Interaction picture for a charged particle in electromagnetic field

The gauge freedom for scalar and vector potential is given by

$$\begin{aligned} \Phi' &\to \Phi - \partial_t \chi \\ \boldsymbol{A}' &\to \boldsymbol{A} - \boldsymbol{\nabla}\chi \end{aligned} \tag{1}$$

where $\chi = \chi(\boldsymbol{r}, t)$ is some scalar function. The Schröedinger Hamiltonian for a particle in an electromagnetic field is given by

$$H = \frac{1}{2m}\left[\boldsymbol{p} + e\boldsymbol{A}\right]^2 - e\Phi + V(\boldsymbol{r}) \tag{2}$$

We can utilize the gauge freedom by moving into an interaction picture with respect to $R \equiv e^{-ie\chi/\hbar}$. We have

$$H' = RHR^\dagger + i\hbar(\partial_t R)R^\dagger \tag{3}$$

The second term is simply

$$\begin{aligned} i\hbar(\partial_t R)R^\dagger &= i\hbar\partial_t\left(e^{-ie\chi/\hbar}\right)e^{ie\chi\hbar} \\ &= e\partial_t\chi \end{aligned} \tag{4}$$

Meanwhile,

$$e^{-ie\chi/\hbar}\left[-e\Phi + V(\boldsymbol{r})\right]e^{ie\chi/\hbar} = -e\Phi + V(\boldsymbol{r}) \tag{5}$$

so that

$$R\left[-e\Phi + V(\boldsymbol{r})\right]R^\dagger + i\hbar\left(\partial_t R\right)R^\dagger = -e\left(\Phi - \partial_t\chi\right) + V(\boldsymbol{r}) \equiv -e\Phi' + V(\boldsymbol{r}) \tag{6}$$

By using $\boldsymbol{p} = -i\hbar\boldsymbol{\nabla}$, we can write

$$\begin{aligned} \left[\boldsymbol{p} + e\boldsymbol{A}\right]^2 e^{ie\chi/\hbar}\psi &= \left[p^2 + e\boldsymbol{p}\cdot\boldsymbol{A} + e\boldsymbol{A}\cdot\boldsymbol{p} + e^2A^2\right]e^{ie\chi/\hbar}\psi \\ &= -\hbar^2\nabla^2\left(e^{ie\chi/\hbar}\psi\right) - ie\hbar\boldsymbol{\nabla}\cdot\left(\boldsymbol{A}e^{ie\chi/\hbar}\psi\right) - ie\hbar\boldsymbol{A}\cdot\boldsymbol{\nabla}\left(e^{ie\chi/\hbar}\psi\right) + e^2A^2e^{ie\chi/\hbar}\psi \end{aligned} \tag{7}$$

Now,

$$\begin{aligned} \boldsymbol{\nabla}\left(e^{ie\chi/\hbar}\psi\right) &= \psi\boldsymbol{\nabla}e^{ie\chi/\hbar} + e^{ie\chi/\hbar}\boldsymbol{\nabla}\psi \\ &= \frac{ie}{\hbar}e^{ie\chi/\hbar}\left(\boldsymbol{\nabla}\chi\right)\psi + e^{ie\chi/\hbar}\boldsymbol{\nabla}\psi \end{aligned} \tag{8}$$

which gives

$$\boldsymbol{A}\cdot\boldsymbol{\nabla}\left(e^{ie\chi/\hbar}\psi\right) = \frac{ie}{\hbar}e^{ie\chi/\hbar}\left(\boldsymbol{A}\cdot\boldsymbol{\nabla}\chi\right)\psi + e^{ie\chi/\hbar}\boldsymbol{A}\cdot\boldsymbol{\nabla}\psi \tag{9}$$

and

$$\begin{aligned} \nabla^2\left(e^{ie\chi/\hbar}\psi\right) &= \frac{ie}{\hbar}\boldsymbol{\nabla}\cdot\left(e^{ie\chi/\hbar}\psi\boldsymbol{\nabla}\chi\right) + \boldsymbol{\nabla}\cdot\left(e^{ie\chi/\hbar}\boldsymbol{\nabla}\psi\right) \\ &= \frac{ie}{\hbar}\left(\nabla^2\chi\right)e^{ie\chi/\hbar}\psi + \frac{ie}{\hbar}\left(\boldsymbol{\nabla}\chi\right)\cdot\boldsymbol{\nabla}\left(e^{ie\chi/\hbar}\psi\right) + e^{ie\chi/\hbar}\nabla^2\psi + \boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}e^{ie\chi/\hbar} \\ &= \frac{ie}{\hbar}\left(\nabla^2\chi\right)e^{ie\chi/\hbar}\psi - \frac{e^2}{\hbar^2}\left(\boldsymbol{\nabla}\chi\right)^2e^{ie\chi/\hbar}\psi + \frac{ie}{\hbar}e^{ie\chi/\hbar}\left(\boldsymbol{\nabla}\chi\right)\cdot\boldsymbol{\nabla}\psi + e^{ie\chi/\hbar}\nabla^2\psi + \frac{ie}{\hbar}e^{ie\chi/\hbar}\left(\boldsymbol{\nabla}\chi\right)\cdot\left(\boldsymbol{\nabla}\psi\right) \end{aligned} \tag{10}$$

Furthermore,

$$\begin{aligned} \boldsymbol{\nabla}\cdot\left(\boldsymbol{A}e^{ie\chi/\hbar}\psi\right) &= (\boldsymbol{\nabla}\cdot\boldsymbol{A})e^{ie\chi/\hbar}\psi + \boldsymbol{A}\cdot\boldsymbol{\nabla}\left(e^{ie\chi/\hbar}\psi\right) \\ &= (\boldsymbol{\nabla}\cdot\boldsymbol{A})e^{ie\chi/\hbar}\psi + \frac{ie}{\hbar}e^{ie\chi/\hbar}\left(\boldsymbol{A}\cdot\boldsymbol{\nabla}\chi\right)\psi + e^{ie\chi/\hbar}\boldsymbol{A}\cdot\boldsymbol{\nabla}\psi \end{aligned} \tag{11}$$

Substituting these back into (5) and multiplying by $e^{-ie\chi/\hbar}$, we find that

$$\begin{aligned} e^{-ie\chi/\hbar}\left[\boldsymbol{p} + e\boldsymbol{A}\right]^2 e^{ie\chi/\hbar}\psi = -\hbar^2 &\left[\frac{ie}{\hbar}\left(\nabla^2\chi\right)\psi - \frac{e^2}{\hbar^2}\left(\boldsymbol{\nabla}\chi\right)^2\psi + \frac{2ie}{\hbar}\left(\boldsymbol{\nabla}\chi\right)\cdot\boldsymbol{\nabla}\psi + \nabla^2\psi + \frac{ie}{\hbar}\left(\boldsymbol{\nabla}\chi\right)\cdot\boldsymbol{\nabla}\psi\right] \\ &- ie\hbar\left[(\boldsymbol{\nabla}\cdot\boldsymbol{A})\psi + \frac{ie}{\hbar}\left(\boldsymbol{A}\cdot\boldsymbol{\nabla}\chi\right)\psi + \boldsymbol{A}\cdot\boldsymbol{\nabla}\psi\right] \\ &- ie\hbar\left[\frac{ie}{\hbar}\left(\boldsymbol{A}\cdot\boldsymbol{\nabla}\chi\right)\psi + \boldsymbol{A}\cdot\boldsymbol{\nabla}\psi\right] \\ &+ e^2A^2\psi \end{aligned} \tag{12}$$

Notice all the terms containing χ. We can write

$$\begin{aligned}(\boldsymbol{p}\cdot e\boldsymbol{\nabla}\chi)\,\psi &= -ie\hbar\boldsymbol{\nabla}\cdot(\psi\boldsymbol{\nabla}\chi)\\ &= -ie\hbar\left(\nabla^2\chi\right)\psi - ie\hbar\boldsymbol{\nabla}\chi\cdot\boldsymbol{\nabla}\psi\end{aligned} \tag{13}$$

and

$$(e\boldsymbol{\nabla}\chi\cdot\boldsymbol{p})\,\psi = -ie\hbar\boldsymbol{\nabla}\chi\cdot\boldsymbol{\nabla}\psi \tag{14}$$

All that is left now is to collect terms and make the appropriate substitutions to find that

$$\begin{aligned}e^{-ie\chi/\hbar}\left[\boldsymbol{p}+e\boldsymbol{A}\right]^2 e^{ie\chi/\hbar}\psi &= \left\{-\hbar^2\nabla^2\psi\right\}\\ &\quad+\left\{\left[-ie\hbar\left(\boldsymbol{\nabla}\cdot\boldsymbol{A}\right)\psi - ie\hbar\boldsymbol{A}\cdot\boldsymbol{\nabla}\psi\right]+\left[-ie\hbar\left(\nabla^2\chi\right)\psi - ie\hbar\boldsymbol{\nabla}\chi\cdot\boldsymbol{\nabla}\psi\right]\right\}\\ &\quad+\left\{\left[-ie\hbar\boldsymbol{A}\cdot\boldsymbol{\nabla}\psi\right]+\left[-ie\hbar\boldsymbol{\nabla}\chi\cdot\boldsymbol{\nabla}\psi\right]\right\}\\ &\quad+\left\{\left[e^2A^2\psi\right]+\left[e^2\left(\boldsymbol{A}\cdot\boldsymbol{\nabla}\chi\right)\psi\right]+\left[e^2\left(\boldsymbol{A}\cdot\boldsymbol{\nabla}\chi\right)\psi\right]+\left[e^2\left(\boldsymbol{\nabla}\chi\right)^2\psi\right]\right\}\\ &\equiv p^2\psi+\left\{\boldsymbol{p}\cdot\left(\boldsymbol{e}\boldsymbol{A}\psi\right)+\boldsymbol{p}\cdot\left(\psi e\boldsymbol{\nabla}\chi\right)\right\}+\left\{e\left(\boldsymbol{A}\cdot\boldsymbol{p}\right)\psi+\left(e\boldsymbol{\nabla}\chi\cdot\boldsymbol{p}\right)\psi\right\}+\left\{e\left(\boldsymbol{A}+\boldsymbol{\nabla}\chi\right)\right\}^2\psi\\ &= p^2\psi+\left\{\boldsymbol{p}\cdot e\left(\boldsymbol{A}+\boldsymbol{\nabla}\chi\right)\right\}\psi+\left\{e\left(\boldsymbol{A}+\boldsymbol{\nabla}\chi\right)\cdot\boldsymbol{p}\right\}\psi+\left\{e\left(\boldsymbol{A}+\boldsymbol{\nabla}\chi\right)\right\}^2\psi\\ &\equiv\left[\boldsymbol{p}+e\boldsymbol{A}'\right]^2\psi\\ R\left[\boldsymbol{p}+e\boldsymbol{A}\right]^2R^\dagger &\equiv\left[\boldsymbol{p}+e\boldsymbol{A}'\right]^2\end{aligned} \tag{15}$$

Putting this result and (6) into (3), we finally obtain

$$H' = \frac{1}{2m}\left[\boldsymbol{p}+e\boldsymbol{A}'\right]^2 - e\Phi' + V\left(\boldsymbol{r}\right) \tag{16}$$