\gamma}$$

$$C_+ = \frac{1}{\gamma} \frac{\lambda_- - E_- - \frac{\hbar\omega}{2}}{\lambda_- - \lambda_+}$$

$$C_- = \frac{1}{\gamma} \frac{\lambda_+ - E_1 - \frac{\hbar\omega}{2}}{\lambda_+ - \lambda_-}$$

It follow that

$$|\Psi_s(t)\rangle = U^+(t)\,|\Psi'(t)\rangle =$$

$$C_+\begin{pmatrix} \gamma e^{(i\frac{\omega}{2} - i\frac{\lambda_+}{\hbar})t} \\ (\lambda_+ - E_- - \frac{\hbar\omega}{2})e^{(-\frac{i\omega}{2} - i\frac{\lambda_+}{\hbar})t} \end{pmatrix} +$$

$$C_-\begin{pmatrix} \gamma(e^{(i\frac{\omega}{2} - i\frac{\lambda_-}{\hbar})t} \\ (\lambda_- - E_1 - \frac{\hbar\omega}{2})e^{(-i\frac{\omega}{2} - i\frac{\lambda_-}{\hbar})t} \end{pmatrix}$$

we can use this to read off the probabilities

$$P(1) = c_+^2 \gamma^2 + c_-^2 \gamma^2 + c_+ c_- \gamma^2 \left(e^{i \frac{\lambda_+ - \lambda_-}{\hbar} t} + e^{-\frac{\lambda_+ - \lambda_-}{\hbar} t}\right)$$

$$= \gamma^2 \left(c_+^2 + c_-^2 + 2 c_+ c_- \cos\left(\frac{\lambda_+ - \lambda_-}{\hbar} t\right)\right)$$

$$P(2) = \left(\lambda_+ - E - \frac{\hbar\omega}{2}\right)^2 c_+^2 + \left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right)^2 c_-^2$$

$$2 c_+ c_- \left(\lambda_+ - E_1 - \frac{\hbar\omega}{2}\right)\left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right) \cos\left(\frac{\lambda_+ - \lambda}{\hbar} t\right)$$

The interesting case is $P(2)$

$$c_+^2 \left(\lambda_+ - E_1 - \frac{\hbar\omega}{2}\right)^2 = \frac{1}{\gamma^2} \frac{\left(\lambda_+ - E_+ - \frac{\hbar\omega}{2}\right)^2 \left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right)^2}{(\lambda_- - \lambda_+)^2}$$

$$c_-^2 \left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right)^2 = \frac{1}{\gamma^2} \frac{\left(\lambda_+ - E_1 - \frac{\hbar\omega}{2}\right)^2 \left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right)^2}{(\lambda_+ - \lambda_-)^2}$$

$$c_+ c_- \left(\lambda_+ - E_1 - \frac{\hbar\omega}{2}\right)\left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right) =$$

$$-\frac{1}{\gamma^2} \frac{\left(\lambda_+ - E_1 - \frac{\hbar\omega}{2}\right)^2 \left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right)^2}{(\lambda_+ - \lambda_-)^2}$$

$$P(2) = \frac{2}{\gamma^2} \frac{\left(\lambda_+ - E_1 - \frac{\hbar\omega}{2}\right)^2 \left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right)^2}{(\lambda_+ - \lambda_-)^2} \left(1 - \cos\left(\frac{\lambda_+ - \lambda_-}{\hbar} t\right)\right)$$

$$= \frac{4}{\gamma^2} \cdot \frac{\left(\lambda_+ - E_1 - \frac{\hbar\omega}{2}\right)^2 \left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right)^2}{(\lambda_+ - \lambda_-)^2} \sin^2\left(\frac{\lambda_+ - \lambda_-}{2\hbar} t\right)$$

$$\lambda_+ - E_1 - \frac{\hbar\omega}{2} = \frac{1}{2}(E_2 - E_1 - \hbar\omega) + \frac{1}{2}\sqrt{}$$

$$\lambda_- - E_1 - \frac{\hbar\omega}{2} = \frac{1}{2}(E_2 - E_1 - \hbar\omega) - \frac{1}{2}\sqrt{}$$

$$\left(\lambda_+ - E_1 - \frac{\hbar\omega}{2}\right)\left(\lambda_- - E_1 - \frac{\hbar\omega}{2}\right) =$$

$$\frac{1}{4}\left[(E_2 - E_1 - \hbar\omega)^2 - \left((E_1 + E_2)^2 - 4\left(E_1 + \frac{\hbar\omega}{2}\right)\left(E_2 - \frac{\hbar\omega}{2}\right) + 4\gamma^2 + \hbar^2\omega^2\right)\right.$$

$$\frac{1}{4}\left[(E_2 - E_1 - \hbar\omega)^2 - (E_2 - E_1 - \hbar\omega)^2 - 4\gamma^2 \right] = -\gamma^2$$

This means

$$P(2) = 4\,\frac{(-\gamma^2)^2}{\gamma^2}\,\frac{\sin^2\left(\frac{\lambda_+ - \lambda_-}{2\hbar}t\right)}{(\lambda_+ - \lambda_-)^2} = \gamma^2\,\frac{\sin^2\left(\frac{\lambda_+ - \lambda_-}{2\hbar}t\right)}{\left(\frac{\lambda_+ - \lambda_-}{2}\right)^2}$$

where $\lambda_+ - \lambda_- = \sqrt{(E_1 - E_2 + \hbar\omega)^2 + 4\gamma^2}$

For small γ $\quad \lambda_+ - \lambda_- \rightarrow$

$$2\gamma\sqrt{\frac{(E_1 - E_2 + \hbar\omega)^2}{4\gamma^2} + 1} \simeq (E_1 - E_2 + \hbar\omega)\left(1 + \frac{1}{2}\,\frac{4\gamma^2}{(E_1 - E_2 + \hbar\omega)^2} + \cdots\right)$$

$$P(2) \rightarrow \gamma^2\,\frac{\sin^2\left(\frac{E_1 - E_2 + \hbar\omega}{2\hbar}t\right)}{\left(\frac{E_1 - E_2 + \hbar\omega}{2}\right)^2}$$

which is exactly the result that one would obtain using perturbation theory (assumes $2\gamma < (E_1 - E_2 + \hbar\omega)$)

(3) In this case

$$c_1 = 0 - \frac{i}{\hbar}\int_0^t e^{i(E_1 - E_0 - \hbar\omega)t/\hbar} \langle 1|F|0\rangle \, dt$$

$$|c_1|^2 = |\langle 1|F_0|0\rangle|^2 \frac{\sin^2\left(\frac{E_1 - E_0 - \hbar\omega}{2\hbar} t\right)}{\left(\frac{E_0 - E_1 + \hbar\omega}{2}\right)^2}$$

where $E_1 - E_2 = \hbar\sqrt{\frac{k}{m}}$

$$|\langle 1|F_0|0\rangle|^2 \frac{\sin^2\left(\frac{1}{2}\left(\sqrt{\frac{k}{m}} - \omega\right)t\right)}{\hbar\left(\sqrt{\frac{k}{m}} - \omega\right)^2}$$

(4) In this case

exact eigenvalues

$$(\lambda I - H) =$$

$$\det \begin{pmatrix} \lambda - E_1 & 0 & a \\ 0 & \lambda - E_1 & b \\ a^* & b^* & \lambda - E_2 \end{pmatrix}$$

$$(\lambda - E_1)((\lambda - E_1)(\lambda - E_2) - b^* b)$$

$$+ a(0 \cdot b - a^*(\lambda - E_1)) =$$

$$(\lambda - E_1)((\lambda - E_1)(\lambda - E_2) - b^* b - a^* a)$$

$(\lambda - E_1)(\lambda - \alpha_+)(\lambda - \alpha_-)$ where $\alpha_\pm$ are roots of

$$\lambda^2 - (E_1+E_2)\lambda - |b|^2 - |a|^2 + E_1E_2$$

$$\alpha_\pm = \tfrac{1}{2}(E_1+E_2) \pm \tfrac{1}{2}\sqrt{(E_1+E_2)^2 - 4E_1E_2 + 4|b|^2 + 4|a|^2}$$

$$= \tfrac{1}{2}(E_1+E_2) \pm \tfrac{1}{2}(E_1-E_2)\sqrt{1 + \frac{4(|a|^2+|b|^2)}{(E_1-E_2)^2}}$$

eigenvalues are

$$\left.\begin{aligned} \lambda &= E_1 \\ \lambda_\pm &= \tfrac{1}{2}\left[(E_1+E_2) \pm (E_1-E_2)\sqrt{1+\frac{4\,|a|^2+|b|^2}{(E_1-E_2)^2}}\right] \end{aligned}\right\} \text{exact}$$

In perturbation theory for

$$|\psi_0^0\rangle = \begin{pmatrix} \alpha \\ \beta \\ 0 \end{pmatrix} \qquad H_0\begin{pmatrix} \alpha \\ \beta \\ 0 \end{pmatrix} = E_1\begin{pmatrix} \alpha \\ \beta \\ 0 \end{pmatrix}$$

For this vector

$$E_0^2 = \frac{\left|(\alpha\ \beta\ 0)\begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & c \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\right|^2}{E_1-E_2} = \frac{|\alpha a + \beta b|^2}{E_1-E_2}$$

the value depends on the choice α, β of starting vector

while

$$E_2^2 = \frac{\left|(0\,0\,1)\begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & c \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}\right|^2}{E_2-E_1} + \frac{\left|(0\,0\,1)\begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & c \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\right|^2}{E_2-E_1} =$$

In this case

$$E_2^{I} = E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

$$E_1^{I} = E_1 + \frac{|\alpha a + \beta b|^2}{E_1 - E_2} \qquad |\alpha|^2 + |\beta|^2 = 1$$

expanding the exact states

$$\lambda_1 = E_1$$

$$\lambda_+ = E_1 + \frac{1}{4}\frac{4(|a|^2 + |b|^2)}{(E_1 - E_2)} + \cdots \quad E_1 + \frac{|a|^2 + |b|^2}{E_1 - E_2}$$

$$= E_1 + \frac{|a|^2 + |b|^2}{E_1 - E_2}$$

$$\lambda_- = E_2 - \frac{1}{4}\frac{4(|a|^2 + |b|^2)}{(E_1 - E_2)} = E_2 + \frac{|a|^2 + |b|^2}{E_2 - E_1}$$

here we see the perturbative result for E_2 agrees with the exact result

For the other states the perturbative and exact states agree for specific values of α β

$$\lambda_1 \leftrightarrow \alpha = Nb \quad \beta = -Na \qquad 1 = N^2(a^2 + b^2)$$

$$N = \frac{1}{\sqrt{a^2 + b^2}}$$

$$\lambda_+ \leftrightarrow \alpha = \frac{1}{\sqrt{2}} \quad \beta = \frac{i}{\sqrt{2}}$$

(5) $$c\begin{pmatrix}0\\1\end{pmatrix} = \left| \begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}0 & \lambda\\ \lambda & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}\right|^2 \frac{1}{4}\,\frac{\sin^2\left(\frac{E_2-E_1\pm\hbar\omega}{2}t\right)}{\left(\frac{E_2-E_1\pm\hbar\omega}{2}\right)^2}$$

$$= \frac{\lambda^2}{4}\,\frac{\sin^2\left(\frac{E_2-E_1\pm\hbar\omega}{2}t\right)}{\left(\frac{E_2-E_1\pm\hbar\omega}{2}\right)^2}$$

The sign choice is the sign that minimizes $E_2-E_1-\hbar\omega$.

6) In this problem

$$H_0 = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}$$

$$V = -qEz$$

The dipole moment is

$$\bar{p} = q\langle\psi|\bar{r}|\psi\rangle$$

This generally vanishes because $|\psi\rangle$ is an eigenstate of the space reflection operator. The electric field breaks this symmetry so we evaluate $\bar{p}$ in the first order $|\psi\rangle$

$$|\psi\rangle = |\psi^0\rangle + \sum_{n\neq 0} \frac{|\psi_n^0\rangle\langle\psi_n^0|V|\psi_0^0\rangle}{E_0 - E_n}$$

For the hydrogen ground state

$$|000\rangle^{(1)} = |000\rangle^0 + \sum \frac{|n\ell m\rangle\langle n\ell m|(-qEz)|000\rangle}{E_0 - E_{n\ell}}$$

The problem is to compute

$$\langle n\ell m| -qEz|000\rangle =$$

$$-qE\int_0^\infty r^2 dr \int d\Omega\, \psi_{n\ell}(r) Y_m^{\ell *}(\hat{r})\, r\cos\theta\, \psi_{00}(r) Y_0^0(\hat{r})$$

since $Y_0^0 = \frac{1}{\sqrt{4\pi}}$ $Y_0^1 = \sqrt{\frac{3}{4\pi}}\cos\theta$ this becomes

$$-\frac{qE}{\sqrt{3}}\delta_{\ell 0}\delta_{m0}\int_0^\infty r^3 dr\, \psi_{n\ell}(r)\psi_{00}(r)\, dr$$

While these integrals can all be done there is still an infinite sum.

There is a trick for dealing with the infinite sum. Let F be an operator and consider

$$\sum \frac{|nem\rangle\langle nem|[H_0,F]|100\rangle}{E_0-E_{ne}} =$$

$$\sum \frac{|nem\rangle\langle nem|F|000\rangle(E_{ne}-E_0)}{E_{ne}-E_0} =$$

$$-\sum |nem\rangle\langle nem|F|000\rangle =$$

If $\langle 000|F|000\rangle = 0$ then this becomes

$$-F|000\rangle$$

If we can choose F so $[H_0F]|000\rangle = z|000\rangle$ then it will be possible to perform the sum. The problem reduces to finding such an F. For a $|000\rangle$ state of the form e^{-ar} F must satisfy

$$([H_0F]-z)e^{-ar} = 0 = ([P^2/2m, F]-z)e^{-ar}$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2F - \frac{\hbar^2}{m}\vec\nabla F\cdot(-a)\hat r - z\right)e^{-ar} = 0$$

$$\nabla^2F - 2a\frac{\partial F}{\partial r} = -\frac{2m}{\hbar^2}z$$

Let G be given by

$$G = -\left(\frac{r}{2}+\frac{1}{a}\right)z$$

$$\vec\nabla G = -\frac{\hat r}{2}z - \left(\frac{r}{2}+\frac{1}{a}\right)\hat z$$

$$\nabla^2 G = -\frac{z}{r} - \frac{z}{2r} - \frac{z}{2r} = -2\frac{z}{r}$$

$$-2a\frac{\partial G}{\partial r} = -2a\left(-\frac{z}{2} - \left(\frac{r}{2}+\frac{1}{a}\right)\frac{z}{r}\right) = az + az + 2\frac{z}{r}$$

adding these gives

$$2aZ = \nabla^2 G - 2a\frac{\partial G}{\partial r} \quad \text{or}$$

$$-\frac{2m}{\hbar^2} Z = -\frac{2m}{2a}\frac{1}{\hbar^2}\left(\nabla^2 G - 2a\frac{\partial G}{\partial r}\right)$$

thus we let $\quad F = -\frac{m}{a\hbar}\cdot G = \frac{m}{a\hbar}\left(\frac{r}{2}+\frac{1}{a}\right)Z$

$$\therefore \sum_{\neq 000} \frac{|n\ell m\rangle\langle n\ell m|Z|000\rangle}{E_{n\ell} - E_{00}} =$$

$$\sum_{\neq 000} \frac{|n\ell m\rangle\langle n\ell m|[H_0 F]|000\rangle}{E_{n\ell} - E_{00}} =$$

$$-\sum_{\neq 000} |n\ell m\rangle\langle n\ell m|F|000\rangle =$$

$$-\sum_{\neq 000} |n\ell m\rangle\langle n\ell m|\frac{m}{a\hbar}\left(\frac{r}{2}+\frac{1}{a}\right)Z|000\rangle$$

since Z changes the parity of $|000\rangle$ this is orthogonal to $|000\rangle$ — this means we can include $|000\rangle$ in the sum — giving

$$|000'\rangle = |000\rangle - \frac{m}{a\hbar}\left(\frac{r}{2}+\frac{1}{a}\right)Z|000\rangle$$

$$= |000\rangle - F|000\rangle$$

the normalized state is (since $|000\rangle \perp F|000\rangle$ by parity)

$$|000'\rangle = \frac{|000\rangle - F|000\rangle}{\sqrt{1 + \langle 000|FF|000\rangle}}$$

The dipole moment is

$$\bar{p} = e\langle 000^{(1)}| z |000^{(1)}\rangle =$$

$$= e\,\frac{\left(\langle 000| - \langle 000|F\right) z \left(-F|000\rangle + |000\rangle\right)}{1+\langle 000|FF|000\rangle} =$$

$$= -e\,\frac{\langle 000|(zF+Fz)|000\rangle}{1+\langle 000|FF|000\rangle}$$

(because of parity $\langle 000|z|000\rangle = \langle 000|FzF|000\rangle = 0$)

$$= -e\,\frac{\langle 000|\frac{2m}{a\hbar}\left(\frac{r}{2}+\frac{1}{a}\right)z^2|000\rangle}{1+\langle 000|\frac{m^2}{a^2\hbar^2}\left(\frac{r}{2}+\frac{1}{a}\right)^2 z^2|000\rangle}$$

note $\int z^2 f(r)\,dr = \frac{1}{3}\int r^3 f(r)\,dr$ since the xyz integrals are the same

$$= -e\,\frac{\frac{2m}{3a\hbar}\langle 000|\left(\frac{r^3}{2}+\frac{r^2}{a}\right)|000\rangle}{1+\langle 000|\frac{m^2}{3a^2\hbar^2}\left(\frac{r^2}{2}+\frac{r}{a}\right)^2|000\rangle}$$

In this case the integrals are elementary. $\langle r|000\rangle = \sqrt{\frac{a^3}{2}}\,e^{-ar}$

$$\langle 000|r^n|000\rangle = \frac{a^3}{2}\int_0^\infty e^{-2ar}\,r^{n+2}\,dr$$

$$= \frac{a^3}{2}\cdot\frac{1}{(2a)^{n+3}}\,\Gamma(n+3)$$

$$\bar{P} = \frac{\hat{z}(-e)\frac{2m}{3a\hbar}\cdot\frac{a^3}{2}\left(\frac{1}{2(2a)^6}\Gamma(6)+\frac{1}{a(2a)^5}\Gamma(5)\right)}{1+\frac{m^2}{3a^2\hbar^2}\frac{a^3}{2}\left(\frac{1}{4}\frac{1}{(2a)^7}\Gamma(7)+\frac{1}{a}\frac{1}{(2a)^6}\Gamma(6)+\frac{1}{a^2}\frac{1}{(2a)^5}\Gamma(5)\right)}$$

where $\frac{1}{a}$ = bohr radius = $\frac{me^2}{\hbar^2}$