1. Gauge invariance and the Lorentz force

(a)

Schroedinger equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)^2\psi + q\phi\psi$$

Complex conjugate

$$\begin{aligned}
-\mathrm{i}\hbar\frac{\partial\psi^*}{\partial t} =& -\frac{\hbar^2}{2m}\left(\nabla + \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)^2\psi^* + q\phi\psi^*\\
\mathrm{i}\hbar\psi^*\frac{\partial\psi}{\partial t} =& -\psi^*\frac{\hbar^2}{2m}\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)^2\psi + q\phi\psi^*\psi\\
-\mathrm{i}\hbar\psi\frac{\partial\psi^*}{\partial t} =& -\frac{\hbar^2}{2m}\psi\left(\nabla + \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)^2\psi^* + q\phi\psi^*\psi\\
\mathrm{i}\hbar\frac{\partial\psi^*\psi}{\partial t} =& -\psi^*\frac{\hbar^2}{2m}\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)^2\psi + \frac{\hbar^2}{2m}\psi\left(\nabla + \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)^2\psi^*\\
=& -\frac{\hbar^2}{2m}\left(\nabla\left(\psi^*\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)\psi\right) - \left|\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)\psi\right|^2\right)\\
&+\frac{\hbar^2}{2m}\left(\nabla\left(\psi\left(\nabla + \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)\psi^*\right) - \left|\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)\psi\right|^2\right)\\
=&\frac{\hbar^2}{2m}\nabla\left(\psi\left(\nabla + \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)\psi^* - \psi^*\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)\psi\right)\\
\frac{\partial\rho}{\partial t} =&\frac{\hbar}{2m\mathrm{i}}\nabla\left(\psi\left(\nabla + \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)\psi^* - \psi^*\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)\psi\right)\\
=& -\nabla\cdot\vec{j}\\
0 =&\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j}
\end{aligned}$$

(b)

Under time reversal transformation

$$\begin{aligned}
&-\mathrm{i}\hbar\frac{\partial\psi^*}{\partial t} + \frac{\hbar^2}{2m}\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)^2\psi^* - q\phi\psi^*\\
=&\frac{\hbar^2}{2m}\left(\left(\nabla - \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)^2 - \left(\nabla + \frac{\mathrm{i}q}{\hbar c}\vec{A}\right)^2\right)\psi^*\\
\neq&0
\end{aligned}$$

(c)

Derivatives,

$$\begin{aligned}
\frac{\partial L}{\partial\dot{r}_i} =&m\dot{r}_i + \frac{q}{c}A_i\\
\frac{\partial L}{\partial r_i} =& -q\partial_i\phi + \frac{q}{c}\dot{r}_j\partial_i A_j
\end{aligned}$$

Euler-Lagrange equation

$$\begin{aligned}
0 =& m\ddot{r}_i + \frac{q}{c}\frac{\mathrm{d}A_i}{\mathrm{d}t} + q\partial_i\phi - \frac{q}{c}\dot{r}_j\partial_i A_j\\
m\ddot{r}_i =& -\frac{q}{c}\frac{\mathrm{d}A_i}{\mathrm{d}t} - q\partial_i\phi + \frac{q}{c}\dot{r}_j\partial_i A_j\\
=& -q\partial_i\phi - \frac{q}{c}\partial_t A_i - \frac{q}{c}\dot{r}_j\partial_j A_i + \frac{q}{c}\dot{r}_j\partial_i A_j\\
=& qE_i + \frac{q}{c}(\delta_{ln}\delta_{im} - \delta_{lm}\delta_{in})\dot{r}_l\partial_m A_n\\
=& qE_i + \frac{q}{c}\varepsilon_{ilj}\dot{r}_l\varepsilon_{jmn}\partial_m A_n\\
=& qE_i + \frac{q}{c}\varepsilon_{ilj}\dot{r}_l B_j\\
=& qE_i + \frac{q}{c}\left(\vec{v}\times\vec{B}\right)_i
\end{aligned}$$

2.

(a)

(b)

(c)

3.

(a)

Function to minimize

$$\begin{aligned}
E =& \int \mathrm{d}^3r\varphi^* H\varphi - \varepsilon\left(\int \mathrm{d}^3r\varphi^*\varphi - 1\right)\\
=& \int \mathrm{d}^3r(\alpha\psi_A + \beta\psi_B)\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r_{1A}} - \frac{e^2}{r_{1B}} + \frac{e^2}{R}\right)(\alpha\psi_A + \beta\psi_B)\\
& - \varepsilon\left(\int \mathrm{d}^3r(\alpha\psi_A + \beta\psi_B)^2 - 1\right)
\end{aligned}$$

Expanding derivative around the center of the wavefunctions

$$\begin{aligned}
E =& \alpha\int \mathrm{d}^3r(\alpha\psi_A + \beta\psi_B)\left(E_{1s} - \frac{e^2}{r_{1B}} + \frac{e^2}{R}\right)\psi_A\\
& + \beta\int \mathrm{d}^3r(\alpha\psi_A + \beta\psi_B)\left(E_{1s} - \frac{e^2}{r_{1A}} + \frac{e^2}{R}\right)\psi_B\\
& - \varepsilon\left(\int \mathrm{d}^3r(\alpha\psi_A + \beta\psi_B)^2 - 1\right)\\
=& \alpha^2\left(E_{1s} - e^2\int \mathrm{d}^3r\frac{\psi_A^2}{r_{1B}} + \frac{e^2}{R}\right) + \alpha\beta\left(E_{1s}S + \frac{e^2S}{R} - e^2\int \mathrm{d}^3r\frac{\psi_A\psi_B}{r_{1B}}\right)\\
& + \beta^2\left(E_{1s} - e^2\int \mathrm{d}^3r\frac{\psi_B^2}{r_{1A}} + \frac{e^2}{R}\right) + \alpha\beta\left(E_{1s}S + \frac{e^2S}{R} - e^2\int \mathrm{d}^3r\frac{\psi_A\psi_B}{r_{1A}}\right)\\
& - \varepsilon\big(\alpha^2 + 2\alpha\beta S + \beta^2 - 1\big)
\end{aligned}$$

Let $U_1 \equiv \int \mathrm{d}^3 r \frac{\psi_A^2}{r_{1B}} = \int \mathrm{d}^3 r \frac{\psi_B^2}{r_{1A}}$, $U_2 \equiv \int \mathrm{d}^3 r \frac{\psi_A \psi_B}{r_{1A}} = \int \mathrm{d}^3 r \frac{\psi_A \psi_B}{r_{1B}}$

$$
\begin{aligned}
E =&\left(\alpha^2 + \beta^2\right)\left(E_{1s} - e^2 U_1 + \frac{e^2}{R} - \varepsilon\right) + 2\alpha\beta\left(E_{1s} S + \frac{e^2 S}{R} - e^2 U_2 - \varepsilon S\right) - \varepsilon \\
=&-\left(\alpha^2 + \beta^2\right)\left(e^2 U_1 + \zeta\right) - 2\alpha\beta\left(e^2 U_2 + \zeta S\right) - \varepsilon
\end{aligned}
$$

To minimize E

$$
\begin{aligned}
0 =&\alpha^2 + 2\alpha\beta S + \beta^2 - 1 \\
0 =&\alpha\left(e^2 U_1 + \zeta\right) + \beta\left(e^2 U_2 + \zeta S\right) \\
0 =&\beta\left(e^2 U_1 + \zeta\right) + \alpha\left(e^2 U_2 + \zeta S\right)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
V_{AA} =&V_{BB} = e^2 U_1 \\
V_{AB} =&V_{BA} = e^2 U_2
\end{aligned}
$$

(b)

From normalization,

$$
\alpha = \frac{1}{\sqrt{2(1+S)}}
$$

Energy

$$
\begin{aligned}
\varepsilon =&2\alpha^2\left(E_{1s} - e^2 U_1 + \frac{e^2}{R}\right) + 2\alpha^2\left(E_{1s} S + \frac{e^2 S}{R} - e^2 U_2\right) \\
=&\frac{1}{1+S}\left(\left(E_{1s} + \frac{e^2}{R}\right)(1+S) - e^2 U_1 - e^2 U_2\right) \\
=&E_{1s} + \frac{e^2}{R} - \frac{e^2}{1 + (1 + \rho + \rho^2/3)\mathrm{e}^{-\rho}}\left(\frac{1}{R}\left(1 - (1+\rho)\mathrm{e}^{-2\rho}\right) + \frac{1}{a_0}(1+\rho)\mathrm{e}^{-\rho}\right) \\
f =&\frac{1 - 2\rho^2/3 + (1+\rho)\mathrm{e}^{-\rho}}{1 + (1 + \rho + \rho^2/3)\mathrm{e}^{-\rho}}\mathrm{e}^{-\rho}
\end{aligned}
$$

(c)

4.

(a)

(b)

(c)

(d)