Review Topics & Formulas for Unit 6

Lorentz *pondermotive* form for Newton's $\mathbf{F}=M\mathbf{a}=M\dot{\mathbf{v}}=M\ddot{\mathbf{R}}$ equation for a mass M of charge e.

$$M\frac{d\mathbf{v}}{dt}=\mathbf{F}=e(\mathbf{E}+\mathbf{v}\times\mathbf{B}) \qquad (17.1.1)$$

Velocity is $\mathbf{v}=\dot{\mathbf{R}}$. *Scalar potential field* $\Phi=\Phi(\mathbf{R},t)$ and a *vector potential field* $\mathbf{A}=\mathbf{A}(\mathbf{R},t)$ use Maxwell's.

$$\mathbf{E}=-\nabla\Phi-\frac{\partial\mathbf{A}}{\partial t},\qquad \mathbf{B}=\nabla\times\mathbf{A} \qquad (17.1.2)$$

Canonical electromagnetic Lagrange equations.

$$\frac{d}{dt}\frac{\partial L}{\partial\mathbf{v}}=\frac{d}{dt}\frac{\partial}{\partial\mathbf{v}}\left(\frac{1}{2}M\mathbf{v}\bullet\mathbf{v}-(e\Phi-\mathbf{v}\bullet e\mathbf{A})\right)=\nabla(e\Phi-\mathbf{v}\bullet e\mathbf{A})=\frac{\partial L}{\partial\mathbf{R}} \qquad (17.1.5c)$$

Here the *electromagnetic Lagrangian* is

$$L=L(\mathbf{R},\mathbf{v},t)=\frac{1}{2}M\mathbf{v}\bullet\mathbf{v}-\left(e\Phi(\mathbf{R},t)-\mathbf{v}\bullet e\mathbf{A}(\mathbf{R},t)\right) \qquad (17.1.5d)$$

The *canonical electromagnetic momentum* is

$$\mathbf{P}=\frac{\partial L}{\partial\mathbf{v}}=\frac{\partial}{\partial\mathbf{v}}\left(\frac{1}{2}m\mathbf{v}\bullet\mathbf{v}-\left(e\Phi(\mathbf{R},t)-\mathbf{v}\bullet e\mathbf{A}(\mathbf{R},t)\right)\right)=m\mathbf{v}+e\mathbf{A}(\mathbf{R},t) \qquad (17.1.5e)$$

Electromagnetic Hamiltonian function.

$$H=\frac{1}{2M}\left(\mathbf{P}-e\mathbf{A}(\mathbf{R},t)\right)\bullet\left(\mathbf{P}-e\mathbf{A}(\mathbf{R},t)\right)+e\Phi(\mathbf{R},t)\quad\begin{pmatrix}\text{Formally}\\ \text{correct}\end{pmatrix} \qquad (17.1.10a)$$

$$H=\frac{\mathbf{P}\bullet\mathbf{P}}{2M}-\frac{e}{2M}(\mathbf{P}\bullet\mathbf{A}+\mathbf{A}\bullet\mathbf{P})+\frac{e^2}{2M}\mathbf{A}\bullet\mathbf{A}+e\Phi(\mathbf{R},t) \qquad (17.1.10b)$$

Schrodinger's equation is non-relativistic.

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi=\left[\frac{(P-q\mathbf{A})^2}{2M}+V(\mathbf{R})\right]\psi=\left[\frac{(\hbar\nabla/i-q\mathbf{A})^2}{2M}+V(\mathbf{R})\right]\psi. \qquad (17.1.15a)$$

$$i\hbar\frac{\partial\psi}{\partial t}=\left[\frac{-\hbar^2\nabla^2}{2M}+i\frac{q\hbar}{M}\mathbf{A}\bullet\nabla+\frac{q^2}{2M}\mathbf{A}\bullet\mathbf{A}+V(\mathbf{R})\right]\psi. \qquad (17.1.15b)$$

Boost $\mathbf{B}(-qA)=e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}$ by momentum $-q\mathbf{A}$.

$\mathbf{B}\mathbf{p}\mathbf{B}^\dagger=\mathbf{B}(\mathbf{P}-q\mathbf{A}\mathbf{1})\mathbf{B}^\dagger=\mathbf{P}=\mathbf{p}+q\mathbf{A}\mathbf{1}$ (17.1.16a) $\qquad$ $\mathbf{B}^\dagger\mathbf{P}\mathbf{B}=\mathbf{B}^\dagger(\mathbf{p}+q\mathbf{A}\mathbf{1})\mathbf{B}=\mathbf{p}=\mathbf{P}-q\mathbf{A}\mathbf{1}$ (17.1.16b)

New position ket $|\mathbf{r}\rangle$ relates to old $|\mathbf{R}\rangle=\mathbf{B}|\mathbf{r}\rangle$ as follows.

$$|\mathbf{r}\rangle=\mathbf{B}^\dagger|\mathbf{R}\rangle\ ,\quad |\mathbf{R}\rangle=\mathbf{B}|\mathbf{r}\rangle\ ,\quad \langle\mathbf{r}|=\langle\mathbf{R}|\,\mathbf{B}\ ,\quad \langle\mathbf{R}|=\langle\mathbf{r}|\,\mathbf{B}^\dagger\ . \qquad (17.1.17a)$$

A wavefunction $\psi(\mathbf{R})=\langle\mathbf{R}|\psi\rangle$ of any state $|\psi\rangle$ times $B=e^{-iq\mathbf{A}\bullet\mathbf{R}/\hbar}$ gives wave $\psi(\mathbf{r})=\langle\mathbf{r}|\psi\rangle$ in $\mathbf{r}$-basis.

$$\psi(\mathbf{r})=\langle\mathbf{r}|\psi\rangle=\langle\mathbf{R}|\,\mathbf{B}|\psi\rangle=\langle\mathbf{R}|\,e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}|\psi\rangle=e^{-iq\mathbf{A}\bullet\mathbf{R}/\hbar}\psi(\mathbf{R})=\psi^B(\mathbf{R})\ . \qquad (17.1.17b)$$

An electric dipole potential $-q\mathbf{E}\bullet\mathbf{r}$ arises from $B\ \partial\psi(R)/\partial t$ and Maxwell equation $\mathbf{E}=-\partial\mathbf{A}/\partial t$.

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[\frac{-\hbar^2\nabla_{\mathbf{r}}{}^2}{2M}+V(\mathbf{r})-q\mathbf{E}(t)\bullet\mathbf{r}\right]\psi(\mathbf{r},t) \qquad (17.1.20c)$$

Time-dependent (non-autonomous) Hamiltonian.

$$\mathbf{H}(t) = \mathbf{H}_0 + \mathbf{V}(t) = \mathbf{H}_0 + \mathbf{H}_I \qquad (18.1.1a)$$

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle=\mathbf{H}(t)\left|\Psi(t)\right\rangle=\left(\mathbf{H}_0+\mathbf{V}(t)\right)\left|\Psi(t)\right\rangle \qquad (18.1.1b)$$

Eigenstates of the unperturbed part $\mathbf{H}_0$ of the Hamiltonian.

$$\mathbf{H}_0|\varepsilon_k\rangle = \varepsilon_k|\varepsilon_k\rangle = \hbar\omega_k\,|\varepsilon_k\rangle \qquad (18.1.3)$$

$$\left|\Psi(t)\right\rangle=\sum_k e^{-i\omega_k t}\left|\varepsilon_k\right\rangle c_k(t) \qquad (18.1.5)$$

$$i\hbar\frac{\partial c_j(t)}{\partial t}=\sum_k e^{i(\omega_j-\omega_k)t}\left\langle\varepsilon_j\right|\mathbf{V}(t)\left|\varepsilon_k\right\rangle c_k(t)=\sum_k V_{jk}(t)c_k(t) \qquad (18.1.10b)$$

The *(j,k)*-coupling time dependence is a modulation by $\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle$ of the transition beat phasor $e^{i\Omega_{jk}}$.

$$V_{jk}(t) = e^{i\Omega_{jk}}\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle = e^{i(\omega_j-\omega_k)t}\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle \qquad (18.1.10c)$$

The time variation of the state amplitude of general state $|\Psi(t)\rangle$ in (18.1.5) is

$$\langle\varepsilon_k|\Psi(t)\rangle = e^{-i\omega_k t}\,c_k(t)\ . \qquad (18.1.10d)$$

Iterative solution:

$$c_k(0)=\delta_{k1}=c_k^{(0)}. \qquad (18.1.11)$$

$$c_j^{(1)}(t)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 V_{j1}(t_1) \qquad (18.1.13)$$

$$c_j^{(2)}(t)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 V_{j1}(t_1)+\frac{1}{(i\hbar)^2}\sum_k\int_0^t dt_2 V_{jk}(t_2)\int_0^{t_2} dt_1 V_{k1}(t_1) \qquad (18.1.14b)$$

$$c_j^{(3)}(t)=c_j^{(2)}(t)+\frac{1}{(i\hbar)^3}\sum_{k,k'}\int_0^t dt_3 V_{jk'}(t_3)\int_0^{t_3} dt_2 V_{k'k}(t_2)\int_0^{t_2} dt_1 V_{k1}(t_1) \qquad (18.1.15)$$

$$c_j^{(1)}(t)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 V_{j1}^c(t_1)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 \mathrm{e}^{i\Omega_{j1}}\,\langle\varepsilon_j\,|\,\mathbf{V}^c(t_1)\,|\,\varepsilon_1\rangle \qquad (18.2.5a)$$

The key quantities are the beats or *(j←1)-transition frequencies* Ω_{j1} and *(j←1)-dipole matrix elements* r_{j1}.

$$\Omega_{j1}=\omega_j-\omega_1. \qquad r_{j1} = \mathbf{e}\bullet\langle j|\,\mathbf{r}\,|1\rangle \qquad (18.2.5b)$$

It is helpful to rewrite the amplitudes $c_j^{(1)}(t)$ as follows (Here: $E_o=2|a|\omega$ appears again.)

$$c_j^{(1)}(t) = \delta_{j1} + \frac{q\,r_{j1}E_0}{2\hbar}\left[e^{i\phi}S\left(\Delta^{\uparrow},t\right) + e^{-i\phi}S\left(\Delta^{\downarrow},t\right)\right], \qquad (18.2.5e)$$

using an important *spectral amplitude function S(Δ,t)* of an angular frequency *detuning parameter Δ*

$$S(\Delta,t) = \int_0^t d\tau\, e^{i\tau\Delta} = \frac{e^{it\Delta/2}\sin(t\Delta/2)}{\Delta/2}. \qquad (18.2.5f)$$

Total transition probability $\Sigma(t) = \int_{-\infty}^{\infty} d\Delta \left|S(\Delta,t)\right|^2 = \int_{-\infty}^{\infty} d\Delta \frac{\sin^2(t\Delta/2)}{(\Delta/2)^2}.$ (18.2.10a)

Fermi's golden rule for constant transition rates. $\Sigma(t) = \int_{-\infty}^{\infty} d\Delta \left|S(\Delta,t)\right|^2 = 2\pi \cdot t$ (18.2.10d)

Oscillator strength and dipole response

$$\begin{aligned}\langle x\rangle &= \sum_{j=1} \frac{2\Omega_{j1}\left|r_{j1}\right|^2 M}{\hbar}\left(\frac{qE_0}{M}\frac{\cos\omega t - \cos\Omega_{j1}t}{\Omega_{j1}^2 - \omega^2}\right) \\ &= \sum_{j=1} \quad f_{j1} \quad \cdot \quad x_{classical}\end{aligned} \qquad (18.3.5a)$$

Lorentz-atomic-oscillator frequency $\omega_0 = \Omega_{j1} = \omega_j - \omega_1$. (18.3.5b)

This is the *(j←1)-transition frequency* Ω_{j1} or quantum beat driven by stimulus frequency $\omega_S = \omega$.

(j←1)-oscillator strength f_{j1} $f_{j1} = \frac{2\Omega_{j1}\left|r_{j1}\right|^2 M}{\hbar}$ (18.3.5d)

Thomas-Reiche-Kuhn sum rule for oscillator strength. This holds for any H_0 eigenstate $|1\rangle$.

$$\sum_{j=1} f_{j1} = \sum_{j=1} 2\langle 1|x|j\rangle\langle j|p|1\rangle/\hbar i = 2\langle 1|xp|1\rangle/\hbar i = -2\langle 1|px|1\rangle/\hbar i = 1 \qquad (18.3.10a)$$

Quantum eigenstate virial theorem that is similar to the classical viral theorem.

$$\langle KE\rangle = \langle m|\frac{p^2}{2M}|m\rangle = \frac{P}{2}\langle m|V\cdot x^P|m\rangle = \frac{P}{2}\langle PE\rangle \qquad (18.3.10c)$$