March 7, 1980

Weinberg quasi-particle, Schmidt method
Dirac and Pauli equations
Kubo response formula

More Weinberg: Suppose one has a system described by $H = H_0 + V$ having a bound state: $H|B\rangle = -B|B\rangle$ where $B<0$. Normally one thinks of H_0 as describing a free particle, e.g. $H_0 = \frac{-1}{2m}\Delta$, so that H_0 has only continuous spectrum $H_0|\underset{\sim}{k}\rangle = \frac{k^2}{2m}|\underset{\sim}{k}\rangle$ located on the positive real axis. But Weinberg has in mind the fact that H_0 isn't really known; it describes the free particles we see before and after collisions, and so there might be a new elementary particle involved in the interaction that we want included in our bare Hamiltonian. So the problem is how does one tell whether the bound state (think of it as the deuteron) is composite (made up of a neutron + proton bound together) or a new elementary particle, which will be a discrete eigenvector for H_0 not in the continuous spectrum.

Here's how one distinguishes the possibilities: If there is an elementary particle, i.e. descrete state for H_0: $H_0|B_0\rangle = -B_0|B_0\rangle$ that must be used to get $|B\rangle$, then one should have $\langle B_0|B\rangle \neq 0$, so assuming $|\underset{\sim}{k}\rangle, |B_0\rangle$ are a complete family of eigen-states for H_0, one has

$$1 = |\langle B_0|B\rangle|^2 + \int d\underset{\sim}{k}\, |\langle \underset{\sim}{k}|B\rangle|^2 \quad > \int d\underset{\sim}{k}\, |\langle \underset{\sim}{k}|B\rangle|^2$$

From $(H_0+V)|B\rangle = -B|B\rangle$ we have

$$-B\langle \underset{\sim}{k}|B\rangle = \langle \underset{\sim}{k}|(H_0+V)|B\rangle = \frac{k^2}{2m}\langle \underset{\sim}{k}|B\rangle + \langle \underset{\sim}{k}|V|B\rangle$$

or

$$\langle \underset{\sim}{k}|B\rangle = \frac{\langle \underset{\sim}{k}|V|B\rangle}{\frac{k^2}{2m} + B}$$

So we get the sum rule

$$1 = \underbrace{|\langle B_0 | B \rangle|^2}_{Z} + \int d\underset{\sim}{k} \frac{|\langle \underset{\sim}{k} | V | B \rangle|^2}{\left(\frac{k^2}{2m} + B\right)^2}$$

Therefore there is an elementary particle [redacted] involved in $|B\rangle$, when the integral is < 1.

Summarize: If one has a system described by $H = H_0 + V$ with a bound state, then the bare Hamiltonian H_0 might have a discrete eigenvector which evolves into the bound state as the interaction is turned on. It seems that Weinberg has a way to adjoin a quasi-particle to the bare Hilbert space so as to achieve this situation.

The next thing to do is to look at the situation where the elementary particle, or quasi-particle exists. Let's consider the Hilbert space $\tilde{\mathcal{H}} = \mathcal{H} \oplus \mathbb{C}|0\rangle$ where

$$\tilde{H}_0 = \left(\begin{array}{c|c} H_0 & 0 \\ \hline 0 & E_0 \end{array}\right) \qquad E_0 < 0$$

and H_0 has the continuous spectrum of the standard variety: $H_0 |\underset{\sim}{k}\rangle = \frac{k^2}{2m} |\underset{\sim}{k}\rangle$. Then $|0\rangle$ is the ground state for $\tilde{H}_0$. We suppose given an interaction $\tilde{V}$. Now notice that we have the very nice situation where the lowest eigenvalue of $\tilde{H}_0$ has been split away from the [redacted] rest of the spectrum, which is the sort of thing we used when we did [redacted] the R.S. series.

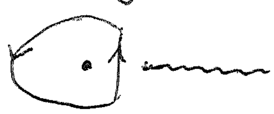
Let's review this a little. If $|\Psi_n\rangle$ are a basis for the eigenstate of $\tilde{H}$, then

$$\frac{1}{W-\tilde{H}} = \sum \frac{|\Psi_n\rangle\langle\Psi_n|}{W-E_n'}$$

so that $\langle\Phi_0|\frac{1}{W-\tilde{H}}|\Phi_0\rangle = \frac{|\langle\Psi_0|\Phi_0\rangle|^2}{W-E_0'} +$ analytic fn with singularities to the right of E_0'.

Hence the normalization constant $Z = |\langle\Psi_0|\Phi_0\rangle|^2$ is the residue of $\langle\Phi_0|\frac{1}{W-\tilde{H}}|\Phi\rangle$

$$Z = \frac{1}{2\pi i}\oint \langle 0|\frac{1}{W-\tilde{H}}|0\rangle\, dW$$



and so it can be easily evaluated as a series. This is something I missed earlier.

I conclude that I can compute the new ground energy and normalization constant, formally via diagrams using for free propagator

$$\frac{1}{W-\tilde{H}_0} = \begin{pmatrix} \frac{1}{W-H_0} & 0 \\ 0 & \frac{1}{W-E_0} \end{pmatrix}$$

and using for interaction

$$\tilde{V} = \left(\begin{array}{c|c} V_1 & * \\ \hline * & * \end{array}\right).$$

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We have $\tilde{H} = \tilde{H}_0 + \tilde{V}$ where

$$\tilde{H}_0 = \left(\begin{array}{c|c} H_0 & 0 \\ \hline 0 & E_0 \end{array}\right) \quad \text{operates on } \tilde{\mathcal{H}} = \mathcal{H} \oplus \mathbb{C}\underset{\text{unit vector}}{|B_0\rangle}$$

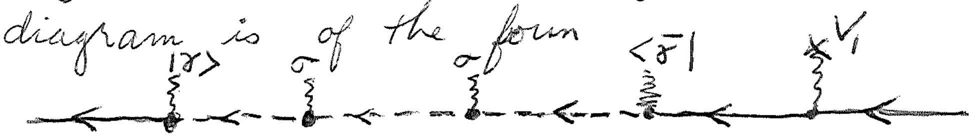
and

$$\tilde{V} = \left(\begin{array}{c|c} V_1 & |\gamma\rangle \\ \hline \langle\bar{\gamma}| & \sigma \end{array}\right) \qquad \sigma \text{ is a constant.}$$

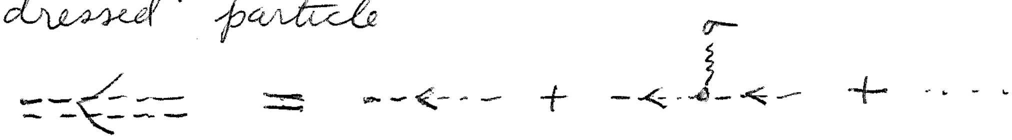
We compute $\frac{1}{W-\tilde{H}}$ using diagrams which come from the expansion

$$\frac{1}{W-\tilde{H}} = \frac{1}{W-\tilde{H}_0} + \frac{1}{W-\tilde{H}_0}\tilde{V}\frac{1}{W-\tilde{H}_0} + \cdots\cdots$$

There will be two kinds of "bare particles", those in $\mathcal{H}$ governed by $\frac{1}{W-H_0}$ and $|B_0\rangle$ governed by $\frac{1}{W-E_0}$. A typical diagram is of the form



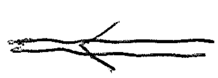
where the solid line denotes a bare particle in $\mathcal{H}$ and a dotted line denotes the bare particle $|B_0\rangle$. It is possible to combine together all iterates of a single bare propogator into a "dressed" particle



$$= \frac{1}{W-E_0} + \frac{1}{W-E_0}\sigma\frac{1}{W-E_0} + \cdots$$

$$= \left(1 - \frac{1}{W-E_0}\sigma\right)^{-1}\frac{1}{W-E_0} = \frac{1}{W-E_0-\sigma}$$

and



$$= \frac{1}{W-H_0} + \frac{1}{W-H_0}V_1\frac{1}{W-H_0} +$$

$$= \frac{1}{W-(H_0+V_1)}$$

If we use these combined diagrams, it's equivalent to working with the splitting

$$\tilde{H} = \left(\begin{array}{c|c} H_0 + V_1 & 0 \\ \hline 0 & E_0 + \sigma \end{array}\right) + \left(\begin{array}{c|c} 0 & |\gamma\rangle \\ \hline \langle\bar{\gamma}| & 0 \end{array}\right)$$

Physically $\tilde{H}$ [redacted] is the Hamiltonian describing a system whose "visible" states are [redacted] in $\mathcal{H}$. Hence one is interested in the matrix elements of $\frac{1}{W-\tilde{H}}$ between states in $\mathcal{H}$. These can be described by diagrams with free propagator $\frac{1}{W-H_0}$ and with interaction the sum of V_1 and going to $|B_0\rangle$ propagating there and coming back. Thus interactions are

or

Hence

$$\frac{1}{W-\tilde{H}} \underset{\text{to } \mathcal{H}}{\text{restricted}} = \frac{1}{W-H_0} + \frac{1}{W-H_0}\left(V_1 + |\gamma\rangle \frac{1}{W-E_0-\sigma}\langle\bar{\gamma}|\right)\frac{1}{W-H_0}$$
$$+ \cdots\cdots$$

which is sort of the resolvant of H_0 with the energy-dependent interaction

$$V_1 + |\gamma\rangle \frac{1}{W-(E_0+\sigma)}\langle\bar{\gamma}|$$

This is still very confused! However Weinberg has another angle – the Schmidt method:

The Schmidt method is used to construct the resolvant $\frac{1}{1-\,\text{[redacted]}K}$ when the geometric series doesn't converge.

Here K is supposed to be compact and the non-convergence is due to K having eigenvalues not in the unit disk.

Start with a bound state for $H = H_0 + V$:

$$(H_0 + V)|B\rangle = E|B\rangle \qquad \langle B|B\rangle = 1.$$

or

$$(E - H_0)|B\rangle = V|B\rangle$$

$$|B\rangle = (E-H_0)^{-1} V |B\rangle$$

so that $|B\rangle$ is an eigenvector for $K = (E-H_0)^{-1}V$ with eigenvalue $= 1$. According to the Schmidt method you want to remove from K the projection operator P which is the residue of $\frac{1}{W-K}$ at $W = 1$. (I'm assuming 1 is a simple eigenvalue for K to keep things simple.)

$$P = \frac{1}{2\pi i} \oint_{\substack{\text{circle} \\ \text{around } 1}} \frac{dW}{W-K}$$

P projects onto $\mathbb{C}|B\rangle$.

$$(E - H_0)|B\rangle = V|B\rangle$$

$$\Rightarrow \langle B|(E - H_0) = \langle B|V$$

$$\Rightarrow \langle B|V = \langle B|\underbrace{V(E-H_0)^{-1}V}_{K}$$

$$\Rightarrow \langle B|V \text{ is a left eigenvector for } K$$

If $\langle B|V|B\rangle \neq 0$, then it seems that

$$P = \frac{|B\rangle\langle B|V}{\langle B|V|B\rangle} \qquad \text{since} \quad KP = P = PK \quad \text{and} \quad P^2 = P$$

We want to replace K by $K - P$ or

$V = (E - H_0)K$ by $V_1 = (E-H_0)(K-P) = V - \frac{V|B\rangle\langle B|V}{\langle B|V|B\rangle}$

Note that $V_1|B\rangle = 0$ and $\langle B|V_1 = 0$
whence V_1 is a self-adjoint operator working in the orthogonal complement of $|B\rangle$.

I think what Weinberg does is to understand the Schmidt method via his $\tilde{H}, \tilde{\mathcal{H}}$ construction as follows. We start with $H = H_0 + V$ on $\mathcal{H}$ having the bound state $|B\rangle$ which, let's assume, is the only thing preventing convergence of the Born series at the energy E. Then construct $\tilde{H} = \tilde{H}_0 + \tilde{V}$ on $\tilde{\mathcal{H}} = \mathcal{H} \oplus \mathbb{C}|B_0\rangle$ in a suitable way. We have to choose E_0 and $\tilde{V} = \left(\begin{array}{c|c} V_1 & |\gamma\rangle \\ \hline \langle\bar{\gamma}| & \sigma \end{array}\right)$. We want to take V_1 as at the top of this page: $V_1 = V - \frac{V|B\rangle\langle B|V}{\langle B|V|B\rangle}$
so that combined with $(E-H_0)^{-1}$
it gives a convergent Born series, i.e. $K_1 = (E-H_0)^{-1}V_1$ has all eigenvalues inside S^1. It remains to choose $|\gamma\rangle$ and/or σ. We do this so that the operator

$$\frac{1}{W - \tilde{H}} \text{ between states of } \mathcal{H} = \frac{1}{W-H_0} + \frac{1}{W-H_0}\left(V_1 + |\gamma\rangle \frac{1}{W-(E_0+\sigma)}\langle\bar{\gamma}|\right)\frac{1}{W-H_0} +$$

coincides with $\frac{1}{W-H} = \frac{1}{W-H_0} + \frac{1}{W-H_0}(V)\frac{1}{W-H_0} + \cdots$

Thus we want

$$V = V_1 + |\gamma\rangle \frac{1}{W-(E_0+\sigma)}\langle\bar{\gamma}|$$

which is clearly impossible for all W, although we can do it for $W = E$. So we want

$$\frac{V|B\rangle\langle B|V}{\langle B|V|B\rangle} = |\gamma\rangle \frac{1}{W-(E_0+\sigma)} \langle\tilde{\gamma}|$$

at least for $W=E$. Clearly this can be done; moreover if $E_0+\sigma \ll 0$, then the W variation is negligible.

The point of the Schmidt method seems to be as follows. Suppose we want ~~to~~ compute

$$\frac{1}{1-K} = 1 + K + K^2 + \cdots$$

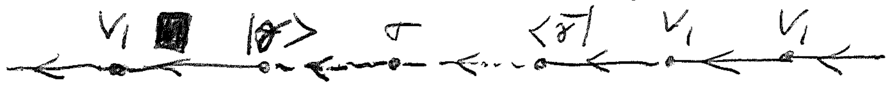
but the series doesn't converge because K has one eigenvalue outside S^1. Then we remove from K a rank 1 operator to get $K_1 = K - |\gamma\rangle\langle\tilde{\gamma}|$, where $\|K_1\| < 1$ and so we can compute $\frac{1}{1-K_1}$ by a geometric series. Then we use

$$\frac{1}{1-K} = \left(1 - \frac{1}{1-K_1}(K-K_1)\right)^{-1} \frac{1}{1-K_1}$$

March 9, 1980

Weinberg's construction: $\tilde{H} = \left(\begin{array}{c|c} H_0 & 0 \\ \hline 0 & E_0 \end{array}\right)$ on $\tilde{\mathcal{H}} = \mathcal{H} \oplus \mathbb{C}|B_0\rangle$

$\tilde{V} = \left(\begin{array}{c|c} V_1 & |\gamma\rangle \\ \hline \langle\tilde{\gamma}| & \sigma \end{array}\right)$. To compute matrix elements of $\frac{1}{W-\tilde{H}}$ we use diagrams looking like



One can combine iterates of the free propagators to get

$$\Leftarrow \;=\; \leftarrow \;+\; \leftarrow\overset{V_1}{\bullet}\leftarrow \;+\; \cdots\cdots$$

$$= \frac{1}{W-(H_0+V_1)}$$

$$\Leftarrow\!\!\!-\,-\,- \;=\; \frac{1}{W-(E_0+\sigma)}$$

and this amounts to breaking $\tilde{H}$ up differently:

$$\tilde{H} = \left(\begin{array}{c|c} H_0+V_1 & 0 \\ \hline 0 & E_0+\sigma \end{array}\right) + \left(\begin{array}{c|c} 0 & |\gamma\rangle \\ \hline \langle\tilde{\gamma}| & 0 \end{array}\right)$$

Of particular interest is the matrix elements of $\frac{1}{W-\tilde{H}}$ between states of $\mathcal{H}$: Put $in_1 : \mathcal{H} \hookrightarrow \tilde{\mathcal{H}}$, $\begin{array}{l} H_1 = H_0 + V_1 \\ E_1 = E_0 + \sigma \end{array}$

$$in_1^* \frac{1}{W-\tilde{H}} in_1 = \frac{1}{W-H_1} + \underbrace{\frac{1}{W-H_1}|\gamma\rangle\frac{1}{W-(E_0+\sigma)}\langle\tilde{\gamma}|}\frac{1}{W-H_1} + \cdots\cdots$$

$$= \left[1-(W-H_1)^{-1}\frac{|\gamma\rangle\langle\tilde{\gamma}|}{W-E_1}\right]^{-1}(W-H_1)^{-1}$$

$$= \left[(W-H_1)\left(1-(W-H_1)^{-1}\frac{|\gamma\rangle\langle\tilde{\gamma}|}{W-E_1}\right)\right]^{-1}$$

$$= \left(W-H_1-\frac{|\gamma\rangle\langle\tilde{\gamma}|}{W-E_1}\right)^{-1}$$

$$= \frac{1}{W-H_1-\frac{|\gamma\rangle\langle\tilde{\gamma}|}{W-E_1}}$$

Notice that this is not in the form $\dfrac{1}{W - \text{some operator}}$ but that it is sort of like the beginning of a continued fraction.

Schmidt method: Let $K = K_1 + |\gamma\rangle\langle\bar{\gamma}|$. Then

$$\frac{1}{1-K} = \frac{1}{1-K_1-(K-K_1)} = \frac{1}{1-\frac{1}{1-K_1}(K-K_1)} \cdot \frac{1}{1-K_1}$$

Recall how to invert $I -$ a rank 1 operator.

$$\frac{1}{1-|\alpha\rangle\langle\bar{\alpha}|} = 1 + |\alpha\rangle\langle\bar{\alpha}| + |\alpha\rangle\langle\bar{\alpha}|\alpha\rangle\langle\bar{\alpha}| + \cdots\cdots$$

$$= 1 + \frac{|\alpha\rangle\langle\bar{\alpha}|}{1-\langle\bar{\alpha}|\alpha\rangle}$$

So one has

$$\frac{1}{1-\frac{1}{1-K_1}(K-K_1)} = \frac{1}{1-\frac{1}{1-K_1}|\gamma\rangle\langle\bar{\gamma}|}$$

$$= 1 + \frac{1}{1-\langle\bar{\gamma}|\frac{1}{1-K_1}|\gamma\rangle} \cdot \frac{1}{1-K_1}|\gamma\rangle\langle\bar{\gamma}|$$

so

$$\boxed{\frac{1}{1-K} = \frac{1}{1-K_1} + \frac{1}{1-\langle\bar{\gamma}|\frac{1}{1-K_1}|\gamma\rangle} \frac{1}{1-K_1}|\gamma\rangle\langle\bar{\gamma}|\frac{1}{1-K_1}}$$

Let's redo this for $H = H_1 +$ rank 1 operator, i.e.
$H = H_0 + V_1 + \dfrac{V|B\rangle\langle B|V}{\langle B|V|B\rangle}$ as on page 672. Say $H = H_1 + |\alpha\rangle\langle\bar{\alpha}|$.
Then

$$\boxed{\begin{aligned}\frac{1}{W-H} &= \frac{1}{1-\frac{1}{W-H_1}|\alpha\rangle\langle\bar{\alpha}|} \cdot \frac{1}{W-H_1} \\ &= \frac{1}{W-H_1} + \frac{1}{W-H_1}|\alpha\rangle \frac{1}{1-\langle\bar{\alpha}|\frac{1}{W-H_1}|\alpha\rangle} \langle\bar{\alpha}|\frac{1}{W-H_1}\end{aligned}}$$

This should be compared to the analogous formula for the $\tilde{H}$ situation:

$$in_1^* \frac{1}{W-\tilde{H}} in_1 = \left(1-(W-H_1)^{-1}\frac{|\gamma\rangle\langle\tilde{\gamma}|}{W-E_1}\right)^{-1}(W-H_1)^{-1}$$

$$= \frac{1}{W-H_1} + \frac{1}{W-H_1}|\gamma\rangle\left[\frac{1}{W-E_1}\,\frac{1}{1-\frac{\langle\tilde{\gamma}|(W-H_1)^{-1}|\gamma\rangle}{W-E_1}}\right]\langle\tilde{\gamma}|\frac{1}{W-H_1}$$

$$\boxed{in_1^* \frac{1}{W-\tilde{H}} in_1 = \frac{1}{W-H_1} + \frac{1}{W-H_1}|\gamma\rangle \frac{1}{W-E_1-\langle\tilde{\gamma}|\frac{1}{W-H_1}|\gamma\rangle}\langle\tilde{\gamma}|\frac{1}{W-H_1}}$$

Note that this expression approaches the one on the bottom of the preceding page provided one lets $-E_1 \to \infty$ with

$$\frac{|\gamma\rangle\langle\tilde{\gamma}|}{-E_1} \longrightarrow |\kappa\rangle\langle\tilde{\kappa}|$$

However it doesn't seem that the Weinberg $\tilde{\mathcal{H}}$ construction is motivated by the Schmidt method. What I mean is that the Schmidt method is carried out directly on $H = H_0 + V$ in the Hilbert space $\mathcal{H}$, and amounts to the splitting $H = \underbrace{H_0 + V_1}_{H_1} + |\kappa\rangle\langle\tilde{\kappa}|$, plus knowledge of the propagator for H_1. There seems to be no point in introducing $\tilde{\mathcal{H}}$ that I can see in order to "explain" the Schmidt method.

March 10, 1980

We would like next to understand the response of an electron gas to an external electromagnetic field. We treat the electrons as non-interacting, so its really a problem of understanding how to describe the response of a single electron and then second quantizing things. This will involve me with Pauli's spin formalism, and ultimately the Dirac equation. Review formulas - this time check units and put in c.

Lorentz law $\quad \underbrace{F}_{\frac{gr\,cm}{sec^2}} = \underbrace{e}_{coul.}(\underbrace{\vec{E}}_{\frac{gr\,cm}{sec^2 coul}} + v \times \underbrace{B}_{\frac{gr}{sec\,coul}})$

$$\boxed{\nabla \cdot B = 0} \Longrightarrow \boxed{B = \nabla \times \underbrace{A}_{\frac{gr\,cm}{sec\,coul}}}$$

$$\boxed{\nabla \times E = -\frac{\partial B}{\partial t}} \qquad \text{this checks unit-wise}$$

$$= -\frac{\partial}{\partial t}(\nabla \times A)$$

ϕ should be measured in ergs/coul. $= \frac{gr\,cm^2}{sec^2 coul}$

$$\boxed{\underbrace{E}_{\frac{gr\,cm}{sec^2 coul}} = -\nabla\phi - \underbrace{\frac{\partial A}{\partial t}}_{\frac{gr\,cm}{sec^2 coul}\ \checkmark}}$$

So the above formulas do not involve c.

Relativistic Lagrangian: $\quad L = -m\sqrt{1-v^2} - e(\phi - \underbrace{v\cdot A}_{\frac{cm}{sec}\frac{gr\,cm}{sec\,coul}})$ OK

for $c=1$. $\quad p = \frac{\partial L}{\partial v} = \frac{mv}{\sqrt{1-v^2}} + eA$

For general c

$$L = -mc^2\sqrt{1-v^2/c^2} - e(\phi - v\cdot A)$$

$$p = \frac{mv}{\sqrt{1-v^2/c^2}} + eA \qquad eA - \frac{g\,cm}{sec} \text{ momentum.}$$

$$H = pv - L = \frac{mv^2}{\sqrt{\ }} + e\cancel{v\cdot A} + mc^2\sqrt{\ \ } + e(\phi - \cancel{v\cdot A})$$

$$= \frac{mc^2}{\sqrt{1-(v/c)^2}} + e\phi$$

$$H = c\sqrt{(p-eA)^2 + m^2c^2} + e\phi \qquad \text{rel. Hamiltonian}$$

$$\approx mc^2 + \frac{(p-eA)^2}{2m} + e\phi \qquad \text{as } c \to \infty.$$

Now $\dfrac{(p-eA)^2}{2m} + e\phi \approx \dfrac{p^2}{2m} + e(\phi - \frac{p}{m}\cdot A)$ ignoring $\dfrac{e^2A^2}{2m}$ term

so for weak A, the extra energy due to A is

$$e(\phi - \tfrac{p}{m}\cdot A) = e(\phi - v\cdot A)$$

If we have a fluid of independent particles, we add this up over all the particles and we get

$$e\int \big(\rho(x)\phi(x) - j(x)\cdot A(x)\big)\, dx$$

where ρ = particle density and j = particle current density.

The above considerations are in classical mechanics. Let's now pass to a quantum particle described by a wave function ψ and Hamiltonian $H_0 = \dfrac{p^2}{2m}$, $p = \dfrac{\hbar}{i}\nabla$. Then $\rho = |\psi|^2$ is the particle density in this state so that

$$\int e|\psi|^2\phi\, dx = \langle\psi|e\phi|\psi\rangle$$

is the electrostatic energy. Derive particle current density

$$\partial_t |\psi|^2 = \bar\psi\left(-\tfrac{i}{\hbar}H_0\psi\right) + \overline{\left(-\tfrac{i}{\hbar}H_0\psi\right)}\psi$$

$$= \bar\psi\left(+\tfrac{i}{\hbar}\tfrac{\hbar^2}{2m}\Delta\psi\right) + \tfrac{i}{\hbar}\tfrac{-\hbar^2}{2m}\Delta\bar\psi\cdot\psi$$

$$= i\frac{\hbar}{2m}\left[\bar\psi\,\Delta\psi - \Delta\bar\psi\cdot\psi\right]$$

$$= i\frac{\hbar}{2m}\nabla\cdot\left(\bar\psi\,\nabla\psi - (\nabla\bar\psi)\psi\right)$$

so $\quad \partial_t |\psi|^2 + \nabla\cdot\vec{j} = 0$ provided we put

$$\vec{j} = \frac{1}{2m}\left[\bar{\psi}\left(\frac{\hbar}{i}\vec{\nabla}\psi\right) + \overline{\left(\frac{\hbar}{i}\vec{\nabla}\psi\right)}\psi\right]$$

whence

$$\int(\vec{j}\cdot A)\,dx = \frac{1}{2m}\int\left(\bar{\psi}\left(A\cdot\frac{\hbar}{i}\nabla\psi\right) + \overline{\left(\frac{\hbar}{i}\nabla\psi\right)}\cdot A\psi\right)dx$$

$$= \frac{1}{2m}\langle\psi|\,A\cdot p + p\cdot A\,|\psi\rangle = \langle\psi|\,\frac{A\cdot p + p\cdot A}{2m}\,|\psi\rangle$$

Thus

$$e\int\left(\rho(x)\phi(x) - j(x)\cdot A(x)\right)dx = \langle\psi|\,e\left(\phi - \frac{A\cdot p + p\cdot A}{2m}\right)|\psi\rangle$$

March 12, 1980

The problem is to understand the response of charged particles to an external EM field. Classically the extra energy acquired by a charged particle moving thru a weak EM field is $e(\phi - v \cdot A)$, so for a fluid of charged particles all having charge e the interaction energy is

$$e \int [\rho(x)\phi(x) - j(x)\cdot A(x)]\, dx$$

We found this to be consistent with the probabilistic interpretation of a wave function:

$$\rho(x) = |\psi(x)|^2$$
$$j(x) = \frac{\hbar}{i\,2m}\left(\bar{\psi}\,\nabla\psi - \overline{\nabla\psi}\,\psi\right)$$

$$e\int[\rho(x)\,\phi(x) - j(x)\cdot A(x)]\,dx = \left\langle \psi \middle| e\left(\phi \quad \frac{p\cdot A + A\cdot p}{2m}\right) \middle| \psi \right\rangle$$

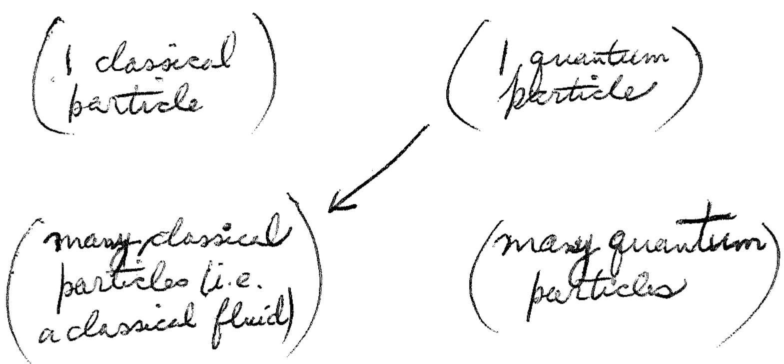
What's mysterious here is the fact that the formula

$$\rho(x) = |\psi(x)|^2$$

which is an equality of numbers will get replaced by

$$\rho(x) = \psi(x)^* \psi(x)$$

an equality of operators after second quantization.



There seems to be a strange arrow called the "hydro-dynamic interpretation" of a wave function, which allows one to interpret a quantum wave function classically. This reminds me vaguely of ~~[illegible]~~ Dold-Thom.

Does there exist a version of Dold-Thom with complex amplitudes?

March 14, 1980

Time to understand spin and the Dirac equation. The Dirac equation is

$$\frac{\hbar i}{c}\frac{\partial \psi}{\partial t} = \left(\alpha \cdot \frac{\hbar}{i}\nabla + \beta mc\right)\psi$$

where $\alpha_1, \alpha_2, \alpha_3, \beta$ satisfy

$$\alpha_i^2 = \beta^2 = I$$
$$\{\alpha_i, \alpha_j\} = 0, \quad i \neq j$$
$$\{\alpha_i, \beta\} = 0.$$

If I put $\alpha_4 = \beta$, then the matrices α_i generate a 2-group of order 32 which is an extension $\tilde{V}$ of an elementary ab 2-gp V of rank 4 by $\mathbb{Z}/2 = \{\pm I\}$. $\tilde{V}$ is generated by $\alpha_1, \ldots, \alpha_4$ which anti-commute and have order 2. The commutator pairing $S^2 V \to \mathbb{F}_2$ has the matrix

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

which is non-singular, so I know from earlier work how to construct the irred. repns of $\tilde{V}$. One takes a max. abelian subgroup $\tilde{W}$ (e.g. gen. by $\alpha_1\alpha_2$, $\alpha_3\alpha_4$) and then a character of $\tilde{W}$ which sends -1 to $-I$, and then induces this character up to $\tilde{V}$ to get an irred repn of dim 4 over $\mathbb{C}$. Since $|\tilde{V}| = 32 = 16 + 4^2$, ($16$ = characters of V) this 4 dim repn. is the unique irreducible repn of $\tilde{V}$ on which the center is non-trivial. So we see there is only one representation for the Dirac matrices.

The simplest representation is obtained as follows. Begin by representing β as a diagonal matrix

$$\beta = \left(\begin{array}{c|c} I & 0 \\ \hline 0 & -I \end{array}\right)$$

where the blocks have to be of equal size, since β is conjugate to $-\beta$. Any matrix anti-commuting with β has the form $\left(\begin{array}{c|c} 0 & B \\ \hline C & 0 \end{array}\right)$. Since $\begin{pmatrix} 0 & B \\ C & 0 \end{pmatrix}\begin{pmatrix} 0 & B' \\ C' & 0 \end{pmatrix} = \left(\begin{array}{c|c} BC' & 0 \\ \hline 0 & CB' \end{array}\right)$

if we want matrices $\alpha_1, \alpha_2, \alpha_3$ to have square I, the simplest thing to do is to take $B = C$ and then look for a representation of the subgroup gen. by $\alpha_1, \alpha_2, \alpha_3$. Thus one puts

$$\alpha_i = \left(\begin{array}{c|c} 0 & \sigma_i \\ \hline \sigma_i & 0 \end{array}\right) \qquad i = 1, 2, 3$$

where the σ_i anti-commute and are of order 2.
Then try the same thing

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

but this time you can't represent both σ_1, σ_2 in the form $\left(\begin{array}{c|c} 0 & B \\ \hline B & 0 \end{array}\right)$ with B a scalar, so the standard choice is

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Let's return to the Dirac equation

$$\frac{\hbar i}{c}\frac{\partial \psi}{\partial t} = \left(\alpha \cdot \frac{\hbar}{i}\nabla + \beta mc\right)\psi$$

and take the limit as $c \longrightarrow \infty$. First look what happens to plane wave solutions

$$\psi(x,t) = e^{i(k \cdot x - \omega t)}\, v$$

$$\frac{\hbar\omega}{c} v = (\alpha \cdot \hbar k + \beta mc) v$$

or if $\varepsilon = \hbar\omega$, $p = \hbar k$, then

$$\frac{\varepsilon}{c} v = (\alpha \cdot p + \beta mc) v$$

hence $\frac{\varepsilon}{c}$ is an eigenvalue for the matrix $(\alpha\cdot p+\beta mc)$. Since $(\alpha\cdot p+\beta mc)^2 = p^2+m^2c^2$ we get the relation

$$\frac{\varepsilon}{c} = \pm\sqrt{p^2+m^2c^2}$$

For positive energy $\varepsilon = c\sqrt{p^2+m^2c^2} \approx mc^2+\frac{p^2}{2m}$. The corresponding eigenvector form a 2-dimensional space. Therefore, for a given momentum p there are two eigenstates with positive energy, and two eigenstates of negative energy.

$$\left(\alpha\cdot p+\beta mc\right) = \begin{pmatrix} mc & \sigma\cdot p \\ \sigma\cdot p & -mc \end{pmatrix}$$

$$0 = \left(\left(\alpha\cdot p+\beta mc\right) - \sqrt{p^2+m^2c^2}\right)v = \begin{pmatrix} \underbrace{mc-\sqrt{p^2+m^2c^2}}_{\approx \frac{p^2}{2mc}} & \sigma\cdot p \\ \sigma\cdot p & -mc-\sqrt{p^2+m^2c^2} \end{pmatrix} v$$

If we write $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ where v_i is a 2-dim'l vector, then for v to be an eigenvector says

$$(\sigma\cdot p)v_1 = \underbrace{\left(+mc+\sqrt{p^2+m^2c^2}\right)}_{\approx +2mc} v_2$$

It follows that v_1 can be arbitrarily prescribed, and then v_2 solved for. As $c\to\infty$ we have

$$(cv_2) \longrightarrow +\frac{1}{2m}(\sigma\cdot p)v_1$$

and hence

$$\psi = e^{i\left(\frac{p}{\hbar}x-\frac{\varepsilon}{\hbar}t\right)} v \approx e^{-i\frac{mc^2}{\hbar}t}\, e^{i\left(\frac{p}{\hbar}\cdot x-\frac{p^2}{\hbar 2m}t\right)} \begin{pmatrix} v_1 \\ O(\frac{1}{c}) \end{pmatrix}.$$

Therefore if we replace ψ by $e^{-i/\hbar (mc^2)t}\tilde{\psi}$ in Dirac's equation we get

$$\frac{\hbar i}{c}\frac{\partial \tilde\psi}{\partial t} = \left(\alpha\cdot\frac{\hbar}{i}\nabla + \beta mc - mc\right)\tilde\psi$$

or

$$\hbar i\frac{\partial \tilde\psi}{\partial t} = c\begin{pmatrix} 0 & \sigma\cdot\frac{\hbar}{i}\nabla \\ \sigma\cdot\frac{\hbar\nabla}{i} & -2mc\end{pmatrix}\tilde\psi$$

$$\hbar i\frac{\partial \tilde\psi_1}{\partial t} = \left(\sigma\cdot\frac{\hbar}{i}\nabla\right)(c\tilde\psi_2)$$

$$\frac{1}{c}\hbar i\frac{\partial \tilde\psi_2}{\partial t} = \left(\sigma\cdot\frac{\hbar}{i}\nabla\right)\tilde\psi_1 - 2m(c\tilde\psi_2)$$

So $\quad c\tilde\psi_2 = \frac{1}{2m}\left(\sigma\cdot\frac{\hbar}{i}\nabla\right)\tilde\psi_1 + O\left(\frac{1}{c^2}\right)$

so $\quad \tilde\psi \longrightarrow \begin{pmatrix}\psi_1\\0\end{pmatrix}$ where $\quad \hbar i\frac{\partial\psi_1}{\partial t} = \frac{1}{2m}\left(\sigma\cdot\frac{\hbar}{i}\nabla\right)^2\psi_1$

$$\sigma\cdot\nabla = \sigma_1\frac{\partial}{\partial x_1} + \sigma_2\frac{\partial}{\partial x_2} + \sigma_3\frac{\partial}{\partial x_3}$$

$$(\sigma\cdot\nabla)^2 = \begin{pmatrix}\Delta & 0\\ 0 & \Delta\end{pmatrix}$$

so we see that $\quad \hbar i\frac{\partial\psi_1}{\partial t} = \frac{-\hbar^2}{2m}\Delta\psi_1 \quad$ and both components of ψ_1 satisfy the ordinary Schroedinger eqn.

Suppose now we have an external EM field given by $(\phi, \vec A)$. The standard recipe is to replace

$$p \longmapsto p - eA \qquad \varepsilon \longmapsto \varepsilon - e\phi$$

so the Dirac equation becomes

$$\frac{1}{c}\left(\hbar i\frac{\partial}{\partial t} - e\phi\right)\psi = \left(\alpha\cdot\left(\frac{\hbar}{i}\nabla - eA\right) + \beta mc\right)\psi$$

$$\left(\hbar i\frac{\partial}{\partial t} - e\phi\right)\begin{pmatrix}\tilde\psi_1\\ \tilde\psi_2\end{pmatrix} = c\begin{pmatrix}0 & \sigma\cdot(p-eA)\\ \sigma\cdot(p-eA) & -2mc\end{pmatrix}\begin{pmatrix}\tilde\psi_1\\ \tilde\psi_2\end{pmatrix}$$

and so as $c \to \infty$, $c\tilde{\psi}_2 = \frac{1}{2m}\sigma\cdot(p-eA)\tilde{\psi}_1$

and $\tilde{\psi} \to \begin{pmatrix}\psi_1\\0\end{pmatrix}$ where

$$\left(\hbar i\frac{\partial}{\partial t} - e\phi\right)\psi_1 = \frac{1}{2m}\left(\sigma\cdot(p-eA)\right)^2\psi_1$$

Now $$\sigma\cdot(p-eA) = \sum_j \sigma_j\left(\frac{\hbar}{i}\frac{\partial}{\partial x_j} - eA_j\right)$$

so $$\left(\sigma\cdot(p-eA)\right)^2 = \sum_{j,k}\sigma_j\sigma_k\left(\frac{\hbar}{i}\frac{\partial}{\partial x_j} - eA_j\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x_k} - eA_k\right)$$

$$= \sum_j\left(\frac{\hbar}{i}\frac{\partial}{\partial x_j} - eA_j\right)^2 - \sum_{j\neq k}\sigma_j\sigma_k\, e\frac{\hbar}{i}\frac{\partial A_k}{\partial x_j}$$

The last term is the interesting one. First notice that

$$\sigma_1\sigma_2\sigma_3 = \begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&-i\\i&0\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix} = \begin{pmatrix}i&0\\0&-i\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix} = \begin{pmatrix}i&0\\0&i\end{pmatrix}$$

so that $\boxed{\sigma_1\sigma_2 = i\sigma_3}$ together with all cyclic permutations of this. Also from $\nabla\times A = B$ we have

$$\sigma_1\sigma_2\frac{\partial A_2}{\partial x_1} + \sigma_2\sigma_1\frac{\partial A_1}{\partial x_2} = i\sigma_3 B_3$$

Thus $$\sum_{j\neq k}\sigma_j\sigma_k\frac{\partial A_k}{\partial x_j} = i\,\sigma\cdot B$$ and so the limiting form of the Dirac equation becomes the Pauli equation

$$\boxed{\left(\hbar i\frac{\partial}{\partial t} - e\phi\right)\psi_1 = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - eA\right)^2 - \frac{e\hbar}{2m}\sigma\cdot B\right]\psi_1}$$

The Dirac equation has a hydro-dynamic interpretation with $\rho = \psi^*\psi$. Let's compute the current density

$$\frac{\partial}{\partial t}\rho = \psi^*\frac{1}{\hbar i}H\psi + \left(\frac{1}{\hbar i}H\psi\right)^*\psi \qquad H = e\phi + c(\alpha\cdot p + \beta mc)$$

$$= \frac{1}{\hbar i}\left(\psi^* \, c\alpha\cdot p\psi \; (p\psi)^*\cdot c\alpha\psi\right)$$

$$= - \left(\psi^* c\alpha\cdot\nabla\psi + \nabla\psi^*\cdot c\alpha\psi\right) = -\nabla\cdot\left(\psi^* c\alpha\psi\right)$$

hence $\boxed{j_k = \psi^* c\alpha_k \psi}$

or

$$j_k = (\psi_1^* \; \psi_2^*)\begin{pmatrix} 0 & c\sigma_k \\ c\sigma_k & 0 \end{pmatrix}\begin{pmatrix}\psi_1 \\ \psi_2\end{pmatrix} = \psi_1^*\sigma_k c\psi_2 + c\psi_2^*\sigma_k\psi_1$$

Now suppose we let $c \to \infty$; we have seen ψ_1 converges and $c\psi_2$ converges to

$$c\psi_2 \to \frac{1}{2m}\,\sigma\cdot(p-eA)\psi_1$$ preceding page

Hence j_k becomes

$$j_k = \frac{1}{2m}\left[\psi_1^*\sigma_k\,\sigma\cdot(p-eA)\psi_1 + \left(\sigma\cdot(p-eA)\psi_1\right)^*\sigma_k\psi_1\right]$$

Now

$$\psi_1^*\sigma_k \sum_j \sigma_j A_j\psi_1 + \left(\sum_j \sigma_j A_j\psi_1\right)^*\sigma_k\psi_1$$

$$= \psi_1^*\sum_j \underbrace{(\sigma_k\sigma_j + \sigma_j\sigma_k)}_{2\delta_{jk}} A_j\psi_1 = 2A_k\,\psi_1^*\psi_1$$

Put

$$\tilde{j}_k = \sum_j\left(\psi_1^*\sigma_k\sigma_j\frac{\partial\psi_1}{\partial x_j} - \frac{\partial\psi_1^*}{\partial x_j}\sigma_j\sigma_k\psi_1\right)\cdot\frac{\hbar}{2mi}$$

Then $\frac{2mi}{\hbar}\nabla\cdot\tilde{j} = \sum_{k,j} \frac{\partial}{\partial x_k}\left(\psi_1^*\sigma_k\sigma_j\frac{\partial\psi_1}{\partial x_j} - \frac{\partial\psi_1^*}{\partial x_j}\sigma_j\sigma_k\psi_1\right)$

$$= \sum_{k,j}\psi_1^*\sigma_k\sigma_j\frac{\partial^2\psi_1}{\partial x_k\partial x_j} - \frac{\partial^2\psi_1^*}{\partial x_k\partial x_j}\sigma_j\sigma_k\psi_1$$

$$= \psi_1^*\Delta\psi_1 - \Delta\psi_1^*\psi_1$$

$$= \nabla\cdot\left(\psi_1^*\nabla\psi_1 - \nabla\psi_1^*\psi_1\right)$$

Thus $\tilde{j}$ differs by a curl from the current $\frac{\hbar}{2mi}(\psi^*\nabla\psi - \nabla\psi^*\psi)$ associated to a "point" electron.

It seems that the magnetic moment of the electron due to its spin doesn't affect the probability current, because it is a zeroth order hermitian operator.

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The Dirac equation with field (ϕ, A) is

$$\left(\hbar i \frac{\partial}{\partial t} - e\phi\right)\psi = c\begin{pmatrix} 0 & \sigma\cdot(p-eA) \\ \sigma\cdot(p-eA) & -2mc \end{pmatrix}\psi \qquad \psi = \begin{pmatrix}\psi_1 \\ \psi_2\end{pmatrix}$$

where we have removed mc^2 already from the energy. Letting $c \to \infty$ we get

$$c\psi_2 = \frac{1}{2m}\sigma\cdot(p-eA)\psi_1$$

$$\left(\hbar i\frac{\partial}{\partial t} - e\phi\right)\psi_1 = \sigma\cdot(p-eA)\psi_2 = \frac{1}{2m}\left[\sigma\cdot(p-eA)\right]^2\psi_1 \qquad \text{Pauli equation}$$

The particle + current densities for the Dirac eqn are

$$\rho = \psi^*\psi \qquad j_k = \psi^* c\alpha_k\psi = (\psi_1^* \; \psi_2^*)\begin{pmatrix} 0 & c\sigma_k \\ c\sigma_k & 0\end{pmatrix}\begin{pmatrix}\psi_1 \\ \psi_2\end{pmatrix}$$

$$= \psi_1^*\sigma_k c\psi_2 + c\psi_2^*\sigma_k\psi_1$$

and in the limit as $c \to \infty$, they become

$$\rho = \psi_1^*\psi_1 \qquad j_k = \psi_1^*\sigma_k\frac{1}{2m}\left[\sigma\cdot(p-eA)\right]\psi_1 + \frac{1}{2m}\left(\left[\sigma\cdot(p-eA)\right]\psi_1\right)^*\sigma_k\psi_1$$

To simplify the sequel we replace ψ_1 by ψ, so that now ψ is a 2-component wave function.

$$j_k = \psi^*\sigma_k\frac{\hbar}{2mi}\sigma_j\frac{\partial\psi}{\partial x_j} - \frac{\hbar}{2mi}\frac{\partial\psi^*}{\partial x_j}\sigma_j\sigma_k\psi$$

summed over j

$$-\frac{e}{2m}\psi^*\sigma_k\sigma_j A_j\psi - \frac{e}{2m}\psi^*\sigma_j\sigma_k A_j\psi$$

[redacted]

$$j_k = \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x_k} - \frac{\partial\psi^*}{\partial x_k}\psi\right) - \frac{e}{2m}\psi^*\sum_j \underbrace{(\sigma_k\sigma_j+\sigma_j\sigma_k)}_{2\delta_{jk}}A_j\psi$$

$$\frac{\hbar}{2mi}\underbrace{\sum_{j\neq k}{}' \psi^*\sigma_k\sigma_j\frac{\partial\psi}{\partial x_j} - \frac{\partial\psi^*}{\partial x_j}\underbrace{\sigma_j\sigma_k}_{-\sigma_k\sigma_j}\psi}$$

If $k=1$ $\qquad Q_i = \psi^*\sigma_i\psi$

$$\sum_{j\neq k}\frac{\partial}{\partial x_j}\left(\psi^*\sigma_k\sigma_j\psi\right) = i\left(\frac{\partial Q_3}{\partial x_2} - \frac{\partial Q_2}{\partial x_3}\right)$$

Thus

$$\boxed{j_k = \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x_k} - \frac{\partial\psi^*}{\partial x_k}\psi\right) - \frac{e}{m}A_k\psi^*\psi + \frac{\hbar}{2m}\left[\nabla\times(\psi^*\sigma\psi)\right]_k}$$

It follows easily that

$$\int e(\phi\rho - A\cdot j)\,dx = \left\langle\psi\middle| e\phi - \frac{e}{2m}(A\cdot p + p\cdot A) + \frac{e^2A^2}{m}\ \frac{\hbar e}{2m}B\cdot\sigma\middle|\psi\right\rangle$$

is the extra energy due to the presence of the field. NO should be $\frac{e^2A^2}{2m}$

The above is slightly mysterious because there seem to be two distinct roads leading to the same place. (not quite) Let me illustrate them with the scalar electron. Without field, the energy relation is $E = \frac{p^2}{2m}$ leading to

$$\hbar i\frac{\partial\psi}{\partial t} = \frac{p^2}{2m}\psi.$$

With field the Schröd. eqn. is

$$\hbar i\frac{\partial\psi}{\partial t} = \left[e\phi + \frac{(p-eA)^2}{2m}\right]\psi$$

So $\qquad H = H_0 + H_{ext}\qquad$ where the extra energy is

$$H_{ext} = e\phi - e\frac{p\cdot A + A\cdot p}{2m} + \frac{e^2A^2}{2m}$$

Hence the extra energy in the ~~state~~ ψ is

$$\langle \psi | H_{ext} | \psi \rangle = \langle \psi | e\phi - \frac{e}{2m}(p\cdot A + A\cdot p) + \frac{e^2}{2m}A^2 | \psi \rangle$$

On the other hand one has prob. density $\rho = \psi^*\psi$ and assuming ψ satisfies the Schroed. eqn. one [redacted] finds

$$\partial_t(\psi^*\psi) = -\nabla\cdot\underbrace{\left[\frac{\hbar}{2mi}(\psi^*\nabla\psi - \nabla\psi^*\psi) - \frac{e}{m}A\psi^*\psi\right]}_{j}$$

so we define j to be:

But then

$$\int e(\phi\rho - j\cdot A)\,dx = \langle \psi | e\phi - \frac{e}{2m}(A\cdot p + p\cdot A) + \frac{e^2}{m}A^2 | \psi \rangle$$

which fails by a factor of 2 to be the extra energy! So it's not true that $\int e(\phi\cdot\rho - j\cdot A)\,dx$ is the extra energy, although <u>this seems to be correct</u> to the first order in (ϕ, A).

However in the case of the Dirac equation

$$\hbar i \frac{\partial\psi}{\partial t} = \underbrace{\left(e\phi + c\alpha\cdot(p - eA) + \beta mc^2 - mc^2\right)}_{H = H_0 + H_{ext}}\psi$$

we have seen $\rho = \psi^*\psi$, $j = \psi^* c\alpha\psi$.

where

$$H_{ext} = e\phi - c\alpha\cdot eA.$$

Then

$$\int e(\phi\rho - A\cdot j)\,dx = \langle \psi | e\phi - eA\cdot c\alpha | \psi \rangle = \langle \psi | H_{ext} | \psi \rangle.$$

Paradox: Why can't we let $c \to \infty$ in this and get a non-relativistic equality? The answer is that

$$\langle \psi | H_0 | \psi \rangle = \langle \psi | c\alpha\cdot p + \beta mc^2 - mc^2 | \psi \rangle$$

$$= \int (\psi_1^* \ \psi_2^*)\begin{pmatrix} 0 & c\sigma\cdot p \\ c\sigma\cdot p & -2mc^2 \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

Say two space-time dims so that $\sigma = 1$

$$\to \langle \psi_1^* | p\,\tfrac{1}{2m}(p - eA) | \psi_1 \rangle + \langle \tfrac{1}{2m}(p - eA)\psi_1 | p\psi_1 \rangle$$
$$- 2m \langle \tfrac{1}{2m}(p - eA)\psi_1 | \tfrac{1}{2m}(p - eA)\psi_1 \rangle$$

$$= \langle \psi_1^* | \frac{p^2}{2m} - \frac{e^2A^2}{2m} | \psi_1 \rangle$$

Hence the energy of the Dirac field due to (ϕ, A), namely $\langle \psi | H | \psi \rangle - \langle \psi | H_0 | \psi \rangle = \langle \psi | H_{ext} | \psi \rangle$, is not the same as the energy of the Pauli field due to A, namely $\langle \psi_1 | e\phi - \frac{e}{2m}(p \cdot A + A \cdot p) + \frac{e^2A^2}{2m} | \psi_1 \rangle$ because of the A-dependence hidden in $\langle \psi | H_0 | \psi \rangle$.

<u>Summary:</u> For the Dirac equation the extra energy change due to (ϕ, A) is

$$\int e(\phi\rho - A \cdot j)\, dx$$

but this is not true for the Pauli equation or for the scalar electron equation, <u>because there is a missing</u> quadratic factor in A.

The next project is 2nd quantization. The goal is as follows - we have an electron gas, we apply an external field (ϕ, A) and we want to understand the response of the gas. The simplest case we looked at already - namely we introduce an impurity at a point

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Kubo formula: One has a system described by a Schroed. eqn.

$$\frac{\partial \psi}{\partial t} = \frac{1}{i} H_0 \psi$$

where (usually) H_0 is time-independent. If A is an operator and $\psi(t) = e^{-iH_0 t}\psi_0$, [redacted] then the value of A in the state $\psi(t)$ is

$$\langle A\rangle(t) = \langle \psi(t) | A | \psi(t)\rangle = \langle \psi_0 | e^{iH_0 t} A e^{-iH_0 t} | \psi_0\rangle$$

If ψ_0 is an H_0 eigenstate, e.g. the ground state, then $\langle A\rangle(t)$ is time-independent.

Now ones considers a small time-dependent perturbation

$$H = H_0 + \delta H$$

where $\delta H(t)$ vanishes for $t \leq 0$. Let $U(t,t')$ be the propagator for

$$\frac{\partial \psi}{\partial t} = \frac{1}{i} H\psi$$

and let $\tilde{\psi}(t) = U(t,0)\psi_0$. Then we want to determine

$$\delta\langle A\rangle(t) = \langle \widetilde{A(t)}\rangle - \langle A(t)\rangle$$

$$= \langle \psi_0 | U(0,t) A\, U(t,0) | \psi_0\rangle - \langle \psi_0 | e^{iH_0 t} A e^{-iH_0 t} | \psi_0\rangle$$

Proceed as follows:

$$e^{iH_0 t} U(t,0) = I - i\int_0^t \delta H(t_1)\, dt_1 \quad + \text{ 2nd order}$$

denotes $e^{iH_0 t_1} \delta H_{\text{at } t_1} e^{-iH_0 t_1}$

[redacted] $$\widetilde{A(t)} \overset{\text{defn}}{=} U(0,t) A U(t,0)$$

$$= U(0,t) e^{-iH_0 t} A(t) e^{iH_0 t} U(t,0)$$

$$= \left(I + i\int_0^t \delta H(t_1)\, dt_1\right) A(t) \left(I - i\int_0^t \delta H(t_1)\, dt_1\right)$$

$$= A(t) + i\int_0^t [\delta H(t_1), A(t)]\, dt_1$$

The preceding [redacted] can be slightly generalized by allowing

$\delta H = 0$ for $t \ll 0$, and then

$$\widetilde{A(t)} = A(t) + i \int_{-\infty}^{t} [\delta H(t_1), A(t)]\, dt_1$$

March 17, 1980

The problem is still to compute the response of an independent particle gas to a weak varying field. Recall the Kubo derivation: Under the perturbation $H = H_0 + \delta H(t)$, $\delta H(t) = 0$ for $t \ll 0$, the ground state eigenfunction for H_0: $\Psi_0(t) = e^{-iH_0 t}\Psi_0$ becomes

$$\Psi(t) = \Psi_0(t) + \int_{-\infty}^{t} e^{-iH_0(t-t_1)}\frac{1}{i}\delta H(t_1)\Psi_0(t_1)\,dt_1$$

to first order. Hence

$$\delta\langle A(t)\rangle = \langle\Psi(t)|A|\Psi(t)\rangle - \langle\Psi_0(t)|A|\Psi_0(t)\rangle$$

$$= \langle\Psi_0(t)|A\frac{1}{i}\int_{-\infty}^{t} e^{-iH_0(t-t_1)}\,\delta H(t_1)\,e^{-iH_0 t_1}|\Psi_0\rangle\,dt_1$$

$$-\frac{1}{i}\int_{-\infty}^{t}\langle\Psi_0|e^{iH_0 t_1}\delta H(t_1)e^{iH_0(t-t_1)}A\,e^{-iH_0 t}|\Psi_0\rangle dt_1$$

$$= \frac{1}{i}\int_{-\infty}^{t}\langle\Psi_0|\,[A(t),\widetilde{\delta H}(t_1)]\,|\Psi_0\rangle\,dt_1 \qquad \begin{array}{l} A(t) = e^{iH_0 t}Ae^{-iH_0 t} \\ \widetilde{\delta H}(t) = e^{iH_0 t}\delta H(t)e^{-iH_0 t}\end{array}$$

For the fermion gas we take $A = \rho(x) = \psi^*(x)\psi(x)$, whence

$$A(t) = \psi^*(xt)\psi(xt) \quad \text{where}$$

$$\psi(xt) = \sum_\alpha u_\alpha(x)e^{-i\varepsilon_\alpha t}a_\alpha$$

u_α = orth. basis of eigenfns for H_0
$H_0 u_\alpha = \varepsilon_\alpha u_\alpha$

Similarly $\delta H(t)$ is the 1-particle operator associated to multiplication by $V(x,t)$:

$$\delta H(t) = \int\psi^*(x)\,V(x,t)\,\psi(x)\,dx$$

$$\widetilde{\delta H}(t) = \int\psi^*(xt)\,V(xt)\,\psi(xt)\,dx$$

Thus we have

$$\delta\langle\rho(xt)\rangle = \int_{-\infty}^{t}\frac{1}{i}\langle\Psi_0|\,[\psi^*(xt)\psi(xt),\int\psi^*(x_1t_1)\,V(x_1t_1)\,\psi(x_1t_1)\,dx_1]|\Psi_0\rangle dt_1$$

$$= \int_{-\infty}^{t}dt_1\int dx_1\,R(xt,x_1t_1)\,V(x_1t_1)$$

where $$R(xt, x_1t_1) = \frac{1}{i}\theta(t-t_1)\langle\Phi_0|\,[\psi^*(xt)\psi(xt), \psi^*(x_1t_1)\psi(x_1t_1)]\,|\Phi_0\rangle$$
is some sort of retarded Green's function.

Let's now review what we know about these multiple Green's functions. First work with imaginary time.

$$G(t,t') = \text{inverse of } \frac{d}{dt} + H_0 \quad \text{with suitable boundary conditions determined by } \varepsilon_F$$

$$= \begin{cases} e^{-H_0(t-t')}P_+ & t > t' \\ -e^{-H_0(t-t')}P_- & t < t' \end{cases}$$

Moreover

$$G(t,t') = \langle\Phi_0|\,T[\psi(t)\psi^*(t')]\,|\Phi_0\rangle$$

$\psi(t) = \sum u_\alpha a_\alpha$ has suppressed indices i.e. $\psi(xt) = \sum u_\alpha(x) a_\alpha$

Also I recall

$$G(t,t') = \frac{\displaystyle\oint e^{-\int \psi^*(\frac{d}{dt}+H_0)\psi\, dt}\ \psi(t)\psi^*(t')}{\displaystyle\oint e^{-\int \psi^*(\frac{d}{dt}+H_0)\psi\, dt}}$$

for a suitable notion of fermi-integration, which becomes well-defined when $\left(\frac{d}{dt}+H_0\right)^{-1}$ is specified (usually $\varepsilon_F = 0$, so the inverse is the inverse in L^2)

Now I am going to need real-time versions. We want
$$G(t,t') = \left(i\frac{d}{dt} - H_0\right)^{-1}$$

so that
$$\left(i\frac{d}{dt} - H_0\right)^{-1} e^{-i\omega t}\psi = e^{-i\omega t}\frac{1}{\omega - H_0}\psi$$

Hence

$$G(t,t') = \begin{cases} -i\, e^{-iH_0(t-t')} P_+ & t > t' \\ +i\, e^{-iH_0(t-t')} P_- & t < t' \end{cases}$$

$$= -i \langle T[\psi(t)\, \psi^*(t')] \rangle$$