Derivation of the Gauge Invariant Schrödinger Equation in Magnetic Field

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1 Introduction

We want to now derive a gauge invariant form of the Schrödinger Equation for a particle in an electromagnetic field, which eradicates the gauge-dependent Ψ and $\mathbf{A}$ in favour of ρ, $\mathbf{J}$ and E.

We know that:

$$\rho \stackrel{\text{def}}{=} |\Psi|^2 = \Psi^*\Psi \tag{1}$$

$$\text{and } \mathbf{J} \stackrel{\text{def}}{=} \frac{1}{2m}\Psi^*\left(-\imath\hbar\nabla - \frac{e}{c}\mathbf{A}\right)\Psi + \frac{1}{2m}\Psi\left(\imath\hbar\nabla - \frac{e}{c}\mathbf{A}\right)\Psi^* \tag{2}$$

And we want to obtain the following gauge invariant version of the Schrödinger equation, dubbed the GISE:

$$\frac{\partial}{\partial t}\left(\frac{m\mathbf{J}}{\rho}\right) = \nabla\left[\frac{\hbar^2}{4m\rho}\nabla^2\rho - \frac{\hbar^2}{8m\rho^2}(\nabla\rho)^2 - \frac{m\mathbf{J}^2}{2\rho^2}\right] + e\mathbf{E} \tag{3}$$

There are 5 main steps in this procedure:

Section 2 Rewriting Ψ in terms of ρ and θ

Section 3 Replacing vector potential with electric field and scalar potential

Section 4 Inputting the Schrödinger equation, and rearranging both right hand side (Section 4.1) and the left hand side (Section 4.2)

Section 5 Refactoring back into $\mathbf{J}$

2 Rewriting Ψ in terms of ρ and θ

We can convert $\mathbf{J}$ into a more useful more using θ defined by:

$$\Psi = \sqrt{\rho}\,e^{\imath\theta} \tag{4}$$

Then $\mathbf{J}$ becomes:

$$
\begin{aligned}
\mathbf{J} &= \frac{1}{2m}\left[\Psi^*\left(-\imath\hbar\nabla\right)\Psi + \Psi\left(\imath\hbar\nabla\right)\Psi^*\right] - \frac{e}{mc}\rho\mathbf{A} && (5)\\
&= \frac{1}{2m}\left[\sqrt{\rho}e^{-\imath\theta}\left(-\imath\hbar\nabla\right)\sqrt{\rho}e^{\imath\theta} + \sqrt{\rho}e^{\imath\theta}\left(\imath\hbar\nabla\right)\sqrt{\rho}e^{-\imath\theta}\right] - \frac{e}{mc}\rho\mathbf{A} && (6)\\
&= \frac{\imath\hbar}{2m}\left[-\sqrt{\rho}e^{-\imath\theta}\nabla\left(\sqrt{\rho}e^{\imath\theta}\right) + \sqrt{\rho}e^{\imath\theta}\nabla\left(\sqrt{\rho}e^{-\imath\hbar}\right)\right] - \frac{e}{mc}\rho\mathbf{A} && (7)
\end{aligned}
$$

We can simply this by using the product rule:

$$
\begin{aligned}
\nabla\left(\sqrt{\rho}e^{\imath\theta}\right) &= \nabla\left(\sqrt{\rho}\right)e^{\imath\theta} + \sqrt{\rho}\nabla\left(e^{\imath\theta}\right) && (8)\\
&= \frac{\nabla\rho}{2\sqrt{\rho}}e^{\imath\theta} + \imath\nabla\theta\sqrt{\rho}e^{\imath\theta} && (9)\\
\text{and } \nabla\left(\sqrt{\rho}e^{-\imath\theta}\right) &= \nabla\left(\sqrt{\rho}\right)e^{-\imath\theta} + \sqrt{\rho}\nabla\left(e^{-\imath\theta}\right) && (10)\\
&= \frac{\nabla\rho}{2\sqrt{\rho}}e^{-\imath\theta} - \imath\nabla\theta\sqrt{\rho}e^{-\imath\theta} && (11)
\end{aligned}
$$

Thus $\mathbf{J}$ becomes:

$$
\begin{aligned}
\mathbf{J} = \frac{\imath\hbar}{2m}&\left[-\sqrt{\rho}e^{-\imath\theta}\left(\frac{\nabla\rho}{2\sqrt{\rho}}e^{\imath\theta} + \imath\nabla\theta\sqrt{\rho}e^{\imath\theta}\right)\right] + && (12)\\
\frac{\imath\hbar}{2m}&\left[\sqrt{\rho}e^{\imath\theta}\left(\frac{\nabla\rho}{2\sqrt{\rho}}e^{-\imath\theta} - \imath\nabla\theta\sqrt{\rho}e^{-\imath\theta}\right)\right] - \frac{e}{mc}\rho\mathbf{A} && (13)\\
= \frac{\imath\hbar}{2m}&\left[-\frac{\nabla\rho}{2} - \imath\rho\nabla\theta + \frac{\nabla\rho}{2} - \imath\rho\nabla\theta\right] - \frac{e}{mc}\rho\mathbf{A} && (14)\\
= \frac{\imath\hbar}{2m}&\left(-2\imath\rho\nabla\theta\right) - \frac{e}{mc}\rho\mathbf{A} && (15)\\
= \frac{\hbar}{m}&\rho\left(\nabla\theta - \frac{e}{\hbar c}\mathbf{A}\right) && (16)
\end{aligned}
$$

Now that we've got $\mathbf{J}$ in this useful form, we can calculate the LHS of the equation we want to derive, Equation 3:

$$
\begin{aligned}
\frac{\partial}{\partial t}\left(\frac{m\mathbf{J}}{\rho}\right) &= \frac{\partial}{\partial t}\left(\hbar\left[\nabla\theta - \frac{e}{\hbar c}\mathbf{A}\right]\right) && (17)\\
&= \hbar\frac{\partial}{\partial t}\left(\nabla\theta\right) - \frac{e}{c}\frac{\partial}{\partial t}\left(\mathbf{A}\right) && (18)
\end{aligned}
$$

As $\frac{\partial(\nabla f)}{\partial t} = \nabla\left(\frac{\partial f}{\partial t}\right)$ for well-behaved f, we can write this as:

$$
\frac{\partial}{\partial t}\left(\frac{m\mathbf{J}}{\rho}\right) = \hbar\nabla\dot{\theta} - \frac{e}{c}\dot{\mathbf{A}} \tag{19}
$$

Where $\dot{f} \stackrel{\text{def}}{=} \frac{\partial f}{\partial t}$.

3 Replacing vector potential with electric field and scalar potential

Now we can use the important equation for the electric field, $\mathbf{E}$, in terms of the vector potential, $\mathbf{A}$, and the scalar potential, ϕ:

$$\mathbf{E} = -\frac{1}{c}\dot{\mathbf{A}} - \nabla\phi \tag{20}$$

$$\Rightarrow \quad \dot{\mathbf{A}} = -c\mathbf{E} - c\nabla\phi \tag{21}$$

Our expression for the LHS of the GISE can then be written:

$$\frac{\partial}{\partial t}\left(\frac{m\mathbf{J}}{\rho}\right) = \hbar\nabla\dot{\theta} + e\mathbf{E} + e\nabla\phi \tag{22}$$

4 Inputting the Schrödinger equation

We now recognise that $\dot{\theta}$ can be given by the Schrödinger equation:

$$\imath\hbar\dot{\Psi} = \frac{1}{2m}\left(-\imath\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2\Psi + e\phi\Psi \tag{23}$$

But first we need to rearrange the Schrödinger equation into a form more useful to us, involving θ and ρ instead of Ψ.

To do this, we can start by expanding the round brackets:

$$\begin{aligned}\left(-\imath\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2\Psi &= \left(-\imath\hbar\nabla\right)^2\Psi + \frac{e^2}{c^2}A^2\Psi &(24)\\ &\quad + \left(\imath\hbar\nabla\right)\cdot\left(\frac{e}{c}\mathbf{A}\right)\Psi + \left(\frac{e}{c}\mathbf{A}\right)\cdot\left(\imath\hbar\nabla\right)\Psi &(25)\\ &= -\hbar^2\nabla^2\Psi + \frac{e^2}{c^2}A^2\Psi + \frac{\imath\hbar e}{c}\nabla\cdot\left(\mathbf{A}\Psi\right) + \frac{\imath\hbar e}{c}\mathbf{A}\cdot\nabla\Psi &(26)\\ &= -\hbar^2\nabla^2\Psi + \frac{e^2}{c^2}A^2\Psi + \frac{\imath\hbar e}{c}\left(\nabla\cdot\mathbf{A}\right)\Psi + \frac{2\imath\hbar e}{c}\mathbf{A}\cdot\nabla\Psi &(27)\end{aligned}$$

By choice of gauge, $\nabla\cdot\mathbf{A} = 0$, so:

$$\left(-\imath\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2\Psi = -\hbar^2\nabla^2\Psi + \frac{e^2}{c^2}A^2\Psi + \frac{2\imath\hbar e}{c}\mathbf{A}\cdot\nabla\Psi \tag{28}$$

4.1 Right Hand Side (RHS)

So now we can start replacing Ψ with $\sqrt{\rho}e^{\imath\theta}$ in parts:

$$
\begin{aligned}
\nabla\Psi &= \nabla\left(\sqrt{\rho}e^{\imath\theta}\right) && (29)\\
&= \nabla\left(\sqrt{\rho}\right)e^{\imath\theta} + \sqrt{\rho}\nabla\left(e^{\imath\theta}\right) && (30)\\
&= \frac{\nabla\rho}{2\sqrt{\rho}}e^{\imath\theta} + \imath\nabla\theta\sqrt{\rho}e^{\imath\theta} && (31)\\
&= \Psi\left(\frac{\nabla\rho}{2\rho} + \imath\nabla\theta\right) && (32)
\end{aligned}
$$

This means that:

$$
\begin{aligned}
\nabla^2\Psi &= \nabla\left[\Psi\left(\frac{\nabla\rho}{2\rho} + \imath\nabla\theta\right)\right] && (33)\\
&= \nabla\Psi\left(\frac{\nabla\rho}{2\rho} + \imath\nabla\theta\right) + \Psi\left(\nabla\left[\frac{\nabla\rho}{2\rho}\right] + \imath\nabla^2\theta\right) && (34)\\
&= \nabla\Psi\left(\frac{\nabla\rho}{2\rho} + \imath\nabla\theta\right) + \Psi\left(\frac{\nabla^2\rho}{2\rho} + \frac{\nabla\rho}{2}\nabla\left(\frac{1}{\rho}\right) + \imath\nabla^2\theta\right) && (35)\\
&= \nabla\Psi\left(\frac{\nabla\rho}{2\rho} + \imath\nabla\theta\right) + \Psi\left(\frac{\nabla^2\rho}{2\rho} - \frac{[\nabla\rho]^2}{2\rho^2} + \imath\nabla^2\theta\right) && (36)
\end{aligned}
$$

Using Equation 32, we can expand this first term:

$$
\begin{aligned}
\nabla\Psi\left(\frac{\nabla\rho}{2\rho} + \imath\nabla\theta\right) &= \Psi\left(\frac{\nabla\rho}{2\rho} + \imath\nabla\theta\right)^2 && (37)\\
&= \Psi\left(\frac{[\nabla\rho]^2}{4\rho^2} - [\nabla\theta]^2 + \imath\frac{\nabla\rho\cdot\nabla\theta}{\rho}\right) && (38)
\end{aligned}
$$

Thus, inputting Equation 38 into the equation for $\nabla^2\Psi$ gives:

$$
\nabla^2\Psi = \Psi\left[\frac{\nabla^2\rho}{2\rho} - \frac{(\nabla\rho)^2}{4\rho^2} - (\nabla\theta)^2 + \imath\nabla^2\theta + \imath\frac{\nabla\rho\cdot\nabla\theta}{\rho}\right] \qquad (39)
$$

Now that we have both $\nabla\Psi$ and $\nabla^2\Psi$, we know that the round bracket squared term in the Schrödinger equation is:

$$\left(-\imath\hbar\nabla-\frac{e}{c}\mathbf{A}\right)^2\Psi=-\hbar^2\Psi\left[\frac{\nabla^2\rho}{2\rho}-\frac{(\nabla\rho)^2}{4\rho^2}-(\nabla\theta)^2+\imath\nabla^2\theta+\imath\frac{\nabla\rho\cdot\nabla\theta}{\rho}\right]$$

$$+\frac{e^2}{c^2}A^2\Psi+\frac{2\imath\hbar e}{c}\mathbf{A}\cdot\left(\frac{\nabla\rho}{2\rho}+\imath\nabla\theta\right)\Psi \tag{40}$$

$$=\Psi\Bigg[-\hbar^2\frac{\nabla^2\rho}{2\rho}+\hbar^2\frac{(\nabla\rho)^2}{4\rho^2}+\hbar^2(\nabla\theta)^2-\imath\hbar^2\nabla^2\theta$$

$$-\imath\hbar^2\frac{\nabla\rho\cdot\nabla\theta}{\rho}+\frac{e^2}{c^2}A^2+\frac{\imath\hbar e}{c}\mathbf{A}\cdot\frac{\nabla\rho}{\rho} \tag{41}$$

$$-\frac{2\hbar e}{c}\mathbf{A}\cdot\nabla\theta\Bigg] \tag{42}$$

Then the full RHS of the Schrödinger equation is given by the monolithic expression:

$$\mathrm{RHS}=\Psi\Bigg[-\frac{\hbar^2}{2m}\frac{\nabla^2\rho}{2\rho}+\frac{\hbar^2}{2m}\frac{(\nabla\rho)^2}{4\rho^2}+\frac{\hbar^2}{2m}(\nabla\theta)^2-\imath\frac{\hbar^2}{2m}\nabla^2\theta$$

$$-\imath\frac{\hbar^2}{2m}\frac{\nabla\rho\cdot\nabla\theta}{\rho}+\frac{e^2}{2mc^2}A^2+\frac{\imath\hbar e}{2mc}\mathbf{A}\cdot\frac{\nabla\rho}{\rho} \tag{43}$$

$$-\frac{\hbar e}{mc}\mathbf{A}\cdot\nabla\theta+e\phi\Bigg]$$

4.2 Left Hand Side (LHS)

Now that we've sufficiently expanded out the RHS of the Schrödinger equation, let's look at the left hand side. By the same logic that $\nabla\Psi=\Psi\left(\frac{\nabla\rho}{2\rho}+\imath\nabla\theta\right)$:

$$\dot{\Psi}=\Psi\left(\frac{\dot{\rho}}{2\rho}+\imath\dot{\theta}\right) \tag{44}$$

Inputting this into the LHS of Schrödinger gives:

$$\imath\hbar\dot{\Psi}=\imath\hbar\Psi\left(\frac{\dot{\rho}}{2\rho}+\imath\dot{\theta}\right) \tag{45}$$

We can eliminate the $\dot{\rho}$ using the continuity equation:

$$\dot{\rho}+\nabla\cdot\mathbf{J}=0 \tag{46}$$

This gives for the LHS:

$$\imath\hbar\dot{\Psi}=\imath\hbar\Psi\left(-\frac{\nabla\cdot\mathbf{J}}{2\rho}+\imath\dot{\theta}\right) \tag{47}$$

We can simply the divergence of $\mathbf{J}$ using Equation 16:

$$
\begin{aligned}
\nabla \cdot \mathbf{J} &= \nabla \cdot \left[\frac{\hbar}{m} \rho \left(\nabla\theta - \frac{e}{\hbar c}\mathbf{A} \right) \right] && (48) \\
&= \frac{\hbar}{m} \left[\nabla\rho \cdot \left(\nabla\theta - \frac{e}{\hbar c}\mathbf{A} \right) + \rho \left(\nabla^2\theta - \frac{e}{\hbar c}\nabla \cdot \mathbf{A} \right) \right] && (49)
\end{aligned}
$$

Again by the choice of the Coulomb gauge, $\nabla \cdot \mathbf{A} = 0$, so:

$$
\begin{aligned}
\nabla \cdot \mathbf{J} &= \frac{\hbar}{m} \left[\nabla\rho \cdot \nabla\theta - \frac{e}{\hbar c}\mathbf{A} \cdot \nabla\rho + \rho\nabla^2\theta \right] && (50) \\
&= \frac{\hbar}{m} \nabla\rho \cdot \nabla\theta - \frac{e}{mc}\mathbf{A} \cdot \nabla\rho + \frac{\hbar}{m}\rho\nabla^2\theta && (51)
\end{aligned}
$$

So the LHS of the Schrödinger equation in full is:

$$
\begin{aligned}
\text{LHS} &= \imath\hbar\dot{\Psi} && (52) \\
&= \imath\hbar\Psi \left[-\frac{\hbar}{m}\frac{\nabla\rho \cdot \nabla\theta}{2\rho} + \frac{e}{mc}\mathbf{A} \cdot \frac{\nabla\rho}{2\rho} - \frac{\hbar}{2m}\nabla^2\theta + \imath\dot{\theta} \right] && (53) \\
&= \Psi \left[-\imath\frac{\hbar^2}{2m}\frac{\nabla\rho \cdot \nabla\theta}{\rho} + \imath\frac{\hbar e}{2mc}\mathbf{A} \cdot \frac{\nabla\rho}{\rho} - \imath\frac{\hbar^2}{2m}\nabla^2\theta - \hbar\dot{\theta} \right] && (54)
\end{aligned}
$$

4.3 Setting LHS and RHS equal to each other

As the title of this subsection suggests, what we do next is, not illogically, set both the LHS and the RHS of the rearranged and monolithic Schrödinger equation equal to each other. Here it is, but I'll warn you in advance that it's not pretty:

$$
\begin{aligned}
\text{LHS} &= \Psi \left[-\imath\frac{\hbar^2}{2m}\frac{\nabla\rho \cdot \nabla\theta}{\rho} + \imath\frac{\hbar e}{2mc}\mathbf{A} \cdot \frac{\nabla\rho}{\rho} - \imath\frac{\hbar^2}{2m}\nabla^2\theta - \hbar\dot{\theta} \right] && (55) \\
= \text{RHS} &= \Psi \Bigg[-\frac{\hbar^2}{2m}\frac{\nabla^2\rho}{2\rho} + \frac{\hbar^2}{2m}\frac{(\nabla\rho)^2}{4\rho^2} + \frac{\hbar^2}{2m}(\nabla\theta)^2 - \imath\frac{\hbar^2}{2m}\nabla^2\theta \\
&\qquad - \imath\frac{\hbar^2}{2m}\frac{\nabla\rho \cdot \nabla\theta}{\rho} + \frac{e^2}{2mc^2}A^2 + \imath\frac{\hbar e}{2mc}\mathbf{A} \cdot \frac{\nabla\rho}{\rho} && (56) \\
&\qquad - \frac{\hbar e}{mc}\mathbf{A} \cdot \nabla\theta + e\phi \Bigg]
\end{aligned}
$$

Immediately we can cancel the Ψ on both sides, as well as the $-\imath\frac{\hbar^2}{2m}\frac{\nabla\rho\cdot\nabla\theta}{\rho}$ terms, the $\imath\frac{\hbar e}{2mc}\mathbf{A} \cdot \frac{\nabla\rho}{\rho}$ terms and the $-\imath\frac{\hbar^2}{2m}\nabla^2\theta$ terms. This cuts the equation down somewhat to:

$$
\begin{aligned}
-\hbar\dot{\theta} = & -\frac{\hbar^2}{4m}\frac{\nabla^2\rho}{\rho} + \frac{\hbar^2}{8m}\frac{(\nabla\rho)^2}{\rho^2} + \frac{\hbar^2}{2m}(\nabla\theta)^2 + \frac{e^2}{2mc^2}A^2 \\
& - \frac{\hbar e}{mc}\mathbf{A}\cdot\nabla\theta + e\phi \qquad (57)
\end{aligned}
$$

$$
\hbar\dot{\theta} + e\phi = \frac{\hbar^2}{4m}\frac{\nabla^2\rho}{\rho} - \frac{\hbar^2}{8m}\frac{(\nabla\rho)^2}{\rho^2} - \frac{\hbar^2}{2m}(\nabla\theta)^2 - \frac{e^2}{2mc^2}A^2 + \frac{\hbar e}{mc}\mathbf{A}\cdot\nabla\theta \qquad (58)
$$

Taking the gradient of both sides of this equation gets us back to something that should look familiar from Section 3:

$$
\begin{aligned}
\hbar\nabla\dot{\theta} + e\nabla\phi = \nabla\Bigg[& \frac{\hbar^2}{4m}\frac{\nabla^2\rho}{\rho} - \frac{\hbar^2}{8m}\frac{(\nabla\rho)^2}{\rho^2} - \frac{\hbar^2}{2m}(\nabla\theta)^2 \\
& - \frac{e^2}{2mc^2}A^2 + \frac{\hbar e}{mc}\mathbf{A}\cdot\nabla\theta\Bigg] \qquad (59)
\end{aligned}
$$

We now substitute the left hand side of this into Equation 22 to get:

$$
\begin{aligned}
\frac{\partial}{\partial t}\left(\frac{m\mathbf{J}}{\rho}\right) &= \hbar\nabla\dot{\theta} + e\nabla\phi + e\mathbf{E} \qquad (60) \\
&= \nabla\Bigg[\frac{\hbar^2}{4m}\frac{\nabla^2\rho}{\rho} - \frac{\hbar^2}{8m}\frac{(\nabla\rho)^2}{\rho^2} - \frac{\hbar^2}{2m}(\nabla\theta)^2 \\
&\qquad - \frac{e^2}{2mc^2}A^2 + \frac{\hbar e}{mc}\mathbf{A}\cdot\nabla\theta\Bigg] + e\mathbf{E} \qquad (61)
\end{aligned}
$$

This is very close to the final gauge invariant form that we want, but we've still got the gauge variant $\mathbf{A}$ in there.

5 Refactoring back into J

We want to gather together our terms in θ and $\mathbf{A}$ into something gauge invariant, to eradicate all of this non-physicality in the equations. To do this, let's look at what $-\frac{m\mathbf{J}^2}{2\rho^2}$ expands out to:

$$
\begin{aligned}
-\frac{m\mathbf{J}}{2\rho^2} &= -\frac{\hbar^2}{2m}\left[\nabla\theta - \frac{e}{\hbar c}\mathbf{A}\right]^2 \qquad (62) \\
&= -\frac{\hbar^2}{2m}\left[(\nabla\theta)^2 + \frac{e^2}{\hbar^2 c^2}A^2 - \frac{2e}{\hbar c}\mathbf{A}\cdot\nabla\theta\right] \qquad (63) \\
&= -\frac{\hbar^2}{2m}(\nabla\theta)^2 - \frac{e^2}{2mc^2}A^2 + \frac{\hbar e}{mc}\mathbf{A}\cdot\nabla\theta \qquad (64)
\end{aligned}
$$

We now recognise this as the θ and $\mathbf{A}$ terms in Equation 61, allowing us to finally write out Schrödinger's equation in a gauge invariant form:

$$\frac{\partial}{\partial t}\left(\frac{m\mathbf{J}}{\rho}\right) = \nabla\left[\frac{\hbar^2}{4m\rho}\nabla^2\rho - \frac{\hbar^2}{8m\rho^2}\left(\nabla\rho\right)^2 - \frac{m\mathbf{J}^2}{2\rho^2}\right] + e\mathbf{E} \tag{65}$$

6 Conclusion

In conclusion, we've used but four key facts:

Definition of phase:

$$\Psi = \sqrt{\rho}e^{\imath\theta}$$

Definition of vector potential:

$$\mathbf{E} = -\frac{1}{c}\dot{\mathbf{A}} - \nabla\phi$$

Continuity equation:

$$\dot{\rho} + \nabla\cdot\mathbf{J} = 0$$

Schrödinger's equation:

$$\imath\hbar\dot{\Psi} = \frac{1}{2m}\left(-\imath\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2\Psi + e\phi\Psi$$

Using these, we've gone from the standard Schrödinger equation, which involves gauge dependent terms Ψ and $\mathbf{A}$, to a gauge invariant form, involving only the probability density ρ, the probability density $\mathbf{J}$ and the electric field, $\mathbf{E}$, all of which are gauge-independent observable quantities.

Note: The above calculations were all performed using CGS units. To do this in SI is a simple matter of replacing all $\frac{e}{c}\mathbf{A}$ with $e\mathbf{A}$. It doesn't actually matter in terms of the final answer you get, because all the factors of $\mathbf{A}$ cancel.