

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

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

(b)

Under time reversal transformation

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

(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

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

2.

(a)

(b)

(c)

3.

(a)

Function to minimize

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

Expanding derivative around the center of the wavefunctions

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

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

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

To minimize E

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

Therefore,

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

(b)

(c)

4.

(a)

(b)

(c)

(d)