An example of gauge transformation

The non-relativistic Schrödinger equation of a charged particle interacting with electromagnetic field is

$$i\hbar\frac{\partial\psi(t,\mathbf{x})}{\partial t} = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\boldsymbol{\nabla} - q\mathbf{A}\right)^2 + qV\right]\psi(t,\mathbf{x}). \tag{1}$$

Apply the gauge transformation:

$$\begin{aligned} V \to V' &= V - \frac{\partial\chi(t,\mathbf{x})}{\partial t}, \\ \mathbf{A} \to \mathbf{A}' &= \mathbf{A} + \boldsymbol{\nabla}\chi(t,\mathbf{x}), \\ \psi(t,\mathbf{x}) \to \psi'(t,\mathbf{x}) &= \exp\left[\frac{iq}{\hbar}\chi(t,\mathbf{x})\right]\psi(t,\mathbf{x}). \end{aligned} \tag{2}$$

1. Expand the original equation:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi' &= \left[\frac{1}{2m}\left(\frac{\hbar}{i}\boldsymbol{\nabla} - q\mathbf{A}'\right)^2 + qV'\right]\psi' \\ &= -\frac{\hbar^2}{2m}\nabla^2\psi' + \frac{iq\hbar}{2m}\left[\boldsymbol{\nabla}\cdot(\mathbf{A}'\psi') + \mathbf{A}'\cdot\boldsymbol{\nabla}\psi'\right] + \left(\frac{q^2}{2m}\mathbf{A}'^2 + qV'\right)\psi' \\ &= \left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{iq\hbar}{2m}\left(\boldsymbol{\nabla}\cdot\mathbf{A}' + 2\mathbf{A}'\cdot\boldsymbol{\nabla}\right) + \frac{q^2}{2m}\mathbf{A}'^2 + qV'\right]\psi' \end{aligned} \tag{3}$$

2. Apply the gauge transformation on the electromagnetic field:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi' = \Bigg[&-\frac{\hbar^2}{2m}\nabla^2 + \frac{iq\hbar}{2m}\left(\boldsymbol{\nabla}\cdot\mathbf{A} + 2\mathbf{A}\cdot\boldsymbol{\nabla} + \nabla^2\chi + 2\boldsymbol{\nabla}\chi\cdot\boldsymbol{\nabla}\right) \\ &+ \frac{q^2}{2m}\left(\mathbf{A}^2 + 2\mathbf{A}\cdot\boldsymbol{\nabla}\chi + (\boldsymbol{\nabla}\chi)^2\right) + q\left(V - \frac{\partial}{\partial t}\chi\right)\Bigg]\psi'. \end{aligned} \tag{4}$$

3. Apply the gauge transformation on the wave function:

$$
\begin{aligned}
i\hbar\left(\frac{iq}{\hbar}\frac{\partial\chi}{\partial t}\psi+\frac{\partial}{\partial t}\psi\right) = &-\frac{iq\hbar}{2m}\left[\frac{iq}{\hbar}\psi(\boldsymbol{\nabla}\chi)^2+\boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\chi+\psi\nabla^2\chi\right] \\
&-\frac{\hbar^2}{2m}\left[\frac{iq}{\hbar}\boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\chi+\nabla^2\psi\right] \\
&+\frac{iq\hbar}{2m}\Big[(\boldsymbol{\nabla}\cdot\mathbf{A})\psi+\frac{2iq}{\hbar}\psi\mathbf{A}\cdot\boldsymbol{\nabla}\chi+2\mathbf{A}\cdot\boldsymbol{\nabla}\psi \\
&\qquad+\psi\nabla^2\chi+\frac{2iq}{\hbar}\psi(\boldsymbol{\nabla}\chi)^2+2\boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\chi\Big] \\
&+\frac{q^2}{2m}\left[\mathbf{A}^2\psi+2\psi\mathbf{A}\cdot\boldsymbol{\nabla}\chi+\psi(\boldsymbol{\nabla}\chi)^2\right] \\
&+qV\psi-q\frac{\partial\chi}{\partial t}\psi
\end{aligned}
\tag{5}
$$

$$\Downarrow$$

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi = &\left[-\frac{\hbar^2}{2m}\nabla^2+\frac{iq\hbar}{2m}\left(\boldsymbol{\nabla}\cdot\mathbf{A}+2\mathbf{A}\cdot\boldsymbol{\nabla}\right)+\frac{q^2}{2m}\mathbf{A}^2+qV\right]\psi \\
&+\frac{q^2}{2m}\psi(\boldsymbol{\nabla}\chi)^2-2\cdot\frac{q^2}{2m}\psi(\boldsymbol{\nabla}\chi)^2+\frac{q^2}{2m}\psi(\boldsymbol{\nabla}\chi)^2 \\
&-\frac{iq\hbar}{2m}\boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\chi-\frac{iq\hbar}{2m}\boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\chi+2\cdot\frac{iq\hbar}{2m}\boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\chi \\
&-\frac{iq\hbar}{2m}\psi\nabla^2\chi+\frac{iq\hbar}{2m}\psi\nabla^2\chi \\
&-\frac{q^2}{m}\psi\mathbf{A}\cdot\boldsymbol{\nabla}\chi+\frac{q^2}{m}\psi\mathbf{A}\cdot\boldsymbol{\nabla}\chi\,,
\end{aligned}
\tag{6}
$$

which finally becomes

$$
i\hbar\frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\nabla^2+\frac{iq\hbar}{2m}\left(\boldsymbol{\nabla}\cdot\mathbf{A}+2\mathbf{A}\cdot\boldsymbol{\nabla}\right)+\frac{q^2}{2m}\mathbf{A}^2+qV\right]\psi. \tag{7}
$$

This equation coincide with equation (3).