

- ① [15 pts]. For a particle (q, m) in an EM field specified by a 4-potential $(A_\mu) = (\vec{A}, i\phi)$, the Klein-Gordon wave equation and continuity equation are $[\psi(x_\mu) = (t, i\vec{x})] \dots$

$$\left[\left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu \right)^2 - k_0^2 \right] \psi = 0, \quad \text{w/ } k_0 = mc/\hbar;$$

$$\left[\partial S_\mu / \partial x_\mu = 0, \quad \text{w/ } S_\mu = \frac{\hbar}{2im} \left[\psi^* \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu \right) \psi - \text{C.C.} \right] \right]$$

Consider the gauge transformation: $A_\mu \rightarrow A'_\mu = A_\mu + \partial\eta / \partial x_\mu$, η = arbitrary fcn.

Given that $\psi \rightarrow \psi' = \psi \exp[i(q/\hbar c)\eta]$ under this transform, show that: (A) S_μ is gauge invariant, and: (B) the KG Eqn itself is gauge covariant (form-invariant).

- ② [15 pts]. Consider a particle of mass m in a 3D attractive spherical potential well of depth V and radius a . Using the Klein-Gordon Eqn for S-states only (set the orbital ℓ momentum $\ell=0$), find the minimum well depth V_{KG} which just barely binds the particle. State your answer in terms of the well-known result from the Schrödinger Eqn, viz: $V_s = \pi^2 \hbar^2 / 8ma^2$. Interpret the difference between V_{KG} and V_s .

- ③ [15 pts]. A Schrödinger-type form for the free-particle Klein-Gordon Eqn can be manufactured as follows. Define a fcn ξ via: $(mc^2)\xi = i\hbar \partial\psi / \partial t$. Then the KG Eqn is: $\frac{1}{m} [\vec{p}^2 + (mc)^2] \psi = i\hbar \partial\xi / \partial t$. Next, define a two-component wavefunction by: $\Psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \psi + \xi \\ \psi - \xi \end{pmatrix}$. In these terms, show the KG Eqn can be written as:

$$i\hbar \partial\Psi / \partial t = \mathcal{H} \Psi, \quad \text{w/ } \mathcal{H} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \frac{\vec{p}^2}{2m}.$$

Notice that this "Hamiltonian" \mathcal{H} is not Hermitian. For nonrelativistic particles ($\vec{p}^2/2m \ll mc^2$), evidently ψ_+ is the solution for positive energy states $E \approx +mc^2$, while ψ_- is the solution for negative energy states $E \approx (-)mc^2$. Now show that the KG "probability density": $\rho = -(\hbar/mc^2) \text{Im}[\psi^* (\partial\psi / \partial t)]$, class notes p. fs 16, can be written as a charge density: $\tilde{\rho} = q\rho = q\{|\psi_+|^2 - |\psi_-|^2\}$. Then (+)ve energy solutions (ψ_+ dominant) have $\tilde{\rho} \doteq +q$, while (-)ve energy solutions (ψ_- dominant) have $\tilde{\rho} \doteq (-)q$. We will see that the Dirac Eqn has similar features.

(17) [15 pts]. KG Eqn under a gauge transform: invariance of S_μ , covariance of KG Eq.

(A) 1. The KG current for a mass m & charge q in an external EM potential A_μ has components
 $\rightarrow S_\mu = (\hbar/2im) [\psi^* (\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu) \psi - \text{C.C.}]$, (1)

as cited. Under a gauge transform by an arbitrary scalar fcn $\eta = \eta(x_\mu)$

$$\rightarrow A_\mu \rightarrow A'_\mu = A_\mu + (\partial\eta/\partial x_\mu), \quad \psi \rightarrow \psi' = \psi e^{i(q/\hbar c)\eta}, \quad (2)$$

we note that $\partial\psi/\partial x_\mu$ transforms as...

$$\frac{\partial}{\partial x_\mu} \psi \rightarrow \frac{\partial}{\partial x_\mu} \psi' = \frac{\partial}{\partial x_\mu} \psi e^{i(q/\hbar c)\eta} = e^{i(q/\hbar c)\eta} \left[\frac{\partial}{\partial x_\mu} + \frac{iq}{\hbar c} \left(\frac{\partial\eta}{\partial x_\mu} \right) \right] \psi \quad (3)$$

$$\begin{aligned} \xrightarrow{S_\mu} \psi^* \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu \right) \psi &\rightarrow \psi'^* \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A'_\mu \right) \psi' = \int \text{assume } \eta \text{ is a real fcn} \\ &= \underbrace{\left(\psi^* e^{-i(q/\hbar c)\eta} \right)}_{\text{product} \equiv 1} \underbrace{e^{i(q/\hbar c)\eta}}_{\text{cancel}} \left[\frac{\partial}{\partial x_\mu} + \frac{iq}{\hbar c} \left(\frac{\partial\eta}{\partial x_\mu} \right) - \frac{iq}{\hbar c} \left(A_\mu + \frac{\partial\eta}{\partial x_\mu} \right) \right] \psi \\ &= \psi^* \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu \right) \psi \leftarrow \text{this quantity is invariant under gauge transf.} \end{aligned} \quad (4)$$

From this, it is evident that S_μ of Eq. (1) is gauge invariant, since the C.C. transforms the same way: $S_\mu \rightarrow S'_\mu \equiv S_\mu$, under the gauge transform of Eq. (2).

2. To establish gauge covariance for the KG Eqn in A_μ , i.e. for

$$(B) \rightarrow \left[\left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu \right)^2 - k_0^2 \right] \psi = 0, \quad (5)$$

we need to show that the same form of the eqn holds when $(A_\mu, \psi) \rightarrow (A'_\mu, \psi')$ via Eq. (2). That is, we must show Eq. (5) also holds with A_μ replaced by A'_μ and ψ replaced by ψ' , w/o any additional terms.

3. We already know from Eq. (3) that...

$$\left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A'_\mu \right) \psi' = e^{i(q/\hbar c)\eta} \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu \right) \psi. \quad (6)$$

Applying the LHS operator a second time, we find...

$$\left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A'_\mu\right)^2 \psi' = \left[\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} \left(A_\mu + \frac{\partial \eta}{\partial x_\mu}\right)\right] \left\{ e^{i(q/\hbar c)\eta} \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu\right) \psi \right\}. \quad (7)$$

... the $\frac{\partial}{\partial x_\mu}$ here operates on each of the three factors in the $\{ \}$, so we get...

$$\begin{aligned} \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A'_\mu\right)^2 \psi' &= e^{i(q/\hbar c)\eta} \left[\frac{\partial}{\partial x_\mu} \left(\frac{iq}{\hbar c} \frac{\partial \eta}{\partial x_\mu} \right) \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu\right) \psi + \right. \\ &\quad \left. + e^{i(q/\hbar c)\eta} \frac{\partial}{\partial x_\mu} \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu\right) \psi - e^{i(q/\hbar c)\eta} \frac{iq}{\hbar c} \left(A_\mu + \frac{\partial \eta}{\partial x_\mu}\right) \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu\right) \psi \right] \end{aligned} \quad (8)$$

term ①
②
③
④

There is no need to perform the differentiation in term ②. Note that term ① is cancelled altogether by term ④. Then, by combining terms ② & ③, we have...

$$\left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A'_\mu\right)^2 \psi' = e^{i(q/\hbar c)\eta} \left[\left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu\right) \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu\right) \psi \right] = e^{i(q/\hbar c)\eta} \left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu\right)^2 \psi.$$

4. On the basis of Eq.(9), we can say the gauge-transformed LHS of Eq.(5) will look like... [note: $k_0^2 \psi' = e^{i(q/\hbar c)\eta} k_0^2 \psi$]... (9)

$$\left[\left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A'_\mu\right)^2 - k_0^2 \right] \psi' = e^{i(q/\hbar c)\eta} \underbrace{\left[\left(\frac{\partial}{\partial x_\mu} - \frac{iq}{\hbar c} A_\mu\right)^2 - k_0^2 \right]}_0 \psi = 0. \quad (10)$$

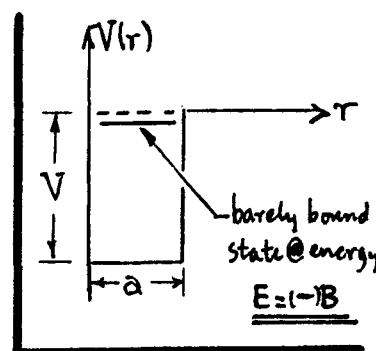
The indicated $[]\psi = 0$ because of (5), i.e. that is the original (untransformed) KG Eqn. So we have shown gauge covariance of the KG Eqn, i.e. if it is true that $[(\partial/\partial x_\mu - i(q/\hbar c)A_\mu)^2 - k_0^2]\psi = 0$, then also $[(\partial/\partial x_\mu - i(q/\hbar c)A'_\mu)^2 - k_0^2]\psi' = 0$.

- QED -

(18) [15 pts]. Particle in a 3D spherical well $[V, a]$: barely bound in a KG S-state.

1. The spherical potential well is ...

$$V(r) = \begin{cases} -V, \text{ const, for } 0 \leq r \leq a; \\ 0, \text{ for } r > a. \end{cases} \quad (1)$$



... and we seek a barely bound S-state ($l=0$) @ energy $E = (-)B \rightarrow 0$ near the top of the well. If the radial wavefn is written as $\psi(r) = \frac{1}{r} R(r)$, then the radial wave eqns are (for $l=0$)...

$$\left\{ \begin{array}{l} \text{SCHRÖDINGER : } \frac{d^2 R}{dr^2} + \frac{2m}{\hbar^2} [E - V(r)] R = 0, \\ \text{KLEIN-GORDON : } \frac{d^2 R}{dr^2} + \frac{2m}{\hbar^2} [E - V(r)] \left\{ 1 + \frac{E - V(r)}{2mc^2} \right\} R = 0. \end{array} \right. \quad (2)$$

Here E is the conventional eigen-energy of the problem (i.e. $E = \text{total energy} - mc^2$). The KG Eqn has the characteristic relativistic correction $(E - V)/2mc^2$ in the $\{ \}$, and in the limit $c \rightarrow \infty$, the KG Eqn reduces to the Schrödinger form.

2. We are looking for a bound state $\approx E = (-)B$, and in Eqs (2): $V(r) = -V$, @ $r \leq a$.

Then the eqns are of the form...

$$\underline{0 \leq r \leq a} : \underline{\frac{d^2 R}{dr^2} + \alpha^2 R = 0}, \quad \approx \alpha = \alpha_s = \left[\frac{2m}{\hbar^2} (V - B) \right]^{1/2}, \text{ for S. Eq. ;} \quad (3)$$

$$\alpha = \alpha_K = \left[\frac{2m}{\hbar^2} (V - B) \left\{ 1 + \frac{V - B}{2mc^2} \right\} \right]^{1/2}, \text{ for KG Eq.}$$

$$\underline{r \geq a} : \underline{\frac{d^2 R}{dr^2} - \beta^2 R = 0}, \quad \approx \beta = \beta_s = [2mB/\hbar^2]^{1/2}, \text{ for S. Eq. ;} \quad (4)$$

$$\beta = \beta_K = \left[\frac{2mB}{\hbar^2} \left\{ 1 - \frac{B}{2mc^2} \right\} \right]^{1/2}, \text{ for KG Eq.}$$

In both cases, the acceptable solutions ($\approx \psi$ finite @ $r=0$ and $\psi \rightarrow 0$ as $r \rightarrow \infty$) are

$$\rightarrow 0 \leq r \leq a : R(r) = A \sin \alpha r ; \quad r \geq a : R(r) = C e^{-\beta r}. \quad (5)$$

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A & C are consts in Eq. (5). We impose the condition that R & dR/dr be continuous at $r=a$... this gives a quantization condition on the energies B , as...

$$\rightarrow \lim_{r \rightarrow a^-} \left[\frac{1}{R} \left(\frac{dR}{dr} \right) \right] = \lim_{r \rightarrow a^+} \left[\frac{1}{R} \left(\frac{dR}{dr} \right) \right] \Rightarrow \boxed{\alpha \cot \alpha a = (-1) \beta}. \quad (6)$$

Solutions to this (transcendental) equation -- for the α & β assignments in Eqs. (3) & (4) -- will specify discrete values of the binding B in terms of well parameters.

3. For a barely bound particle, $B \rightarrow 0$, and in Eq. (6) $\beta \rightarrow 0$ for both the S.Eq. and KG Eq. [ref. Eq. (4)]. So we want...

$$\left\{ \begin{array}{l} \text{barely bound} \\ \text{state: } B \rightarrow 0 \end{array} \right\} \beta \rightarrow 0 \Rightarrow \alpha \cot \alpha a \rightarrow 0, \text{ and: } \underline{\underline{\alpha a \rightarrow \pi/2}}. \quad (7)$$

With the α -values in Eq. (2), this condition gives the minimum well depth V which will just barely bind the particle in an S -state. For the two cases...

$$\underline{\text{S.Eq.}}: \alpha_s a = \left[\frac{2m}{\hbar^2} (V_s - \overset{0}{\cancel{B}}) \right]^{1/2} a = \frac{\pi}{2} \Rightarrow \boxed{V_s = \pi^2 \hbar^2 / 8ma^2}. \quad (8)$$

$$\underline{\text{KG Eq.}}: \alpha_k a = \left[\frac{2m}{\hbar^2} (V_k - \overset{0}{\cancel{B}}) \left\{ 1 + \frac{V_k - \overset{0}{\cancel{B}}}{2mc^2} \right\} \right]^{1/2} = \frac{\pi}{2} \Rightarrow V_k \left\{ 1 + \frac{V_k}{2mc^2} \right\} = V_s$$

$$\text{or } \boxed{V_k = mc^2 \left\{ \left[1 + \frac{2V_s}{mc^2} \right]^{1/2} - 1 \right\} \stackrel{V_s \ll mc^2}{\approx} V_s \left[1 - \frac{1}{2} (V_s/mc^2) \right]}. \quad (9)$$

We see that the min. KG binding $V_k < V_s$ in the nonrelativistic limit. In fact $V_k < V_s$ at all finite values of mc^2 . In effect, relativistic effects reduce the Schrödinger value $V_s = \pi^2 \hbar^2 / 8ma^2$. A way to think about this is that V_s scales as $1/m$, so heavier particles are easier to bind (for a given size a). And, we know that a relativistic particle shows: $\vec{p} = m\vec{v} \rightarrow (m/\sqrt{1-(v/c)^2})\vec{v}$ for its momentum... in effect its mass increases: $m \rightarrow m/\sqrt{1-(v/c)^2}$. So, expect V_s decreases due to relativistic corrections, and thus $V_k < V_s$.

¶ The nonrelativistic approx is reasonable since $V_s \sim mc^2$ only if the well size $a \sim \hbar/mc$, the particle's Compton wavelength. Wells this small rarely occur in nature.

①⑨ [15pts]. KG Eqn: two-component formulation; identification of charge density.

1. The free-particle KG Eqn can be written as

$$\rightarrow c^2 [\vec{p}^2 + (mc)^2] \psi = (i\hbar \frac{\partial}{\partial t})^2 \psi, \quad \text{w/ } \vec{p} = -i\hbar \vec{\nabla}. \quad (1)$$

If we define a new fn ξ by: $(mc^2)\xi = i\hbar \partial\psi/\partial t$, then Eq. (1) becomes

$$\rightarrow \frac{1}{m} [\vec{p}^2 + (mc)^2] \psi = i\hbar \frac{\partial \xi}{\partial t}. \quad (2)$$

We have therefore split the 2nd order KG Eqn into two 1st order pieces, viz.

$$\rightarrow i\hbar \frac{\partial \psi}{\partial t} = (mc^2)\xi, \quad \text{and} \quad i\hbar \frac{\partial \xi}{\partial t} = (mc^2)\psi + (\vec{p}^2/m)\psi. \quad (3)$$

These can already be written in a Hamiltonian form, as...

$$\left\{ \begin{array}{l} \underline{\text{if}}: \Phi = \begin{pmatrix} \psi \\ \xi \end{pmatrix}, \quad \underline{\text{then}}: i\hbar \partial\Phi/\partial t = K\Phi, \\ \text{where: } K = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} mc^2 + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \frac{\vec{p}^2}{m}. \end{array} \right\} \quad (4)$$

K is not Hermitian, since $K^\dagger = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} mc^2 + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \frac{\vec{p}^2}{m} \neq K$.

2. We transform Φ in Eq. (4) to a new wavefn Ψ , as defined by...

$$\left\{ \begin{array}{l} \Psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \psi + \xi \\ \psi - \xi \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \psi \\ \xi \end{pmatrix}; \\ \text{i.e. } \Psi = U\Phi, \quad \text{with: } U = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \end{array} \right\} \quad (5)$$

It is easy to show that the inverse of U is

$$U^{-1} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \text{with: } U^{-1}U = UU^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (6)$$

We see that $U^{-1} = 2U^\dagger$, so U is quasi-unitary. In any case, with U in hand, we can easily transform Eq. (4) to the Ψ representation.

3. Multiply through Eq. (4) on the left by U . Then...

$$\begin{cases} i\hbar \frac{\partial}{\partial t} U\Phi = UK\Phi = (UKU^{-1})U\Phi, \\ \text{or } i\hbar \frac{\partial \Psi}{\partial t} = \mathcal{H}\Psi, \quad \Psi = U\Phi \quad \mathcal{H} = UKU^{-1}. \end{cases} \quad (7)$$

This is the desired Hamiltonian form for $\Psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$, with \mathcal{H} given by

$$\mathcal{H} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} mc^2 + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \frac{\vec{p}^2}{m} \right\} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$\text{or } \boxed{\mathcal{H} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \frac{\vec{p}^2}{2m}}, \text{ as required.} \quad (8)$$

Evidently \mathcal{H} is not Hermitian, since $\mathcal{H}^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \frac{\vec{p}^2}{2m} \neq \mathcal{H}$. When the Newtonian K.E. $\vec{p}^2/2m \ll mc^2$, however, the eigenvalues of \mathcal{H} are the (+)ve and (-)ve energy solutions $\pm mc^2$, with associated eigenfns ψ_\pm .

4. The main utility in this formulation of the KG Eqn is to provide a rational interpretation of the probability density $\rho = -(\hbar/mc^2) \text{Im}[\psi^*(\partial\psi/\partial t)]$. Multiply by the charge q of m (q could be (+)ve, or zero), so we are looking at...

$$\rightarrow \tilde{\rho} = -(q\hbar/mc^2) \text{Im}[\psi^*(\partial\psi/\partial t)]. \quad (9)$$

Our transform has been to: $\psi_\pm = \frac{1}{2}(\psi \pm \xi)$, so: $\psi = \psi_+ + \psi_-$, and: $\xi = \psi_+ - \psi_- = (i\hbar/mc^2) \partial\psi/\partial t$. The charge density in Eq. (9) is therefore...

$$\begin{aligned} \tilde{\rho} &= -\left(\frac{q\hbar}{mc^2}\right) \text{Im}[(\psi_+ + \psi_-)^* \frac{mc^2}{i\hbar} (\psi_+ - \psi_-)] = q \text{Im}[i(\psi_+^* + \psi_-^*)(\psi_+ - \psi_-)] \\ &= q \text{Im}\left[i \underbrace{(|\psi_+|^2 - |\psi_-|^2)}_{(1)} - i \underbrace{(\psi_+^* \psi_- - \psi_+ \psi_-^*)}_{(2)}\right] \end{aligned}$$

term (1) is pure real and contributes; term (2) is pure imaginary and does not contribute

i.e., $\boxed{\tilde{\rho} = q(|\psi_+|^2 - |\psi_-|^2)}, \text{ as required.} \quad (10)$

The (+)ve energy solutions (ψ_+ dominant) show $\tilde{\rho} = +q$; the (-)ve energy solutions have $\tilde{\rho} = (-)q$. These are interpreted in Dirac theory as particle-antiparticle modes.

* If \vec{p} is not an operator, eigenvalues of \mathcal{H} of Eq. are $\pm \sqrt{(mc^2)^2 + (\vec{p}c)^2}$.