1. Gauge invariance and the Lorentz force

(a)

Schroedinger equation

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

Complex conjugate

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

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

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

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

$$= -\frac{\hbar^2}{2m}\left(\nabla\left(\psi^*\left(\nabla - \frac{iq}{\hbar c}\vec{A}\right)\psi\right) - \left|\left(\nabla - \frac{iq}{\hbar c}\vec{A}\right)\psi\right|^2\right)$$

$$+ \frac{\hbar^2}{2m}\left(\nabla\left(\psi\left(\nabla + \frac{iq}{\hbar c}\vec{A}\right)\psi^*\right) - \left|\left(\nabla - \frac{iq}{\hbar c}\vec{A}\right)\psi\right|^2\right)$$

$$= \frac{\hbar^2}{2m}\nabla\left(\psi\left(\nabla + \frac{iq}{\hbar c}\vec{A}\right)\psi^* - \psi^*\left(\nabla - \frac{iq}{\hbar c}\vec{A}\right)\psi\right)$$

$$\frac{\partial \rho}{\partial t} = \frac{\hbar}{2mi}\nabla\left(\psi\left(\nabla + \frac{iq}{\hbar c}\vec{A}\right)\psi^* - \psi^*\left(\nabla - \frac{iq}{\hbar c}\vec{A}\right)\psi\right)$$

$$= -\nabla \cdot \vec{j}$$

$$0 = \frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j}$$

(b)

Under time reversal transformation

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

$$= \frac{\hbar^2}{2m}\left(\left(\nabla - \frac{iq}{\hbar c}\vec{A}\right)^2 - \left(\nabla + \frac{iq}{\hbar c}\vec{A}\right)^2\right)\psi^*$$

$$\neq 0$$

(c)

Derivatives,

$$\frac{\partial L}{\partial \dot{r}_i} = m\dot{r}_i + \frac{q}{c}A_i$$

$$\frac{\partial L}{\partial r_i} = -q\partial_i\phi + \frac{q}{c}\dot{r}_j\partial_i A_j$$

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

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

Expanding derivative around the center of the wavefunctions

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

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

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

To minimize E

$$0 = \alpha^2 + 2\alpha\beta S + \beta^2 - 1$$
$$0 = \alpha(e^2 U_1 + \zeta) + \beta(e^2 U_2 + \zeta S)$$
$$0 = \beta(e^2 U_1 + \zeta) + \alpha(e^2 U_2 + \zeta S)$$

Therefore,

$$V_{AA} = V_{BB} = e^2 U_1$$
$$V_{AB} = V_{BA} = e^2 U_2$$

(b)

From normalization,

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

Energy

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

(c)

Effective "force"

$$F = -\frac{\mathrm{d}\varepsilon}{\mathrm{d}R}$$
$$\frac{Fa_0^2}{e^2} = -\frac{\mathrm{d}}{\mathrm{d}\rho}\frac{f}{\rho}$$
$$= -\frac{\mathrm{d}}{\mathrm{d}\rho}\frac{(3 - 2\rho^2)\mathrm{e}^{-\rho} + (3 + 3\rho)\mathrm{e}^{-2\rho}}{3\rho + (3\rho + 3\rho^2 + \rho^3)\mathrm{e}^{-\rho}}$$
$$= \mathrm{e}^{-\rho}\frac{\left(3\rho + (3\rho + 3\rho^2 + \rho^3)\mathrm{e}^{-\rho}\right)\left((3 + 4\rho - 2\rho^2) + (3 + 6\rho)\mathrm{e}^{-\rho}\right)}{(3\rho + (3\rho + 3\rho^2 + \rho^3)\mathrm{e}^{-\rho})^2}$$
$$+ \mathrm{e}^{-\rho}\frac{\left((3 - 2\rho^2) + (3 + 3\rho)\mathrm{e}^{-\rho}\right)\left(3 + (3 + 3\rho - \rho^3)\mathrm{e}^{-\rho}\right)}{(3\rho + (3\rho + 3\rho^2 + \rho^3)\mathrm{e}^{-\rho})^2}$$

$$\frac{Fa_0^2}{e^2}e^\rho\big(3\rho + \big(3\rho + 3\rho^2 + \rho^3\big)e^{-\rho}\big)^2$$
$$=3\big(3 + 3\rho + 2\rho^2 - 2\rho^3\big) + \big(18 + 36\rho + 44\rho^2 - 2\rho^4\big)e^{-\rho} + 3\big(3 + 9\rho + 12\rho^2 + 6\rho^3 + \rho^4\big)e^{-2\rho}$$

4.

(a)

Eigenvalue equation

$$(\varepsilon - \lambda)^2 = t^2$$
$$\varepsilon - \lambda = \pm t$$
$$\lambda = \varepsilon \pm t$$

Eigenvectors $r_1|R\rangle + r_2|R'\rangle$

$$0 = (\varepsilon - \lambda)r_1 - tr_2$$
$$r_2 = \mp r_1$$

Normalized eigenvectors

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|R\rangle + \mp|R'\rangle)$$

(b)

(c)

(d)