FORMULA SHEET

Free-space unnormalized Gaussian wavepacket:

$$\psi(x,t) \;=\; \int_{-\infty}^{\infty} A(k)\, e^{ikx}\, e^{-i\omega(k)t}\, \frac{dk}{2\pi}$$

$$A(k) = \sqrt{2\pi L^2} e^{-k^2L^2/2}$$

$$\psi(x,t) \;=\; \frac{1}{(1+i\hbar t/mL^2)^{1/2}}\, e^{-x^2/2L^2(1+i\hbar t/mL^2)}$$

$$\Delta x^2(t) \;=\; \Delta x^2(0) \;+\; \frac{\Delta p^2(0)}{m^2}t^2$$

Heisenberg uncertainty relations:

$$\Delta x \Delta p \;\geq\; \frac{\hbar}{2} \qquad\qquad \Delta E \Delta t \;\geq\; \frac{\hbar}{2}$$

Operators:

$$\hat{x} \;=\; x \;=\; i\frac{\partial}{\partial k}$$

$$\hat{p} \;=\; -i\hbar\frac{\partial}{\partial x} \;=\; \hbar k$$

$$\hat{E} \;=\; i\hbar\frac{\partial}{\partial t}$$

$$\hat{H} \;=\; \frac{\hat{p}^2}{2m} \;+\; V(\hat{x}) \;=\; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \;+\; V(x)$$

Schrodinger equation, probability amplitudes:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) \;=\; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) \;+\; V(x)\psi(x,t)$$

$$P(x,t) \;=\; |\psi(x,t)|^2$$

Time-independent simple harmonic oscillator:

$$E\psi(x) \;=\; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) \;+\; \frac{1}{2}m\omega_0^2x^2\psi(x)$$

SHO Ground State

$$\phi_0(x) \;=\; \left[\frac{m\omega_0}{\hbar\pi}\right]^{1/4} e^{-m\omega_0x^2/2\hbar}$$

$$E \;=\; \frac{1}{2}\hbar\omega_0$$

$$\Delta x \;=\; \sqrt{\frac{\hbar}{2m\omega_0}} \qquad\qquad \Delta p \;=\; \sqrt{\frac{m\hbar\omega_0}{2}}$$

$$\Delta x\Delta p \;=\; \frac{\hbar}{2}$$

Simple harmonic oscillator excited states:

$$\phi_n(x) \;=\; \left[\frac{m\omega_0}{\pi\hbar}\right]^{1/4} \frac{1}{\sqrt{2^n n!}}\, e^{-\frac{1}{2}\frac{m\omega_0}{\hbar}x^2}\, H_n\left(\sqrt{\frac{m\omega_0}{\hbar}}x\right)$$

$$E_n \;=\; \hbar\omega_0\,(n \;+\; \frac{1}{2})$$

SHO classical states:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) \;=\; -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) \;+\; \frac{1}{2}m\omega_0^2x^2\psi(x,t)$$

$$\psi(x,t) \;=\; \left[\frac{m\omega_0}{\hbar\pi}\right]^{1/4} e^{-i\Theta(t)}\, e^{iP(t)[x-X(t)]/\hbar}\, e^{-\frac{1}{2}\frac{m\omega_0}{\hbar}[x-X(t)]^2}$$

$$\frac{d}{dt}X(t) \;=\; \frac{P(t)}{m} \qquad\qquad \frac{d}{dt}P(t) \;=\; -m\omega_0^2X(t)$$

$$\hbar\frac{d}{dt}\Theta(t) \;=\; \frac{1}{2}\hbar\omega_0 \;-\; \frac{P^2(t)}{2m} \;+\; \frac{1}{2}m\omega_0^2X^2(t)$$

Expectation values:

$$\langle\hat{Q}\rangle \;=\; \frac{\int_{\infty}^{\infty} \psi^*(x,t)\hat{Q}\psi(x,t)\,dx}{\int_{\infty}^{\infty} \psi^*(x,t)\psi(x,t)\,dx}$$

Dirac notation:

$$\langle\psi(x,t)|\hat{Q}|\psi(x,t)\rangle \;=\; \int_{\infty}^{\infty} \psi^*(x,t)\hat{Q}\psi(x,t)\,dx$$

$$\langle\hat{Q}\rangle \;=\; \frac{\langle\psi(x,t)|\hat{Q}|\psi(x,t)\rangle}{\langle\psi(x,t)|\psi(x,t)\rangle}$$

$$|\psi(x,t)\rangle \;=\; \psi(x,t)$$

$$\langle\psi(x,t)| \;=\; \int_{-\infty}^{\infty} \psi^*(x,t)\,[\;\;\cdots\;\;]\,dx$$

Ehrenfest Theorem:

$$\frac{d}{dt}\langle\hat{Q}\rangle \;=\; \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle \;+\; \frac{1}{i\hbar}\langle[\hat{Q},\hat{H}]\rangle$$

Commutators:

$$[\hat{A},\hat{B}] \;=\; \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$[\hat{A},\hat{A}] \;=\; 0$$

$$[\hat{x},\hat{p}] \;=\; i\hbar$$

$$[\hat{x},\hat{H}] \;=\; \frac{\hbar^2}{m}\frac{\partial}{\partial x} \;=\; i\frac{\hbar}{m}\hat{p}$$

$$[\hat{p},\hat{H}] \;=\; -i\hbar\frac{\partial V}{\partial x}$$

Creation and annihilation operators:

$$\hat{a} \;=\; \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega_0}{\hbar}}x \;+\; \sqrt{\frac{\hbar}{m\omega_0}}\frac{d}{dx}\right] \qquad\qquad \hat{a}^\dagger \;=\; \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega_0}{\hbar}}x \;-\; \sqrt{\frac{\hbar}{m\omega_0}}\frac{d}{dx}\right]$$

$$\hat{a}\phi_n(x) \;=\; \sqrt{n}\,\phi_{n-1}(x) \qquad\qquad \hat{a}^\dagger\phi_n(x) \;=\; \sqrt{n+1}\,\phi_{n+1}(x)$$

$$\hat{x} \;=\; \sqrt{\frac{\hbar}{2m\omega_0}}\,(\hat{a}^\dagger + \hat{a}) \qquad\qquad \hat{p} \;=\; i\sqrt{\frac{m\hbar\omega_0}{2}}\,(\hat{a}^\dagger - \hat{a})$$

$$[\hat{a},\hat{a}^\dagger] \;=\; 1$$

Classical state expansion:

For the special case where $X(0) = X_0$, with $P(0) = 0$ and $\Theta(0) = 0$, we can write

$$\left[\frac{m\omega_0}{\hbar\pi}\right]^{\frac{1}{4}} e^{-\frac{m\omega_0}{2\hbar}(x-X_0)^2} \;=\; e^{-z^2/2}\sum_n \frac{1}{\sqrt{n!}}\, z^n\, \phi_n(x)$$

$$X_0 = \sqrt{\frac{2\hbar}{m\omega_0}}z$$

LC Circuit:

Classical equations:

$$\frac{d}{dt}v(t) = \frac{1}{C}i(t) \qquad\qquad \frac{d}{dt}i(t) = -\frac{1}{L}v(t)$$

$$E = \frac{1}{2}Li^2(t) + \frac{1}{2}Cv^2(t)$$

Quantum equations:

$$i\hbar\frac{\partial}{\partial t}\psi(v,t) = -\frac{\hbar^2}{2LC^2}\frac{\partial^2}{\partial v^2}\psi(v,t) + \frac{1}{2}Cv^2\psi(v,t)$$

$$\hat{v} \;=\; v \qquad\qquad \hat{i} = -i\frac{\hbar}{LC}\frac{\partial}{\partial v}$$

$$\psi_n(v) = \left[\frac{C}{\pi\hbar\omega_0}\right]^{1/4} \frac{1}{\sqrt{2^n n!}}\, H_n\left(\sqrt{\frac{C}{\hbar\omega_0}}v\right)\, e^{-\frac{C}{2\hbar\omega_0}v^2}$$

$$E_n \;=\; \hbar\omega_0\left(n + \frac{1}{2}\right)$$

Time-independent Schrödinger equation:

$$\psi(x,t) \;=\; e^{-iEt/\hbar}\,\phi(x)$$

$$E\phi(x) \;=\; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) \;+\; V(x)\phi(x)$$

$$\langle\phi_i|\phi_j\rangle \;=\; 0 \quad \text{if } E_i \neq E_j$$

Eigenfunction expansion:

$$\psi(x,t) \;=\; \sum_j a_j\, \phi_j(x)\, e^{-iE_jt/\hbar}$$

$$\hat{H}\phi_j \;=\; E_j\phi_j$$

$$a_j \;=\; \langle\phi_j(x)|\psi(x,0)\rangle$$

Continuity of probability and probability flux:

$$\frac{\partial}{\partial t}P(\mathbf{r},t) \;+\; \nabla\cdot\mathbf{J_p}(\mathbf{r},t) \;=\; 0$$

$$\mathbf{J_p}(\mathbf{r},t) \;=\; \frac{\hbar}{2mi}\Big[\psi^*(\mathbf{r},t)\nabla\psi(\mathbf{r},t) \;-\; \psi(\mathbf{r},t)\nabla\psi^*(\mathbf{r},t)\Big]$$

Infinite square well:

$$E\phi(x) \;=\; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) \;+\; V(x)\phi(x)$$

$$V(x) \;=\; \begin{cases} \infty & \text{for } x < 0 \\ 0 & \text{for } 0 \leq x \leq L \\ \infty & \text{for } x > L \end{cases}$$

$$\phi_n(x) \;=\; \sqrt{\frac{2}{L}}\,\sin(n\pi x/L)$$

$$E_n \;=\; \frac{\hbar^2\pi^2n^2}{2mL^2}$$

WKB Approximation:

Normalized Schrödinger equation:

$$\epsilon\psi(y) \;=\; -\frac{d^2}{dy^2}\psi(y) \;+\; v(y)\psi(y)$$

Oscillatory solutions:

$$\psi(y) \;=\; \begin{cases} \frac{e^{\pm i\phi(y)}}{\sqrt{\eta(y)}} \\ \frac{\sin\phi(y)}{\sqrt{\eta(y)}} \\ \frac{\cos\phi(y)}{\sqrt{\eta(y)}} \end{cases}$$

with

$$\frac{d}{dy}\phi(y) \;=\; \eta(y)$$

WKB representation (exact):

$$\epsilon \;=\; -\eta^{\frac{1}{2}}(y)\frac{d^2}{dy^2}\eta^{-\frac{1}{2}}(y) \;+\; v(y) \;+\; \eta^2(y)$$

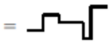
WKB approximation for allowed regions:

$$\eta(y) \;=\; \pm\sqrt{\epsilon - v(y)}$$

WKB approximate eigenvalue equation for bound states

$$\phi(y_{max}) - \phi(y_{min}) \;=\; \int_{y_{min}}^{y_{max}} \sqrt{\epsilon - v(y)}\,dy \;=\; \begin{cases} n\pi & \text{2 hard boundaries} \\ \left(n-\frac{1}{4}\right)\pi & \text{1 hard boundary, 1 soft boundar} \\ \left(n-\frac{1}{2}\right)\pi & \text{2 soft boundaries} \end{cases}$$

Piece-wise linear potentials:

$V(x) \;=$ 

In allowed regions:

$$k \;=\; \sqrt{\frac{2m(E-V)}{\hbar^2}} \qquad \psi(x) \;=\; Ae^{ikx} \;+\; Be^{-ikx}$$

In forbidden regions:

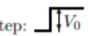
$$\kappa \;=\; \sqrt{\frac{2m(V-E)}{\hbar^2}} \qquad \psi(x) \;=\; Ae^{\kappa x} \;+\; Be^{-\kappa x}$$

Matching point and slope:

$$\psi(x_-) \;=\; \psi(x_+)$$

$$\frac{d\psi(x_-)}{dx} \;=\; \frac{d\psi(x_+)}{dx}$$

Single step:

Single step: 

$$\psi(x) \;=\; \begin{cases} e^{ik_ix} \;+\; \frac{k_i - k_f}{k_i + k_f}e^{-ik_ix} & \text{for } x \leq 0 \\ \frac{2k_i}{k_i + k_f}e^{ik_tx} & \text{for } x > 0 \end{cases}$$

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

Exponential solutions:

$$\psi(y) \;=\; \begin{cases} \frac{e^{+\theta(y)}}{\sqrt{\zeta(y)}} \\ \frac{\sinh\theta(y)}{\sqrt{\zeta(y)}} \\ \frac{\cosh\theta(y)}{\sqrt{\zeta(y)}} \end{cases}$$

with

$$\frac{d}{dy}\theta(y) \;=\; \zeta(y)$$

WKB representation (exact):

$$\epsilon \;=\; -\zeta^{\frac{1}{2}}(y)\frac{d^2}{dy^2}\zeta^{-\frac{1}{2}}(y) \;+\; v(y) \;-\; \zeta^2(y)$$

WKB approximation for forbidden regions:

$$\zeta(y) \;=\; \sqrt{v(y) - \epsilon}$$

Gamow approximation for transmission through a smooth barrier:

$$T \approx e^{-2G} \qquad\qquad G \;=\; \int_{y_{min}}^{y_{max}} \sqrt{v(y) - \epsilon}\,dy$$

Without normalization:

$$G \;=\; \int_{x_{min}}^{x_{max}} \sqrt{\frac{2m[V(x) - E]}{\hbar^2}}\,dx$$

Variational Method:

$$E\psi(x) \;=\; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) \;+\; V(x)\psi(x) \;=\; H\psi(x)$$

Trial solution:

$$\psi(x) \;\approx\; \psi_t[\alpha,\beta,\cdots]$$

$$\epsilon_t[\alpha,\beta,\cdots] \;=\; \langle\, \psi_t[\alpha,\beta,\cdots] \mid H \mid \psi_t[\alpha,\beta,\cdots]\, \rangle$$

Optimization:

$$\frac{\partial}{\partial\alpha}\epsilon_t \;=\; 0 \qquad\qquad \frac{\partial}{\partial\beta}\epsilon_t \;=\; 0 \qquad\qquad \cdots$$

Finite Basis Expansions:

$$E\psi(x) \;=\; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) \;+\; V(x)\psi(x) \;=\; H\psi(x)$$

Trial solution (orthonormal basis u_j):

$$\psi \;=\; \sum_j a_j\; u_j$$

$$E\begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix} = \begin{pmatrix} H_{11} & \cdots & H_{1N} \\ \vdots & \vdots & \vdots \\ H_{N1} & \cdots & H_{NN} \end{pmatrix}\begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$$

$$H_{ij} \;=\; \langle\; \phi_i \mid H \mid \phi_j \;\rangle$$

Static Two-Level Model:

$$E\psi(x) \;=\; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) \;+\; V(x)\psi(x) \;=\; H\psi(x)$$

Trial solution (orthonormal basis u_j):

$$\psi \;=\; c_1\, u_1 \;+\; c_2\, u_2$$

$$E\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} H_1 & V_{12} \\ V_{21} & H_2 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$E_- \;=\; \frac{H_1+H_2}{2} \;-\; \frac{1}{2}\sqrt{(H_2-H_1)^2+4|V_{12}|^2}$$

$$E_+ \;=\; \frac{H_1+H_2}{2} \;+\; \frac{1}{2}\sqrt{(H_2-H_1)^2+4|V_{12}|^2}$$

$$e_{\mathbf{k},\sigma}(t) \;\sim\; e^{-i\omega_{\mathbf{k}}t} \qquad \omega_{\mathbf{k}} \;=\; \frac{1}{\sqrt{\epsilon_0\mu_0}}|\mathbf{k}| \;=\; c|\mathbf{k}|$$

Periodic boundary conditions:

$$\mathbf{k} \;=\; \mathbf{i}_x\frac{2\pi n_x}{L} \;+\; \mathbf{i}_y\frac{2\pi n_y}{L} \;+\; \mathbf{i}_z\frac{2\pi n_z}{L}$$

where

$$n_x \;=\; 0,\;\; \pm 1,\;\; \pm 2,\;\; \cdots$$

$$n_y \;=\; 0,\;\; \pm 1,\;\; \pm 2,\;\; \cdots$$

$$n_z \;=\; 0,\;\; \pm 1,\;\; \pm 2,\;\; \cdots$$

Quantized fields and operators

$$\hat{\mathbf{E}}(\mathbf{r}) \;=\; \sum_\sigma\sum_{\mathbf{k}} \mathbf{i}_\sigma \sqrt{\frac{\hbar\omega_{\mathbf{k},\sigma}}{2\epsilon_0 L^3}}\left[\hat{a}_{\mathbf{k},\sigma}\, e^{i\mathbf{k}\cdot\mathbf{r}} \;+\; \hat{a}^\dagger_{\mathbf{k},\sigma}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\right]$$

$$\hat{\mathbf{H}}(\mathbf{r}) \;=\; \sum_\sigma\sum_{\mathbf{k}} (\mathbf{i}_{\mathbf{k}}\times\mathbf{i}_\sigma) \sqrt{\frac{\hbar\omega_{\mathbf{k},\sigma}}{2\mu_0 L^3}}\left[\hat{a}_{\mathbf{k},\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} \;+\; \hat{a}^\dagger_{\mathbf{k},\sigma} e^{-i\mathbf{k}\cdot\mathbf{r}}\right]$$

$$\hat{H} \;=\; \int \frac{1}{2}\epsilon_0|\hat{\mathbf{E}}(\mathbf{r})|^2 \;+\; \frac{1}{2}\mu_0|\hat{\mathbf{H}}(\mathbf{r})|^2\; d^3\mathbf{r} \qquad \hat{H} \;=\; \sum_\sigma\sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}\left(\hat{a}^\dagger_{\mathbf{k},\sigma}\hat{a}_{\mathbf{k},\sigma}+\frac{1}{2}\right)$$

Vector potential operator

$$\mu_0\hat{\mathbf{H}}(\mathbf{r}) \;=\; \nabla\times\hat{\mathbf{H}}(\mathbf{r})$$

$$\nabla\cdot\hat{\mathbf{A}}(\mathbf{r}) \;=\; 0$$

$$\hat{\mathbf{A}}(\mathbf{r}) \;=\; -i\sum_\sigma\sum_{\mathbf{k}} \mathbf{i}_\sigma \sqrt{\frac{\hbar}{2\omega_{\mathbf{k}}\epsilon_0 L^3}}\left[\hat{a}_{\mathbf{k},\sigma}\, e^{i\mathbf{k}\cdot\mathbf{r}} \;-\; \hat{a}^\dagger_{\mathbf{k},\sigma}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\right]$$

Bound state solutions:

$$\Phi \;=\; \prod_{\mathbf{k},\sigma}\frac{(\hat{a}^\dagger_{\mathbf{k},\sigma})^{n_{\mathbf{k},\sigma}}}{\sqrt{n_{\mathbf{k},\sigma}!}}|\Phi_0\rangle$$

where $|\Phi_0\rangle$ is the ground state.
Hamiltonian with classical source:

$$\hat{H} \;=\; \int \frac{1}{2}\epsilon_0|\hat{\mathbf{E}}(\mathbf{r})|^2 \;+\; \frac{1}{2}\mu_0|\hat{\mathbf{H}}(\mathbf{r})|^2\; d^3\mathbf{r} \;-\; \int \mathbf{J}(\mathbf{r},t)\cdot\hat{\mathbf{A}}(\mathbf{r})\; d^3\mathbf{r}$$

Dynamic Two-Level Model:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) \;=\; H_0 \;+\; V(t)\;\psi(x,t)$$

Trial solution (ϕ_1 and ϕ_2 eigenfunctions of H_0):

$$\psi(t) \;=\; c_1(t)\;\phi_1 \;+\; c_2(t)\;\phi_2$$

$$i\hbar\frac{d}{dt}c_1(t) \;=\; \langle\phi_1|H_0|\phi_1\rangle\; c_1(t) \;+\; \langle\phi_1|V(t)|\phi_2\rangle\; c_2(t)$$

$$i\hbar\frac{d}{dt}c_2(t) \;=\; \langle\phi_2|V(t)|\phi_1\rangle\; c_1(t) \;+\; \langle\phi_2|H_0|\phi_2\rangle\; c_2(t)$$

Position and effective momentum in two-level approximation:

$$\langle x\rangle \;=\; \langle\Phi_2|x|\Phi_1\rangle\,[c_2^*(t)c_1(t) \;+\; c_1^*(t)c_2(t)]$$

$$\langle p\rangle \;=\; m\;\omega_0\;\langle\Phi_2|x|\Phi_1\rangle\;\frac{(c_1^*c_2 - c_2^*c_1)}{i}$$

$$\frac{d}{dt}\langle x\rangle \;=\; \frac{\langle p\rangle}{m}$$

$$\frac{d}{dt}\langle p\rangle \;=\; -\,m\;\omega_0^2\;\langle x\rangle \;+\; 2V(t)\;\frac{m\omega_0}{\hbar}\;\langle\Phi_2|x|\Phi_1\rangle\;(|c_2|^2-|c_1|^2)$$

$$\omega \;=\; \frac{(E_2-E_1)}{\hbar}$$

Bloch equations:

$$\frac{d}{dt}Q(t) \;=\; \omega_0 P(t) \;+\; \frac{2\;\mathrm{Im}V_{12}(t)}{\hbar}N(t)$$

$$\frac{d}{dt}P(t) \;=\; -\,\omega_0 Q(t) \;+\; \frac{2\;\mathrm{Re}V_{12}(t)}{\hbar}N(t)$$

$$\frac{d}{dt}N(t) \;=\; -\,\frac{2\;\mathrm{Re}V_{12}(t)}{\hbar}P(t) \;-\; \frac{2\;\mathrm{Im}V_{12}(t)}{\hbar}Q(t)$$

with polarization $[Q(t),P(t)]$ and inversion $[N(t)]$ variables defined as:

$$Q(t) \;=\; c_1^*(t)c_2(t) \;+\; c_2^*(t)c_1(t)$$

$$P(t) \;=\; \frac{1}{i}\Big[c_1^*(t)c_2(t) \;-\; c_2^*(t)c_1(t)\Big]$$

$$N(t) \;=\; |c_2(t)|^2 \;-\; |c_1(t)|^2$$

Particle and field:

$$\hat{H} \;=\; \int \frac{1}{2}\epsilon_0|\hat{\mathbf{E}}(\mathbf{r})|^2 \;+\; \frac{1}{2}\mu_0|\hat{\mathbf{H}}(\mathbf{r})|^2\; d^3\mathbf{r} \;+\; \left[-\frac{\hbar^2\nabla^2}{2m} \;+\; V(\mathbf{r})\right]$$
$$-\;\frac{1}{2}\left[\frac{q\hat{\mathbf{p}}}{m}\cdot\hat{\mathbf{A}}(\mathbf{r}) \;+\; \hat{\mathbf{A}}(\mathbf{r})\cdot\frac{q\hat{\mathbf{p}}}{m}\right]$$

Minimal coupling:

$$\hat{H} \;=\; \int \frac{1}{2}\epsilon_0|\hat{\mathbf{E}}(\mathbf{r})|^2 \;+\; \frac{1}{2}\mu_0|\hat{\mathbf{H}}(\mathbf{r})|^2\; d^3\mathbf{r} \;+\; \left[\frac{|\hat{\mathbf{p}} - q\hat{\mathbf{A}}(\mathbf{r})|^2}{2m} \;+\; V(\mathbf{r})\right]$$

Electric dipole coupling:

$$\hat{H}_{int} \;=\; -\,\hat{\mathbf{d}}\cdot\hat{\mathbf{E}}(\mathbf{r})$$

Magnetic dipole coupling:

$$\hat{H}_{int} \;=\; -\,\hat{\mu}\cdot\hat{\mathbf{H}}(\mathbf{r})$$

Evolution with classical current source:

$$\frac{\partial}{\partial t}\epsilon_0\langle\hat{\mathbf{E}}\rangle \;=\; \nabla\times\langle\hat{\mathbf{H}}\rangle \;-\; \mathbf{J}(\mathbf{r},t)$$

$$\frac{\partial}{\partial t}\mu_0\langle\hat{\mathbf{H}}\rangle \;=\; -\,\nabla\times\langle\hat{\mathbf{E}}\rangle$$

$$\nabla\cdot(\epsilon_0\langle\hat{\mathbf{E}}\rangle) \;=\; 0$$

$$\nabla\cdot(\mu_0\langle\hat{\mathbf{H}}\rangle) \;=\; 0$$

Density of States:

Defining relations:

$$\sum_j \xi_j \;=\; \int g(\epsilon)\;\xi(\epsilon)\;d\epsilon$$

$$N(\epsilon) \;=\; \sum_{\epsilon_j<\epsilon} 1 \;\longrightarrow\; g(\epsilon) \;=\; \frac{dN}{d\epsilon}$$

$$\Delta E \;=\; \frac{dE(n)}{dn}\Delta n \;\longrightarrow\; g(\epsilon) \;\longrightarrow\; \frac{\Delta n}{\Delta E} = \left[\frac{dE}{dn}\right]^{-1}$$

Electrons, 1-D square well, continuum limit:

$$g(\epsilon) \;=\; g_s\sqrt{\frac{mL^2}{2\hbar^2\pi^2\epsilon}}$$

Problems in Several Dimensions:

Separable problems:

$$E\Psi(x,y) \;=\; \Big[\hat{H}_x(x) \;+\; \hat{H}_y(y)\Big]\Psi(x,y)$$

$$\Psi(x,y) \;=\; \phi(x)\psi(y) \qquad E \;=\; E_x \;+\; E_y$$

$$E_x\phi(x) \;=\; \hat{H}_x(x)\phi(x)$$
$$E_y\psi(y) \;=\; \hat{H}_y(y)\psi(y)$$

Eigenfunction expansions:

$$\Psi(x,y,t) \;=\; \sum_j \Phi_j(x,y)\; e^{-iE_jt/\hbar}$$

$$E_j\Phi_j(x,y) \;=\; \hat{H}(x,y)\Phi_j(x,y)$$

Classical EM Fields (resonators):

Classical equations:

$$\frac{\partial}{\partial t}\epsilon_0\mathbf{E}(\mathbf{r},t) = \nabla\times\mathbf{H}(\mathbf{r},t)$$

$$\frac{\partial}{\partial t}\mu_0\mathbf{H}(\mathbf{r},t) = -\nabla\times\mathbf{E}(\mathbf{r},t)$$

$$E = \int \frac{1}{2}\epsilon_0|\mathbf{E}(\mathbf{r})|^2 \;+\; \frac{1}{2}\mu_0|\mathbf{H}(\mathbf{r})|^2\; d^3\mathbf{r}$$

Single mode solution:

$$\mathbf{E}(\mathbf{r},t) = e(t)\mathbf{u}(\mathbf{r}) \qquad \mathbf{H}(\mathbf{r},t) = h(t)\mathbf{v}(\mathbf{r})$$

$$\frac{d}{dt}e(t) \;=\; \frac{1}{\epsilon_0}kh(t) \qquad \frac{d}{dt}h(t) \;=\; -\,\frac{1}{\mu_0}ke(t)$$

$$E \;=\; \frac{1}{2}\epsilon_0 e^2(t)\int|\mathbf{u}|^2d^3\mathbf{r} \;+\; \frac{1}{2}\mu_0 h^2(t)\int|\mathbf{v}|^2d^3\mathbf{r}$$

$$\int|\mathbf{u}(\mathbf{r})|^2d^3\mathbf{r} = L^3 \qquad \int|\mathbf{v}(\mathbf{r})|^2d^3\mathbf{r} = L^3$$

Electrons, 3-D square well, continuum limit:

$$g(\epsilon) \;=\; g_s\frac{\pi}{4}\left(\frac{2mL^2}{\hbar^2\pi^2}\right)^{\frac{3}{2}}\epsilon^{\frac{1}{2}}$$

Photons, 3-D cube, continuum limit:

$$g(\epsilon) \;=\; \frac{L^3}{\pi^2\hbar^3c^3}\epsilon^2$$

Basic Thermodynamics:

Basis: "In thermodynamic equilibrium, all accessible microstates are equally probable."

$$\text{Number of accessible microstates} : \Omega$$

$$\text{Entropy} : S \;=\; k_B\ln\Omega$$

$$\frac{1}{T} \;=\; \left(\frac{\partial S}{\partial E}\right)_{N,V}$$

$$\frac{p}{T} \;=\; \left(\frac{\partial S}{\partial V}\right)_{E,N}$$

$$\frac{\mu}{T} \;=\; -\left(\frac{\partial S}{\partial N}\right)_{E,V}$$

First Law:

$$dE \;=\; TdS \;+\; \mu dN \;-\; pdV$$

Ideal gas law:

$$pV \;=\; Nk_BT$$

Level Occupation:

$$\langle Q\rangle \;=\; \sum_m p_m(T)Q_m$$

$$p_m \;=\; \frac{g_m\; e^{-(E_m-\mu N_m)/k_BT}}{\sum_m\; g_m\; e^{-(E_m-\mu N_m)/k_BT}}$$

Fermi-Dirac Statistics:

$$\langle N\rangle \;=\; \frac{1}{1\;+\;e^{(\epsilon-\mu)/k_BT}}$$

Quantum EM Fields:

Single mode:

$$\hat{E}\psi(e,t) \;=\; \frac{1}{2}\epsilon_0L^3\hat{e}^2 \;+\; \frac{1}{2}\mu_0L^3\hat{h}^2$$

$$i\hbar\frac{\partial}{\partial t}\psi(e,t) \;=\; \left[\;-\frac{\hbar^2\omega_0^2}{2\epsilon_0L^3}\frac{\partial^2}{\partial e^2} + \frac{\epsilon_0L^3}{2}e^2\;\right]\psi(e,t)$$

$$\hat{e} \;=\; e \qquad \hat{h} = -i\hbar\frac{\omega_0c}{L^3}\frac{\partial}{\partial e}$$

$$\phi_n(e) \;=\; \left[\frac{\epsilon_0L^3}{\pi\hbar\omega_0}\right]^{1/4}\frac{1}{\sqrt{2^nn!}}\exp\left\{-\frac{\frac{1}{2}\epsilon_0L^3e^2}{\hbar\omega_0}\right\}H_n\left(\sqrt{\frac{\epsilon_0L^3}{\hbar\omega_0}}e\right)$$

$$E_n \;=\; \hbar\omega_0\left[n+\frac{1}{2}\right]$$

$$\hat{H} \;=\; \hbar\omega_0\left[\hat{a}^\dagger\hat{a}+\frac{1}{2}\right]$$

Multi-mode:

$$\hat{H} \;=\; \sum_j\hbar\omega_j\left[\hat{a}_j^\dagger\hat{a}_j+\frac{1}{2}\right]$$

$$\Psi(e_1,e_2,\cdots) \;=\; \phi_{n_1}(e_1)\phi_{n_2}(e_2)\cdots$$

$$E \;=\; \sum_j\hbar\omega_j\left[n_j+\frac{1}{2}\right]$$

Classical EM Fields (free space):

$$\mathbf{E}(\mathbf{r},t) \;=\; \sum_\sigma\sum_{\mathbf{k}}\mathbf{i}_\sigma\left[\,e_{\mathbf{k},\sigma}(t)\;e^{i\mathbf{k}\cdot\mathbf{r}} \;+\; e^*_{\mathbf{k},\sigma}(t)\;e^{-i\mathbf{k}\cdot\mathbf{r}}\,\right]$$

$$\mathbf{H}(\mathbf{r},t) \;=\; \sum_\sigma\sum_{\mathbf{k}}(\mathbf{i}_{\mathbf{k}}\times\mathbf{i}_\sigma)\left[\,h_{\mathbf{k},\sigma}(t)\;e^{i\mathbf{k}\cdot\mathbf{r}} \;+\; h^*_{\mathbf{k},\sigma}(t)\;e^{-i\mathbf{k}\cdot\mathbf{r}}\,\right]$$

with

$$\mathbf{k}\cdot\mathbf{i}_\sigma \;=\; 0$$

By convention, usually take

Bose-Einstein Statistics:

$$\langle N \rangle = \frac{1}{e^{(\epsilon-\mu)/k_BT} - 1}$$

Donor Statistics:

$$\langle N \rangle = \frac{1}{1 + \frac{1}{2} e^{(E_d-\mu)/k_BT}}$$

Grand Partition Function:

$$Z = \sum_m g_m \, e^{-(E_m - \mu N_m)/k_BT}$$

$$\langle N \rangle = k_BT \frac{\partial}{\partial \mu} \ln Z$$

$$\langle E \rangle = k_BT^2 \frac{\partial}{\partial T} \ln Z + \mu \langle N \rangle$$

Blackbody energy density:

$$u = \frac{1}{L^3} \sum_j \frac{\hbar\omega_j}{e^{\hbar\omega_j/k_BT} - 1} = \int_0^\infty \frac{\epsilon^2}{\pi^2\hbar^3c^3} \frac{\epsilon}{e^{\epsilon/k_BT} - 1} \, d$$

Metals:

Determination of Fermi level:

$$n_e = \frac{1}{L^3} \sum_j f_{FD}(\epsilon_j) = \frac{1}{L^3} \int g(\epsilon) \frac{1}{1 + e^{(\epsilon-\mu)/k_BT}} d\epsilon$$

Electrons in a box:

$$\mu(T) = \mu(0) \left[1 - \frac{\pi^2}{12} \left(\frac{k_BT}{\mu(0)} \right)^2 + \cdots \right]$$

Averages near the Fermi surface:

$$\langle \xi \rangle = \int_0^\infty g(\epsilon)\xi(\epsilon) \, f_{FD}(\epsilon) \, d\epsilon$$

$$= \int_0^{E_F} g(\epsilon)\xi(\epsilon) \, d\epsilon + \frac{\pi^2}{6} (k_BT)^2 \left(\frac{d(g\xi)}{d\epsilon} \right)_{E_F} + \cdots$$

Electronic energy density:

$$u = u(0) + \frac{\pi^2}{6L^3} (k_BT)^2 g(E_F) + \cdots$$

Semiconductors:

Density of states near band gap:

$$g_C(\epsilon) = \frac{\pi}{2} \left(\frac{2m_e^* L^2}{\hbar^2\pi^2} \right)^{\frac{3}{2}} (\epsilon - E_C)^{\frac{1}{2}}$$

$$g_V(\epsilon) = \frac{\pi}{2} \left(\frac{2m_h^* L^2}{\hbar^2\pi^2} \right)^{\frac{3}{2}} (E_V - \epsilon)^{\frac{1}{2}}$$

Carrier densities:

$$n = \frac{1}{L^3} \int g_C(\epsilon) \frac{1}{1 + e^{(\epsilon-\mu)/k_BT}} d\epsilon$$

$$\approx N_C(T) \, e^{-(E_C-\mu)/k_BT}$$

$$N_C(T) = 2 \left(\frac{m_e^* kT}{2\pi\hbar^2} \right)^{\frac{3}{2}}$$

$$p = \frac{1}{L^3} \int_{-\infty}^{E_V} g_V(\epsilon) \frac{1}{1 + e^{-(\epsilon-\mu)/k_BT}} d\epsilon$$

$$\approx N_V(T) \, e^{(E_V-\mu)/k_BT}$$

$$N_V(T) = 2 \left(\frac{m_h^* kT}{2\pi\hbar^2} \right)^{\frac{3}{2}}$$

Equilibrium, undoped semiconductor:

$$n(T) = p(T) = n_i(T) = \sqrt{N_C(T)N_V(T)} \, e^{-E_g/2k_BT}$$

Doped semiconductor:

$$N_d^+ + p - n = 0$$

$$N_d \frac{1}{1 + 2\exp[-(E_d - \mu)/k_BT]} + N_V(T) \, e^{(E_V-\mu)/k_BT}$$

$$- N_C(T) \, e^{-(E_C-\mu)/k_BT} = 0$$

$$np = n_i^2 \qquad n \neq p$$

Classical Hydrogen Atom:

Coulomb potential:

$$V(|\mathbf{r}_2 - \mathbf{r}_1) = -\frac{e^2}{4\pi\epsilon_0|\mathbf{r}_2 - \mathbf{r}_1|}$$

Newton's laws:

$$\frac{d\mathbf{r}_1}{dt} = \frac{\mathbf{p}_1}{m_1} \qquad \frac{d\mathbf{r}_2}{dt} = \frac{\mathbf{p}_2}{m_2}$$

$$\frac{d\mathbf{p}_1}{dt} = -\nabla_1 V \qquad \frac{d\mathbf{p}_2}{dt} = -\nabla_2 V$$

Energy:

$$E = \frac{|\mathbf{p}_1|^2}{2m_1} + \frac{|\mathbf{p}_2|^2}{2m_2} + V(|\mathbf{r}_2 - \mathbf{r}_1)$$

Coordinate transformation:

$$\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1 \qquad \mathbf{R} = \frac{m_1}{M}\mathbf{r}_1 + \frac{m_2}{M}\mathbf{r}_2$$

$$\mathbf{p} = \frac{\mu}{m_2}\mathbf{p}_2 - \frac{\mu}{m_1}\mathbf{p}_1 \qquad \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$$

Newton's laws, center of mass, relative coordinates:

$$\frac{d\mathbf{r}}{dt} = \frac{\mathbf{p}}{\mu} \qquad \frac{d\mathbf{R}}{dt} = \frac{\mathbf{P}}{M}$$

$$\frac{d\mathbf{p}}{dt} = -\nabla V(|\mathbf{r}|) \qquad \frac{d\mathbf{P}}{dt} = 0$$

Energy:

$$E = \frac{|\mathbf{P}|^2}{2M} + \frac{|\mathbf{p}|^2}{2\mu} + V(|\mathbf{r}|)$$

Angular momentum:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \qquad \frac{d}{dt}\mathbf{L} = 0$$

Newton's laws for the radial coordinate:

$$\mu \frac{dr}{dt} = p$$

$$\frac{dp}{dt} = -\frac{d}{dr} \left[V(r) + \frac{|\mathbf{L}|^2}{2\mu r^2} \right]$$

Energy associated with relative motion:

$$E = \frac{p^2}{2\mu} + V(r) + \frac{|\mathbf{L}|^2}{2\mu r^2}$$

Quantum Hydrogen Atom:

Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}_1, \mathbf{r}_2, t)$$

$$= \left[-\frac{\hbar^2\nabla_1^2}{2m_1} - \frac{\hbar^2\nabla_2^2}{2m_2} - \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_2 - \mathbf{r}_1|} \right] \Psi(\mathbf{r}_1, \mathbf{r}_2, t)$$

Eigenfunction expansion:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \sum_j c_j \, e^{-iE_jt/\hbar} \, \Phi_j(\mathbf{r}_1, \mathbf{r}_2)$$

$$E_j \Phi_j(\mathbf{r}_1, \mathbf{r}_2)$$

$$= \left[-\frac{\hbar^2\nabla_1^2}{2m_1} - \frac{\hbar^2\nabla_2^2}{2m_2} - \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_2 - \mathbf{r}_1|} \right] \Phi_j(\mathbf{r}_1, \mathbf{r}_2)$$

Center of mass, relative coordinate separation:

$$E\Phi(\mathbf{r}, \mathbf{R}) = \left[-\frac{\hbar^2\nabla_{\mathbf{R}}^2}{2M} - \frac{\hbar^2\nabla_{\mathbf{r}}^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0|\mathbf{r}|} \right] \Phi(\mathbf{r}, \mathbf{R})$$

$$\Phi(\mathbf{r}, \mathbf{R}) = e^{i\mathbf{K}\cdot\mathbf{R}}$$

$$E = \frac{\hbar^2|\mathbf{K}|^2}{2M} + E_r$$

Relative problem ($\mathbf{K} = 0$)

$$E\psi(\mathbf{r}) = \left[-\frac{\hbar^2\nabla^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0|\mathbf{r}|} \right] \psi(\mathbf{r})$$

Ground state solution:

$$\psi_{1s}(\mathbf{r}) = \frac{1}{\sqrt{\pi a_\mu^3}} e^{-r/a_\mu}$$

$$\frac{1}{a_\mu} = \frac{\mu e^2}{4\pi\epsilon_0\hbar^2} = \frac{\mu}{m_e} \frac{1}{a_0}$$

$$E_{1s} = -\frac{\mu e^4}{32\pi^2\epsilon_0^2\hbar^2} = -\frac{\mu}{m_e} I_H = -I_\mu$$

Hydrogen constants:

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = 0.529 \text{ Å}$$

$$I_H = \frac{m_e e^4}{32\pi^2\epsilon_0^2\hbar^2} = 13.6058 \text{ eV}$$

Radial and Angular Separation:

$$|\hat{\mathbf{p}}|^2 = -\hbar^2\nabla^2 = \hat{p}^2 + \frac{|\hat{\mathbf{L}}|^2}{r^2}$$

$$\hat{p}^2 = -\hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$$

$$|\hat{\mathbf{L}}|^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

Schrodinger equation:

$$E\psi(r, \theta, \phi) = \left[\frac{\hat{p}^2}{2\mu} + \frac{|\hat{\mathbf{L}}(\theta, \phi)|^2}{2\mu r^2} + V(r) \right] \psi(r, \theta, \phi)$$

Separated solutions:

$$\psi_{nlm}(r, \theta, \phi) = \frac{P(r)}{r} Y_{lm}(\theta, \phi)$$

Spherical harmonics:

$$|\hat{\mathbf{L}}(\theta, \phi)|^2 Y_{lm}(\theta, \phi) = \hbar^2 l(l+1) Y_{lm}(\theta, \phi)$$

$$Y_{lm}(\theta, \phi) = (-1)^{m+|m|/2} \left[\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!} \right]^{\frac{1}{2}} P_l^{|m|}(\cos\theta) \, e^{im\phi}$$

$$\langle Y_{lm} | Y_{l'm'} \rangle = \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin\theta \, Y_{lm}^*(\theta, \phi) \, Y_{l'm'}(\theta, \phi) = \delta_{ll'}\delta_{mm'}$$

l	m	$Y_{lm}(\theta, \phi)$	x, y, z-representation
0	0	$\frac{1}{\sqrt{4\pi}}$	$\frac{1}{\sqrt{4\pi}}$
1	0	$\sqrt{\frac{3}{4\pi}} \cos\theta$	$\sqrt{\frac{3}{4\pi}} \frac{z}{r}$
1	± 1	$\mp\sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi}$	$\mp\sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$
2	0	$\sqrt{\frac{5}{16\pi}} (2\cos^2\theta - \sin^2\theta)$	$\sqrt{\frac{5}{16\pi}} \frac{2z^2 - x^2 - y^2}{r^2}$
2	± 1	$\mp\sqrt{\frac{15}{8\pi}} \sin\theta\cos\theta e^{\pm i\phi}$	$\mp\sqrt{\frac{15}{8\pi}} \frac{z(x \pm iy)}{r^2}$
2	± 2	$\sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\phi}$	$\sqrt{\frac{15}{32\pi}} \frac{(x \pm iy)^2}{r^2}$

Final 2017 Problem 3 12/12/19

Quantum system in thermal equilibrium with an infinite reservoir under conditions where energy is exchanged but not particles or volume

$$P_j(T) = \frac{\Omega_j e^{-E_j/k_BT}}{\sum_k \Omega_k e^{-E_k/k_BT}}$$

thermal expectation value of a quantity $Q_j = Q(E_j)$ is then

$$\langle\langle Q\rangle\rangle = \frac{\sum_j Q_j \Omega_j e^{-E_j/k_BT}}{\sum_j \Omega_j e^{-E_j/k_BT}}$$

Suppose an infinite thermal reservoir is not available, & the quantum system must make due with a distinctly finite reservoir made of an ideal gas.

a) Find an expression for T_j by expanding the entropy to second order. In this case the occupation probability can be written as:

$$P_j(T) = \frac{\Omega_j e^{-E_j/k_BT_j}}{\sum_k \Omega_k e^{-E_k/k_BT_k}}$$

where the occupation probability is reduced due to a loss of energy from the reservoir. Find an expression for T_j in terms of the

$$P_1(N_1, E_1, V_1) = \frac{\Omega_1(N_1, E_1, V_1)\Omega_R(N-N_1, E-E_1, V-V_1)}{\sum_{E_1'} \Omega_1(N_1, E_1', V_1)\Omega_R(N-N_1, E-E_1', V-V_1)}$$

if we suppress the number & volume part of the problem:

$$P_1(E_1) = \frac{\Omega_1(E_1)\Omega_R(E-E_1)}{\sum_{E_1'} \Omega_1(E_1')\Omega_R(E-E_1')}$$

We can use a Taylor series approximation to second order to write

$$S_R(E-E_1) = S_R(E) - E_1\left(\frac{dS_R}{dE}\right)_E + \frac{1}{2}E_1^2\left(\frac{d^2S_R}{dE^2}\right)_E$$

We make use of Sackur-Tetrode entropy for ideal gas:

$$S_{ST}(N,E,V) = Nk_B\left\{\frac{3}{2}\ln\frac{E}{N} - \ln\frac{N}{V} + \frac{3}{2}\ln\frac{M}{3\pi\hbar^2} + \frac{5}{2}\right\}$$

$$\boxed{\text{remember } \frac{d}{dx}\ln(x) = \frac{1}{x}}$$

$$\left(\frac{\partial S_{ST}}{\partial E}\right)_{N,V} = \frac{3}{2}\frac{Nk_B}{E} \qquad \left(\frac{\partial^2 S_{ST}}{\partial E^2}\right)_{N,V} = -\frac{3}{2}\frac{Nk_B}{E^2}$$

$$E = \frac{3}{2}Nk_BT \Rightarrow \left(\frac{\partial S_{ST}}{\partial E}\right)_{N,V} = \frac{1}{T} \qquad \left(\frac{\partial^2 S_{ST}}{\partial E^2}\right)_{N,V} = -\frac{3}{2}\frac{Nk_B}{(\frac{3}{2}Nk_BT)^2} = -\frac{2}{3}\frac{1}{Nk_BT^2}$$

$$S_R(E-E_1) = S_R(E) - \frac{E_1}{T} - \frac{1}{3}\frac{E_1^2}{Nk_BT^2}$$

$$P_1(E_1) = \frac{\Omega_1(E_1)\exp\left\{\frac{-E_1}{k_BT} - \frac{1}{3}\frac{E_1^2}{N(k_BT)^2}\right\}}{\sum_{E_1'}\Omega_1(E_1')\exp\left\{\frac{-E_1'}{k_BT} - \frac{1}{3}\frac{(E_1')^2}{N(k_BT)^2}\right\}} \qquad \Omega_R = e^{S_R/k_B}$$

For this to be written in the form specified, we require:

$$\frac{E_j}{k_BT_j} = \frac{E_j}{k_BT} + \frac{1}{3}\frac{E_j^2}{N(k_BT)^2} \qquad \frac{1}{T_j} = \frac{1}{T} + \frac{1}{3}\frac{E_j}{Nk_BT} = \frac{1}{T}\left(1 + \frac{1}{3}\frac{E_j}{Nk_BT}\right)$$

$$T_j = \frac{T}{1 + \frac{1}{3}\frac{E_j}{Nk_BT}}$$

b) Find an expression for the occupation probability $P_j(T)$ based on the Sackur-Tetrode entropy directly.

$$P_1(E_1) = \frac{\Omega_1(E_1)\Omega_R(E-E_1)}{\sum_{E_1'}\Omega_1(E_1')\Omega_R(E-E_1')}$$

$$\Omega_R(E,V) = e^{S_{ST}(N,E,V)} = \exp\left\{N\left[\frac{3}{2}\ln\frac{E}{N} - \ln\frac{N}{V} + \frac{3}{2}\ln\frac{M}{3\pi\hbar^2} + \frac{5}{2}\right]\right\}$$

$$= \left(\frac{E}{N}\right)^{3N/2}\left(\frac{V}{N}\right)^N\left(\frac{M}{3\pi\hbar^2}\right)^{3N/2}\left(\frac{5}{2}\right)^N$$

for a specific level j: We can use this to write:

$$P_1(E_1) = \frac{\Omega_1(E_1)(E-E_1)^{3N/2}}{\sum_{E_1'}\Omega_1(E_1')(E-E_1')^{3N/2}} \quad \text{or} \quad P_j = \frac{\Omega_j(\frac{3}{2}Nk_BT - E_j)^{3N/2}}{\sum_k \Omega_k(\frac{3}{2}Nk_BT - E_k)^{3N/2}}$$

Pset 13 Question 1 12/16/19

Modeling the absorption of He into a small metal sample. Identical He atoms, K absorption sites in metal. Absorption energy: ΔE where $+\Delta E$ means energy is required for helium to go into solid.

$$\Omega(N,E,V) = \sum_{N_1,E_1,V_1} \Omega_1(N_1,E_1,V_1)\,\Omega_2(N-N_1, E-E_1, V-V_1)$$

Hint: $\frac{\theta}{1-\theta} = p f(T)$

For the helium atom in the gas phase, we can estimate # of accessible micro states using Sackur-Tetrode ideal gas entropy:

$$\Omega_2(N_2,E_2,V_2) = N_2 k_B \left\{ \frac{3}{2}\ln\frac{E_2}{N_2} - \ln\frac{N_2}{V_2} + \frac{3}{2}\ln\frac{M}{3\pi\hbar^2} + \frac{5}{2} \right\}$$

We assume pressure is small so volume change ~~can~~ is negligible

---

a) Use ~~a~~ the model to find a general expression for probability that the metals contains exactly N_1 helium atoms.

$$P_1(N_1) = \frac{\Omega_1(N_1,E_1,V_1)\,\Omega_2(N-N_1, E-E_1, V-V_1)}{\sum_{N_1'}\sum_{E_1}\sum_{V_1} \Omega_1(N_1', E_1, V_1)\,\Omega_2(N-N_1', E-E_1, V-V_1)}$$

$$= \frac{\Omega_1(N_1)\,\Omega_2(N-N_1, E-N_1\Delta E)}{\sum_{N_1'} \Omega_1(N_1')\,\Omega_2(N-N_1', E-N_1'\Delta E)}$$

b) Find a specific formula for probability there are N_1 absorbed helium atoms in terms of gas temperature T & chemical potential μ of helium in the gas.

$$S_{ST}(N-N_1, E-N_1\Delta E, V) = S_{ST}(N,E,V) - N_1\underbrace{\left(\frac{\partial S_T}{\partial N}\right)_{E,V}}_{=-\frac{\mu}{T}} - N_1\Delta E\underbrace{\left(\frac{\partial S_T}{\partial E}\right)_{N,V}}_{=\frac{1}{T}} + \ldots$$

(This is because $f(x_0+\delta x) = f(x_0) + \delta x\left(\frac{df}{dx}\right)_{x_0} + \frac{1}{2}\delta x^2\left(\frac{d^2f}{dx^2}\right)_{x_0} + \ldots$)

$$\longrightarrow S_T(N,E,V) + N_1'\frac{\mu}{T} - N_1'\frac{\Delta E}{T}$$

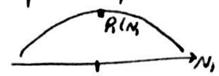
$$\Omega_2(N_2,E_2,V_2) = e^{\left[-\frac{N_1(\Delta E-\mu)}{k_BT} + \frac{S_2(N,E,V)}{k_B}\right]} = \Omega_2(N,E,V)\,e^{-\frac{N_1(\Delta E-\mu)}{k_BT}}$$

$$p = \frac{\Omega_1(N_1)\,\cancel{\Omega_2(N,E,V)}\,e^{-N_1(\Delta E-\mu)/k_BT}}{\sum_{N_1}\Omega_1(N_1')\,\cancel{\Omega_2(N,E,V)}\,e^{-N_1'\frac{\Delta E-\mu}{k_BT}}} = \frac{\Omega_1(N_1)\,e^{-N_1(\Delta E-\mu)/k_BT}}{\sum_{N_1'}\Omega_1(N_1')\,e^{-N_1'(\Delta E-\mu)/k_BT}}$$

$$= \boxed{\frac{\binom{K}{N_1}\exp\left\{-N_1\frac{\Delta E-\mu}{k_BT}\right\}}{\sum_{N_1'}\binom{K}{N_1'}\exp\left\{-N_1'\frac{\Delta E-\mu}{k_BT}\right\}}}$$

c) Determine N_1 that corresponds to the most probable state of the combined system. Express answer in terms of μ & θ defined by $\theta = \frac{N_1}{K}$

Hint: Solve for $p(N_1) = p(N_1+1)$



$$\frac{\partial}{\partial N_1}P_1(N_1) = 0$$

$$P_1(N_1) = p(N_1+1)$$

$$\Omega_1(N_1)\,e^{-N_1(\Delta E-\mu)/k_BT} = \Omega_1(N_1+1)\,e^{\left(-(N_1+1)\frac{\Delta E-\mu}{k_BT}\right)}$$

$$\Longrightarrow e^{\frac{\Delta E-\mu}{k_BT}} = \frac{\binom{K}{N_1+1}}{\binom{K}{N_1}} = \frac{K-N_1}{N_1+1} \qquad \text{assume } N_1 \gg 1 \Rightarrow \theta = \frac{N_1}{K}$$

$$(N_1+1) = (K-N_1)\exp\left\{-\frac{\Delta E-\mu}{k_BT}\right\} \qquad \theta = \frac{N_1}{K} \qquad \frac{\theta}{1-\theta} = \exp\left\{-\frac{\Delta E-\mu}{k_BT}\right\}$$

(this is an absorption isotherm written in terms of chemical potential)

d) Evaluate the chemical potential of the ideal gas to find an expression for the absorbed fraction θ as a function of gas pressure & temp

$$\frac{-\mu}{T} = \left(\frac{\partial S_{ST}}{\partial N}\right)_{E,V} = k_B\left\{\frac{3}{2}\ln\frac{E}{N} - \ln\frac{N}{V} + \frac{3}{2}\ln\frac{M}{3\pi\hbar^2} + \frac{5}{2}\right\} - \frac{3}{2}k_B - k_B$$

$$\frac{E}{N} \to \frac{3}{2}k_BT \quad \frac{N}{V} \to \frac{p}{k_BT} \Rightarrow \quad = k_B\left\{\frac{3}{2}\ln\frac{E}{N} - \ln\frac{N}{V} + \frac{3}{2}\ln\frac{M}{3\pi\hbar^2}\right\}$$

$$= k_B\left\{\frac{3}{2}\ln\left(\frac{Mk_BT}{2\pi\hbar^2}\right) - \ln\left(\frac{p}{k_BT}\right)\right\}$$

$$\exp\left\{-\frac{\mu}{k_BT}\right\} = \left(\frac{Mk_BT}{2\pi\hbar^2}\right)^{3/2}\left(\frac{p}{k_BT}\right)^{-1} \qquad \frac{\theta}{1-\theta} = \exp\left\{-\frac{\Delta E}{k_BT}\right\}\left(\frac{2\pi\hbar^2}{Mk_BT}\right)^{3/2}\left(\frac{p}{k_BT}\right)$$

Pset 12 Problem 1 12/13/19

Two systems in equilibrium at diff. temperatures T_1 & T_2, pressures p_1 & p_2, & potentials μ_1 & μ_2. They are then brought into contact with each other, & allowed to exchange energy, volume, & particles.

→ Does the entropy of the total system increase, decrease, or stay the same during the contact & subsequent equilibration?

total # of accessible microstates initially

$$\Omega_{before}(N, E, V) = \Omega_1(N_1, E_1, V_1)\,\Omega_2(N_2, E_2, V_2)$$

$N = N_1 + N_2$ $\quad E = E_1 + E_2$ $\quad V = V_1 + V_2$

$$\Omega_{after}(N, E, V) = \sum_{N_1}\sum_{E_1}\sum_{V_1}\Omega_1(N_1, E_1, V_1)\,\Omega_2(N-N_1, E-E_1, V-V_1)$$

We can see that the before state is going to be one of the terms in the summation for the number of accessible microstates after they are combined. Since the entropy is:

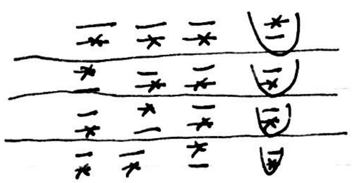
$$S = K_B \ln \Omega$$

by argument, we expect the entropy to increase, but it is possible for the # of accessible microstates to remain the same in special cases.

Pset 12 problem 4 12/13/19

a) Reservoir contains 3 two-level systems, one unit of energy $E = \hbar\omega_0$ above ground state for oscillator & 2-level system.

Compare the excitation probability p_n of the states of the oscillator.



n	Ω
0	1
1	3

$\Omega_0 = \binom{3}{0} = 1$ ⇒ excited state in oscillator

$\Omega_1 = \binom{3}{1} = 3$ ⇒ not excited state in oscillator

$P_0 = \frac{\Omega_1}{\Omega_0 + \Omega_1} = \frac{3}{4}$ $\quad P_1 = \frac{\Omega_0}{\Omega_0 + \Omega_1} = \frac{1}{4}$

b) Now reservoir contains seven 2-level systems. Two units of energy $E = 2\hbar\omega_0$ ~~Compare excitation~~ above ground state for oscillator & 2-level system. Compare excitation probability p_n of the states of the oscillator.

$\Omega_0 = 1$ (all are in oscillator) $\quad \Omega_1 = \binom{7}{1} = 7$ (1 in oscillator) $\quad \Omega_2 = \binom{7}{2} = 21$ (0 in oscillator)

$P_2 = \frac{\Omega_0}{\Omega_0 + \Omega_1 + \Omega_2} = \frac{1}{29}$ $\quad P_1 = \frac{\Omega_1}{\Omega_0 + \Omega_1 + \Omega_2} = \frac{7}{29}$ $\quad P_0 = \frac{\Omega_2}{\Omega_0 + \Omega_1 + \Omega_2} = \frac{21}{29}$

c) Estimate the temperature T associated with the reservoir when the oscillator is in the ground state for configurations described in part a & part b.

Recall for a very large reservoir, we would expect:

$$\frac{P_1}{P_0} = e^{-\hbar\omega_0/K_BT}$$

pt. a) $\frac{1/4}{3/4} = \frac{1}{3} = e^{-\hbar\omega_0/K_BT}$

pt. b) $\frac{7/29}{21/29} = \frac{1}{3} = e^{-\hbar\omega_0/K_BT}$

$$\ln\left(\tfrac{1}{3}\right) = -\hbar\omega_0/K_BT \rightarrow \frac{\hbar\omega_0}{\ln(3)K_B} = T$$

d) If the total energy $E = m\hbar\omega_0$ is present in $4m-1$ two-level systems estimate the temperature according to:

$$\frac{1}{T} = \frac{\partial S}{\partial E} = K_B\frac{\partial}{\partial E}\ln\Omega \approx K_B\left[\frac{\ln\Omega(n=0) - \ln\Omega(n=1)}{\hbar\omega_0}\right]$$

$\Omega(n=m) = \binom{4m-1}{m}$ $\quad \frac{P_1}{P_0} = \frac{\Omega_{m-1}}{\Omega_m}$

$\Omega(n=m-1) = \binom{4m-1}{m-1}$

$$\ln\left(\frac{\Omega_m}{\Omega_{m-1}}\right) = \ln\left(\frac{\binom{4m-1}{m}}{\binom{4m-1}{m-1}}\right) = \frac{\hbar\omega_0}{K_BT} \Rightarrow K_BT = \frac{\hbar\omega_0}{\ln 3}$$

e) Fill in entries in the following table

Ratio	3 two-level	7 two-level	$4m-1$ two-level	Infinite reservoir
P_1/P_0	1/3	1/3	1/3	1/3
P_2/P_1	0	1/7	$\frac{\binom{4m-1}{m-2}}{\binom{4m-1}{m-1}} = \frac{m-1}{3m+1}$	1/3

The ratio P_2/P_1 is less than 1/3 because the reservoir is depleted, & hence the temperature is lower, the more energy goes into the oscillator.

Final 2018 Problem 4 12/16/19

At low temp. rare gas atoms can form weak bonds associated with Van der Waals interaction. For He & Ne, body so weak $l=0$ ground state of HeNe molecule is bound, but none of rotational states $l>0$ are bound.

→ in this problem, we are interested in developing an isotherm for formation of HeNe ground state dimer.

total # of accessible microstates:

volume is fixed. binding energy of HeNe is ΔE

$$\Omega(N_{He}, N_{Ne}, E, V) =$$

$$\sum_{N_1}\sum_{E_1}\sum_{E_2} \Omega_{HeNe}(N_1, E_1 + N_1\Delta E, V)\,\Omega_{He}(N_{He}-N_1, E_2, V)\,\Omega_{Ne}(N_{Ne}-N_1, E-E_1-E_2, V)$$

a) Show constraints from finding most probable configuration is consistent with: $T_{He} = T_{Ne} = T_{HeNe}$ and: $\mu_{HeNe} = \text{constant} + \mu_{He} + \mu_{Ne}$

Find the constant value.

optimize by N_1. Also optimize by E_1

$$\frac{\partial}{\partial N_1}\left(\Omega_{HeNe}(N_1, E_1+N_1\Delta E, V)\,\Omega_{He}(N_{He}-N_1, E_2, V)\,\Omega_{Ne}(N_{Ne}-N_1, E-E_1-E_2, V)\right)_{E_1,E_2,V} = 0$$

by chain rule:

$$\Rightarrow \left(\frac{\partial}{\partial N_1}\Omega_{HeNe}(N_1, E_1+N_1\Delta E, V)\right)_{E,V}\Omega_{He}(N_{He}-N_1, E_2, V)\,\Omega_{Ne}(N_{Ne}-N_1, E-E_1-E_2, V)$$

$$+\,\Omega_{HeNe}(N_1, E, V)\left(\frac{\partial}{\partial N_1}\Omega_{He}(N_{He}+N_1, E_2, V)\right)_{E_2,V}(\ldots \text{ too lazy to write here}) = 0$$

$$= \left(\frac{\partial}{\partial N_1}\ln\Omega_{HeNe}(N_1, E_1+N_1\Delta E, V)\right)_{E_1,V} + \left(\frac{\partial}{\partial N_1}\ln\Omega_{He}(N_{He}-N_1, E_2, V)\right)_{E_2,V} + \left(\frac{\partial}{\partial N_1}\ln\Omega_{Ne}(N_{Ne}-N_1, E-E_1-E_2, V)\right)_{E_1,E_2,V} = 0$$

$$= \left(\frac{\partial}{\partial N_1}S_{HeNe}(N_1, E_1+N_1\Delta E, V)\right)_{E_1,V} + \left(\frac{\partial}{\partial N_1}S_{He}(N_{He}-N_1, E_2, V)\right)_{E_2,V} + \left(\frac{\partial}{\partial N_1}\ln\Omega_{Ne}(N_{Ne}-N_1, E-E_1-E_2, V)\right)_{E_1,E_2,V} = 0$$

$$\frac{-\mu_{HeNe}}{T_{HeNe}} + \frac{\Delta E}{T_{HeNe}} + \frac{\mu_{He}}{T_{He}} + \frac{\mu_{Ne}}{T_{Ne}} = 0$$

Optimize by E_1: $\frac{\partial}{\partial E_1}(\ldots) = 0$ } gets you $\frac{1}{T_{HeNe}} = \frac{1}{T_{Ne}}$

Optimize by E_2: $\frac{\partial}{\partial E_2}(\ldots) = 0$ } gets you $\frac{1}{T_{HeNe}} = \frac{1}{T_{He}}$

$$\Rightarrow \boxed{\mu_{HeNe} = \Delta E + \mu_{He} + \mu_{Ne}}$$

b) Make use of the ideal gas chemical potential to derive an isotherm for molecular HeNe. The isotherm shall be of the form:

$$\frac{n_{HeNe}}{n_{He}n_{Ne}} = F(T, M_{He}, M_{Ne}, M_{HeNe}) \quad \text{where } n_{He} = \frac{N_{He}}{V}\quad n_{Ne} = \frac{N_{Ne}}{V}\quad n_{HeNe} = \frac{N_{HeNe}}{V}$$

Chemical potential from Sakur-Tetrode entropy:

$$\frac{-\mu}{k_BT} = \frac{3}{2}\ln\frac{E}{N} - \ln\frac{N}{V} + \frac{3}{2}\ln\frac{M}{3\pi\hbar^2}$$

$$\Rightarrow -k_BT\left[\frac{3}{2}\ln\frac{E_{HeNe}}{N_{HeNe}} - \ln\frac{N_{HeNe}}{V} + \frac{3}{2}\ln\frac{M_{HeNe}}{3\pi\hbar^2}\right] = \Delta E - k_BT\left[\frac{3}{2}\ln\frac{E_{He}}{N_{He}} - \ln\frac{N_{He}}{V} + \frac{3}{2}\ln\frac{M_{He}}{3\pi\hbar^2}\right] - k_BT\left[\frac{3}{2}\ln\frac{E_{Ne}}{N_{Ne}} - \ln\frac{N_{Ne}}{V} + \frac{3}{2}\ln\frac{M_{Ne}}{3\pi\hbar^2}\right]$$

plug in $E = \frac{3}{2}Nk_BT$, we get: $\frac{3}{2}\ln\left(\frac{3}{2}k_BT\right) - \ln n_{HeNe} + \frac{3}{2}\ln\frac{M_{HeNe}}{3\pi\hbar^2}$

$$= \frac{-\Delta E}{k_BT} + \frac{3}{2}\ln\left(\frac{3}{2}k_BT\right) - \ln n_{He} + \frac{3}{2}\ln\frac{M_{He}}{3\pi\hbar^2} + \frac{3}{2}\ln\left(\frac{3}{2}k_BT\right) - \ln n_{Ne} + \frac{3}{2}\ln\frac{M_{Ne}}{3\pi\hbar^2}$$

Simplified to: $\frac{\Delta E}{k_BT} + \frac{3}{2}\ln\frac{3\pi\hbar^2 M_{HeNe}}{M_{He}M_{Ne}} = \ln\frac{n_{HeNe}}{n_{He}n_{Ne}} + \frac{3}{2}\ln\left(\frac{3}{2}k_BT\right)$

$$\exp\left\{\frac{\Delta E}{k_BT}\right\}\left(\frac{3\pi\hbar^2 M_{HeNe}}{M_{He}M_{Ne}}\right)^{3/2} = \frac{n_{HeNe}}{n_{He}n_{Ne}}\left(\frac{3}{2}k_BT\right)^{3/2}$$

Rewritten as: $\frac{n_{HeNe}}{n_{He}n_{Ne}} = \exp\left\{\frac{\Delta E}{k_BT}\right\}\left(\frac{3\pi\hbar^2 M_{HeNe}}{M_{He}M_{Ne}}\right)^{3/2}\left(\frac{3}{2}k_BT\right)^{-3/2} = \left(\frac{2\pi\hbar^2 M_{HeNe}}{M_{He}M_{Ne}k_BT}\right)^{3/2}\exp\left\{\frac{\Delta E}{k_BT}\right\}$

Pset 11 Problem 2

$$\hat{H}(x,y,z) = \hat{H}_x(x) + \hat{H}_y(y) + \hat{H}_z(z)$$

a) show density of states is of form:

$$g(E) = (g_x * g_y * g_z)(E)$$

$$E = E_x + E_y \qquad g(E) = \int_{-\infty}^{\infty}dE_x\int_{-\infty}^{\infty}dE_y\left\{g_x(E_x)\,g_y(E_y)\,\delta(E_x+E_y-E)\right\}$$

$$= \underbrace{\int_{-\infty}^{\infty} g_x(E-E_y)\,g_y(E_y)\,dE_y = (g_x \otimes g_y)(E)}_{\text{definition of convolution}}$$

For 3D,

$$g(E) = \int_{-\infty}^{\infty}dE_x\int_{-\infty}^{\infty}dE_y\int_{-\infty}^{\infty}dE_z\left\{g_x(E_x)\,g_y(E_y)\,g(E_z)\,\delta(E_x+E_y+E_z-E)\right\}$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g_x(E-E_y-E_z)\,g_y(E_y)\,g_z(E_z)\,dE_y\,dE_z$$

$$= \int_{-\infty}^{\infty}(g_x\otimes g_y)(E-E_z)\,g_z(E_z)\,dE_z = (g_x\otimes g_y\otimes g_z)(E)$$

b) determine density of states for a cubic 3D square well by using 1D density of states & convolutions.

$$g_x(E) = \begin{cases} 0 & E<0 \\ \sqrt{\frac{mL^2}{2\hbar^2\pi^2 E_x}} & 0<E_x \end{cases}$$

$\Rightarrow$ 2D density of states: $(g_x\otimes g_y)(E) = \int_{-\infty}^{\infty} g_x(E-E_y)\,g_y(E_y)\,dE_y$

$$= \int_0^E\sqrt{\frac{mL^2}{2\hbar^2\pi^2(E-E_y)}}\sqrt{\frac{mL^2}{2\hbar^2\pi^2E_y}}\,dE_y = \frac{mL^2}{2\hbar^2\pi^2}\int_0^E\frac{1}{\sqrt{E_y(E-E_y)}}\,dE_y = \frac{mL^2}{2\hbar^2\pi}$$

$$g(E) = \int_{-\infty}^{\infty}(g_x\otimes g_y)(E-E_z)\,g_z(E_z)\,dE_z = \int_0^E\frac{mL^2}{2\hbar^2\pi}\sqrt{\frac{mL^2}{2\hbar^2\pi^2E_z}}\,dE_z = \left(\frac{mL^2}{2\hbar^2\pi^2}\right)^{3/2}\pi\int_0^E\frac{1}{\sqrt{E_z}}\,dE_z$$

$$= \frac{\pi}{4}\left(\frac{2mL^2}{\hbar^2\pi^2}\right)^{3/2}\sqrt{E}$$

c) density of states (in the continuum approximation) associated with the Hamiltonian in three dimensions $\hat{H} = \frac{|\hat{p}|^2}{2m} + \frac{1}{2}m\omega_0^2(x^2+y^2)$

$$g_x(E) = g_y(E) = \frac{1}{\hbar\omega_0} \qquad (g_x\otimes g_y)(E) = \int_0^E\frac{1}{(\hbar\omega_0)^2}\,dE_y = \frac{E}{(\hbar\omega_0)^2}$$

$$g_z(E_z) = 2\frac{dn}{dE} = \sqrt{\frac{mL^2}{\hbar^2 2\pi^2 E_z}} \qquad E_n = \frac{\hbar^2k_n^2}{2m} \qquad k_n = \frac{2\pi n}{L} \quad n = 0, \pm1, \pm2$$

$$g(E) = \int_{-\infty}^{\infty}(g_x\otimes g_y)(E-E_z)\,g_z(E_z)\,dE_z \qquad E_n = \frac{\hbar^2(2\pi)^2}{2mL^2}n^2$$

$$= \int_0^E\frac{E-E_z}{(\hbar\omega_0)^2}\sqrt{\frac{mL^2}{2\hbar^2\pi^2E_z}}\,dE_z = \frac{1}{(\hbar\omega_0)^2}\sqrt{\frac{mL^2}{2\hbar^2\pi^2}}\,\frac{4}{3}E^{3/2} \qquad dE = \frac{\hbar^2(2\pi)^2}{2mL^2}2n\,dn$$

Final 2018 Question 1 12/11/19

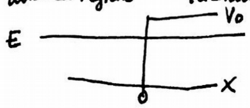
A particle is incident on a finite barrier & reflects.

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) \qquad \text{where } E<V_0$$

$$V(x) = \begin{cases} 0 & x<0 \\ V_0 & 0<x \end{cases} \qquad \psi(x) = \begin{cases} e^{ikx} + re^{-ikx} & x<0 \\ Ae^{-\beta x} & 0<x \end{cases}$$

a) Determine k & β in terms of the model parameters.

allowed regions forbidden regions



$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \beta = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

b) Find expressions for coefficients r & A.

$\psi^{I} = \psi^{II}$ at $x=0$ $\Rightarrow e^{ikx} + re^{-ikx} = Ae^{-\beta x} \Rightarrow 1+r = A$

$\psi'_{I}(0) = \psi'_{II}(0) \quad ike^{ikx} - ikre^{-ikx} = -\beta Ae^{-\beta x} \Rightarrow ik(1-r) = -\beta A$

$1+r = \frac{ik(1-r)}{-\beta} \quad \cancel{\frac{1+r}{1-r} = \frac{ik}{-\beta}} \quad 1+r = \frac{ik-ikr}{-\beta} \quad -\beta - \beta r = ik - ikr \Rightarrow \boxed{r = \frac{ik+\beta}{ik-\beta}}$

$A - 1 = \frac{-\beta A - ik}{-ik} \quad -Aik + ik = -\beta A - ik \Rightarrow A = \frac{-2ik}{\beta - ik} = \boxed{\frac{2ik}{ik-\beta}}$

c) We are interested in when barrier height could be determined from low energy measurements where $E \ll V_0$. Sol'n can be written as:

$$|\psi(x)|^2\big|_{x<0} \rightarrow = 4\sin^2\left(kx - \frac{\theta}{2}\right) \qquad \frac{\theta}{2} \text{ is a phase shift}$$

Find expression for $\theta/2$ in terms of E & V_0 when $E \ll V_0$

* Recall that:

$1 - \cos(2a) = 2\sin^2(a)$

$\frac{1+\epsilon}{1-\epsilon} = 1 + 2\epsilon + 2\epsilon^2 + \ldots$

Reflection always occurs: $R = |r|^2 = 1$

$$|\psi(x)|^2\big|_{x<0} = |e^{ikx} + re^{-ikx}|^2 = (e^{-ikx} + r^*e^{ikx})(e^{ikx} + re^{-ikx})$$
$$= 2 + r^*e^{2ikx} + re^{-2ikx}$$

If $E \ll V_0$, then $\beta \gg k$.

$$\Rightarrow r = \frac{-\beta + ik}{\beta - ik} \rightarrow -\left(1 + 2i\frac{k}{\beta} + \ldots\right)$$

interpretted as phase shift:

$r \rightarrow -e^{i\theta} = -(1 + i\theta + \ldots)$

with $\theta = 2\frac{k}{\beta}$

$$|\psi(x)|^2\big|_{x<0} \rightarrow 2 - e^{-i\theta}e^{2ikx} - e^{i\theta}re^{-2ikx}$$
$$= 2 - e^{i(2kx-\theta)} - e^{-i(2kx-\theta)}$$
$$= 2 - 2\cos(2kx - \theta) = 2 - 2[1 - 2\sin^2(kx - \theta/2)] = 4\sin^2(kx - \theta/2) = 4\sin^2\left(kx - \frac{k}{\beta}\right)$$

Write in terms of E & V_0:

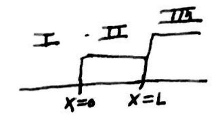
$$|\psi(x)|^2\big|_{x<0} \rightarrow 4\sin^2\left(kx - \sqrt{\frac{E}{V_0 - E}}\right)$$

Conclusion: barrier height can be determined from measurements of phase shift at different energies.

Final 2017 Question 1 12/11/19

Particle incident on a double step potential

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \qquad V(x) = \begin{cases} 0 & x<0 \\ V_0 & 0<x<L \\ V_0 & L<x \end{cases}$$



Interested in: $E\psi(x) = \hat{H}\psi(x)$ with $\psi(x)$:

$$\psi(x) = \begin{cases} e^{ik_1x} + re^{-ik_1x} & x<0 & \text{Region I} \\ ae^{ik_2x} + be^{-ik_2x} & 0<x<L & \text{Region II} \\ te^{ik_3x} & L<x & \text{Region III} \end{cases}$$

a) Find k_1, k_2, & k_3 in terms of energy E

$$E_I = \frac{\hbar^2k_1^2}{2m} \qquad E_{II} = \frac{\hbar^2k_2^2}{2m} + V_0 \qquad E_{III} = \frac{\hbar^2k_3^2}{2m} + V_0$$

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} \qquad k_3 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

b) Obtain constraints on $r, a, b,$ & t from imposing boundary conditions at $x=0$ & $x=L$

$\psi_{I}(0) = \psi_{II}(0) \Rightarrow 1 + r = a + b$

$\psi'_{I}(0) = \psi'_{II}(0) \Rightarrow ik_1 - rik_1 = ik_2a - ik_2b \quad = ik_1(1-r) = ik_2(a-b)$

$\psi_{II}(L) = \psi_{III}(L) \Rightarrow ae^{ik_2L} + be^{-ik_2L} = te^{ik_3L}$

$\psi'_{II}(L) = \psi'_{III}(L) \Rightarrow ik_2ae^{ik_2L} - ik_2be^{-ik_2L} = ik_3te^{ik_3L}$

$$\begin{array}{rl} & \frac{a}{t}e^{ik_2L} + \frac{b}{t}e^{-ik_2L} = e^{ik_3L} \\ + & \frac{a}{t}e^{ik_2L} - \frac{b}{t}e^{-ik_2L} = \frac{k_3}{k_2}e^{ik_3L} \\ \hline & 2\frac{a}{t}e^{ik_2L} = \left(1 + \frac{k_3}{k_2}\right)e^{ik_3L} \end{array} \qquad \begin{array}{rl} & \frac{a}{t}e^{ik_2L} + \frac{b}{t}e^{-ik_2L} = e^{ik_3L} \\ - & \frac{a}{t}e^{ik_2L} - \frac{b}{t}e^{-ik_2L} = \frac{k_3}{k_2}e^{ik_3L} \\ \hline & 2\frac{b}{t}e^{-ik_2L} = \left(1 - \frac{k_3}{k_2}\right)e^{ik_3L} \end{array}$$

c) Find an expression for r in terms of k_1, k_2, k_3. Your analysis will be simpler if you work with $1/t$, r/t, a/t, & b/t as variables.

$$\begin{array}{rl} & \frac{1}{t} + \frac{r}{t} = \frac{a}{t} + \frac{b}{t} \\ + & \frac{1}{t} - \frac{r}{t} = \frac{k_2}{k_1}\left(\frac{a}{t} - \frac{b}{t}\right) \\ \hline & 2\frac{1}{t} = \frac{a}{t}\left(1 + \frac{k_2}{k_1}\right) + \frac{b}{t}\left(1 - \frac{k_2}{k_1}\right) \end{array} \qquad \begin{array}{rl} & \frac{1}{t} + \frac{r}{t} = \frac{a}{t} + \frac{b}{t} \\ - & \frac{1}{t} - \frac{r}{t} = \frac{k_2}{k_1}\left(\frac{a}{t} - \frac{b}{t}\right) \\ \hline & 2\frac{r}{t} = \frac{a}{t}\left(1 - \frac{k_2}{k_1}\right) + \frac{b}{t}\left(1 + \frac{k_2}{k_1}\right) \end{array}$$

$$r = \frac{\frac{a}{t}\left(1 - \frac{k_2}{k_1}\right) + \frac{b}{t}\left(1 + \frac{k_2}{k_1}\right)}{\frac{a}{t}\left(1 + \frac{k_2}{k_1}\right) + \frac{b}{t}\left(1 - \frac{k_2}{k_1}\right)} = \frac{\frac{1}{2}e^{i(k_3-k_2)L}\left(1 + \frac{k_3}{k_2}\right)\left(1 - \frac{k_2}{k_1}\right) + \frac{1}{2}e^{i(k_3+k_2)L}\left(1 - \frac{k_3}{k_2}\right)\left(1 + \frac{k_2}{k_1}\right)}{\frac{1}{2}e^{i(k_3-k_2)L}\left(1 + \frac{k_3}{k_2}\right)\left(1 + \frac{k_2}{k_1}\right) + \frac{1}{2}e^{i(k_3+k_2)L}(k_2-k_3)(k_1-k_2)}$$

$$= \frac{e^{-ik_2L}(k_2+k_3)(k_1-k_2) + e^{ik_2L}(k_2-k_3)(k_1+k_2)}{e^{-ik_2L}(k_2+k_3)(k_1+k_2) + e^{ik_2L}(k_2-k_3)(k_1-k_2)}$$

Bound/ step-wise potential

d) Find conditions under which the reflection coefficient is zero.
Find constraints on k_3/k_2 & k_2/k_1 & $k_2 L$

$$e^{-ik_2L}(k_2+k_3)(k_1-k_2)+e^{ik_2L}(k_2-k_3)(k_1+k_2)=0$$

rewrite as:
$$e^{2ik_2L} = -\frac{(k_2+k_3)(k_1-k_2)}{(k_2-k_3)(k_1+k_2)} = -\frac{(1+\frac{k_3}{k_2})(1-\frac{k_2}{k_1})}{(1-\frac{k_3}{k_2})(1+\frac{k_2}{k_1})}$$
this is a k_1

suppose $\eta = \frac{k_3}{k_2}=\frac{k_2}{k_1}$

$$e^{2ik_2L} = -\frac{(1+\eta)(1-\eta)}{(1-\eta)(1+\eta)} = -1$$

We require also that:
$2k_2L=\pi(2n+1)$
or $k_2L=\pi(n+\frac12)$

also there is no reflection if $k_1=k_2=k_3$

Final 2018 Problem 2 12/12/19

Particle in a simple harmonic oscillator described by:
$$\hat H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac12 m\omega_0^2x^2 - F(t)x$$

identity: $\cos(2\theta)=\cos^2\theta-\sin^2(\theta)$

a) In the special case that the force is constant
$F(t)=F_0$

Determine the ground state energy & eigenfunction.

time-independent Schrödinger eqn:
$$E\psi(x)=\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+\frac12 m\omega_0^2x^2 - F_0x\right]\psi(x)$$

We know harmonic oscillator has a restoring force $F_0 = kX_0 = m\omega_0^2X_0$
$$\frac12 m\omega_0^2x^2 - F_0x = \frac12 m\omega_0^2\left[x^2-2x\frac{F_0}{m\omega_0^2}\right]\quad X_0=\frac{F_0}{m\omega_0^2}$$
$$=\frac12 m\omega_0^2\left[\left(x-\frac{F_0}{m\omega_0^2}\right)^2-\left(\frac{F_0}{m\omega_0^2}\right)^2\right] = \frac12 m\omega_0^2\left[(x-X_0)^2-X_0^2\right]$$
$$E\psi(x)=\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+\frac12 m\omega_0^2(x-X_0)^2-\frac12 m\omega_0^2X_0^2\right]\psi(x)$$

ground state soln is
$$\psi(x)=\phi_0(x-X_0)=\left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4}\exp\left\{-\frac{m\omega_0}{2\hbar}(x-X_0)^2\right\}$$
associated eigenvalue is
$$E=\frac12\hbar\omega_0-\frac12 m\omega_0^2X_0^2 = \frac12\hbar\omega_0 - \frac12 m\omega_0^2\left(\frac{F_0}{m\omega_0^2}\right)^2 = \frac12\hbar\omega_0-\frac{F_0^2}{2(m\omega_0^2)^2}$$

b) In the event the force is a δ-function
$F(t)=P_0\delta(t)$ & particle is at rest, find $\Psi(x,t)$ for $t>0$
$$\Psi(x,t)=\left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4}e^{-i\theta(t)}\exp\left\{i\frac{P(t)[x-X(t)]}{\hbar}\right\}\exp\left\{-\frac{m\omega_0}{2\hbar}(x-X(t))^2\right\}$$
$\frac{d}{dt}X(t)=\frac{P(t)}{m}$ $\frac{d}{dt}P(t)=-m\omega_0^2X(t)+F(t)$ $\hbar\frac{d}{dt}\theta(t)=\frac12\hbar\omega_0-\frac{P^2(t)}{2m}+\frac12 m\omega_0^2X^2$

At $t=0$, we know that $X(0)=0$ & $P(0)=0$. determine initial impulse: $-F(t)X(t)$
$$\int_{0^-}^{0^+}\frac{d}{dt'}P(t')dt' = P(0^+)-P(0^-)=\int_{0^-}^{0^+}-m\omega_0^2X(t')+P_0\delta(t')dt' = P_0$$

Forced SHO

For $t>0$: $\frac{d}{dt}X(t)=\frac{P(t)}{m}$ $\frac{d}{dt}P(t)=-m\omega_0^2X(t)$

subject to $X(0)=0$ $P(0)=P_0$

$X(t)=X_0\sin(\omega_0t)$
$P(t)=P_0\cos(\omega_0t)$

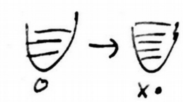
Newton's laws are satisfied if:
$$\frac{d}{dt}X(t)=\omega_0X_0\cos(\omega_0t)=\frac{P_0\cos(\omega_0t)}{m}$$
$$X_0=\frac{P_0}{m\omega_0}$$

for phase, we have $t>0$
$$\hbar\frac{d}{dt}\theta(t)=\frac12\hbar\omega_0-\frac{P^2(t)}{2m}+\frac12 m\omega_0^2X^2(t) = \frac12\hbar\omega_0-\frac{P_0^2}{2m}\cos(2\omega_0t)$$
$$\theta(t)-\theta(0)=-\frac12\omega_0t-\frac{P_0^2}{4m\hbar\omega_0}\sin(2\omega_0t)$$

2016 Final 12/17/19

A forced harmonic oscillator: $\hat H=-\frac{d^2}{dy^2}+y^2-f_0y$
normalized
Find ground state eigenfunction & eigenvalue.

$$E\psi=\left[-\frac{d^2}{dy^2}+y^2-f_0y\right]\psi(x)$$



$$\phi_0(y-y_0)=\frac{1}{\pi^{1/4}}e^{-(y-y_0)^2/2}$$

$f_0=ky_0 \Rightarrow E=\frac12\hbar\omega_0+y_0^2$

PSet 4 Question 3 12/17/19

Consider a simple harmonic oscillator with static force constant
$$\hat H=\frac{\hat p^2}{2m}+\frac12m\omega_0^2x^2-F_0x$$

a) Determine the ground state energy & eigenfunction by assuming a trial soln of form: $\psi(x)=e^{-\beta(x-X_0)^2/2}$

We take derivative $\frac{d}{dx}e^{-\beta(x-X_0)^2/2}=-\beta(x-X_0)e^{-\beta(x-X_0)^2/2}$
$$\frac{d^2}{dx^2}e^{-\beta(x-X_0)^2/2}=(\beta^2(x-X_0)^2-\beta)=e^{-\beta(x-X_0)^2/2}$$

insert into time-independent Schrödinger eqn
$$E\psi(x)=\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+\frac12m\omega_0^2x^2\psi(x)-F_0x\psi(x)$$
to obtain
$$Ee^{-\beta(x-X_0)^2/2}=-\frac{\hbar^2}{2m}(\beta^2(x-X_0)^2-\beta)e^{-\beta(x-X_0)^2}+\frac12m\omega_0^2x^2e^{-\beta(x-X_0)^2/2}-F_0xe^{-\beta(x-X_0)^2/2}$$

We can match terms to write: $E=\frac{\hbar^2\beta}{2m}-\frac{\hbar^2\beta^2X_0^2}{2m}$ $0=\frac{\hbar^2}{2m}\beta^2 2xX_0-F_0x$
$$0=-\frac{\hbar^2\beta^2}{2m}x^2+\frac12m\omega_0^2x^2$$

We solve the x^2 constraint to get:
$\beta=\frac{m\omega_0}{\hbar}$ $X_0=\frac{F_0}{m\omega_0^2}$
$$\Rightarrow E=\frac12\hbar\omega_0-\frac12m\omega_0^2X_0^2=\frac12\hbar\omega_0-\frac{F_0^2}{2m\omega_0^2}$$

b) Find expressions for the eigenfunctions & eigenvalues in general

In this case, we simplify things by writing the potential as a shifted parabolic potential plus a constant offset:
$$\frac12m\omega_0^2x^2-F_0=\frac12m\omega_0^2(x-X_0)^2-\frac12m\omega_0^2X_0^2$$
$m\omega_0^2xX_0=F_0x$ $X_0=\frac{F_0}{m\omega_0^2}$

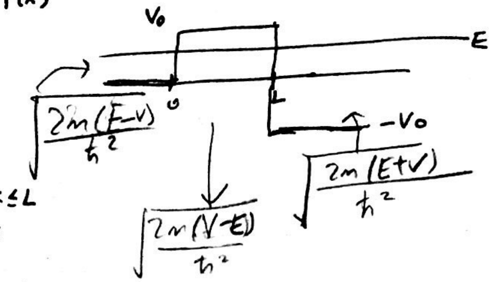
The time-independent Schrödinger eqn becomes:
$$E\psi(x)=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+\frac12m\omega_0^2(x-X_0)^2\psi(x)-\frac12m\omega_0^2X_0^2\psi(x)$$

We expect solns just to be shifted SHO according to:
$\psi_n(x)=\phi_n(x-X_0)$ $E_n=\hbar\omega_0(n+\frac12)-\frac12m\omega_0^2X_0^2$

Exam 2016 Problem 2 12/17/19

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x)$$

$$V(x) = \begin{cases} 0 & x<0 \\ V_0 & 0\le x\le L \\ -V_0 & L<x \end{cases}$$



$$\psi = \begin{cases} e^{ik_i x} + re^{-ik_i x} & x<0 \\ ae^{\gamma x} + be^{-\gamma x} & 0\le x\le L \\ te^{ik_f x} & L<x \end{cases}$$

a) $\psi_I(0) = \psi_{II}(0) = 1 + r = a + b$

$\psi_I'(0) = \psi_{II}'(0) = ik_i - rik_i = a\gamma - \gamma b$

$\psi_{II}(L) = \psi_{III}(L) = ae^{\gamma L} + be^{-\gamma L} = te^{ik_f L}$

$\psi_{II}'(L) = \psi_{III}'(L) = a\gamma e^{\gamma L} - \gamma b e^{-\gamma L} = ik_f t e^{ik_f L}$

b) $\frac{a}{t}e^{\gamma L} + \frac{b}{t}e^{-\gamma L} = e^{ik_f L}$

$\frac{a}{t}e^{\gamma L} - \frac{b}{t}e^{-\gamma L} = \frac{ik_f}{\gamma}e^{ik_f L}$ $\Longrightarrow$ $-$

$+$ $2\frac{a}{t}e^{\gamma t} = \left(\frac{ik_f}{\gamma}+1\right)e^{ik_f L}$ $\qquad 2\frac{b}{t}e^{-\gamma L} = \left(1-\frac{ik_f}{\gamma}\right)e^{ik_f L}$

c) $\frac{1}{t} + \frac{r}{t} = \frac{a}{t} + \frac{b}{t}$ $\qquad \frac{(1-r)}{t}ik_i = \frac{(a-b)\gamma}{t}$

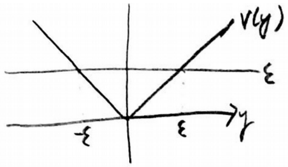
$+$ $\frac{1}{t} - \frac{r}{t} = \frac{a\gamma}{tik_i} - \frac{b\gamma}{tik_i}$ $\Longrightarrow$ $+$

$\frac{2r}{t} = \left(1-\frac{\gamma}{ik_i}\right)\frac{a}{t} + \frac{b}{t}\left(1+\frac{\gamma}{ik_i}\right)$ $\qquad \frac{2}{t} = \frac{a}{t}\left(1+\frac{\gamma}{ik_i}\right) + \frac{b}{t}\left(1-\frac{\gamma}{ik_i}\right)$

$$r = \frac{\left(1-\frac{\gamma}{ik_i}\right)\frac{a}{t} + \left(1+\frac{\gamma}{ik_i}\right)\frac{b}{t}}{\left(1+\frac{\gamma}{ik_i}\right)\frac{a}{t} + \left(1-\frac{\gamma}{ik_i}\right)\frac{b}{t}} = \frac{\left(1-\frac{\gamma}{ik_i}\right)\left(\frac{ik_f}{\gamma}+1\right)\frac{e^{ik_f L-\gamma t}}{2} + \left(1+\frac{\gamma}{ik_i}\right)\left(1-\frac{ik_f}{\gamma}\right)\frac{e^{ik_f L+\gamma L}}{2}}{\left(1+\frac{\gamma}{ik_i}\right)\left(\frac{ik_f}{\gamma}+1\right)\frac{e^{ik_f L-\gamma t}}{2} + \left(1-\frac{\gamma}{ik_i}\right)\left(1-\frac{ik_f}{\gamma}\right)\frac{e^{ik_f L+\gamma L}}{2}}$$

?

d) $1 - r^2 = T$ $\qquad e^{ik_f L+\gamma L} \Rightarrow e^{\gamma L}$



Consider: $\epsilon\psi(y) = -\frac{d^2}{dy^2}\psi(y) + |y|\psi(y)$ $\qquad \frac{96+15}{100} =$

Use WKB to develop a formula for the energy eigenvalues

$\psi(y) \sim \frac{\sin\phi(y)}{\sqrt{\eta}}$ $\qquad \frac{d\phi}{dy} = \eta = \sqrt{\epsilon - V(y)}$ $\qquad \phi(y_{max}) - \phi(y_{min}) = \int_{-\epsilon}^{\epsilon}\eta\, dy$

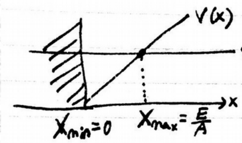
$2\int_0^{\epsilon}\sqrt{\epsilon - y}\, dy = 2\left[\frac{-2}{3}(\epsilon-y)^{3/2}\Big|_0^{\epsilon}\right] = \frac{4}{3}\epsilon^{3/2}$

$(m+1)\pi - \frac{\pi}{2} = (m+\frac{1}{2})\pi = \frac{4}{3}\epsilon^{3/2}$ $\qquad \epsilon_m = \left(\frac{3}{4}(m+\frac{1}{2})\pi\right)^{2/3}$ ✓

m starts from 0 $\quad$ soft boundaries

Pset 11 problem 18 12/17/19

$\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$ $\qquad V(x) = \begin{cases}\infty & x<0 \\ Ax & 0<x\end{cases}$



$\eta(x) = \sqrt{\frac{2m(E-V(x))}{\hbar^2}}$ $\qquad \phi(X_{max}) - \phi(X_{min}) = \int_{X_{min}}^{X_{max}}\eta(x)\,dx = (n+1)\pi - \frac{\pi}{4} = (n+\frac{3}{4})\pi$

$\sqrt{\frac{2m}{\hbar^2}}\int_0^{E/A}\sqrt{E-Ax}\,dx = \left[\frac{-2}{3}(E-Ax)^{3/2}\Big|_0^{E/A}\right]\sqrt{\frac{2m}{\hbar^2}}$

$= \frac{2}{3A}E^{3/2}\sqrt{\frac{2m}{\hbar^2}} = (n+\frac{3}{4})\pi$

$n = \frac{2}{3A\pi}E^{3/2}\sqrt{\frac{2m}{\hbar^2}} - \frac{3}{4}$

$\frac{dn}{dE} = \frac{3}{2}\frac{2}{3A\pi}E^{1/2}\sqrt{\frac{2m}{\hbar^2}} = \boxed{\frac{1}{A\pi}E^{1/2}\sqrt{\frac{2m}{\hbar^2}}}$

Quiz 2016 Problem 5 12/17/19

$\hat{H} = \frac{|\hat{p}|^2}{2M} + Mgz + V(x,y)$ $\qquad V(x,y) = \begin{cases}0 & 0\le x\le L,\ 0\le y\le L \\ \infty & \text{otherwise}\end{cases}$ $\qquad z<0$ potential is infinite

a) $\Psi(x,y,z) = X(x)Y(y)Z(z)$ Find $X(x)$, $Y(y)$, $Z(z)$ time-independent Schrödinger eqn

$X: \frac{p_x^2}{2M} + V(x)$ $\qquad y \to \frac{p_y^2}{2M} + V(y)$ $\qquad z \to \frac{p_z^2}{2M} + Mgz$

$E\psi = \left[\frac{p_x^2}{2m} + V(x)\right]\psi = \left[\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi$

b) ~~[illegible]~~ Find exact eigenfunctions $X(x)$ & $Y(y)$ & Eigenvalues E_x & E_y

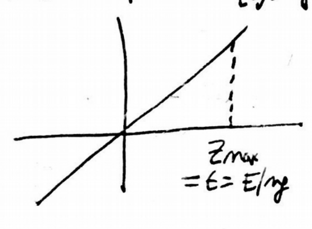
$X(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ $\qquad Y_y = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi y}{L}\right)$

$E_x = \frac{\hbar^2\pi^2 n_x^2}{2mL^2}$ $\qquad E_y = \frac{n^2\pi^2 n_y^2}{2mL^2}$

c) WKB example $\qquad \eta(y) = \sqrt{\frac{2m(E-Mgz)}{\hbar^2}}$ $\qquad \phi(z_{max}) - \phi(z_{min}) = \int_0^{6}\eta\, dy$

$= \sqrt{\frac{2m}{\hbar^2}}\int_0^{E/mg}\sqrt{E-mgz}\,dz$ $\qquad u = -Mgz$, $du = -Mg\,dz$

$\left(\sqrt{\frac{2m}{2\hbar^2}}\right)\frac{-2}{3mg}(E-Mgz)^{3/2}\Big|_0^{E/mg} = \frac{-2}{3mg}E^{3/2}\sqrt{\frac{2m}{\hbar^2}}$



$\Rightarrow \sqrt{\frac{2m}{\hbar^2}}\left(\frac{-2}{3mg}\right)E^{3/2} = (n-\frac{1}{4})\pi$

$\Rightarrow n = \frac{-2}{3mg}\pi E^{3/2}\sqrt{\frac{2m}{\hbar^2}} + \frac{1}{4}$

One more bound problem / WKB

Pset 7, Questions 2 and 3

Variational Method

Consider the normalized Schrödinger equation

$$\epsilon\psi(y) = -\frac{d^2}{dy^2}\psi(y) + v(y)\psi(y)$$

with a potential given by

$$v(y) = \begin{cases} \infty & y < 0 \\ y^3 & y > 0 \end{cases}$$

We are interested in developing an approximate ground state wavefunction and estimate for the eigenvalue. Assume that the unnormalized trial wavefunction is

$$\psi_t(y) = ye^{-\beta y^2/2}$$

for $y > 0$, and 0 for $y < 0$.

(a) Determine an expression for the variational energy ϵ_t as a function of the variational parameter β.

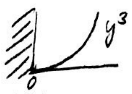
(b) Find the value of β which minimizes the trial energy.

(c) What is the resulting estimate for the ground state energy?

Problem

$$\epsilon\psi(y) = -\frac{d^2}{dy^2}\psi(y) + v(y)\psi(y) \qquad v(y) = \begin{cases} \infty & y<0 \\ y^3 & y>0 \end{cases} \qquad \psi_t(y) = ye^{-\beta y^2/2}$$

a) $\hat{H} = v(y) - \frac{d^2}{dy^2}$ $\quad E_t = \frac{\langle\psi_t|\hat{H}|\psi_t\rangle}{\langle\psi_t|\psi_t\rangle}$ ← normalize



$$\langle\psi_t|\hat{H}|\psi_t\rangle = \int_{-\infty}^{\infty}\left(ye^{-\beta y^2/2}\right)^* \hat{H}\left(ye^{-\beta y^2/2}\right)dy = \int_0^\infty ye^{-\beta y^2/2}\left(v(y)\,ye^{-\beta y^2/2} - \frac{d^2}{dy^2}ye^{-\beta y^2/2}\right)dy$$

$$= \underbrace{\int_0^\infty ye^{-\beta y^2/2}\,v(y)\,ye^{-\beta y^2/2}dy}_{PE} + \underbrace{\int_0^\infty ye^{-\beta y^2/2}\left(-\frac{d^2}{dy^2}ye^{-\beta y^2/2}\right)dy}_{KE}$$

$$= \frac{1}{\beta^3} + \frac{3}{8}\sqrt{\frac{\pi}{\beta}} = \frac{1}{\beta^3} + \frac{3}{8}\sqrt{\frac{\pi}{\beta}}$$

$$\langle\psi_t|\psi_t\rangle = \int_0^\infty \psi_t\psi_t\,dy = \int_0^\infty y^2e^{-\beta y^2}dy$$

$$E_t = \frac{\langle\psi_t|\hat{H}|\psi_t\rangle}{\langle\psi_t|\psi_t\rangle} = \frac{4}{\sqrt{\pi}}\left(\frac{1}{\beta^3} + \frac{3}{8}\sqrt{\frac{\pi}{\beta}}\right)\beta^{3/2}$$

b) We need to see $\frac{dE_t}{d\beta} = 0$ & then solve for β

$$\frac{d}{d\beta}\left(\frac{4}{\sqrt{\pi}}\left(\frac{1}{\beta^3} + \frac{3}{8}\sqrt{\frac{\pi}{\beta}}\right)\beta^{3/2}\right) = \frac{6}{\sqrt{\pi}}\left(\frac{1}{\beta^3} + \frac{3}{8}\sqrt{\frac{\pi}{\beta}}\right)\sqrt{\beta} + \frac{4}{\sqrt{\pi}}\left(-\frac{3}{\beta^4} - \frac{3}{16}\frac{\sqrt{\pi}}{\beta^{3/2}}\right)\beta^{3/2} = 0$$

$$\Rightarrow \boxed{\beta = \left(\frac{2^4}{\pi}\right)^{1/5}}$$

c) We substitute β into E_t:

$$\frac{4}{\sqrt{\pi}}\left(\frac{1}{\left(\frac{2^4}{\pi}\right)^{3/5}} + \frac{3}{8}\sqrt{\frac{\pi}{\left(\frac{2^4}{\pi}\right)^{1/5}}}\right)\left(\frac{2^4}{\pi}\right)^{3/10} = \frac{5}{(2\pi)^{1/5}} = 3.46206$$

this is only ≈ 0.01 off from $\epsilon = 3.45056$

Problem 3

We are interested in finding an approximate solution for the time-independent Schrödinger equation

$$E\psi(x) = \hat{H}\psi(x)$$

In this case, we would like to use a trial wavefunction composed of two basis states

$$\psi_t(x) = c_1u_1(x) + c_2u_2(x)$$

Unfortunately, $u_1(x)$ and $u_2(x)$ in this case are not orthogonal or normalized. To make things simpler, assume that $\hat{H}$, $u_1(x)$ and $u_2(x)$ are all real, as well as c_1 and c_2.

Use the variational principle to find constraints on c_1 and c_2 consistent with energy minimization. Make sure that the trial energy is properly normalized in your solution.

Problem 3 25/25

$$\psi_t = C_1u_1(x) + C_2u_2(x)$$

$$E_t = \frac{\langle\psi_t|\hat{H}|\psi_t\rangle}{\langle\psi_t|\psi_t\rangle} = \frac{\langle C_1u_1 + C_2u_2|\hat{H}|C_1u_1 + C_2u_2\rangle}{\langle C_1u_1 + C_2u_2|C_1u_1 + C_2u_2\rangle}$$

$$= \frac{C_1^*C_1\langle u_1|H|u_1\rangle + C_2^*C_2\langle u_2|H|u_2\rangle + C_1^*C_2\langle u_1|\hat{H}|u_2\rangle + C_2^*C_1\langle u_2|\hat{H}|u_1\rangle}{C_1^*C_1\langle u_1|u_1\rangle + C_2^*C_2\langle u_2|u_2\rangle + C_1^*C_2\langle u_1|u_2\rangle + C_2^*C_1\langle u_2|u_1\rangle}$$

$$= \frac{C_1^*C_1H_{11} + C_2^*C_2H_{22} + C_1^*C_2H_{12} + C_2^*C_1H_{21}}{C_1^*C_1O_{11} + C_2^*C_2O_{22} + C_1^*C_2O_{12} + C_2^*C_1O_{21}}$$

H_{jk} Real
O_{jk} Real
C_j Real

$$= \frac{C_1^2H_{11} + C_2^2H_{22} + 2C_1C_2H_{12}}{C_1^2O_{11} + C_2^2O_{22} + 2C_1C_2O_{12}}$$

$H_{12} = H_{21}$
$O_{12} = O_{21}$

$$\frac{\partial}{\partial C_1}E_t = 0 \qquad \frac{\partial}{\partial C_2}E_t = 0$$

$$E_t = \frac{C_1^2H_{11} + C_2^2H_{22} + 2C_1C_2H_{12}}{C_1^2O_{11} + C_2^2O_{22} + 2C_1C_2O_{12}}, \qquad \left.\begin{aligned}\frac{\partial E_t}{\partial C_1} &= \frac{2C_1H_{11} + 0 + 2C_2H_{12}}{den} \\ &- \frac{Num}{den^2}\frac{\partial}{\partial C_1}(den)\end{aligned}\right\} = 0$$

$$2C_1H_{11} + 2C_2H_{12} = \frac{Num}{dnom}\left(2C_1O_{11} + 2C_2O_{12}\right)$$

$$= C_1H_{11} + C_2H_{12} = \frac{Num}{den}(C_1O_{11} + C_2O_{12}) \qquad E_t = \frac{Num}{Den}$$

$$H_{11}C_1 + H_{12}C_2 = E_t(O_{11}C_1 + O_{12}C_2)$$
$$H_{22}C_2 + H_{21}C_1 = E_t(O_{22}C_2 + O_{21}C_1)$$

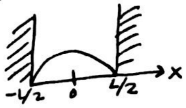
$$\boxed{\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22}\end{bmatrix}\begin{bmatrix} C_1 \\ C_2\end{bmatrix} = E\begin{bmatrix} O_{11} & O_{12} \\ O_{21} & O_{22}\end{bmatrix}\begin{bmatrix} C_1 \\ C_2\end{bmatrix}} \Rightarrow \boxed{E\,\bar{\bar{O}}\,\bar{C} = \bar{\bar{H}}\,\bar{C}}$$

Pset 7 Question 5 12/16/19

Square well augmented by a uniform force term described by Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}_{square}(x) - F_0 x$$

where $\hat{V}_{square}(x) = \begin{cases} \infty & x < -L/2 \\ 0 & -L/2 \le x \le L/2 \\ \infty & L/2 < x \end{cases}$



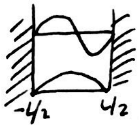
$\psi = \begin{cases} 0 & x < -L/2 \\ \cos(kx) & -L/2 \le x \le L/2 \\ 0 & x > L/2 \end{cases}$

a) Determine the ground state wave function & eigenvalue of the square well when $F_0 = 0$.

$\boxed{\phi_1(x) = \sqrt{\tfrac{2}{L}}\cos\left(\tfrac{\pi x}{L}\right)}$ $\quad E\psi = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + 0 \quad E\cos(kx) = +k^2\cos(kx)\frac{\hbar^2}{2m}$

$\cos(k(-\tfrac{L}{2})) = 0 \quad k(-\tfrac{L}{2}) = \tfrac{\pi}{2} \quad \Rightarrow k = \tfrac{\pi}{L}$ $\quad \Rightarrow E_F = \frac{\hbar^2(\frac{\pi}{L})^2}{2m} = \boxed{\frac{\hbar^2\pi^2}{2mL}}$

b) Determine the first excited state wave function $\phi_1(x)$ and eigenvalue E_1 of the square well when $F_0 = 0$.



$\boxed{\phi_2 = \sqrt{\tfrac{2}{L}}\sin(kx) = \sqrt{\tfrac{2}{L}}\sin\left(\tfrac{2\pi x}{L}\right)}$ $\quad \sin(k(\tfrac{L}{2})) = 0 \quad k\tfrac{L}{2} = \pi \quad k = \tfrac{2\pi}{L}$

$E_2 = \frac{(\frac{2\pi}{L})^2\hbar^2}{2m} = \boxed{\frac{4\hbar^2\pi^2}{2mL^2}}$

c) Construct a two-state Hamiltonian that approximates the Hamiltonian above when $F_0 \neq 0$.

$$\begin{bmatrix} \langle\phi_1|H|\phi_1\rangle & \langle\phi_1|H|\phi_2\rangle \\ \langle\phi_2|H|\phi_1\rangle & \langle\phi_2|H|\phi_2\rangle \end{bmatrix} = \begin{bmatrix} \frac{\hbar^2\pi^2}{2mL} = E_1 & \langle\phi_1|H|\phi_2\rangle \\ \langle\phi_2|H|\phi_1\rangle & \frac{4\hbar^2\pi^2}{2mL^2} = E_2 \end{bmatrix} \quad (?)$$

From pset ~~sol~~: $\langle\phi_1|\hat{H}|\phi_2\rangle = \frac{2}{L}\int_{-L/2}^{L/2}\cos\left(\frac{\pi x}{L}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{sq} - F_0(x)\right)\sin\left(\frac{2\pi x}{L}\right)dx - F_0(x)\sin\left(\frac{2\pi x}{L}\right)$

$= -\frac{2}{L}F_0\int_{-L/2}^{L/2}\cos\left(\frac{\pi x}{L}\right) x \sin\left(\frac{2\pi x}{L}\right)dx$

these are two equal!

$\langle\phi_2|\hat{H}|\phi_1\rangle = \frac{2}{L}\int_{-L/2}^{L/2}\sin\left(\frac{2\pi x}{L}\right)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{sq} - F_0 x\right]\cos\left(\frac{\pi x}{L}\right)dx$

$= -\frac{2}{L}F_0\int_{-L/2}^{L/2}\sin\left(\frac{2\pi x}{L}\right) x \cos\left(\frac{\pi x}{L}\right)dx$

From pset solutions:

In general for an N-level model, we can write: $\hat{H}_N = \sum_{j=1}^{N}\sum_{k=1}^{N}|\phi_j\rangle\langle\phi_j|\hat{H}|\phi_k\rangle\langle\phi_k|$

$\Rightarrow \hat{H}_2 = |\phi_1\rangle H_{11}\langle\phi_1| + |\phi_2\rangle H_{22}\langle\phi_2|$

$- |\phi_1\rangle\langle\phi_1|F_0 x|\phi_2\rangle\langle\phi_2|$ $\qquad$ apparently $\langle\phi_1|x|\phi_2\rangle = \langle\phi_2|x|\phi_1\rangle = \frac{16}{9\pi^2}L$

$- |\phi_2\rangle\langle\phi_2|F_0 x|\phi_1\rangle\langle\phi_1|$

$\Rightarrow \hat{H}_{2\text{-level}} = |\phi_1\rangle H_{11}\langle\phi_1| + |\phi_2\rangle H_{22}\langle\phi_2| - \frac{16}{9\pi^2}F_0 L\left(|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|\right)$

Pset 8 Question 3 12/17/19

Consider a square well with a time-dependent uniform force term described by Hamiltonian: $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}_{square}(x) - F(t)x$

$\hat{V}_{square} = \begin{cases} \infty & x < -L/2 \\ 0 & -L/2 \le x \le L/2 \\ \infty & L/2 < x \end{cases}$

Assume we make use of a two-state model based on lowest two states.

a) Find evolution eqns for $\langle x\rangle$ & $\langle\hat{p}\rangle$ within the two-state approximation.

We expect Ehrenfest's theorem eqns of form:

$$\frac{d}{dt}\langle x\rangle = \frac{\langle\hat{p}\rangle}{m} \qquad \frac{d}{dt}\langle\hat{p}\rangle = -m\omega_0^2\langle x\rangle + 2\frac{m\omega_0}{\hbar}\langle\phi_1|x|\phi_2\rangle^2 F(t)\left(|C_1(t)|^2 - |C_2(t)|^2\right)$$

b) Determine $\langle x\rangle$ for ground state in special case that $F(t) = F_0$, assuming perturbation is weak.

If perturbation is weak, $|C_1|^2$ can be taken as close to 1, we can approximate:

$$\frac{d}{dt}\langle\hat{p}\rangle \to -m\omega_0^2\langle x\rangle + 2\frac{m\omega_0}{\hbar}\langle\phi_1|x|\phi_2\rangle^2 F_0$$

This allows for a steady-state ~~soln~~ condition to determine expectation value $\langle x\rangle$ for ground state w/ uniform force

$$0 = -m\omega_0^2\langle x\rangle + 2\frac{m\omega_0}{\hbar}\langle\phi_1|x|\phi_2\rangle^2 F_0$$

$$\langle x\rangle = \frac{2}{\hbar\omega_0}\langle\phi_1|x|\phi_2\rangle^2 F_0$$

c) Assume force is weak so two-level approximation should be applicable w/ sinusoidal force: $F(t) = F_0\cos(\omega t)$ where $\hbar\omega \ll E_3$

E_3 is the energy of third state of unperturbed well; interactions between the ground state & first excited state should dominate. Determine the Rabi oscillation frequency on resonance in this case.

$$F(t) = F_0\cos(\omega t) = F_0\underbrace{\frac{e^{i\omega t} + e^{-i\omega t}}{2}}_{\text{derived from Euler formula}}$$

Idea: one term corresponds to increasing the energy by $\hbar\omega$ & the other corresponds to decreasing the energy by $\hbar\omega$. Associated 2-level system keeping both terms:

$\hat{H} = |\phi_1\rangle H_{11}\langle\phi_1| + |\phi_2\rangle H_{22}\langle\phi_2| - F_0\cos(\omega t)\langle\phi_1|x|\phi_2\rangle\left[|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|\right]$

With this approach, we can write: $H_{12}(t) = H_{21}(t) = -F_0\cos(\omega t)\langle\phi_1|x|\phi_2\rangle$

Exact sol'n can be obtained in event that: $H_{12}(t) = V_0 e^{i\omega t}$

If we assume $H_{22} - H_{11} > 0$ & $\hbar\omega > 0$, we expect domin. part of interaction to be:

$H_{12}(t) \to -F_0\frac{e^{i\omega t}}{2}\langle\phi_1|x|\phi_2\rangle$

$H_{21}(t) \to -F_0\frac{e^{-i\omega t}}{2}\langle\phi_1|x|\phi_2\rangle$

$$\hbar\Omega(\omega) = \sqrt{(H_{22} - H_{11} - \hbar\omega)^2 + 4\left(\frac{F_0\langle\phi_1|x|\phi_2\rangle}{2}\right)^2}$$

$H_{22} - H_{11} = 4\frac{\hbar^2\pi^2}{2mL^2} - \frac{\hbar^2\pi^2}{2mL^2} = 3\frac{\hbar^2\pi^2}{2mL^2}$

Rabi freq on resonance is $\quad \Omega \to \frac{|F_0\langle\phi_1|x|\phi_2\rangle|}{\hbar}$ when $\omega \to \frac{H_{22} - H_{11}}{\hbar}$

Two level systems forced stuff

Consider a classical state which at $t = 0$ is given by

$$\psi(x,0) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}} e^{i\frac{p_0}{\hbar}x} e^{-\frac{m\omega_0}{2\hbar}x^2}$$

We would like to develop an expansion of this function in terms of the SHO eigenfunctions; in particular, we would like an expansion of the form

$$\psi(x,0) = \sum_n a_n \phi_n(x)$$

We know that the expansion coefficients can be computed in principle from

$$a_n = \langle \phi_n | \psi(x,0) \rangle$$

Unfortunately, the associated integrals are difficult to do in general. In this problem we are interested in the possibility of making use of the creation and annihilation operators to achieve an expansion of this kind.

Problem 5

$$\Psi(x,0) = \left(\frac{m\omega_0}{\hbar\pi}\right)^{1/4} e^{i\frac{p_0}{\hbar}x} e^{\frac{-m\omega_0}{2\hbar}x^2} = \sum_n a_n \phi_n(x)$$

10

a) $\Psi(x,0) = \hat{Q}\phi_0$ find $\hat{Q}$ using $\hat{a}$ & $\hat{a}^+$

$\hat{Q} = e^{i\frac{p_0}{\hbar}\hat{x}}$ where $\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}}(\hat{a}+\hat{a}^+)$

plugging in $\hat{x}$ $\Rightarrow \boxed{\hat{Q} = e^{\frac{ip_0}{\hbar}\sqrt{\frac{\hbar}{2m\omega_0}}(\hat{a}+\hat{a}^+)}} = e^{iz_0(\hat{a}+\hat{a}^+)}$ ✓ where we define $z_0 = \frac{p_0}{\hbar}\sqrt{\frac{\hbar}{2m\omega_0}}$

b) Baker-Campbell-Hausdorff formula:

$$e^{\hat{x}+\hat{y}} = e^{\hat{x}}e^{\hat{y}}e^{-\frac{1}{2}[\hat{x},\hat{y}]}e^{\frac{1}{6}(2[\hat{y},[\hat{x},\hat{y}]]+[\hat{x},[\hat{y},\hat{x}]])}\ldots$$ ✓

$$\hat{Q} = e^{iz_0(\hat{a}^++\hat{a})} = e^{iz_0\hat{a}^+}e^{iz_0\hat{a}}e^{iz_0(-\frac{1}{2})[\hat{a}^+,\hat{a}]}\cancel{e^{\frac{1}{6}(0)}}$$

$$\Rightarrow \boxed{\hat{Q} = e^{iz_0\hat{a}^+}e^{iz_0\hat{a}}e^{-\frac{z_0^2}{2}}}$$ ✓

c) $a_n = \langle \phi_n | \Psi(x,0) \rangle$

$e^x = 1 + x + \frac{x^2}{2!} + \ldots = \sum_{n=0}^{\infty}\frac{x^n}{n!}$ ✓

$$\hat{Q}|\phi_0\rangle = e^{-\frac{z_0^2}{2}}e^{iz_0\hat{a}^+}(1 + \underbrace{iz_0\hat{a} + \frac{(iz_0)^2}{2!}\hat{a}^2 + \ldots}_{=0 \text{ (destruction operator is being used on the ground state)}})|\phi_0\rangle$$

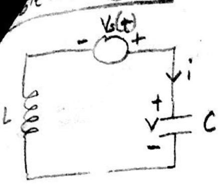
$$= e^{-z_0^2/2}e^{iz_0\hat{a}^+}\phi_0$$

$$= e^{-\frac{z_0^2}{2}}\sum\frac{(iz_0)^n(a^+)^n}{n!} = e^{-\frac{z_0^2}{2}}\sum_n\frac{(iz_0)^n\phi_n\sqrt{n!}}{n!} = e^{-\frac{z_0^2}{2}}\sum_n\frac{\phi_n(iz_0)^n}{\sqrt{n!}}$$ ✓

$$a_n = \langle\phi_n|\hat{Q}|\phi_0\rangle = \langle\phi_n|e^{-z_0^2/2}\sum_n\frac{(iz_0)^n}{\sqrt{n!}}|\phi_n\rangle = \boxed{e^{-z_0^2/2}\left(\frac{(iz_0)^n}{\sqrt{n!}}\right)}$$ ✓

d) $P_n = |a_n|^2 = \frac{e^{-z_0^2}}{n!}(iz_0)^{2n}$ poisson distribution ✓

Problem 3



C $+$ $-$ $V_c(t)$, $i(t)$, $i(t) = C\frac{dv}{dt}$

L $+$ $-$ $V_L(t) = -L\frac{di}{dt}$

+10

a) $V_L = V - V_s = -L\frac{di}{dt} \Rightarrow V_s = V - V_L = V + L\frac{di}{dt}$

$\boxed{V_s(t) = V(t) + L\frac{di}{dt}}$ ✓ $i(t) = C\frac{dV}{dt}$ ✓ $\Rightarrow \boxed{\frac{d}{dt}V(t) = \frac{1}{C}i(t)}$

b) Classical SHO ✓ Quantum LC-Circuit

$\hat{p} = -i\hbar\frac{\partial}{\partial x}$

$\hat{i} = -i\hbar\omega_0^2\frac{\partial}{\partial V}$

$\frac{d}{dt}x(t) = \frac{p(t)}{m} \longleftrightarrow \frac{d}{dt}V(t) = \frac{i(t)}{C}$

$\frac{d}{dt}p(t) = -m\omega_0^2x(t) + F(t) \leftrightarrow \frac{d}{dt}i(t) = \frac{-V(t)}{L} + \frac{V_s(t)}{L}$

$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2x^2 - F(t)x \leftrightarrow \boxed{\hat{H} = \frac{1}{2}L\hat{i}^2 + \frac{1}{2}C\hat{V}^2 - C'V_s(t)V}$ ✓

Finding constant C' using Ehrenfest's theorem

$$\frac{d}{dt}\langle\hat{i}\rangle = \langle\cancel{\frac{\partial\hat{i}}{\partial t}}\rangle + \frac{1}{i\hbar}\langle[\hat{i},\hat{H}]\rangle = \frac{1}{i\hbar}\langle[\hat{i}, \cancel{\frac{1}{2}L\hat{i}^2} + \frac{1}{2}CV^2 - C'V_s(t)V]\rangle$$

$$[\hat{i}, -C'V_sV]f = C'\left[-i\hbar\omega_0^2\frac{\partial}{\partial V}((-V_sV)f) + V_sV\left(-i\hbar\omega_0^2\frac{\partial}{\partial V}f\right)\right]$$

$$= -C'i\hbar\omega_0^2\left[\frac{\partial}{\partial V}((-V_sV)f) + V_sV\frac{\partial}{\partial V}f\right]$$

$$= -C'i\hbar\omega_0^2\left[-V_sf + \cancel{(-V_sV)\frac{\partial f}{\partial V}} \cancel{+ V_sV\frac{\partial f}{\partial V}}\right]$$

$[\hat{i}, -C'V_sV] = C'i\hbar\omega_0^2V_s$ $\quad \frac{d}{dt}\langle\hat{i}\rangle = C'\omega_0^2\cancel{V_s} = \frac{V_s(t)}{L} \leftarrow \frac{d}{dt}i(t) = \frac{-V(t)}{L} + \frac{V_s(t)}{L}$

$\Rightarrow \boxed{C' = \frac{1}{L\omega_0^2}}$

$\boxed{\frac{1}{i\hbar}\langle[\hat{i}, \frac{1}{2}CV^2]\rangle \quad [\hat{i}, \frac{1}{2}CV^2] = \frac{1}{2}C[\hat{i},V^2]}$ $= C'\omega_0^2$

$\frac{1}{2}C[\hat{i},V^2] = \frac{1}{2}C([\hat{i},V]V - V[\hat{i},V])$

$[\hat{i},V] = -[V,\hat{i}] = -i\hbar\omega_0^2$

$\rightarrow = -CVi\hbar\omega_0^2$

$\frac{1}{i\hbar}\langle[\hat{i},\frac{1}{2}CV^2]\rangle = -CV\omega_0^2$

$= -\frac{\langle V\rangle}{L}$

c) Show: $\frac{d}{dt}\langle V\rangle = \frac{1}{i\hbar}\langle[V,\hat{H}]\rangle = \frac{\langle\hat{i}\rangle}{C}$

From part b.

$\frac{1}{i\hbar}\langle[\hat{i}, -C'V_s(t)V]\rangle = C'\omega_0^2V_s$, where $C' = \frac{1}{L\omega_0^2}$ & $C = \frac{1}{L}$

$\boxed{\frac{d}{dt}\langle\hat{i}\rangle = \frac{1}{i\hbar}\langle[\hat{i},\hat{H}]\rangle = V_sC - \frac{\langle\hat{V}\rangle}{L}}$

$\boxed{\frac{d}{dt}\langle\hat{i}\rangle = \frac{1}{i\hbar}\langle[\hat{i},\frac{1}{2}CV^2 - C'V_s(t)V\rangle = CV_s - \frac{\langle V\rangle}{L}}$ ✓

$$\frac{d}{dt}\langle V\rangle = \frac{1}{i\hbar}\langle[V, \frac{1}{2}L\hat{i}^2 + \cancel{\frac{1}{2}CV^2} - \cancel{C'V_s(t)}V]\rangle$$

$\frac{1}{2}L[V,\hat{i}^2] \Rightarrow [V,\hat{i}^2] = [V,\hat{i}]\hat{i} + \hat{i}[V,\hat{i}]$ $\Rightarrow [V,\hat{i}]f = V\hat{i}f - \hat{i}Vf = V(-i\hbar\omega_0^2\frac{\partial}{\partial V}f) + i\hbar\omega_0^2\frac{\partial}{\partial V}(Vf)$

$= \cancel{-Vi\hbar\omega_0^2\frac{\partial}{\partial V}f} + i\hbar\omega_0^2f \cancel{+ i\hbar\omega_0^2V\frac{\partial}{\partial V}f} \Rightarrow [V,\hat{i}] = i\hbar\omega_0^2$ ✓

$\frac{1}{2}L[V,\hat{i}^2] = \frac{1}{2}L(i\hbar\omega_0^2\hat{i} + \hat{i}\,i\hbar\omega_0^2)$

$= i\hbar\omega_0^2L\hat{i}$

$\boxed{\frac{d}{dt} = \omega_0^2L\langle\hat{i}\rangle \quad C' = \frac{1}{L\omega_0^2} \Rightarrow \frac{d}{dt} = \frac{\langle\hat{i}\rangle}{C}}$ ✓

$\boxed{\text{Both } \frac{d}{dt}\langle V\rangle \text{ and } \frac{d}{dt}\langle\hat{i}\rangle \text{ check out according to Ehrenfest's theorem}}$

(d) Find a classical state solution in terms of $V(t)$, $I(t)$ and $\Theta(t)$, and determine the associated constraints.

d) $$\Psi(x,t) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} e^{-i\theta(t)} e^{i\frac{p(t)}{\hbar}(x-X(t))} e^{-\frac{1}{2}\frac{m\omega_0}{\hbar}(x-X(t))^2}$$

$$\Psi(0,t) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} e^{-i\theta(t)} e^{\frac{iI(t)}{\hbar\omega_0^2}(V-V(t))} e^{-\frac{1}{2}\frac{C}{\hbar\omega_0}(V-V(t))^2}$$

End of prev. problem

Blown up of part you can't see

$$\boxed{\begin{aligned}
&\frac{d}{dt}X(t) = \frac{p(t)}{m} \longleftrightarrow \frac{d}{dt}V(t) = \frac{I(t)}{C}\\
&\frac{d}{dt}p(t) = -m\omega_0^2 X(t) + F(t) \longleftrightarrow \frac{d}{dt}I(t) = -\frac{V(t)}{L} + \frac{V_s(t)}{L}\\
&\hbar\frac{d}{dt}\theta(t) = \frac{1}{2}\hbar\omega_0 - \frac{p^2(t)}{2m} + \frac{1}{2}m\omega_0^2 X^2(t) - F(t)X(t) \leftrightarrow \hbar\frac{d}{dt}\theta(t) = \frac{1}{2}\hbar\omega_0 - \frac{1}{2}LI^2 + \frac{1}{2}CV^2 - CV_s(t)V(t)
\end{aligned}}$$

$[\hat{I}, -C'V_sV] = C'i\hbar\omega_0^2 V_s$

$\frac{d}{dt}\langle \hat{I}\rangle = C$

$\Rightarrow \boxed{C' = \frac{1}{L\omega_0^2}}$

$\boxed{\frac{1}{i\hbar}\langle[\hat{I}, \frac{1}{2}CV^2]\rangle}$ $= C'\omega_0^2$

$[\hat{I}, \frac{1}{2}CV^2] = \frac{1}{2}C[\hat{I}, V^2]$

$\frac{1}{2}C[\hat{I}, V^2] = \frac{1}{2}C([\hat{I}, V]V - V[\hat{I}, V])$

$[\hat{I}, V] = -[V, \hat{I}] = -i\hbar\omega_0^2$

$\rightarrow = -CVi\hbar\omega_0^2$

$\frac{1}{i\hbar}\langle[\hat{I}, \frac{1}{2}CV^2]\rangle = -CV\omega_0^2 = -\frac{\langle V\rangle}{L}$

$$\frac{d}{dt}\langle V\rangle = \frac{1}{i\hbar}\langle[V, \hat{H}]\rangle = \frac{\langle \hat{I}\rangle}{C}$$

$$\boxed{\frac{d}{dt}\langle \hat{I}\rangle = \frac{1}{i\hbar}\langle[\hat{I}, \hat{H}]\rangle = V_sC - \frac{\langle\hat{V}\rangle}{L}}$$

From part b.

$\frac{1}{i\hbar}\langle[\hat{I}, -C'V_s(t)V]\rangle$

$= C'\omega_0^2 V_s$, where

$C = \frac{1}{L\omega_0^2}$ & $C = \frac{1}{L}$

$= \frac{1}{i\hbar}\langle[V, \frac{1}{2}L\hat{I}^2 + \frac{1}{2}CV^2 - \cancel{C'V_s(t)V}]\rangle$

$\boxed{\frac{d}{dt}\langle \hat{I}\rangle = \frac{1}{i\hbar}\langle[\hat{I}, \frac{1}{2}CV^2 - C'V_s(t)V = CV_s - \frac{\langle V\rangle}{L}}$

$[V, \hat{I}]f = V\hat{I}f - \hat{I}Vf = V(-i\hbar\omega_0^2\frac{\partial}{\partial V}f$

LC, nonlinear capacitor and inductor
Ehrenfest's theorem

In this problem we are concerned with the development of a quantum mechanical model for an LC-circuit with a nonlinear capacitor. For the classical version of the problem we can write circuit equations of the form

$$v(t) = -L\frac{d}{dt}i(t)$$

$$i(t) = \frac{d}{dt}q(t)$$

where $i(t)$ is the classical current, where $v(t)$ is the classical voltage, and where $q(t)$ is the charge on the capacitor. We can write for the total classical energy

$$E = \frac{1}{2}Li^2(t) + E_q(q(t))$$

where $E_q(t)$ is the electrostatic energy of the capacitor. The voltage in this case is derived from the derivative of the stored energy with respect to charge

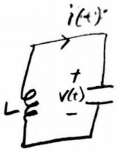
$$v = \frac{d}{dq}E_q(q)$$

a) $\frac{d}{dt}q(t) = i(t) \longleftrightarrow \frac{d}{dt}x(t) = \frac{p(t)}{m}$ $\quad$ LC $\quad$ $i(t) \leftrightarrow p(t)$

$\frac{d}{dt}i(t) = -\frac{1}{L}\frac{d}{dq}E_q(q(t)) \longleftrightarrow \frac{d}{dt}p(t) = -\frac{d}{dx}V(x(t))$

$E = \frac{1}{2}Li^2(t) + E_q(q(t)) \longleftrightarrow E = \frac{p^2(t)}{2m} + V(x(t))$

$\hat{H} = \frac{1}{2}L\hat{i}^2 + E_q(q) \longleftrightarrow \hat{H} = \frac{\hat{p}^2}{2m} + V(x)$



b) $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ $\quad$ $\hat{i} = -Ai\hbar\frac{\partial}{\partial q}$

Finding constant A using Ehrenfest's theorem

$\frac{d}{dt}\langle q\rangle = \langle\cancel{\frac{\partial q}{\partial t}}\rangle^{0} + \frac{1}{i\hbar}\langle[q,\hat{H}]\rangle = \frac{1}{i\hbar}\langle[q, \frac{1}{2}L\hat{i}^2 + \cancel{E_q(q)}^{0}]\rangle$

$[q, \frac{1}{2}L\hat{i}^2] = \frac{1}{2}L[q,\hat{i}^2] = \frac{1}{2}L([q,\hat{i}]\hat{i} + \hat{i}[q,\hat{i}])$

$[q,\hat{i}]f = q\hat{i}f - \hat{i}qf = q(-Ai\hbar\frac{\partial f}{\partial q}) + Ai\hbar\frac{\partial}{\partial q}(qf)$

$[q,\hat{i}] = Ai\hbar \Leftarrow = \cancel{-qAi\hbar\frac{\partial f}{\partial q}} + Ai\hbar f + \cancel{Ai\hbar q\frac{\partial}{\partial q}f} = Ai\hbar f$

$\to \frac{1}{2}L(Ai\hbar\hat{i} + \hat{i}Ai\hbar) = Li\hbar A\hat{i}$

$\frac{d}{dt}\langle q\rangle = \frac{1}{\cancel{i\hbar}}\langle L\cancel{i\hbar}A\hat{i}\rangle = LA\langle\hat{i}\rangle \Rightarrow \boxed{A = \frac{1}{L}}$

$\boxed{\hat{i} = -\frac{i\hbar}{L}\frac{\partial}{\partial q}}$ $\quad$ $\boxed{\hat{H} = \frac{1}{2}L\hat{i}^2 + E_q(q) \text{ where } \hat{i} = -\frac{i\hbar}{L}\frac{\partial}{\partial q}}$

c) $\frac{d}{dt}\langle\hat{i}\rangle = \langle\cancel{\frac{\partial\hat{i}}{\partial t}}\rangle^{0} + \frac{1}{i\hbar}\langle[\hat{i},H]\rangle = \frac{1}{i\hbar}\langle[\hat{i}, \cancel{\frac{1}{2}L\hat{i}^2} + E_q(q)]\rangle$

$[\hat{i}, E_q(q)]f(q) = \hat{i}E_q(q)f(q) - E_q(q)\hat{i}f(q) = -\frac{i\hbar}{L}\frac{\partial}{\partial q}(E_q(q)f(q)) + E_q(q)\frac{i\hbar}{L}\frac{\partial}{\partial q}f(q)$

$= -\frac{i\hbar}{L}(\frac{\partial}{\partial q}E_q(q)f + \cancel{E_q(q)\frac{\partial}{\partial q}f(q)}) + \cancel{E_q(q)\frac{i\hbar}{L}\frac{\partial}{\partial q}f(q)}$

$[\hat{i}, E_q(q)] = -\frac{i\hbar}{L}\frac{\partial}{\partial q}E_q(q) \Rightarrow \boxed{\frac{d}{dt}\langle\hat{i}\rangle = -\frac{1}{L}\frac{\partial}{\partial q}E_q(q)}$ this matches with $\frac{d}{dt}i(t) = -\frac{1}{L}\frac{d}{dq}E_q(q(t))$

In this problem we are concerned with the development of a quantum mechanical model for an LC-circuit with a nonlinear inductor. For the classical version of the problem we can write circuit equations of the form

$$i(t) = C\frac{d}{dt}v(t)$$

$$v(t) = -\frac{d}{dt}\lambda(t)$$

where $i(t)$ is the classical current, where $v(t)$ is the classical voltage, and where $\lambda(t)$ is the flux linkage of the inductor. We can write for the total classical energy

$$E = \frac{1}{2}Cv^2(t) + E_L(\lambda(t))$$

where $E_L(\lambda(t))$ is the magnetic energy of the inductor. The current in this case is related to the derivative of the stored magnetic energy with respect to flux linkage

$$i = \frac{d}{d\lambda}E_L(\lambda)$$

$i(t) = C\frac{d}{dt}v(t)$ $\quad$ $E = \frac{1}{2}Cv^2(t) + E_L(\lambda(t))$ $\quad$ $+6/6$

$v(t) = -\frac{d}{dt}\lambda(t)$ $\quad$ $i = \frac{d}{d\lambda}E_L(\lambda)$

a) Classical particle $\qquad$ Nonlinear inductor $\qquad$ $\hat{V} = -i\hbar A\frac{d}{d\lambda}$

$\frac{d}{dt}x(t) = \frac{p(t)}{m}$ $\qquad$ $\frac{d}{dt}\lambda(t) = -V(t)$ $\qquad$ $\hat{p} = -i\hbar\frac{d}{dx}$

$\frac{d}{dt}p(t) = -\frac{d}{dx}V(x(t))$ $\qquad$ $\frac{d}{dt}V(t) = \frac{i(t)}{C} = \frac{1}{C}\frac{d}{d\lambda}E_L(\lambda)$

$\hat{H} = \frac{p^2(t)}{2m} + V(x(t))$ $\qquad$ $\hat{H} = \frac{1}{2}CV^2(t) + E_L(\lambda(t))$

b) $\frac{d}{dt}\langle\lambda\rangle = \langle\cancel{\frac{\partial\lambda}{\partial t}}\rangle^{0} + \frac{1}{i\hbar}\langle[\lambda, \frac{1}{2}CV^2(t) + \cancel{E_L(\lambda(t))}^{0}]\rangle$

$[\lambda, \frac{1}{2}CV^2(t)] = \frac{1}{2}C[\lambda, V^2(t)]$

$[\lambda, V^2] = [\lambda, V]V + V[\lambda, V]$

$[\lambda, V]f = \lambda(-i\hbar A\frac{df}{d\lambda}) + i\hbar A\frac{d}{d\lambda}(\lambda f) = \cancel{-i\hbar\lambda A\frac{df}{d\lambda}} + i\hbar Af + \cancel{i\hbar A\lambda\frac{df}{d\lambda}}$

$[\lambda, V] = i\hbar A \Rightarrow [\lambda, V^2] = 2i\hbar AV \Rightarrow \frac{1}{2}C[\lambda, V^2(t)] = Ci\hbar A\hat{V}$

$\frac{d}{dt}\langle\lambda\rangle = CA\langle\hat{V}\rangle = -\langle\hat{V}\rangle \Rightarrow \boxed{A = -\frac{1}{C}, \; \hat{V} = \frac{i\hbar}{C}\frac{d}{d\lambda}}$

c) $\frac{d}{dt}\langle V\rangle = \langle\cancel{\frac{\partial V}{\partial t}}\rangle^{0} + \frac{1}{i\hbar}\langle[V, \cancel{\frac{1}{2}CV^2}^{0} + E_L(\lambda(t))]\rangle$

$[V, E_L(\lambda(t))]f = VE_L(\lambda(t))f - E_L(\lambda(t))Vf$

$= \frac{i\hbar}{C}\frac{d}{d\lambda}(E_L(\lambda(t))f) - E_L(\lambda(t))\frac{i\hbar}{C}\frac{df}{d\lambda}$

$= \frac{i\hbar}{C}\frac{dE_L(\lambda(t))}{d\lambda}f + \cancel{\frac{i\hbar}{C}E_L(\lambda(t))\frac{df}{d\lambda}} - \cancel{\frac{i\hbar}{C}E_L(\lambda(t))\frac{df}{d\lambda}}$

$\boxed{\frac{d}{dt}\langle V\rangle = \frac{1}{C}\langle\frac{dE_L(\lambda(t))}{d\lambda}\rangle = \frac{\langle i\rangle}{C}}$

There are a great many papers in the literature that focus on a model of a harmonic oscillator with a dynamical mass, with a Hamiltonian given by

$$\hat{H} = e^{-\gamma t}\frac{\hat{p}^2}{2m} + e^{\gamma t}\frac{1}{2}m\omega_0^2 x^2$$

a) $\frac{d^2}{dt^2}\langle x\rangle + A\frac{d}{dt}\langle x\rangle + B\langle x\rangle + C = 0$ Use Ehrenfest's theorem to find a second order evolution equation to $\langle x\rangle$ of the form:

$$\frac{d}{dt}\langle x\rangle = \left\langle \frac{\partial x}{\partial t}\right\rangle^{\to 0} + \frac{1}{i\hbar}\left\langle [\hat{x}, e^{-\gamma t}\frac{\hat{p}^2}{2m} + \cancel{e^{\gamma t}\frac{1}{2}m\omega_0^2x^2}^{\,0}]\right\rangle$$

$$= \frac{e^{-\gamma t}}{2m(i\hbar)}\langle[\hat{x},\hat{p}^2]\rangle \Rightarrow [\hat{x},\hat{p}^2] = \underbrace{[\hat{x},\hat{p}]}_{i\hbar}\hat{p} + \hat{p}[\hat{x},\hat{p}]$$

$$= \frac{\cancel{2}\cancel{i\hbar} e^{-\gamma t}}{\cancel{2}m\cancel{(i\hbar)}}\langle\hat{p}\rangle = \frac{e^{-\gamma t}}{m}\langle\hat{p}\rangle \qquad = i\hbar\hat{p} + \hat{p}i\hbar = 2i\hbar\hat{p}$$

$$\frac{d^2}{dt^2}\langle x\rangle = \frac{d}{dt}\left(\frac{e^{-\gamma t}}{m}\langle\hat{p}\rangle\right) = \underbrace{\left\langle\frac{d}{dt}\left(\frac{e^{-\gamma t}}{m}\hat{p}\right)\right\rangle}_{= -\gamma e^{-\gamma t}\frac{\langle\hat{p}\rangle}{m}} + \frac{1}{i\hbar}\frac{e^{-\gamma t}}{m}\langle[\hat{p},\hat{H}]\rangle$$

$$[\hat{p},\hat{H}] = [\hat{p}, \cancel{e^{-\gamma t}\frac{\hat{p}^2}{2m}}^{\,0} + e^{\gamma t}\tfrac{1}{2}m\omega_0^2x^2]$$

$$= [\hat{p}, e^{\gamma t}\tfrac{1}{2}m\omega_0^2x^2]f = \hat{p}[e^{\gamma t}\tfrac{1}{2}m\omega_0^2x^2(f)] - e^{\gamma t}\tfrac{1}{2}m\omega_0^2x^2\hat{p}(f)$$

$\hat{p} = -i\hbar\frac{\partial}{\partial x}$ $\quad -i\hbar\left[\frac{\partial}{\partial x}e^{\gamma t}\tfrac{1}{2}m\omega_0^2x^2\right]f + \cancel{-i\hbar\left(e^{\gamma t}\tfrac{1}{2}m\omega_0^2x^2\right)\frac{\partial f}{\partial x} - e^{\gamma t}\tfrac{1}{2}m\omega_0^2x^2(-i\hbar)\ldots}$

$$= \left(-i\hbar e^{\gamma t}\cancel{\tfrac{1}{2}}m\omega_0^2\cancel{2}x\right)f \Rightarrow [\hat{p},\hat{H}] = -i\hbar e^{\gamma t}m\omega_0^2 x$$

$$\frac{1}{\cancel{i\hbar}}\frac{\cancel{e^{-\gamma t}}}{\cancel{m}}\cancel{(-i\hbar)}\cancel{e^{\gamma t}}\cancel{m}\omega_0^2\langle\hat{x}\rangle = -\omega_0^2\langle\hat{x}\rangle \Leftarrow \text{this is } \frac{1}{i\hbar}\frac{e^{-\gamma t}}{m}\langle[\hat{p},\hat{H}]\rangle$$

$$\frac{d^2}{dt}\langle x\rangle = -\gamma e^{-\gamma t}\frac{\langle\hat{p}\rangle}{m} - \omega_0^2\langle x\rangle \Rightarrow \frac{d^2}{dt}\langle x\rangle + \gamma e^{-\gamma t}\frac{\langle\hat{p}\rangle}{m} + \omega_0^2\langle x\rangle = 0$$

$$= \frac{d^2}{dt^2}\langle x\rangle + \gamma\frac{d}{dt}\langle x\rangle + \omega_0^2\langle x\rangle = 0 \Rightarrow \boxed{A=\gamma,\ B=\omega_0^2,\ C=0}$$

Question: Consider a version of the model where the decay is very slow $\frac{\gamma}{\omega_0} \ll 1$

b) Hamiltonian can be written this way

$$\hat{H} = \frac{\hat{p}^2}{2(me^{\gamma t})} + \frac{1}{2}[me^{\gamma t}]\omega_0^2x^2 \qquad \frac{\gamma}{\omega_0} \ll 1 \qquad \frac{dm}{dt} \simeq 0$$

$\left(t=0 \quad \hat{H} \approx \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2x^2\right)$

$\left(t=\frac{1}{\gamma} \quad \hat{H} \approx \frac{\hat{p}^2}{2m'} + \frac{1}{2}m'\omega_0^2x^2 \quad m' \simeq em\right)$

$H \to \hat{p}^2/2m + \frac{1}{2}m\omega_0^2x^2$

$t=0 \quad m(0)=m \to \phi_0 = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega_0}{2\hbar}x^2} \quad E = \frac{\hbar\omega_0}{2}$

$t=1/\gamma \quad m(1/\gamma)=me^{\gamma(1/\gamma)} \to \phi_0 = \left(\frac{me\omega_0}{\pi\hbar}\right)^{1/4} e^{-\frac{me\omega_0}{2\hbar}x^2} \quad E = \frac{\hbar\omega_0}{2}$

Use this approximation to determine ground state & approximate energy eigenvalue at $t=0$ & $t=1/\gamma$

$$\psi(x, t=\tfrac{1}{\gamma}) = e^{-i\omega_0 t/2}\left[\frac{(me)\omega_0}{\pi\hbar}\right]^{1/4}\exp\left\{-\frac{1}{2}\frac{[me]\omega_0}{\hbar}x^2\right\}$$

idea: frequency is maintained in this limit.

c) Find an exact sol'n in which the wavefunction could be thought of as being in the ground state for all time (even w/ mass changing in time). Assume that $\gamma < 2\omega_0$.

Assume squeezed state sol'n of form

$$\psi(x,t) = \left[\frac{2a(t)}{\pi}\right]^{1/4} e^{-i\Theta(t)} e^{-a(t)x^2}$$

Time derivative:

$$\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{1}{4a}\frac{da}{dt} - i\frac{d\Theta}{dt} - x^2\frac{da}{dt}\right]\psi(x,t)$$

Spatial derivative:

$$\frac{\partial}{\partial x}\psi(x,t) = -2ax\psi(x,t)$$

$$\frac{d^2}{dx^2}\psi(x,t) = [-2a + 4a^2x^2]\psi(x,t)$$

plug into Shrödinger eq'n & end up with constraint

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -e^{-\gamma t}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + e^{\gamma t}\frac{1}{2}m\omega_0^2x^2\psi(x,t)$$

$$i\hbar\left[-\frac{1}{4a}\frac{da}{dt} - i\frac{d\Theta}{dt} - x^2\frac{da}{dt}\right] = -e^{-\gamma t}\frac{\hbar^2}{2m}[-2a + 4a^2x^2] + e^{\gamma t}\frac{1}{2}m\omega_0^2x^2$$

match terms to obtain

$$\frac{-i\hbar}{4a}\frac{da}{dt} + \hbar\frac{d\Theta}{dt} = e^{-\gamma t}\frac{\hbar^2 a}{m} \qquad i\hbar\frac{da}{dt} = e^{-\gamma t}\frac{2\hbar^2}{m}a^2 - e^{\gamma t}\frac{1}{2}m\omega_0^2$$

$$a(t) = \frac{m\omega_0}{2\hbar}e^{\gamma t}\eta \Rightarrow i\hbar\gamma\frac{m\omega_0}{2\hbar}\eta = \frac{2\hbar^2}{m}\left(\frac{m\omega_0\eta}{2\hbar}\right)^2 - \frac{1}{2}m\omega_0^2$$

$$\text{Consistent w/ } \eta^2 - i\frac{\gamma}{\omega_0}\eta - 1 = 0 \Rightarrow \eta = \left[-i\left(\frac{\gamma}{\omega_0}\right) \pm \sqrt{-\left(\frac{\gamma}{\omega_0}\right)^2 - 4}\right]/2$$

choosing $\gamma < 2\omega_0$ allows sqrt to contain a positive # for positive γ $\Leftarrow$

$$\Rightarrow \eta = \sqrt{1-\left(\frac{\gamma}{2\omega_0}\right)^2} - i\left(\frac{\gamma}{2\omega_0}\right)$$

<u>next</u> solve for $\Theta(t)$

$$\hbar\frac{d\Theta}{dt} = \frac{i\hbar}{4a}\frac{da}{dt} + e^{-\gamma t}\frac{\hbar^2 a}{m} \qquad a(t) = \frac{m\omega_0}{2\hbar}e^{\gamma t}\eta \qquad \hbar\frac{d\Theta}{dt} = \frac{i\hbar}{4}\gamma + \frac{\hbar^2}{m}\frac{m\omega_0}{2\hbar}\eta$$

$$= \frac{i\hbar\gamma}{4} + \frac{\hbar\omega_0}{2}\eta$$

$$\Theta(t) = \frac{1}{2}\omega_0\eta t + \frac{i}{4}\gamma t \Leftarrow$$

$$\Rightarrow \Theta(t) = \frac{1}{2}\omega_0\left[\sqrt{1-\left(\frac{\gamma}{2\omega_0}\right)^2} - i\left(\frac{\gamma}{2\omega_0}\right)\right]t + \frac{i}{4}\gamma t$$

$$= \frac{1}{2}\sqrt{\omega_0^2-\gamma^2}\,t$$

Ultimately

$$\psi(x,t) = \left[\frac{m\omega_0 e^{\gamma t}\eta}{\pi\hbar}\right]^{1/4}\exp\left\{-i\frac{1}{2}\sqrt{\omega_0^2-\gamma^2}\,t\right\}\exp\left\{-\frac{m\omega_0 e^{\gamma t}}{2\hbar}x^2\right\}$$

$$\eta = \sqrt{1-\left(\frac{\gamma}{2\omega_0}\right)^2} - i\left(\frac{\gamma}{2\omega_0}\right)$$

LC Circuit dynamic mass

Pset 11 Problem 3 Golden Rule $\omega_0^2 = \frac{1}{LC}$ 12/12/19

LC circuit by adding a bath. $\hat{H} = \hat{H}_{LC} + \hat{H}_{bath} + \hat{H}_{int}$

where $\hat{H}_{LC} = \frac{1}{2}L\hat{i}^2 + \frac{1}{2}Cv^2$ $\quad \hat{H}_{bath} = \sum_j (|\phi_1\rangle H_1 \langle\phi_1| + |\phi_2\rangle H_2 \langle \phi_2|)_j$

assume $\rho(E) = \rho_0$ $\quad \hat{H}_{int} = Av\sum_j (|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|)_j$

a) Classical eqns of motion for LC circuit w/ resistor in series:

$$\frac{d}{dt}v(t) = \frac{1}{C}i(t) \qquad \frac{d}{dt}i(t) = \frac{-1}{L}(v(t) + Ri(t))$$

We can check by working out Ehrenfest's theorem for v & i.

$$\frac{d}{dt}\langle v\rangle = \frac{1}{i\hbar}\langle[v,\hat{H}]\rangle = \frac{1}{i\hbar}\langle[v, \frac{-\hbar^2}{2LC^2}\frac{\partial^2}{\partial v^2}]\rangle = -\left(\frac{\hbar^2}{2LC^2}\right)\frac{1}{i\hbar}\langle -2\frac{\partial}{\partial v}\rangle$$

$$= \frac{1}{C}\langle -\frac{i\hbar}{LC}\frac{\partial}{\partial v}\rangle = \frac{1}{C}\langle\hat{i}\rangle$$

$\swarrow \hat{O}$ contains raising & lowering operators for two level system.

$$\frac{d}{dt}\langle\hat{i}\rangle = \frac{1}{i\hbar}\langle[\hat{i},\hat{H}]\rangle = \frac{1}{i\hbar}\langle[\hat{i}, \tfrac{1}{2}Cv^2]\rangle + \underbrace{\frac{1}{i\hbar}\langle[\hat{i}, v\hat{O}]\rangle}_{=\frac{1}{i\hbar}\left(-\frac{i\hbar}{LC}\right)\langle\frac{\partial}{\partial v}, v\hat{O}\rangle = \frac{-1}{LC}\langle\hat{O}\rangle}$$

$$= -\frac{1}{L}\langle v\rangle - \frac{1}{LC}\langle\hat{O}\rangle$$

This interaction Hamiltonian has the right form to contribute loss the way a resistor would. Would work best if followed that: $-\frac{R}{L}\langle i\rangle = -\frac{1}{LC}\langle\hat{O}\rangle$ or $\langle\hat{O}\rangle = RC\langle\hat{i}\rangle$

b) Find the decay rate for energy loss in case of classical series RLC circuit.

We can estimate the rate of energy loss by solving for the complex frequency at resonance. We assume:

$$v(t) = V_0 e^{-i\omega t} \qquad \frac{d}{dt}i(t) = -\frac{1}{L}v(t) - \frac{R}{L}i(t)$$

$$i(t) = i_0 e^{-i\omega t} \qquad \frac{d^2}{dt^2}i(t) = \frac{-1}{L}\frac{dv(t)}{dt} - \frac{R}{L}\frac{di}{dt}$$

$\uparrow = \frac{1}{C}i(t)$

$$\frac{d^2}{dt^2}i(t) + \frac{1}{LC}i(t) + \frac{R}{L}\frac{di}{dt} = 0$$

$$\Rightarrow s^2 + \frac{R}{L}s + \frac{1}{LC} = \gamma$$

$$s = \frac{-\frac{R}{L} \pm \sqrt{\left(\frac{R}{L}\right)^2 - 4\left(\frac{1}{LC}\right)}}{2} = -\frac{R}{2L} \pm \sqrt{\left(\frac{R}{2L}\right)^2 - \frac{1}{LC}}$$

$$s \approx \pm i\omega_0 - \frac{R}{2L} \qquad i(t) \sim e^{\pm i\omega_0 t}e^{-\frac{R}{2L}t} \sim v(t)$$

$\uparrow \sqrt{\omega_0^2 - \left(\frac{R^2}{L}\right)}$

$$E = \tfrac{1}{2}Cv^2(t) + \tfrac{1}{2}Li^2(t) \sim e^{-\frac{Rt}{L}}$$

~~Year~~ $\gamma \sim \frac{R}{L}$ energy decay rate.

c) Find an expression for the transition matrix element between initial state ~~a~~ w/ one photon in LC circuit & no excited states in the bath, and a final state w/ LC circuit in ground state & one excited bath state.

$$\Psi_i = \underbrace{\psi_1(v)}_{\text{one photon in LC circuit}}\ \underbrace{\Phi_0}_{\text{no excited states in bath}} \qquad \Psi_f = \underbrace{\psi_0(v)}_{\text{LC circuit ground state}}\ \underbrace{(|\phi_2\rangle\langle\phi_1|)_K\Phi_0}_{\text{one excited bath state.}}$$

$\langle\Psi_f|\hat{H}_{int}|\Psi_i\rangle$

$$= \langle\psi_0(v)(|\phi_2\rangle\langle\phi_1|)_K\Phi_0 \,|\, Av\sum_j(|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|)_j \,|\, \psi_1(v)\Phi_0\rangle$$

$$A\langle\psi_0(v)|v|\psi_1(v)\rangle\underbrace{\langle(|\phi_2\rangle\langle\phi_1|)_K\Phi_0|\sum_j(|\phi_1\rangle\langle\phi_2| + |\phi_2\rangle\langle\phi_1|)_j|\Phi_0\rangle}$$

$$= \langle(|\phi_2\rangle\langle\phi_1|)_K\Phi_0|(\cancel{|\phi_1\rangle\langle\phi_2|} + |\phi_2\rangle\langle\phi_1|)_K\Phi_0\rangle$$

because $(|\phi_1\rangle\langle\phi_2|)(|\phi_1\rangle\langle\phi_2|) = 0$

$$= \langle(|\phi_2\rangle\langle\phi_1|)_K\Phi_0|(|\phi_2\rangle\langle\phi_1|)_K\Phi_0\rangle$$

$$A\langle\psi_0(v)|v|\psi_1(v)\rangle = A\langle\psi_0(v)|\sqrt{\frac{\hbar\omega}{2C}}(\hat{a}+\hat{a}^\dagger)|\psi_0(v)\rangle = A\sqrt{\frac{\hbar\omega_0}{2C}}$$

d) Evaluate the decay rate for single oscillator quantum through Golden Rule

$$\Gamma = \frac{2\pi}{\hbar}|\langle\psi_f|V|\psi_i\rangle|^2\rho(E)$$

$$= \boxed{\frac{2\pi}{\hbar}\left|A\sqrt{\frac{\hbar\omega_0}{2C}}\right|^2\rho_0}$$

2005 Final Problem 5 12/16/19

Use the Golden rule to estimate radiative capture rate for a free electron by a proton. $\gamma = \frac{2\pi}{\hbar}|\langle\psi_f|\hat{V}|\psi_i\rangle|^2\rho(E_f)$. When the electron is free, assume it is described by $\psi_i = \frac{e^{ik\cdot r}}{L^{3/2}}$. In the ground state, the electron is given by: $\psi_f = \frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}$

$\hat{V} = -d\cdot\hat{E}(r)$ where $d = -er$ $\quad \psi_i = \psi_i(r)\Phi_0 \quad \psi_f = \psi_f(r)(\hat{a}^\dagger_{k\sigma}\Phi_0)$

Assume wavelength of photon is large compared to size of atom $e^{ik\cdot r} \approx 1$

$$\int e^{ik\cdot r} z e^{-r/a_0}d^3r = -i(32\pi a_0^5)\frac{k_z}{(1+a_0^2|k|^2)^3}$$

Since proton mass $m_p \gg$ electron mass m_e, reduced mass:

$$\mu = \frac{m_e m_p}{m_e + m_p} \approx m_e$$

Emitted photon carries an energy

$$\hbar\omega = E_i - E_f = \frac{\hbar^2k^2}{2m} + \frac{\mu}{m_e}I_H = \frac{\hbar^2k^2}{2m} + I_H$$

density of states:

$$\rho(E_f) = \frac{L^3\omega^2}{\pi^2\hbar c^3}$$

matrix element: $\langle\psi_f|\hat{V}|\psi_i\rangle = -\langle\psi_f|d|\psi_i\rangle\cdot\langle\phi_i|\hat{E}|\phi_f\rangle = -\langle\psi_f|d|\psi_i\rangle\sum_\sigma\sum_k i_\sigma\sqrt{\frac{\hbar\omega}{2\epsilon_0L^3}}\langle\hat{a}^\dagger\Phi_0|\hat{a}+\hat{a}^\dagger|\Phi_0\rangle$

The dipole moment: $\langle\psi_f|d|\psi_i\rangle = -e\langle\psi_f|r|\psi_i\rangle = -e[\langle\psi_f|x|\psi_i\rangle i_x + \langle\psi_f|y|\psi_i\rangle i_y + \langle\psi_f|z|\psi_i\rangle i_z]$

$$= \frac{ie(32\pi a_0^5)}{L^{\frac{3}{2}}\sqrt{\pi a_0^3}(1+a_0^2|k|^2)^3}[k_x i_x + k_y i_y + k_z i_z]$$

Since the electric field can be polarized in arbitrary directions, we need ~~to~~ do an averaging of the matrix element squared over all angles. Let θ be the angle between i_σ and k:

$$|\langle\psi_f|\hat{V}|\psi_i\rangle|^2 = \frac{\hbar\omega}{2\pi a_0^3\epsilon_0L^6}\frac{e^2(32\pi a_0^5)^2|k|^2}{(1+a_0^2|k|^2)^6}\frac{\int_0^{2\pi}d\phi\int_0^\pi d\theta\cos^2\theta\sin\theta\, d\theta}{\int_0^{2\pi}d\phi\int_0^\pi d\theta\sin\theta}$$

$$= \frac{\hbar\omega}{6\pi a_0^3\epsilon_0L^6}\frac{e^2(32\pi a_0^5)^2|k|^2}{(1+a_0^2|k|^2)^3}$$

Therefore the Golden Rule radiative capture rate is $\gamma = \frac{2\pi}{\hbar}|\langle\psi_f|\hat{V}|\psi_i\rangle|^2\rho(E_f)$

$$\boxed{\gamma = \frac{\omega^3a_0^7}{3c^3\hbar\epsilon_0L^3}\frac{e^2 32^2|k|^2}{(1+a_0^2|k|^2)^6}}$$

Problem 4

Dealing with interaction matrix

In this problem we are interested in the Compton scattering of a photon from an electron in free space using a nonrelativistic approximation. We make use of the Hamiltonian

$$\hat{H} = \int \frac{1}{2}\epsilon_0 \hat{\mathbf{E}}(\mathbf{r}) \cdot \hat{\mathbf{E}}(\mathbf{r}) + \frac{1}{2}\mu_0 \hat{\mathbf{H}}(\mathbf{r}) \cdot \hat{\mathbf{H}}(\mathbf{r}) + \frac{\left(\hat{\mathbf{p}} + e\hat{\mathbf{A}}(\mathbf{r})\right) \cdot \left(\hat{\mathbf{p}} + e\hat{\mathbf{A}}(\mathbf{r})\right)}{2m}$$

where we have assumed for the charge of the electron

$$q = -|e| = -e$$

For the initial state we take a free electron state normalized to the volume of a box (making use of periodic boundary conditions for the electron), and a photon according to

$$\Psi_i = \frac{1}{\sqrt{L^3}} e^{i\mathbf{q}_i \cdot \mathbf{r}} \hat{a}^\dagger_{\mathbf{k}_i, \sigma_i} |\Phi_0\rangle$$

and for the final state we have

$$\Psi_f = \frac{1}{\sqrt{L^3}} e^{i\mathbf{q}_f \cdot \mathbf{r}} \hat{a}^\dagger_{\mathbf{k}_f, \sigma_f} |\Phi_0\rangle$$

We require that

$$\mathbf{k}_i \neq \mathbf{k}_f \qquad \mathbf{q}_i \neq \mathbf{q}_f$$

in order to ensure that a scattering event is modeled. Later on we will assume that the electron is initially at rest

$$\mathbf{q}_i \to 0$$

(a) Evaluate the interaction matrix element

$$\langle \Psi_f | \hat{H}_{int} | \Psi_i \rangle = \left\langle \Psi_f \left| \frac{e^2 \hat{\mathbf{A}}(\mathbf{r}) \cdot \hat{\mathbf{A}}(\mathbf{r})}{2m} \right| \Psi_i \right\rangle$$

Note that for photon scattering, there is one photon in the initial state and one photon in the final state, so that terms linear in $\hat{\mathbf{A}}$ will not contribute at lowest order.

(b) (Optional) There are various ways to proceed with the evaluation of the Golden Rule rate. Perhaps the simplest for this calculation is to make use of

$$\gamma = \frac{2\pi}{\hbar} \sum_{\mathbf{q}_f} \sum_{\mathbf{k}_f} \sum_{\sigma_f} |\langle \Psi_f | \hat{H}_{int} | \Psi_i \rangle|^2 \delta(E_i - E_f(\mathbf{q}_f, \mathbf{k}_f))$$

where we assume that a continuum approximation will be made for the evaluation of the δ-function in energy. For this part of the problem, carry out the summation over the final electron momentum $\mathbf{q}_f$.

[redacted]lem 4 + 9/10

$$\hat{H} = \int \tfrac{1}{2}\epsilon_0 \hat{E}(r)\cdot\hat{E}(r) + \tfrac{1}{2}\mu_0 \hat{H}(r)\cdot\hat{H}(r) + \frac{(\hat{p}+e\hat{A}(r))\cdot(\hat{p}+e\hat{A}(r))}{2m}$$

$$\hookrightarrow \frac{\hat{p}\cdot\hat{p}}{2m} + \frac{e\hat{A}\cdot\hat{p}}{m} + \frac{e^2}{2m}\hat{A}\cdot\hat{A}$$

$\Rightarrow$ want $\gamma = \frac{2\pi}{\hbar}|\langle \psi_f | \hat{H}_{int} | \psi_i \rangle|^2 \rho$

$$\Psi_i = \frac{1}{\sqrt{L^3}} e^{i\vec{q}_i\cdot\vec{r}} \hat{a}^+_{k_i\sigma_i}|\Phi_0\rangle \qquad \Psi_f = \frac{1}{\sqrt{L^3}} e^{i\vec{q}_f\cdot\vec{r}} \hat{a}^+_{\vec{k}_f\sigma_f}|\Phi_0\rangle$$

a) $$\langle \Psi_f | \hat{H}_{int} | \Psi_i \rangle = \left\langle \frac{e^{i\vec{q}_f\cdot\vec{r}}}{\sqrt{L^3}} \hat{a}^+_{\vec{k}_f\sigma_f}|\Phi_0 \right| \left[\sum_{k\sigma} \hat{i}_\sigma \sqrt{\frac{\hbar}{2\epsilon_0 L^3 \omega_k}} \frac{[\hat{a}_{k\sigma}e^{i\vec{k}\cdot\vec{r}} \cdot \hat{a}^+_{k\sigma}e^{-i\vec{k}\cdot\vec{r}}]}{i}\right]$$

$$\left[\sum_{k\sigma} \hat{i}_\sigma \sqrt{\frac{\hbar}{2\epsilon_0 L^3 \omega_k}} \frac{[\hat{a}_{k\sigma}e^{i\vec{k}\cdot\vec{r}} - \hat{a}^+_{k\sigma}e^{-i\vec{k}\cdot\vec{r}}]}{i}\right] \left| \frac{e^{i\vec{q}_i\cdot\vec{r}}}{\sqrt{L^3}} a^+_{\vec{k}_i\sigma_i}|\Phi_0 \right\rangle$$

define: $$\vec{A}(\vec{r}) = -i\sum_k \sum_\sigma \hat{i}_\sigma \sqrt{\frac{\hbar}{2\epsilon_0 L^3 \omega_k}} \left(\hat{a}_{k\sigma}e^{i\vec{k}\cdot\vec{r}} - a^+_{k\sigma}e^{-i\vec{k}\cdot\vec{r}}\right) = \hat{A}_+(\vec{r}) + \hat{A}_-(\vec{r})$$

destroy destroy

$$= \frac{e^2}{m}\frac{1}{L^3}\left\langle e^{i\vec{q}_f\cdot\vec{r}} a^+_{\vec{k}_f\sigma_f}|\Phi_0\rangle \right| \hat{A}_+(\vec{r})\cdot\hat{A}_-(\vec{r}) + \hat{A}_-(\vec{r})\hat{A}_+(\vec{r}) \left| e^{i\vec{q}_i\cdot\vec{r}} a^+_{\vec{k}_i\sigma_i}|\Phi_0 \right\rangle$$

$$= \frac{e^2}{m}\frac{1}{L^3}\frac{\hbar}{2\epsilon_0 L^3}\sqrt{\frac{1}{\omega_{k_f}\omega_{k_f}}}\, \hat{i}_{\sigma_i}\cdot\hat{i}_{\sigma_f} \langle \Phi_0|\Phi_0\rangle \int_0^L\int_0^L\int_0^L e^{-i\vec{q}_f\cdot\vec{r}} e^{-i\vec{k}_f\cdot\vec{r}} e^{i\vec{q}_i\cdot\vec{r}} e^{i\vec{k}_i\cdot\vec{r}}\, d^3r$$

$d^3r = dx\,dy\,dz$

q_s & k_s are discrete

$$\Rightarrow \boxed{\frac{e^2}{m}\frac{1}{L^3}\frac{\hbar}{2\epsilon_0}\frac{1}{\sqrt{\omega_{k_i}\omega_{k_f}}}\, \hat{i}_{\sigma_i}\cdot\hat{i}_{\sigma_f}\, \delta_{\vec{q}_i+\vec{k}_i-\vec{q}_f-\vec{k}_f}} \Leftarrow L^3 \delta_{\vec{q}_i+\vec{k}_i-\vec{q}_f-\vec{k}_f}$$

Conservation of momentum $\Rightarrow$ integral $= L^3$

$\Rightarrow$ initial & final momentum of photon conserved

b) $$\gamma = \frac{2\pi}{\hbar}\sum_{q_f}\sum_{k_f}\sum_{\sigma_f} |\langle \Psi_f | \hat{H}_{int} | \Psi_i \rangle|^2 \delta(E_i - E_f(q_f, k_f))$$

$$\rho_{xy}(E) = \int_{-\infty}^{\infty} dE_x \int_{-\infty}^{\infty} dE_y\, \rho_x(E_x)\rho_y(E_y)\delta(E - E_x - E_y)$$

$$E_i = \frac{\hbar^2|\vec{q}_i|^2}{2m} + \hbar c|\vec{k}_i| \qquad E_f = \frac{\hbar^2|q_f|^2}{2m} + \hbar c$$

Sum over $\vec{q}_f$

$$\sum_{\vec{q}_f} |\text{stuff}\ \delta_{\vec{q}_i+\vec{k}_i-\vec{q}_f-\vec{k}_f}|^2 = |\text{stuff}|^2 \Big|_{\vec{q}_f = \vec{q}_i+\vec{k}_i-\vec{k}_f}$$

$$\delta(E_i - E_f(\vec{q}_f, \vec{k}_f)) = \delta\left(\frac{\hbar|\vec{q}_i|^2}{2m} + \hbar c|k_i| - \frac{\hbar^2|\vec{q}_i+\vec{k}_i-\vec{k}_f|^2}{2m} + \hbar c|\vec{k}_f|\right)$$

$q_f \Rightarrow$ electron momentum

$$\gamma = \frac{2\pi}{\hbar}\left[\frac{e^2\hbar}{2\epsilon_0 m L^3}\right]^2 \sum_{k_f}\sum_{\sigma_f} \frac{1}{\omega_{\vec{k}_f}\omega_{\vec{k}_i}} (\hat{i}_{\sigma_k}\cdot\hat{i}_{\sigma_i})^2\, \delta\left(\frac{\hbar|\vec{q}_i|^2}{2m} + \hbar c|\vec{k}_i| - \frac{\hbar^2|\vec{q}_i+\vec{k}_i-\vec{k}_f|^2}{2m} - \hbar c|\vec{k}_f|\right)$$

Pset 10 Problem 1 12/17/19

focus on modes $n_x=1, n_y=1, n_z=0$

$$u(r) = \hat{i}_z 2 \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)$$

$$v(r) = \hat{i}_x \sqrt{2}\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right) - \hat{i}_y \sqrt{2}\cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)$$

a) Show TM is normalized according to $\int |\vec{u}(\vec{r})|^2 d^3r = L^3$ & $\int |v(r)|^2 d^3r = L^3$

Just plug in & chug. Remember: $\int_0^L \int_0^L \int_0^L |u(r)|^2 \, dx\,dy\,dz$

i.e. $\int |\vec{u}(\vec{r})|^2 d^3r = \int_0^L\int_0^L\int_0^L 2^2 \sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{\pi y}{L}\right) dx\,dy\,dz = 4\cdot\left(\frac{1}{2}L\right)\left(\frac{1}{2}L\right)L = L^3$

b) Find expressions for field operators $\hat{\vec{E}}(r)$, $\hat{\vec{H}}(r)$, & $\hat{\vec{A}}(r)$ for this mode in terms of $u(r)$ & $v(r)$. Note that vector potential can be constructed using:

$\mu_0 \hat{H}(r) = \nabla\times\hat{A}(r)$

$\nabla\cdot\hat{A}(r) = 0$

$$\hat{\vec{E}}(r) = \sqrt{\frac{\hbar\omega_0}{2\epsilon_0 L^3}}\,\vec{u}(\vec{r})\,(\hat{a}+\hat{a}^+)$$

$$\hat{\vec{H}}(r) = \sqrt{\frac{\hbar\omega_0}{2\mu_0 L^3}}\,\vec{v}(\vec{r})\left(\frac{\hat{a}-\hat{a}^+}{i}\right)$$

For the vector potential operator, we would expect: $\hat{\vec{A}}(\vec{r}) = \vec{u}(r)\hat{A}$

Plugging into sol'n that connects $\hat{A}(r)$ & $A(r)$; $\mu_0\hat{H}(r) = \mu_0\sqrt{\frac{\hbar\omega_0}{2\mu_0 L^3}}\,\vec{v}(\vec{r})\left(\frac{\hat{a}-\hat{a}^+}{i}\right) = \nabla\times\hat{\vec{A}}(\vec{r}) = \nabla\times[\vec{u}(\vec{r})\hat{A}]$

resonator modes satisfy: $\nabla\times\vec{u}(r) = k\vec{v}(r)$, $\nabla\times\vec{v}(\vec{r}) = k\vec{u}(\vec{r})$

so we can write: $\mu_0\sqrt{\frac{\hbar\omega_0}{2\mu_0 L^3}}\,\vec{v}(r)\left(\frac{\hat{a}-\hat{a}^+}{i}\right) = k\vec{v}(\vec{r})\hat{A}$

conclude: $\hat{A} = \frac{\mu_0}{k}\sqrt{\frac{\hbar\omega_0}{2\mu_0 L^3}}\left(\frac{\hat{a}-\hat{a}^+}{i}\right) = \frac{\mu_0 c}{\omega_0}\sqrt{\frac{\hbar\omega_0}{2\mu_0 L^3}}\left(\frac{\hat{a}-\hat{a}^+}{i}\right) = \sqrt{\frac{\mu_0}{\epsilon_0}}\sqrt{\frac{\hbar}{2\mu_0 L^3\omega_0}}\left(\frac{\hat{a}-\hat{a}^+}{i}\right) = \sqrt{\frac{\hbar}{2\epsilon_0 L^3\omega_0}}\left(\frac{\hat{a}-\hat{a}^+}{i}\right)$

$$\Rightarrow \hat{\vec{A}}(\vec{r}) = \sqrt{\frac{\hbar}{2\epsilon_0\omega_0 L^3}}\,\vec{u}(\vec{r})\left(\frac{\hat{a}-\hat{a}^+}{i}\right)$$

c) Consider a semiclassical approximation in which an electron is treated classically, and the fields are treated quantum mechanically. The Hamiltonian in this case is:

$$\hat{H} = \int \frac{1}{2}\epsilon_0\hat{\vec{E}}(\vec{r})\cdot\hat{\vec{E}}(\vec{r}) + \frac{1}{2}\mu_0\hat{\vec{H}}(\vec{r})\cdot\hat{\vec{H}}(\vec{r})\,d^3\vec{r} - \int\vec{J}(\vec{r},t)\,\hat{\vec{A}}(\vec{r})\,d^3\vec{r}$$

electron trajectory: $z(t) = v_0 t$

associated current density:

$$\vec{J}(\vec{r},t) = \hat{i}_z q v_0\,\delta(x-L/2)\,\delta(y-L/2)\,\delta(z-v_0t)$$

Write down the time-dependent Hamiltonian for the mode in configuration space. Hamiltonian should be in the form: $\hat{H} = [\ldots]\frac{d^2}{de^2} + [\ldots]e^2 + [\ldots]\hat{h}$

For the electromagnetic Hamiltonian, we can write:

$$\int \frac{1}{2}\epsilon_0\hat{\vec{E}}(\vec{r})\cdot\hat{\vec{E}}(\vec{r}) + \frac{1}{2}\epsilon_0\hat{\vec{H}}(\vec{r})\cdot\hat{\vec{H}}(\vec{r})\,d^3\vec{r} = \frac{-(\hbar\omega_0)^2}{2\epsilon_0 L^3}\frac{d^2}{de^2} + \frac{1}{2}\epsilon_0 L^3 e^2$$

For the interaction, we can write:

$$-\int\vec{J}(\vec{r},t)\hat{\vec{A}}(\vec{r})\,d^3\vec{r} = -\int\vec{J}(\vec{r},t)\cdot\sqrt{\frac{\hbar}{2\epsilon_0 L^3\omega_0}}\,\vec{u}(\vec{r})\left(\frac{\hat{a}-\hat{a}^+}{i}\right)d^3\vec{r}$$

$$= -\sqrt{\frac{\hbar}{2\epsilon_0 L^3\omega_0}}\int\vec{J}(\vec{r},t)\cdot\vec{u}(\vec{r})\,d^3\vec{r}\left(\frac{\hat{a}-\hat{a}^+}{i}\right)$$

For the spatial integral, we can write:

$$\int\vec{J}(\vec{r},t)\cdot\vec{u}(\vec{r})\,d^3\vec{r} = \int\left[\hat{i}_z q v_0\delta(x-L/2)\delta(y-L/2)\delta(z-v_0t)\right]\cdot\left[\hat{i}_z 2\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)\right]d^3\vec{r}$$

$$= 2qv_0\left[\int_0^L\delta(x-L/2)\sin\left(\frac{\pi x}{L}\right)dx\right]\left[\int_0^L\delta(y-L/2)\sin\left(\frac{\pi y}{L}\right)dy\right]\left[\int_0^L\delta(z-v_0t)\,dz\right]$$

$$= 2qv_0\left[\sin\left(\frac{\pi}{2}\right)\right]\left[\sin\left(\frac{\pi}{2}\right)\right]\left[\int_0^L\delta(z-v_0t)\,dz\right]$$

The sine term both evaluate to 1 and the last integral evaluates to 1 when the electron is inside the cavity. Consequently, we can write:

$$\int\vec{J}(\vec{r},t)\cdot\vec{u}(\vec{r})\,d^3\vec{r} = 2qv_0 f(t) = 2qv_0\begin{cases}0 & t<0\\ 1 & 0<t<L/v_0\\ 0 & L/v_0<t\end{cases}$$

We can then write the time-dependent Hamiltonian as:

$$\hat{H} = \frac{-(\hbar\omega_0)^2}{2\epsilon_0 L^3}\frac{d^2}{de^2} + \frac{1}{2}\epsilon_0 L^3 e^2 - \sqrt{\frac{\hbar}{2\epsilon_0 L^3\omega_0}}\,2qv_0 f(t)\left(\frac{\hat{a}-\hat{a}^+}{i}\right)$$

We recall that $\hat{h} = -i\frac{\hbar\omega_0 c}{L^3}\frac{d}{de} = \sqrt{\frac{\hbar\omega_0}{2\mu_0 L^3}}\left(\frac{\hat{a}-\hat{a}^+}{i}\right)$

We can write the dynamic Hamiltonian as

$$\boxed{\hat{H} = -\frac{(\hbar\omega_0)^2}{2\epsilon_0 L^3}\frac{d^2}{de^2} + \frac{1}{2}\epsilon_0 L^3 e^2 - 2\sqrt{\frac{\mu_0}{\epsilon_0}}\frac{qv_0}{\omega_0}f(t)\,\hat{h}}$$

d) Find Ehrenfest theorem evolution equations for $\langle e\rangle$ & $\langle\hat{h}\rangle$ for this model.

Without the source present, we know that Ehrenfest equations would be:

$$\frac{d}{dt}\langle e\rangle = \frac{k}{\epsilon_0}\langle\hat{h}\rangle \qquad \frac{d}{dt}\langle\hat{h}\rangle = -\frac{k}{\epsilon_0}\langle e\rangle$$

The only issue is that there is a driving term. We know that $\hat{h}$ commutes with $\hat{h}$ so we would not expect the second Ehrenfest theorem evolution equation to change. However, there will definitely be modification of the first one.

$$\frac{d}{dt}\langle e\rangle = \frac{k}{\epsilon_0}\langle\hat{h}\rangle + \frac{1}{i\hbar}\left\langle\left[e, -2\sqrt{\frac{\mu_0}{\epsilon_0}}\frac{qv_0}{\omega_0}f(t)\,\hat{h}\right]\right\rangle = \frac{k}{\epsilon_0}\langle\hat{h}\rangle - \frac{1}{i\hbar}2\sqrt{\frac{\mu_0}{\epsilon_0}}\frac{qv_0}{\omega_0}f(t)\langle[e,\hat{h}]\rangle$$

We evaluate the commutator: $[e,\hat{h}] = \left[e, -i\frac{\hbar\omega_0 c}{L^3}\frac{d}{de}\right] = i\frac{\hbar\omega_0 c}{L^3}$

This can be used to obtain: $\frac{d}{dt}\langle e\rangle = \frac{k}{\epsilon_0}\langle\hat{h}\rangle - \frac{1}{i\hbar}2\sqrt{\frac{\mu_0}{\epsilon_0}}\frac{qv_0}{\omega_0}f(t)\left[i\frac{\hbar\omega_0 c}{L^3}\right] = \frac{k}{\epsilon_0}\langle\hat{h}\rangle - 2\frac{qv_0}{\epsilon_0 L^3}f(t)$

e) Solve for $\langle e\rangle$ and $\langle\hat{h}\rangle$ for $0\le t\le L/v_0$

assuming model is in ground state initially.

- For $0\le t\le L/v_0$, assume sol'ns of form: $\langle e\rangle = A + B\sin(\omega_0 t) + C\cos(\omega_0 t)$, $\langle\hat{h}\rangle = D + F\sin(\omega_0 t) + G\cos(\omega_0 t)$

plug in to get:

$$\omega_0 B\cos(\omega_0 t) - \omega_0 C\sin(\omega_0 t) = \frac{k}{\epsilon_0}\left[D + F\sin(\omega_0 t) + G\cos(\omega_0 t)\right] - 2\frac{qv_0}{\epsilon_0 L^3}$$

$$\omega_0 F\cos(\omega_0 t) - \omega_0 G\sin(\omega_0 t) = \frac{-k}{\mu_0}\left[A + B\sin(\omega_0 t) + C\cos(\omega_0 t)\right]$$

Match terms & write: $\omega_0 B = \frac{k}{\epsilon_0}G$, $-\omega_0 C = \frac{k}{\epsilon_0}F$, $0 = \frac{k}{\epsilon_0}D - 2\frac{qv_0}{\epsilon_0 L^3}$, $\omega_0 F = -\frac{k}{\mu_0}C$

$-\omega_0 G = \frac{-k}{\mu_0}B$, $0 = A$

Match boundary conditions at $t=0$ leads to: $A + C = 0$, $D + G = 0$

Use this to assign constants: $A=0$, $C=0$, $F=0$, $D = 2\frac{qv_0}{kL^3}$, $G = -2\frac{qv_0}{kL^3}$, $B = \frac{k}{\omega_0\epsilon_0}G = -\sqrt{\frac{\mu_0}{\epsilon_0}}\,2\frac{qv_0}{kL^3}$

$$\langle e\rangle = -\sqrt{\frac{\mu_0}{\epsilon_0}}\,2\frac{qv_0}{kL^3}\sin(\omega_0 t) \qquad \langle\hat{h}\rangle = 2\frac{qv_0}{kL^3}\left(1-\cos(\omega_0 t)\right)$$

f) Making use of (e), what would you expect for the value of $\langle\hat{n}\rangle$ # photons in mode after a single electron passes through? (Hint: would you expect this system to generate a classical state?)

Since there is no loss once electron leaves, we can use expectation value at $t=L/v_0$ to figure out $\langle\hat{n}\rangle$

Classical state generated:

$E_{classical} = \frac{1}{2}\epsilon_0 L^3\langle e\rangle^2 + \frac{1}{2}\mu_0 L^3\langle\hat{h}\rangle^2 = \hbar\omega_0\langle\hat{n}\rangle$

$\langle\hat{n}\rangle = \frac{\frac{1}{2}\epsilon_0 L^3\langle e\rangle^2 + \frac{1}{2}\mu_0 L^3\langle\hat{h}\rangle^2}{\hbar\omega_0}\Big|_{t=L/v_0}$

plug in part (e) & solve:

$$\langle\hat{n}\rangle = \frac{4q^2v_0^2}{\hbar\omega_0^3\epsilon_0 L^3}\left[1-\cos\left(\frac{\omega_0 L}{v_0}\right)\right]$$

Electromagnetic wave resonator

Pset 10, question 2 11/23/19

Consider a model for a charged particle in an electromagnetic field described by Hamiltonian:

$$\hat{H} = \frac{(\hat{p}-qA)\cdot(\hat{p}-qA)}{2m} + q\Phi$$

In the special case that: make use of Ehrenfest's theorem to evaluate $A = \hat{i}_x A_x(z,t)$

$$m\frac{d^2}{dt^2}\langle r\rangle = \langle F\rangle$$

Determine the expected value for force $\langle F\rangle$. You can use the Coulomb gauge

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Hint: may be useful to define canonical momentum: $\hat{\pi} = \hat{p} - qA$

Hint 2: Recall a nonrelativistic charged classical particle in the presence of an electric field & magnetic field is accelerated according to:

$$m\frac{d^2}{dt^2}r(t) = qE + v\times B \qquad \text{where in free space } B = \mu_0 H$$

$$\frac{d}{dt}\langle r\rangle = \frac{1}{i\hbar}\langle[r,\hat{H}]\rangle = \frac{1}{i\hbar}\left\langle\left[r, \frac{|\hat{p}|^2}{2m}\right]\right\rangle - \frac{1}{i\hbar}\left\langle\left[r, \frac{q}{m}A\cdot\hat{p}\right]\right\rangle \text{ in Coulomb gauge}$$

Coulomb Gauge:

$$\hat{H} = \frac{(\hat{\vec{p}}-q\vec{A})(\hat{\vec{p}}-q\vec{A})}{2m} + q\Phi = \frac{\hat{\vec{p}}\cdot\hat{\vec{p}}}{2m} - \frac{(q\vec{A}\hat{\vec{p}} + \hat{\vec{p}}q\vec{A})}{2m} + \frac{q^2\vec{A}\cdot\vec{A}}{2m} + q\Phi$$

From class notes

$$\left(-\frac{q}{m}\vec{A}\cdot\vec{p}\right) \Rightarrow \text{Coulomb Gauge}$$

$$\frac{d}{dt}\langle r\rangle = \frac{1}{i\hbar}\left\langle\left[\hat{i}_x x, -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right]\right\rangle + \frac{1}{i\hbar}\left\langle\left[\hat{i}_y y, -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}\right]\right\rangle + \frac{1}{i\hbar}\left\langle\left[\hat{i}_z z, -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\right]\right\rangle$$

$$+ \frac{1}{i\hbar}\left\langle\left[\hat{i}_x x, i\hbar\frac{q}{m}A_x\frac{\partial}{\partial x}\right]\right\rangle = \left\langle\hat{i}_x\frac{\hat{p}_x}{m}\right\rangle + \left\langle\hat{i}_y\frac{\hat{p}_y}{m}\right\rangle + \left\langle\hat{i}_z\frac{\hat{p}_z}{m}\right\rangle - \left\langle\hat{i}_x\frac{q}{m}A_x\right\rangle$$

$$= \frac{\langle\hat{p}-qA\rangle}{m}$$

easier to work with effective momentum operator: $\hat{\pi} = \hat{p} - qA$

$$\frac{d}{dt}\langle\hat{\pi}\rangle = \left\langle\frac{\partial\hat{\pi}}{\partial t}\right\rangle + \frac{1}{i\hbar}\langle[\hat{\pi},\hat{H}]\rangle$$

$$= \left\langle -q\frac{\partial A}{\partial t}\right\rangle + \frac{1}{i\hbar}\langle[\hat{p}, q\Phi]\rangle + \frac{1}{i\hbar}\left\langle\left[\hat{p}, -\frac{q}{m}A\cdot\hat{p}\right]\right\rangle + \frac{1}{i\hbar}\left\langle\left[\hat{p}, \frac{q^2}{2m}|A|^2\right]\right\rangle + \frac{1}{i\hbar}\left\langle\left[-qA, \frac{|\hat{p}|^2}{2m}\right]\right\rangle$$

$$+ \frac{1}{i\hbar}\left\langle\left[-qA, -\frac{q}{m}A\cdot\hat{p}\right]\right\rangle$$

$$\left\langle -q\frac{\partial A}{\partial t}\right\rangle = qE_T \qquad \frac{1}{i\hbar}\langle[\hat{p}, q\Phi]\rangle = -q\nabla\Phi = qE_L \qquad \frac{1}{i\hbar}\left\langle\left[\hat{p}, -\frac{q}{m}A\cdot\hat{p}\right]\right\rangle = \frac{1}{i\hbar}\left\langle\left[-\hat{i}_z i\hbar\frac{\partial}{\partial z}, i\hbar\frac{q}{m}A_x\frac{\partial}{\partial x}\right]\right\rangle$$

$$= \left\langle\hat{i}_z\frac{\partial A_x}{\partial z}\frac{q}{m}\hat{p}_x\right\rangle$$

$$\frac{1}{i\hbar}\left\langle\left[\hat{p}, \frac{q^2}{2m}|A|^2\right]\right\rangle = \left\langle\frac{-q^2}{m}A_x\frac{\partial A_x}{\partial z}\right\rangle$$

$$\frac{1}{i\hbar}\left\langle\left[-qA, \frac{|\hat{p}|^2}{2m}\right]\right\rangle = \frac{1}{i\hbar}\left\langle\left[-q\hat{i}_x A_x, -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right]\right\rangle = \left\langle -\frac{q}{2m}\hat{i}_x\hat{p}_z\frac{\partial A_z}{\partial z}\right\rangle + \left\langle\frac{-q}{2m}\hat{i}_x\frac{\partial A_x}{\partial z}\hat{p}_z\right\rangle$$

$$\frac{1}{i\hbar}\left\langle\left[-qA, -\frac{q}{m}A\cdot\hat{p}\right]\right\rangle = \left\langle -q\hat{i}_x A_x, \frac{q}{m}A_x\frac{\partial}{\partial x}\right\rangle = 0$$

$$\frac{d}{dt}\langle\hat{\pi}\rangle = qE_T + qE_L + \left\langle\hat{i}_z\frac{\partial A_x}{\partial z}\frac{q}{m}\hat{p}_x\right\rangle + \left\langle\frac{-q^2}{m}A_x\frac{\partial A_x}{\partial z}\right\rangle + \left\langle\frac{-q}{2m}\hat{i}_x\hat{p}_z\frac{\partial A_x}{\partial z}\right\rangle$$

$$+ \left\langle\frac{-q}{2m}\hat{i}_x\frac{\partial A_x}{\partial z}\hat{p}_z\right\rangle$$

$$E = E_L + E_T$$

$$B = \mu_0 H = \nabla\times A = \begin{vmatrix} \hat{i}_x & \hat{i}_y & \hat{i}_z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x(z) & 0 & 0 \end{vmatrix} = \hat{i}_y\frac{\partial A_x}{\partial z}$$

quantum mechanical version:

$$\frac{1}{2}\left(\frac{\hat{p}-qA}{m}\times B - B\times\frac{\hat{p}-qA}{m}\right) = \frac{1}{2}\left(\hat{i}_z\frac{\hat{p}_x - qA_x}{m}B_y - \hat{i}_x\frac{\hat{p}_z}{m}B_y\right)$$

$$-\frac{1}{2}\left(-\hat{i}_z B_y\frac{\hat{p}_x - qA_x}{m} + \hat{i}_x B_y\frac{\hat{p}_z}{m}\right) = \hat{i}_z\frac{\hat{p}_x - qA_x}{m}B_y - \hat{i}_x\frac{\hat{p}_z}{2m}B_y - \hat{i}_x B_y\frac{\hat{p}_z}{2m}$$

Based on this, we conclude that Ehrenfest's theorem is consistent with

$$\frac{d}{dt}\langle\hat{\pi}\rangle = qE + \left\langle\frac{1}{2}\left(\frac{\hat{p}-qA}{m}\times B - B\times\frac{\hat{p}-qA}{m}\right)\right\rangle$$

$$\text{or} \quad \frac{d}{dt}\langle\hat{\pi}\rangle = qE + \left\langle\frac{1}{2}\left(\frac{\hat{\pi}}{m}\times B - B\times\frac{\hat{\pi}}{m}\right)\right\rangle$$

overall, we can write

$$m\frac{d^2}{dt^2}\langle r\rangle = qE + \left\langle\frac{1}{2}\left(\frac{\hat{\pi}}{m}\times B - B\times\frac{\hat{\pi}}{m}\right)\right\rangle$$

Electromagnetic field thing

Pset 9 Question 3 12/17/19

A particle is trapped in an elongated well for which the time-independent Schrödinger equation applies: $E\Psi(x,y,z) = \left[-\frac{\hbar^2\nabla^2}{2m} + V(x,y,z)\right]\Psi(x,y,z)$

$$V(x,y,z) = \begin{cases} Az & 0<x<bz,\ 0<y<bz,\ z>0 \\ \infty & \text{otherwise} \end{cases}$$

Assume an adiabatic sol'n of form: $\Psi(x,y,z) = \phi(x,y,z)\psi(z)$

a) The adiabatic wavefunction $\phi(x,y;z)$ satisfies a parameterized Schrödinger eq'n of the form: $E_{xy}(z)\phi(x,y;z) = \hat{H}_{xy}(x,y;z)\phi(x,y;z)$

Find an expression for $\hat{H}_{xy}(x,y;z)$

We take z as a parameter & write

$$\hat{H}_{xy}(x,y;z) = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right] + V(x,y;z) \quad \text{where } V(x,y;z) = V(x,y;z)$$

b) Determine $\phi(x,y;z)$ & $E_{xy}(z)$ assuming the particle is in adiabatic ground state.

$$E_{xy}(z)\phi(x,y;z) = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]\phi(x,y;z) + V(x,y;z)\,\phi(x,y;z)$$

$$\phi(x,y;z) = \frac{2}{bz}\sin\left(\frac{\pi x}{bz}\right)\sin\left(\frac{\pi y}{bz}\right) \qquad E_{xy}(z) = 2\frac{\hbar^2\pi^2}{2m(bz)^2}$$

c) In the adiabatic approximation $\psi(z)$ satisfies eq'n of form: $E\psi(z) = \hat{H}_z(z)\psi(z)$

Find $\hat{H}_z(z)$

$$E\psi(z) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + Az + E_{xy}(z)\right]\psi(z)$$

$$\hat{H}_z(z) = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + Az + E_{xy}(z) = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + Az + 2\frac{\hbar^2\pi^2}{2m(bz)^2}$$

d) Find approximate shifted SHO sol'n for $\psi(z)$ & for E.

Taylor series for potential in z around minimum:

$$\frac{d}{dz}V_z(z) = 0 = \frac{d}{dz}\left[Az + E_{xy}(z)\right] = \frac{d}{dz}\left[Az + 2\frac{\hbar^2\pi^2}{2m(bz)^2}\right]$$

$$\Rightarrow z_0 = \left(\frac{2\hbar^2\pi^2}{Amb^2}\right)^{1/3}$$

Taylor series in general away from $z=0$:

$$V_z(z) = V_z(z_0) + (z-z_0)\cancel{\frac{dV_z}{dz}\Big|_{z=z_0}}^{\,0} + \frac{1}{2}(z-z_0)^2\frac{d^2V_z}{dz^2}\Big|_{z=z_0} + \ldots$$

$$\hat{H}_z(z) = -\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + V_z(z_0) + \frac{1}{2}(z-z_0)^2\frac{d^2V_z}{dz^2}\Big|_{z=z_0}$$

define shifted variable $z' = z - z_0$

$$m\omega_0^2 = \frac{d^2V_z}{d(z')^2}\Big|_{z=z_0} = \frac{d^2V_z}{dz^2}\Big|_{z=z_0}$$

$$\Rightarrow \psi(z) = \left[\frac{m\omega_0}{\pi\hbar}\right]^{1/4}\exp\left\{-\frac{m\omega_0}{2\hbar}(z')^2\right\} \quad \text{with } E = V_z(z_0) + \frac{1}{2}\hbar\omega_0$$

to find explicit expressions for $V_z(z_0)$ & $\frac{d^2V_z}{dz^2}\Big|_{z=z_0}$, we write:

$$V_z(z_0) = Az_0 + \frac{\hbar^2\pi^2}{mb^2z_0^2} = Az_0\left(\frac{2\hbar^2\pi^2}{Amb^2}\right)^{1/3} + \frac{\hbar^2\pi^2}{mb^2}\left(\frac{Amb^2}{2\hbar^2\pi^2}\right)^{2/3} = (\ldots) = 3A\left(\frac{Amb}{2\hbar^2\pi^2}\right)^{1/3}$$

$$m\omega_0^2 = \frac{d^2V_z}{dz^2}\Big|_{z=z_0} = 3A\left(\frac{Amb^2}{2\hbar^2\pi^2}\right)^{1/3}$$

$$\omega_0 = \sqrt{\frac{1}{m}\frac{d^2V_z}{dz^2}\Big|_{z=z_0}} = \sqrt{\frac{3A}{m}\left(\frac{Amb^2}{2\hbar^2\pi^2}\right)^{1/3}} = \left(\frac{27}{2}\right)^{1/6}\left[\frac{A^2b}{\hbar\pi m}\right]^{1/3}$$

2005 Final Problem 2 12/14/19

a) Determine the ground state energy for an electron with effective mass m_e in a spherical quantum well of radius R.

Same as that for a one-dimensional sq. well:

$$\frac{\hbar^2\pi^2}{2m_eR^2}$$

b) Estimate the total energy for two electrons in the ground state of the same quantum well. Coulomb interaction: $V_c = \frac{e^2}{4\pi\epsilon|r_2-r_1|}$

arbitrary estimate for $|r_2-r_1| \approx \frac{3R}{2}$

$$E = 2E[1s] + \frac{e^2}{6\pi\epsilon R} = \frac{\hbar^2\pi^2}{m_eR^2} + \frac{e^2}{6\pi\epsilon R} \qquad \frac{e^2}{4\pi\epsilon\frac{3R}{2}} = \frac{e^2}{6\pi\epsilon R}$$

c) The ground state energy for the two-electron ground state in the independent particle approximation can be written in the form

$$E_t = 2I[1s] + D[1s,1s]$$

Find $I[1s]$ & $D[1s,1s]$

$$I[1s] = \frac{\hbar^2\pi^2}{2m_eR^2} \quad \text{with definition } \phi_{1s}(r) = \frac{P_{1s}(r)}{\sqrt{4\pi}\,r}$$

$$D[1s,1s] = \iint \phi_{1s}(r)\,\phi_{1s}(s)\frac{e^2}{4\pi\epsilon_0|r-s|}\phi_{1s}(r)\,\phi_{1s}(s)\,d^3r\,d^3s$$

$$= \frac{e^2}{4\pi\epsilon_0}\sum_{lm}\frac{4\pi}{2l+1}\int_0^R dr_1\int_0^R dr_2\,P_{1s}^2(r_1)P_{1s}^2(r_2)\left(\frac{r_<^l}{r_>^{l+1}}\right)\int_0^{2\pi}\int_0^{\pi}Y_{lm}^*(\theta_1,\phi_1)\,d\theta_1\,d\phi_1$$

$$\times\int_0^{2\pi}\int_0^{\pi}Y_{lm}(\theta_2,\phi_2)\,d\theta_2\,d\phi_2 = \frac{e^2}{4\pi\epsilon_0}\int_0^R dr_1\int_0^R dr_2\,P_{1s}^2(r_1)\,P_{1s}^2(r_2)\frac{1}{r_>}$$

d) ~~For the Coulomb potential, 2s state has same energy as 2p state~~

Would you expect the 1s2s states to have higher or lower energy than 1s2p states?

- For Coulomb potential, 2s state has same energy as 2p state.
- potential in this prob. is flat ≈ Coulomb potential w/ parts closer to origin elevated
- 2s state sits closer to origin, energy elevated in this prob & is higher than that of 2p state
- we expect 1s2s to have higher energy than 1s2p state.

Random: multi-D, random hydrogen problem