OPTIONAL

CHARGE PARTICLE IN A E.M. FIELD

THE FORCE DUE TO THE LIGHT ON A CHARGE PARTICLE q ON A POSITION $\bar{r}$ HAVING A VELOCITY $\bar{v}$ IS EXPRESSED BY THE LORENTZ LAW

$$\bar{F} = q\left[\bar{E}(\bar{r},t) + \frac{\bar{v}}{c}\times\bar{B}(\bar{r},t)\right]$$

TO WRITE THE EQUATION OF MOTION, WE MUST OBTAIN THE EQUIVALENT LAGRANGIAN AND HAMILTONIAN. THIS TASK IS EASIER BY USING THE POTENTIAL INSTEAD THAN THE FIELDS,

$$\bar{B}(\bar{r},t) = \nabla\times\bar{A}(\bar{r},t)$$

$$\bar{E}(\bar{r},t) = -\nabla\phi(\bar{r},t) - \frac{1}{c}\frac{\partial\bar{A}(\bar{r},t)}{\partial t}$$

USING THESE RELATIONS INTO THE LORENTZ FORCE LAW THE NEWTON'S EQUATION OF MOTION BECOMES

$$m\frac{d^2\bar{r}}{dt^2} = q\left[-\nabla\phi - \frac{1}{c}\frac{\partial\bar{A}}{\partial t} + \frac{\bar{v}}{c}\times(\nabla\times\bar{A})\right] =$$

$$= q\left\{-\nabla\left(\phi - \frac{1}{c}\dot{A}\cdot\dot{r}\right) - \frac{1}{c}\left[\frac{\partial\bar{A}}{\partial t} + (\dot{r}\cdot\nabla)\bar{A}\right]\right\}$$

THE LAGRANGIAN WHICH YIELDS THE SAME EQUATION OF MOTION IS

$$L(\bar{r},\dot{\bar{r}},t) = \frac{1}{2}m\dot{r}^2 + \frac{q}{c}\dot{A}\cdot\dot{r} - q\phi$$

THE LAGRANGIAN EQUATION OF MOTION

$$\frac{\partial L}{\partial\bar{r}} = \frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\bar{r}}}\right)$$

WHICH USING THE LAGRANGIAN GIVES

$$-q\nabla\left(\phi-\frac{1}{c}\bar{A}\cdot\dot{\bar{r}}\right)-\frac{d}{dt}\left(m\dot{\bar{r}}+\frac{q}{c}\bar{A}\right)=0$$

WHERE THE LAST TERM $dA/dt=\dot{\bar{r}}\cdot\nabla\bar{A}+\frac{\partial\bar{A}}{\partial t}$

(USING THE COULOB GAUGE). THE HAMILTONIAN H (WHICH IS FUNCTION OF $\bar{r},\bar{p}$ AND (IN CASE) t) IS OBTAIN BY THE LEGENDRE TRANSFORMATION

$$H(\bar{r},\bar{p},t)=\dot{\bar{r}}\cdot\bar{p}-L(\bar{r},\dot{\bar{r}},t)$$

WHERE $\bar{p}\equiv\frac{\partial L}{\partial\dot{\bar{r}}}$. FOR THE LAGRANGIAN THE MOMENTUM $\bar{p}$ CONJUGATE TO $\bar{r}$ IS $\bar{p}\equiv\frac{\partial L}{\partial\dot{\bar{r}}}=$

$=m\dot{\bar{r}}+\frac{q}{c}\bar{A}$. NOTE THAT THE MOMENTUM $\bar{p}$ CONJUGATE TO $\bar{r}$ IS NOT EQUAL TO $m\dot{\bar{r}}$ BUT INVOLVES $\bar{A}$. SUBSTITUTING $\dot{\bar{r}}=1/m\left[\bar{p}-(q/c)\bar{A}\right]$

WE OBTAIN THE HAMILTONIAN AS A FUNCTION OF $\bar{r},\bar{p},t$

$$H(\bar{r},\bar{p},t)=\frac{1}{m}\left(\bar{p}-\frac{q}{c}\bar{A}\right)\cdot\bar{p}-\left[\frac{1}{2m}\left(\bar{p}-\frac{q}{c}\bar{A}\right)^2-\right.$$
$$\left.+q\phi+\frac{q}{c}\bar{A}\cdot\frac{1}{m}\left(\bar{p}-\frac{q}{c}\bar{A}\right)\right]$$

THIS EXPRESSION CAN BE SEMPLIFIED AS

$$H(\bar{r},\bar{p},t)=\frac{1}{2m}\left(\bar{p}-\frac{q}{c}\bar{A}\right)^2+q\phi$$

HAMILTON'S EQS. OF MOTION ARE:

$$\dot{\bar{p}} = -\nabla_r H \quad , \quad \dot{\bar{r}} = \nabla_p H \Rightarrow$$

$$\dot{\bar{p}} = -q\nabla\left[\phi(\bar{r},t) - \frac{1}{c}\bar{A}(\bar{r},t)\cdot\dot{\bar{r}}\right]$$

$$\dot{\bar{r}} = \frac{1}{m}\left[\bar{p} - \frac{q}{c}\bar{A}(\bar{r},t)\right].$$

WE CONCLUDE THAT THE HAMILTONIAN H_0 FOR A CHARGE PARTICLE HAVING POTENTIAL ENERGY U (NOT FROM THE E.M. FIELD) GOES OVER TO THE HAMILTONIAN H,

$$H_0 = \bar{p}^2/2m + U \rightarrow H$$

$\boxed{H = \frac{1}{2m}\left(\bar{p} - \frac{q}{c}\bar{A}\right)^2 + q\phi + U}$, i.e. $\bar{p} \rightarrow \bar{p} - (q/c)\bar{A}$. THE QUANTITY $[\bar{p} - (q/c)\bar{A}]/m$

IS CALLED KINETIC VELOCITY. THE ABSORPTION, EMISSION AND SCATTERING OF LIGHT BY MATTER CAN BE TREATED QUANTUM MECHANICALLY IN TERMS OF H UPON TURNING H INTO A Q.M. OPERATOR $\hat{H}$. MOREOVER, BY CONSIDERING THE RADIATION FIELD ITSELF THIS MUST BE ADDED AS A CLASSICAL FIELD OR A QUANTIZEZ FIELD AS SUGGESTED FIRST BY P. DIRAC. IF ADDING TO THE HAMILTONIAN THE QUANTIZED E.M. FIELD WE OBTAIN

$$H_{M+F} = \frac{1}{2m}\left(\bar{p} - \frac{q}{c}\bar{A}\right)^2 + q\phi + U + \sum_{\bar{k}}{}' \sum_{\alpha}{}' \hbar\omega\, n_{\bar{k}\alpha}$$

THIS HAMILTONIAN DESCRIBES THE INTERACTION OF A CHARGE PARTICLE WITH AN

E.M. FIELD. $\bar{A}$ QUANTIZED, AS PREVIOUSLY DESCRIBED, CAN BE EVALUATED IN ITS RADIATION GAUGE, $\phi = 0; \nabla \cdot \bar{A} = 0$. THEREFORE THE TOTAL HAMILTONIAN IS THE SUM OF THREE TERMS

$$H = H_0 + H_{INT} + H_{E.M.}$$

WHERE $H_0 = p^2/2m + U$ IS THE HAMILTONIAN FOR THE CHARGED PARTICLE (ATOM), AND

$$H_{INT} = \frac{-q}{2mc}\left[\bar{p}\cdot\bar{A} + \bar{A}\cdot\bar{p}\right] + \frac{q^2}{2mc^2}\bar{A}^2$$

IS THE HAMILTONIAN FOR THE INTERACTION. IN PARTICULAR THE TERMS $\bar{p}\cdot\bar{A} + \bar{A}\cdot\bar{p}$ COUPLE THE MOMENTUM OF THE CHARGE PARTICLE WITH THE E.M. FIELD. THE TRANSFORMATION OF THE HAMILTONIAN INTO A Q.M. OPERATOR IS AFFECTED IN COORDINATE OPERATION BY MAKING THE REPLACEMENT

$$\bar{p} \rightarrow \left(\frac{\hbar}{i}\right)\nabla$$

SO THE H_{INT} BECOMES $\hat{H}_{INT}$,

$$H_{INT} = \frac{i\hbar q}{2mc}\left[\nabla\cdot\bar{A} + \bar{A}\cdot\nabla\right] + \frac{q^2}{2mc^2}\bar{A}^2$$

THE TERM $\bar{\nabla}\cdot\bar{A} = \bar{A}\cdot\nabla + (\nabla\cdot\bar{A})$, THUS WE OBTAIN

$$H_{INT} = \frac{i\hbar q}{2mc}\left[2\bar{A}\cdot\nabla + (\bar{\nabla}\cdot\bar{A})\right] + \frac{q^2}{2mc^2}\bar{A}^2$$

IN THE RADIATION GAUGE (COULOMB) $\phi = 0$

$\nabla\cdot\bar{A} = 0$

THE INTERACTION HAMILTONIAN BECOMES

$$H_{INT} = \frac{i\hbar q}{mc}\bar{A}\cdot\nabla + \frac{q^2}{2mc^2}\bar{A}^2$$

ABSORPTION AND EMISSION: TIME DEPENDENT PERTURBATION THEORY

CONSIDER A HAMILTONIAN CONTAINING A TIME-DEPENDENT POTENTIAL SO THAT THE FULL HAMILTONIAN CAN BE WRITTEN AS
$H = H_0 + H_{INT}(t)$, BUT $H_0 = T + V_0$ $(H_0 = T + U)$ IS NOT t-DEPENDENT. THE t-DEPENDENT WAVEFUNCTION

$$\Psi(\bar{r}, t)$$

CAN BE EXPANDED IN TERMS OF THE SET { } OF ZERO-ORDER EIGENFUNCTION $\{\psi_k\}$ SATISFYING THE EQUATION

$$H_0 \psi_k(\bar{r}) = E_k \psi_k(\bar{r})$$

IN THE FORM

$$\Psi(\bar{r}, t) = \sum_{k}{}' c_k(t)\psi_k(\bar{r})\, e^{-iE_k t/\hbar}$$

THE $c_k(t)$ ARE TIME DEPENDENT EXPANSION COEFFICIENTS THAT MUST BE COMPUTED. Ψ SATISFIES THE TIME DEPENDENT SCHRÖDINGER EQUATION

$$\left[H_0 + H_{INT}(t)\right]\Psi(\bar{r}, t) = i\hbar \frac{\partial}{\partial t}\Psi(\bar{r}, t)$$

THEREFORE, WE OBTAIN

$$\sum_k{}' c_k(t) H_{INT} \psi_k(\bar{r}) e^{(-iE_k t/\hbar)} = i\hbar \sum_k{}' \psi_k(\bar{r}) e^{(-iE_k t/\hbar)} \frac{dc_k(t)}{dt}$$

TO DETERMINE THE DIFFERENTIAL EQUATIONS FOR THE TIME-DEPENDENT EXPANSION COEFFICIENTS $c_k(t)$ WE CAN MULTIPLY THE ABOVE EQUATION BY $[\psi_k(\bar{r}) e^{-iE_k t/\hbar}]^*$ AND INTEGRATE OVER $\bar{r}$ TO OBTAIN

$$\frac{dc_j(t)}{dt} = \frac{1}{i\hbar} \sum{}' c_k(t) \langle \psi_j | H_{INT}(t) | \psi_k \rangle e^{i(E_j - E_k)t/\hbar}$$

AT $t=0$ ONLY THE INITIAL STATE i IS POPULATED, SO $c_k(t=0) = \delta_{ki}$. WE CAN APPROXIMATE $c_k(t)$ BY THE ZERO-ORDER APPROXIMATION $c_k^{(0)}(t) = \delta_{ki}$

TO OBTAIN THE FIRST-ORDER APPROXIMATION FOR $c_j(t)$: $c_j^{(1)}(t)$

$$c_j^{(1)}(t) = \frac{1}{i\hbar} \int_0^t dt' \langle \psi_j | H_{INT}(t') | \psi_i \rangle \times e^{i(E_j - E_i)t'/\hbar}$$

THE SECOND ORDER APPROXIMATION CAN BY OBTAINED BY SUBSTITUTING THIS EXPRESSION IN THE PREVIOUS EQ.

$$c_j^{(2)}(t) = \frac{1}{i\hbar} \int_0^t dt'' \sum_k{}' \langle \psi_j | H_{INT}(t'') | \psi_k \rangle \times e^{i(E_j - E_k)t''/\hbar} c_k^{(1)}(t'')$$

THIS PROCEDURE CAN BE REPETED TO OBTAIN AN EXPRESSION FOR THE THIRD ORDER APPROXIMATION FOR $C_j(t)$ AND SO ON. THE COEFFICIENT $C_j(t)$ IS THEN GIVEN BY

$$C_j(t) = C_j^{(0)}(t) + C_j^{(1)}(t) + C_j^{(2)}(t) + \dots$$

WE NOW EXPLICITLY CONSIDER A HARMONIC TIME-DEPENDENT INTERACTION HAMILTONIAN OF THE FORM

$$H_{INT}(t) = h(\bar{r})e^{-i\omega t} + h^{+}(r)e^{i\omega t}$$

THIS TERM IS SUDDENLY TURNED ON AT $t=0$ WHEN AN E.M. WAVE (PLANE) INTERACT WITH AN ELECTRON, AND

$$h(\bar{r}) = \frac{e}{mc}\left\{\bar{A}(\bar{r})\cdot\bar{p}\right\}$$ (HERE WE EXPLICITLY EXCLUDE THE ELECTRON-SPIN COUPLING).

THE VECTOR POTENTIAL $\bar{A}(\bar{r},t)$ CAN BE EXPRESSED AS A CLASSICAL FIELD OR IN ITS QUANTIZED FORM. THE TERM

$h(\bar{r})e^{-i\omega t}$ IS RESPONSIBLE FOR ABSORPTION

AND THE $h^{+}(\bar{r})e^{i\omega t}$ IS RESPONSIBLE FOR EMISSION. WE CAN NOW CALCULATE $C_j^{(1)}(t)$

$$C_j^{(1)}(t) = \frac{1}{i\hbar}\int_0^t dt'\left\{\langle\psi_j|h|\psi_i\rangle e^{i(E_j - E_i - \hbar\omega)t'/\hbar} + \right.$$

$$\left. + \langle\psi_j|h^{+}|\psi_i\rangle e^{i(E_j - E_i + \hbar\omega)t'/\hbar}\right.$$

THE INTEGRATION OVER TIME CAN BE PERFORMED AS FOLLOWS

$$\int_0^t dt' e^{i(E_j-E_i-\hbar\omega)t'/\hbar} = e^{i(E_j-E_i-\hbar\omega)t/2\hbar} \times \frac{\sin(E_j-E_i-\hbar\omega)t/2\hbar}{(E_j-E_i-\hbar\omega)/2\hbar}$$

YILDING TO

$$c_j^{(1)}(t) = \frac{1}{\hbar}\left\{\langle\psi_j|h|\psi_i\rangle \times e^{i(E_j-E_i-\hbar\omega)t/2\hbar} \times \frac{\sin[(E_j-E_i-\hbar\omega)t/2\hbar]}{(E_j-E_i-\hbar\omega)/2\hbar} + \langle\psi_j|h^+|\psi_i\rangle\, e^{[i(E_j-E_i+\hbar\omega)t/2\hbar]} \times \frac{\sin[(E_j-E_i+\hbar\omega)t/2\hbar]}{(E_j-E_i+\hbar\omega)/2\hbar}\right\}$$

THE TRANSITION AMPLITUDE $c_j^{(1)}(t)$ FOR GOING FROM THE INITIAL STATE i TO THE FINAL j IS MADE UP OF TWO TERMS. FOR LARGE t THE FIRST TERM WILL CONTRIBUTE SIGNIFICANTLY ONLY WHEN $E_j - E_i - \hbar\omega \approx 0$. THE SECOND WILL CONTRIBUTE ONLY WHEN $E_j - E_i + \hbar\omega \approx 0$. HENCE, THE FIRST TERM IS IMPORTANT FOR ABSORPTION ($E_j \approx E_i + \hbar\omega$) AND THE SECOND FOR EMISSION OF RADIATION $E_j + \hbar\omega \approx E_i$