Quantentheorie II Übung 4

– Sample solutions –

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2. **Gauge invariance and charge conjugation:**

(a) we assume $A'_\mu(x) = A_\mu(x) + \Lambda_\mu(x)$ when $\psi(x)$ transforms as $\psi'(x) = e^{-ie\alpha(x)}\psi(x)$. $A'(x)$ and $\psi'(x)$ should satisfy

$$(i\not\partial + e\not A'(x) - m)\psi'(x) = 0, \tag{1}$$

which becomes

$$\begin{aligned}
&(i\not\partial + e\not A(x) + e\not\Lambda(x) - m)e^{-ie\alpha(x)}\psi(x) \\
&= e(\not\partial\alpha(x))e^{-ie\alpha(x)}\psi(x) + ie^{-ie\alpha(x)}\not\partial\psi(x) + (e\not A(x) + e\not\Lambda - m)e^{-ie\alpha(x)}\psi(x) \\
&= e^{-ie\alpha(x)}\{(i\not\partial + e\not A(x) - m)\psi(x) + e(\not\partial\alpha(x) + \not\Lambda(x))\psi(x)\} \\
&= e^{-ie\alpha(x)}e(\not\partial\alpha(x) + \not\Lambda(x)) \Longleftarrow \text{(Dirac eq.: } (i\not\partial + e\not A(x) - m)\psi(x) = 0) \\
&= 0\,.
\end{aligned} \tag{2}$$

Therefore,

$$\Lambda_\mu(x) = -\partial_\mu\alpha(x)\,. \tag{3}$$

(b) The charge conjugation of ψ is defined as $\psi_c \equiv C\bar\psi^{\mathrm{T}}$, and it describes a particle with the same mass but the opposite charge. The Dirac equation of ψ_c is obtained by changing charge $q = -e \to q = +e$

$$(i\not\partial - e\not A(x) - m)\psi_c(x) = 0 \tag{4}$$

To determine the charge conjugation matrix C, we take the complex conjugation of the Dirac equation

$$\begin{aligned}
&[(i\not\partial + e\not A(x) - m)\psi(x)]^* \\
&= (-i\gamma^{\mu*}\partial_\mu = e\gamma^{\mu*}A_\mu(x) - m)\psi^*(x) \\
&= (-i\gamma^2\gamma^\mu\gamma^2\partial_\mu + e\gamma^2\gamma^\mu\gamma^2A_\mu(x) + m\gamma^2\gamma^2)\psi^* \Longleftarrow (\gamma^{\mu*} = \gamma^2\gamma^\mu\gamma^2\,, (\gamma^i)^2 = -\mathbb{1}_4) \\
&= (-i\gamma^2\gamma^\mu\gamma^2\partial_\mu + e\gamma^2\gamma^\mu\gamma^2A_\mu(x) + m\gamma^2\gamma^2)\gamma^0\bar\psi^{\mathrm{T}} \Longleftarrow (\bar\psi^{\mathrm{T}} = \gamma^0\psi^*) \\
&= \gamma^2(i\not\partial - e\not A(x) - m)\gamma^2\gamma^0\bar\psi^{\mathrm{T}} = 0\,.
\end{aligned} \tag{5}$$

By comparing Eqs. (4) and (5) we can determine

$$\begin{aligned}
&\psi_c \equiv C\bar\psi^{\mathrm{T}} = \gamma^2\gamma^0\bar\psi^{\mathrm{T}}, \\
\Longrightarrow\ & C = \gamma^2\gamma^0\,.
\end{aligned} \tag{6}$$

	a	b	c
K-G	$\hat{L}^2 - \alpha^2$	$2E_K\alpha$	$E_K^2 - M^2$
Schr.	$\hat{L}^2$	$2M\alpha$	$2ME_S$

Table 1: a, b and c are the coefficients of $-r^{-2}$, r^{-1} and r^0 respectively.

3. **Relativistic hydrogen atom (spinless):**

   (a) The Klein-Gordon equation is

$$(iD^\mu iD_\mu - M^2)\psi_K(\vec{r}) = 0\,, \tag{7}$$

where $iD^\mu = i\partial^\mu + eA^\mu$ and $A^0 = \Phi$(time independent), $\vec{A} = 0$. Eq. (7) can be written as

$$(\partial_t^2 - \nabla^2 - 2ie\Phi\partial_t - e^2\Phi^2 + M^2)\psi_K(\vec{r}) = 0\,. \tag{8}$$

After applying the Ansatz, $\psi_K = e^{-i\omega t}\phi_K$, to Eq. (8) we obtain

$$\begin{aligned}
&(\nabla^2 + 2\omega e\Phi + e^2\Phi^2 + \omega^2 - M^2)\phi_K(\vec{r}) \\
&= (\nabla^2 + 2E_K\frac{\alpha}{r} + \frac{\alpha^2}{r^2} + E_K^2 - M^2)\phi_K(\vec{r}) \Longleftarrow \left(e\Phi = \frac{\alpha}{r}\,, E_k = \omega\right) \\
&= (\partial_r^2 + \frac{2}{r}\partial_r - \frac{(\hat{L} - \alpha^2)}{r^2} + 2E_K\frac{\alpha}{r} + E_K^2 - M^2)\phi_K(\vec{r}) \Longleftarrow \left(\nabla^2 = \partial_r^2 + \frac{2}{r}\partial_r - \frac{\hat{L}^2}{r^2}\right) \\
&= 0\,.
\end{aligned} \tag{9}$$

The Schrödinger equation is

$$(\partial_r^2 + \frac{2}{r}\partial_r - \frac{\hat{L}^2}{r^2} + 2M\frac{\alpha}{r} + 2ME_S)\phi_S(\vec{r}) = 0\,. \tag{10}$$

The comparison of Eqs. (9) and (10) is summarized in Table 1. The energy eigenvalues of the Schrödinger equation is $E_S = E_n = -\frac{M\alpha^2}{2n^2}$, where n is a positive integer. The relation of a, b, and c of the Schrödinger equation is

$$\begin{aligned}
&\frac{c}{b} = \frac{E_n}{\alpha} = -\frac{M\alpha}{2n^2} = -\frac{b}{4n^2} \\
&\Longrightarrow c = -\frac{b^2}{4n^2}\,.
\end{aligned} \tag{11}$$

We assume that the coefficients of the Klein-Gordon equation also satisfy the relation in Eq. (11) when the positive integer n is replaced by a non-integer number $\tilde{n}$. Then we obtain

$$\begin{aligned}
&c = -\frac{b^2}{4\tilde{n}^2} \Longrightarrow E_K^2(\tilde{n}) - M^2 = -\frac{E_K^2(\tilde{n})\alpha^2}{\tilde{n}^2} \\
&\Longrightarrow E_K^2(\tilde{n}) = M^2\left(1 + \frac{\alpha^2}{\tilde{n}^2}\right)^{-1}.
\end{aligned} \tag{12}$$

Now we compare the coefficients of $-r^{-2}$ of both equations. From the Schrödinger equation we have $\hat{L} = l(l+1)$ for $l = 0, 1, 2, 3, \cdots$. In the Klein-Gordon equation we define

$$\hat{L}^2 - \alpha^2 \equiv \tilde{l}(\tilde{l}+1)\,, \tag{13}$$

where $\tilde{l}$ is a positive number. We separate the integer and non-integer parts of $\tilde{l}$ such as follows: $\tilde{l} = l + \delta$, for $l = 0, 1, 2, \cdots$ and δ = a positive non-integer. We know from the Schrödinger equation, $\hat{L} = l(l+1)$. We solve Eq. (13) to find $\tilde{l}$ in terms of l and α, which is small and therefore the expansion parameter.

$$\begin{aligned}
\tilde{l}(\tilde{l}+1) &= \hat{L}^2 - \alpha^2 \\
(l+\delta)(l+\delta+1) &= l(l+1) - \alpha^2 \Longleftarrow \; (\hat{L}^2 = l(l+1), \tilde{l} = l+\delta) \\
\therefore \delta_{\pm} &= -\left(l+\frac{1}{2}\right) \pm \sqrt{\left(l+\frac{1}{2}\right)^2 - \alpha^2}\,.
\end{aligned} \tag{14}$$

To obtain the energy eigenvalues in Eq. (12) $\tilde{n}$ should be determined. From the Schrödinger equation we have $n = l + m$, and correspondingly we set $\tilde{n} = \tilde{l} + n'$, and $n = l + n'$ where n' is an integer. After applying Eq. (14) we obtain

$$\begin{aligned}
\tilde{n}^2 &= (\tilde{l} + n')^2 \\
&= \left(-\frac{1}{2} + n' + \sqrt{\left(1+\frac{1}{2}\right)^2 - \alpha^2}\right)^2 \Longleftarrow \; (\tilde{l} = l + \delta_+) \\
&= \left(n - \left(l+\frac{1}{2}\right) + \sqrt{\left(1+\frac{1}{2}\right)^2 - \alpha^2}\right)^2 \Longleftarrow \; (n = l + n') \\
&= n^2 + n - \frac{\alpha^2}{l+\frac{1}{2}} + \mathcal{O}(\alpha^3)\,.
\end{aligned} \tag{15}$$

After combining Eqs. (12) and (15) we obtain the energy eigenvalues of the Klein-Gordon equation

$$\begin{aligned}
E_K(\tilde{n}) &= M\sqrt{\left(1+\frac{\alpha^2}{\tilde{n}^2}\right)^{-1}} \\
&\approx M\sqrt{1 - \frac{\alpha^2}{n^2} - \frac{\alpha^4}{n^3\left(l+\frac{1}{2}\right)} + \frac{\alpha^4}{n^4}} \Longleftarrow \; (\tilde{n}^2 \text{ in Eq. (15) and } \alpha\text{-expansion}) \\
&\approx M\left(n - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{8n^4} - \frac{\alpha^4}{2n^3\left(l+\frac{1}{2}\right)} + \frac{\alpha^4}{2n^4}\right), \\
&\qquad \Longleftarrow \; \left(\sqrt{1+ax+bx^2} = 1 + a\frac{x}{2} + \left(-\frac{a^2}{4} + b\right)\frac{x^2}{2} + \mathcal{O}(x^3)\right) \\
\therefore \quad E_K(\tilde{n}) &= M\left(1 - \frac{\alpha^2}{2n^2} + \alpha^4\left(\frac{3}{8n^4} - \frac{1}{2n^3\left(l+\frac{1}{2}\right)}\right)\right) + \mathcal{O}(\alpha^6)
\end{aligned} \tag{16}$$

4. **Dirac Hamiltonian in non relativistic limit:**

(a) The electric field is homogeneous and time-independent: $\vec{E} = \mathcal{E}\hat{z}$. After applying the Ansatz, $\psi_{\vec{k}}(\vec{x}) = \begin{pmatrix} u(\vec{k}) \\ v(\vec{k}) \end{pmatrix} e^{i\vec{k}\cdot\vec{x}}$ with $\vec{k} = (k_x, k_y, 0)$, $\vec{x} = (x, y, 0)$, the Dirac equation becomes

$$
\begin{aligned}
H_D\psi(\vec{x}) &= \left(\frac{\vec{p}^2}{2m} - \frac{\vec{p}^4}{8m^3} - \frac{2}{4m^2}\vec{E}\cdot(\vec{\sigma}\times\vec{p})\right)\psi(\vec{x}) \\
&= \left(\frac{\vec{k}^2}{2m} - \frac{\vec{k}^4}{8m^3} - \frac{e}{4m^2}\mathcal{E}\begin{pmatrix} 0 & k_y + ik_x \\ k_y - ik_x & 0 \end{pmatrix}\right)\psi(\vec{x}) \\
&\qquad \Longleftarrow\ \vec{p}^2\psi = \vec{k}^2\psi,\ \vec{E}\cdot(\vec{\sigma}\times\vec{p})\psi = \mathcal{E}(\sigma_x k_y - \sigma_y k_x)\psi \\
&= \begin{pmatrix} \epsilon_k & \lambda_k \\ \lambda_k^* & \epsilon_k \end{pmatrix}\begin{pmatrix} u(\vec{k}) \\ v(\vec{k}) \end{pmatrix} e^{-\vec{k}\cdot\vec{x}} \Longleftarrow\ \epsilon_k \equiv \frac{\vec{k}^2}{2m} - \frac{\vec{k}^4}{8m^3}, \\
&\qquad \lambda_k \equiv -\frac{e}{4m^2}\mathcal{E}(k_y + ik_x) \\
&= E_k\psi(\vec{x})
\end{aligned}
$$

$$
\Longrightarrow \text{ Eigenvalue equation: } \begin{pmatrix} \epsilon_k & \lambda_k \\ \lambda_k^* & \epsilon_k \end{pmatrix}\begin{pmatrix} u(\vec{k}) \\ v(\vec{k}) \end{pmatrix} = E_k\begin{pmatrix} u(\vec{k}) \\ v(\vec{k}) \end{pmatrix}
$$

Eigenvalues: $\begin{vmatrix} \epsilon_k - E_k & \lambda_k \\ \lambda_k^* & \epsilon_k - E_k \end{vmatrix} = 0$, $\therefore E_k = \epsilon_k \pm |\lambda_k|$,

Eigenvectors: $\epsilon_k u(\vec{k}) + \lambda v(\vec{k}) = (\epsilon_k \pm |\lambda_k|)u(\vec{k})$

$$
\therefore u(\vec{k}) = \pm\frac{\lambda_k}{|\lambda_k|}v(\vec{k}) = \mp i\,\mathrm{sign}(\mathcal{E})e^{-i\phi}v(\vec{k}) \Longleftarrow (\lambda_k = |\lambda_k|e^{-i\phi}) \tag{17}
$$

(b) $E_k^{\pm} = \frac{\vec{k}^2}{2m} \pm \frac{e}{4m^2}|\mathcal{E}||\vec{k}|$.

i. $k_x > 0$

$$
E_k^{\pm} = \frac{1}{2m}\left(k_x \pm \frac{2|\mathcal{E}|}{4m}\right)^2 - \frac{e^2|\mathcal{E}|^2}{8m^3}. \tag{18}
$$

ii. $k_x < 0$

$$
E_k^{\pm} = \frac{1}{2m}\left(k_x \mp \frac{2|\mathcal{E}|}{4m}\right)^2 - \frac{e^2|\mathcal{E}|^2}{8m^3}. \tag{19}
$$

(c) For $\vec{s} = \frac{\vec{\sigma}}{2}$, $\langle\vec{s}\rangle_{\pm} = \int_{\mathcal{A}} d^2r\psi^\dagger\left(\frac{\vec{\sigma}}{2}\right)\psi$: we consider 2-dimensional movements in the area of $\mathcal{A}$. Using Eq. (17) we set

$$
\psi_k^{\pm}(\vec{x}) = \begin{pmatrix} \mp i\,\mathrm{sign}(\mathcal{E})e^{-i\phi} \\ 1 \end{pmatrix} e^{-i\vec{k}\cdot\vec{r}} \quad \text{(Normalization ignored)}, \tag{20}
$$

$$
\begin{aligned}
\langle s_x \rangle_{\pm} &= \int_{\mathcal{A}} d^2r (\psi_k^{\pm})^{\dagger} s_x \psi_k^{\pm} \\
&= \int_{\mathcal{A}} d^2r (\pm i \ \mathrm{sign}(\mathcal{E}) e^{i\phi}, 1) \frac{1}{2} \sigma^1 \begin{pmatrix} \mp i \ \mathrm{sign}(\mathcal{E}) e^{-i\phi} \\ 1 \end{pmatrix} \\
&= \mp \mathcal{A} \ \mathrm{sign}(\mathcal{E}) \sin\phi = \mp \mathcal{A} \ \mathrm{sign}(\mathcal{E}) \frac{k_y}{|\vec{k}|} \,, \qquad (21)
\end{aligned}
$$

$$
\begin{aligned}
\langle s_y \rangle_{\pm} &= \int_{\mathcal{A}} d^2r (\psi_k^{\pm})^{\dagger} s_y \psi_k^{\pm} \\
&= \int_{\mathcal{A}} d^2r (\pm i \ \mathrm{sign}(\mathcal{E}) e^{i\phi}, 1) \frac{1}{2} \sigma^2 \begin{pmatrix} \mp i \ \mathrm{sign}(\mathcal{E}) e^{-i\phi} \\ 1 \end{pmatrix} \\
&= \pm \mathcal{A} \ \mathrm{sign}(\mathcal{E}) \cos\phi = \pm \mathcal{A} \ \mathrm{sign}(\mathcal{E}) \frac{k_x}{|\vec{k}|} \,, \qquad (22)
\end{aligned}
$$

$$
\begin{aligned}
\langle s_z \rangle_{\pm} &= \int_{\mathcal{A}} d^2r (\psi_k^{\pm})^{\dagger} s_z \psi_k^{\pm} \\
&= \int_{\mathcal{A}} d^2r (\pm i \ \mathrm{sign}(\mathcal{E}) e^{i\phi}, 1) \frac{1}{2} \sigma^3 \begin{pmatrix} \mp i \ \mathrm{sign}(\mathcal{E}) e^{-i\phi} \\ 1 \end{pmatrix} \\
&= \frac{\mathcal{A}}{2} (e^{i\phi} e^{-i\phi} - 1) = 0, \qquad (23)
\end{aligned}
$$

$$
\therefore \quad \langle \vec{s} \rangle_{\pm} = \pm \ \mathrm{sign}(\mathcal{E}) \mathcal{A} \left(\hat{e}_3 \times \frac{\vec{k}}{|\vec{k}|} \right) . \qquad (24)
$$