173(6): Hamiltonian Formulation of Fermion Equation.

It was proven in note 173(3) that the fermion eq. gives the result:

$$E \phi^L = \hat{H} \phi^L \quad -(1)$$

where:

$$\hat{H} = mc^2 + e\phi + \frac{1}{2m} \underline{\sigma} \cdot \underline{\pi} \left(1 - \frac{e\phi}{2mc^2} \right) \underline{\sigma} \cdot \underline{\pi} . \quad -(2)$$

Note carefully that this result corresponds to positive energy,

i.e

$$E = \left(p^2 c^2 + m^2 c^4 \right)^{1/2} \quad -(3)$$

We also have

$$E \phi^R = H \phi^R \quad -(4)$$

and

$$E \psi = H \psi \quad -(5)$$

where

$$\psi = \begin{bmatrix} \psi_1^R & \psi_2^R \\ \psi_1^L & \psi_2^L \end{bmatrix} . \quad -(6)$$

In the position representation eq. (5) is:

$$i\hbar \frac{\partial \psi}{\partial t} = H \psi . \quad -(7)$$

The expectation value of a quantity A is:

$$\langle \hat{A} \rangle = \int \psi^* \hat{A} \psi \, d^3 x \quad -(8)$$

where ψ^+ is the hermitian conjugate of ψ and where ψ^* is the complex conjugate of ψ.

Therefore:

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{d}{dt}\int \psi^*(t)\,\hat{A}\,\psi(t)\,d^3x \quad -(9)$$

The operator $\hat{A}$ acts on the wavefunction $\psi(t)$. The operator $\hat{A}$ itself is independent of time (Atkins, 2nd. ed., page 97) but acquires a time dependence by acting on a time dependent wavefunction. So:

$$\frac{d\langle\hat{A}\rangle}{dt} = \int\left(\frac{\partial\psi^*}{\partial t}\right)\hat{A}\psi\,d^3x + \int\psi^*\hat{A}\left(\frac{\partial\psi}{\partial t}\right)d^3x \quad -(10)$$

by the Leibniz rule.

Now use the time dependent Schroedinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \quad -(11)$$

where $\hat{H}$ is the hamiltonian operator. The complex conjugate of eq. (11) is:

$$-i\hbar\frac{\partial\psi^*}{\partial t} = \hat{H}\psi^* \quad -(12)$$

Therefore using eqs. (11) and (12) in eq. (10):

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{1}{i\hbar}\left(-\int\left(\hat{H}\psi^*\right)\hat{A}\psi\,d^3x + \int\psi^*\hat{A}\left(\hat{H}\psi\right)d^3x\right) \quad -(13)$$

Now use the hermiticity of the hamiltonian operator (Atkins, p. 88, 2nd. ed.):

$$\int\psi^*\hat{H}\psi\,d^3x = \int\left(\hat{H}\psi\right)^*\psi\,d^3x \quad -(14)$$

to find that:

$$\frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i\hbar}\left(-\int \psi^* \hat{H} \hat{A} \psi \, d^3x + \int \psi^* \hat{A} \hat{H} \psi \, d^3x \right) \quad -(15)$$

$$= \frac{1}{i\hbar} \int \psi^* \left(\hat{H}\hat{A} - \hat{A}\hat{H} \right) \psi \, d^3x$$

$$\frac{d}{dt}\langle \hat{A} \rangle = \frac{1}{i\hbar} \langle [\hat{H}, \hat{A}] \rangle . \quad -(15a)$$

So:

$$\boxed{\frac{d\hat{A}}{dt} = -\frac{i}{\hbar}[\hat{H}, \hat{A}]} \quad -(16)$$

Eq. (15a) means that the expectation value is constant in time if $\hat{A}$ commutes with $\hat{H}$. In this case the observable is a constant of motion with conserved expectation values. For a constant of motion:

$$[\hat{H}, \hat{A}] = 0 \quad -(17)$$

For linear momentum in one direction:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x), \quad -(18)$$

$$\hat{p} = \hat{A} = \frac{\hbar}{i}\frac{d}{dx} \quad -(19)$$

Derivatives commute, so:

$$[\hat{H}, \hat{p}] = \frac{\hbar}{i}\left[V(x), \frac{d}{dx} \right] \quad -(20)$$

and

4)

$$[\hat{H}, \hat{p}]\phi = \frac{\hbar}{i}\left[V(x), \frac{d}{dx}\right]\phi$$

$$= \frac{\hbar}{i}\left(V(x)\frac{d\phi}{dx} - \frac{d}{dx}\left(V(x)\phi\right)\right)$$

$$= \frac{\hbar}{i}\left(V(x)\frac{d\phi}{dx} - V(x)\frac{d\phi}{dx} - \frac{dV(x)}{dx}\right)$$

$$= -\frac{\hbar}{i}\frac{dV}{dx} = i\hbar\frac{dV}{dx} \quad -(15)$$

Therefore

$$\frac{d}{dt}\langle\hat{p}\rangle = -\left\langle\frac{d\hat{V}}{dx}\right\rangle = -\frac{dV}{dx} \quad -(16)$$

In classical dynamics, the force is:

$$F = -\frac{dV}{dx}. \quad -(17)$$

so the momentum is constant in the absence of force. This is Newton's first law. From eq. (16):

$$\langle\hat{F}\rangle = \frac{d}{dt}\langle\hat{p}\rangle \quad -(18)$$

which is Newton's second law.

In relativistic mechanics the Newtonian laws are replaced by eq. (3), i.e. by:

$$\underline{p} = \gamma m \underline{v} \quad -(19)$$

$$E = \gamma m c^2 \quad -(20)$$

$$\gamma = \left(1 - \frac{v^2}{c^2}\right)^{-1/2} \quad -(21)$$

5) The hamiltonian for the interaction of the fermion and electromagnetic field is eq. (2), which may be expanded as:

$$\hat{H} = mc^2 + e\phi + \frac{1}{2m}(p - eA)^2 - \frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{B}$$
$$- \frac{e}{4m^2c^2}\underline{\sigma}\cdot\underline{\hat{\pi}}\,\phi\,\underline{\sigma}\cdot\underline{\hat{\pi}} \quad -(22)$$

where

$$\underline{\hat{\pi}} = \underline{\hat{p}} - e\hat{A}, \quad -(23)$$
$$\hat{p} = -i\hbar\underline{\nabla} \,. \quad -(24)$$

The hamiltonian operator $\hat{H}$ of the fermion equation commutes with constants of motion. The last term in eq. (22) may be expanded as follows:

$$\underline{\sigma}\cdot\underline{\hat{\pi}}\,\phi\,\underline{\sigma}\cdot\underline{\hat{\pi}} = \underline{\sigma}\cdot(\underline{\hat{p}} - e\underline{A})\,\phi\,\underline{\sigma}\cdot(\hat{p} - e\underline{A}) \quad -(25)$$
$$= \underline{\sigma}\cdot\underline{\hat{p}}\,\phi\,\underline{\sigma}\cdot\underline{\hat{p}} + \cdots$$
$$= -i\hbar\,\underline{\sigma}\cdot\underline{\nabla}\left(\phi\,\underline{\sigma}\cdot\underline{\hat{p}}\right)$$

Using the Leibniz rule:

$$\underline{\nabla}\left(\phi\,\underline{\sigma}\cdot\underline{\hat{p}}\right) = \underline{\nabla}\phi\cdot(\underline{\sigma}\cdot\underline{\hat{p}}) + \phi\,\underline{\nabla}\,(\underline{\sigma}\cdot\underline{\hat{p}}) \quad -(26)$$

The electric field strength $\underline{E}$ is:

$$\underline{E} = -\underline{\nabla}\phi \quad -(27)$$

6) So:

$$\underline{\sigma} \cdot \hat{\underline{\pi}} \, \phi \, \underline{\sigma} \cdot \hat{\underline{\pi}} = i\hbar \, \underline{\sigma} \cdot \underline{E} \; \underline{\sigma} \cdot \underline{p} + \dots \quad -(28)$$

Now use:

$$\underline{\sigma} \cdot \underline{E} \; \underline{\sigma} \cdot \underline{p} = \underline{E} \cdot \underline{p} + i \underline{\sigma} \cdot \underline{E} \times \underline{p} \quad -(29)$$

So:

$$\underline{\sigma} \cdot \hat{\underline{\pi}} \, \phi \, \underline{\sigma} \cdot \hat{\underline{\pi}} = -\frac{e\hbar}{4m^2c^2} \, \underline{\sigma} \cdot \underline{E} \times \underline{p} + \dots \quad (30)$$

and this is the spin orbit term with the Thomas factor of 2 in the denominator.

Therefore the fermion equation produces:

$$\hat{H} = mc^2 + e\phi + \frac{1}{2m}(p - eA)^2 - \frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B} - \frac{e\hbar}{4m^2c^2} \underline{\sigma} \cdot \underline{E} \times \underline{p} \quad -(31)$$

$$+ \dots$$

The equation of motion for any operator $\hat{A}$ is:

$$\frac{d\langle \hat{A} \rangle}{dt} = -\frac{i}{\hbar} \langle [\hat{H}, \hat{A}] \rangle \quad -(32)$$

There are several other terms in eq. (31), e.g. the Darwin term and crossed electric / magnetic effects.