

Quantum Mechanics 3 - Class Exercise 3

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Cross Section and Scattering Amplitude

Below there is a brief description of the scattering experiment. Imagine a beam of free particles that is fired towards a fixed target. By analyzing the angular distribution of the scattered particles we can learn something about the target and how it interacts with the incoming particles. For example, large deflection angles may indicate a strong interaction.

A particular quantity of interest is the cross section σ , which has units of area. If the beam consists N particles and has area A , then the number of scattered particles, N_s , is given by

$$N_s = N \frac{\sigma}{A}. \quad (1)$$

So σ is a measure for how strong the interactions are. Often we don't have the luxury of covering the entire 4π solid angle with detectors (for example, we can't place a detector at the beam's source), and therefore the angular distribution of σ , that is the differential cross section $d\sigma/d\Omega$, is the measurable quantity.

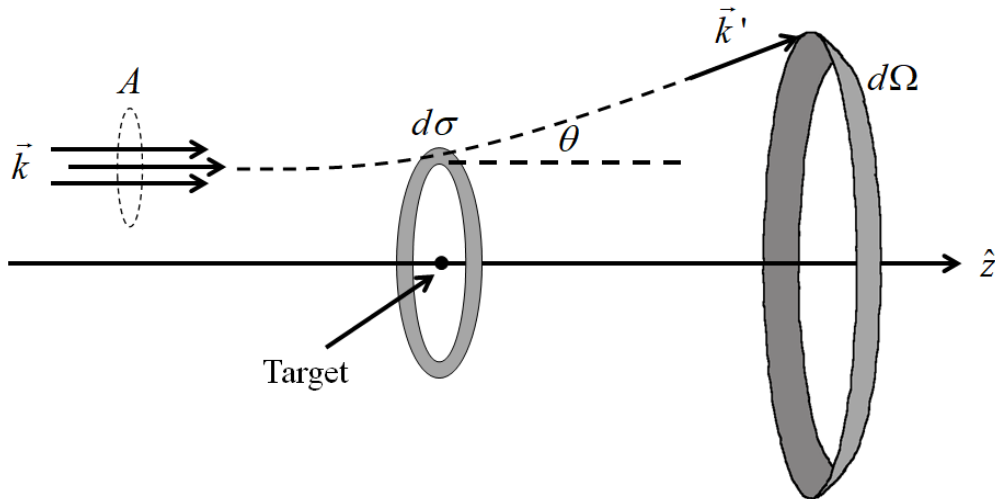


Figure 1: Sketch of the scattering experiment. A beam of particles with momentum $\hbar k \hat{z}$ and area A is fired towards a fixed target. The particles are then deflected by an angle θ and their final momentum is $\hbar \vec{k}'$. Particles that hit the target within the shaded area $d\sigma$ are scattered to a solid angle $d\Omega$.

If the beam is aligned with the z -axis and has momentum $\hbar k$, then you showed in class that the wave-function has the following structure:

$$\psi_k(\vec{r}) = \frac{1}{L^{3/2}} \left[e^{ikz} + f_k(\theta, \phi) \frac{e^{ikr}}{r} \right], \quad (2)$$

where $f_k(\theta, \phi)$ is the scattering amplitude, given by

$$f_k(\theta, \phi) = -\frac{mL^3}{2\pi\hbar^2} \langle \vec{k}' | \hat{V} | \psi_k \rangle = -\frac{mL^{3/2}}{2\pi\hbar^2} \int d^3r' e^{-i\vec{k}' \cdot \vec{r}'} V(\vec{r}') \psi_k(\vec{r}'), \quad (3)$$

where the second equality is under the assumption that the potential depends only on \vec{r} (and not on \vec{p} for instance). Here \vec{k}' is the wave-vector of the scattered particle. It has magnitude k (due to energy conservation) and it points to (θ, ϕ) . In class you proved the important connection

$$\frac{d\sigma}{d\Omega} = |f_k(\theta, \phi)|^2. \quad (4)$$

Thus, by measuring the differential cross section we can probe the potential $V(\vec{r})$.

In the *Born approximation* we approximate $\psi_k(\vec{r}')$ in the RHS of Eq. (3) to $e^{ikz'}/L^{3/2}$, which simplifies the expression for the scattering amplitude:

$$f_k(\theta, \phi) \approx -\frac{m}{2\pi\hbar^2} \int d^3r' e^{i\vec{q} \cdot \vec{r}'} V(\vec{r}') = -\frac{m}{2\pi\hbar^2} \tilde{V}(\vec{q}), \quad (5)$$

where $\vec{q} \equiv \vec{k} - \vec{k}'$ is the momentum transfer and $\tilde{V}(\vec{q})$ is the 3D Fourier transformation of the potential $V(r)$. In the special case of a spherical symmetric potential, we can write:

$$\begin{aligned} \tilde{V}(\vec{q}) &= \int d^3r' e^{i\vec{q}' \cdot \vec{r}'} V(r') = \int_0^\infty r'^2 dr' \int_{-1}^1 d(\cos\theta) \int_0^{2\pi} d\phi e^{iqr' \cos\theta} V(r') \\ &= 2\pi \int_0^\infty r'^2 \frac{e^{iqr'} - e^{-iqr'}}{iqr} V(r') dr' = \frac{4\pi}{q} \int_0^\infty r' \sin(qr') V(r') dr'. \end{aligned} \quad (6)$$

I highly recommend you to remember Eq. (6) instead of deriving it every time. Another useful quantity to remember is

$$q = |\vec{q}| = |\vec{k} - \vec{k}'| = \sqrt{k^2 + k'^2 - 2\vec{k} \cdot \vec{k}'} \underset{k'=k}{=} k\sqrt{2 - 2\cos\theta} = 2k \sin\left(\frac{\theta}{2}\right). \quad (7)$$

Question 1

Find the differential cross section in the Born approximation for the spin-dependent potential

$$V(r) = e^{-ar^2} [A + B\vec{\sigma} \cdot \vec{r}]. \quad (8)$$

Assume that the initial spin is $|\uparrow\rangle$ and sum over all final spins.

Solution

We need to calculate the scattering amplitude

$$f_{k,s,s'}(\theta, \phi) = -\frac{mL^3}{2\pi\hbar^2} \langle \vec{k}', s' | \hat{V} | \psi_{k,s} \rangle \approx -\frac{mL^3}{2\pi\hbar^2} \langle s' | \otimes \langle \vec{k}' | \hat{V} | \vec{k} \rangle \otimes | s \rangle = -\frac{m}{2\pi\hbar^2} \langle s' | \tilde{V}(\vec{q}) | s \rangle. \quad (9)$$

Let us denote $f(r) \equiv e^{-ar^2}$. Then the Fourier transformation of $V(\vec{r})$ is

$$\tilde{V}(\vec{q}) = [A + B\vec{\sigma} \cdot (-i\vec{\nabla}_q)] \tilde{f}(q). \quad (10)$$

It is convenient to calculate $\tilde{f}(q)$ in cartesian coordinates.

$$\tilde{f}(q) = \int d^3r' e^{i\vec{q} \cdot \vec{r}'} f(r') = \prod_{i=1,2,3} \int_{-\infty}^{\infty} dx'_i e^{iq_i x'_i - ax_i'^2} = \prod_{i=1,2,3} \sqrt{\frac{\pi}{a}} e^{-q_i^2/4a} = \left(\frac{\pi}{a}\right)^{3/2} e^{-q^2/4a}. \quad (11)$$

Thus,

$$\begin{aligned} \tilde{V}(\vec{q}) &= [A + B\vec{\sigma} \cdot (-i\vec{\nabla}_q)] \left(\frac{\pi}{a}\right)^{3/2} e^{-q^2/4a} = [A - B\vec{\sigma} \cdot \left(-i\frac{\vec{q}}{2a}\right)] \left(\frac{\pi}{a}\right)^{3/2} e^{-q^2/4a} \\ &= \left(\frac{\pi}{a}\right)^{3/2} e^{-q^2/4a} \begin{bmatrix} A + \frac{iB}{2a}q_z & \frac{iB}{2a}(q_x - iq_y) \\ \frac{iB}{2a}(q_x + iq_y) & A - \frac{iB}{2a}q_z \end{bmatrix}. \end{aligned} \quad (12)$$

We now have everything we need in order to evaluate $d\sigma_{s,s'}/d\Omega$, the differential cross section with initial spin s and final spin s' . Since we are given that $|s\rangle = |\uparrow\rangle$, and we are required to sum over all final spins, then

$$\frac{d\sigma}{d\Omega} = \sum_{s'} |f_{k,s,s'}(\theta, \phi)|^2 = \frac{m^2}{4\pi^2\hbar^4} \left[|\langle \uparrow | \tilde{V}(\vec{q}) | \uparrow \rangle|^2 + |\langle \downarrow | \tilde{V}(\vec{q}) | \uparrow \rangle|^2 \right], \quad (13)$$

which yields

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{\pi m^2}{4\hbar^4 a^3} e^{-q^2/2a} \left(A^2 + \frac{B^2}{4a^2} q^2 \right)}. \quad (14)$$

Question 2

The operator describing the interaction of a spin 1/2 particle with an external field has the form of

$$V(r) = V_0(r) + V_1(r) \vec{\sigma} \cdot \vec{L}, \quad (15)$$

where $\vec{L} = \vec{r} \times \vec{p}$ is the orbital angular momentum. Find the electron scattering amplitude between different spin-states, in the Coulomb field of a nucleus,

$$V_0(r) = \frac{Ze^2}{r}, \quad (16)$$

taking into account the spin-orbital interaction,

$$V_1(r) = \frac{\hbar}{4m^2c^2r} \frac{\partial V_0}{\partial r}. \quad (17)$$

Solution

Here in this problem the potential is a 2×2 matrix in spin-space, and therefore the scattering amplitude that we will consider is also a 2×2 matrix. We use the Born approximated expression for $f_k(\theta, \phi)$ as given by

$$f_k(\theta, \phi) \approx -\frac{mL^3}{2\pi\hbar^2} \langle \vec{k}' | \hat{V} | \vec{k} \rangle = f_0 + f_1. \quad (18)$$

The scattering amplitude has two pieces due to the two terms of $V(\vec{r})$. For

$$f_0 = -\frac{m}{2\pi\hbar^2} \tilde{V}_0(\vec{q}), \quad (19)$$

we can exploit the spherical symmetry and use Eq. (6).

$$\tilde{V}_0(\vec{q}) = \frac{4\pi}{q} \int_0^\infty r \sin(qr) V_0(r) dr = \frac{4\pi Ze^2}{q} \int_0^\infty \sin(qr) dr. \quad (20)$$

Sadly, this integral is not well-defined. However, we can use the Yukawa trick and add to the potential a multiplicative factor of $e^{-\mu r}$ and eventually take $\mu \rightarrow 0$. Now:

$$\begin{aligned} \tilde{V}_0(\vec{q}) &= \frac{4\pi Ze^2}{q} \int_0^\infty \sin(qr) e^{-\mu r} dr = \frac{4\pi Ze^2}{q} \text{Im} \left[\int_0^\infty e^{(iq-\mu)r} dr \right] \\ &= \frac{4\pi Ze^2}{q} \text{Im} \left[-\frac{1}{iq-\mu} \right] = \frac{4\pi Ze^2}{q} \frac{q}{q^2 + \mu^2} \xrightarrow{\mu \rightarrow 0} \frac{4\pi Ze^2}{q^2}. \end{aligned} \quad (21)$$

The second piece is more challenging since we can't use spherical symmetry (due to the \vec{L} term). Moreover, the potential depends on the particle's momentum as well. So we go back to the original definition of f_1 ,

$$\begin{aligned} f_1 &= -\frac{mL^3}{2\pi\hbar^2} \langle \vec{k}' | \hat{V}_1 \vec{\sigma} \cdot \hat{L} | \vec{k} \rangle = -\frac{mL^3}{2\pi\hbar^2} \vec{\sigma} \cdot \langle \vec{k}' | \hat{V}_1 (\hat{r} \times \hat{p}) | \vec{k} \rangle \stackrel{(1)}{=} -\frac{mL^3}{2\pi\hbar^2} \epsilon_{ijk} \sigma_i \langle \vec{k}' | \hat{V}_1 \hat{r}_j \hat{p}_k | \vec{k} \rangle \\ &\stackrel{(2)}{=} -\frac{mL^3}{2\pi\hbar} \epsilon_{ijk} \sigma_i k_k \langle \vec{k}' | \hat{V}_1 \hat{r}_j | \vec{k} \rangle = -\frac{m}{2\pi\hbar} \epsilon_{ijk} \sigma_i k_k \int d^3r e^{i\vec{q}\cdot\vec{r}} V_1(\vec{r}) r_j \\ &= -\frac{m}{2\pi\hbar} \epsilon_{ijk} \sigma_i k_k \left(-i \frac{\partial}{\partial q_j} \right) \tilde{V}_1(\vec{q}) = i \frac{m}{2\pi\hbar} \epsilon_{ijk} \sigma_i k_k \left(\frac{\partial q}{\partial q_j} \frac{\partial}{\partial q} \right) \tilde{V}_1(\vec{q}) \\ &\stackrel{(3)}{=} i \frac{m}{2\pi\hbar q} \epsilon_{ijk} \sigma_i q_j k_k \frac{\partial \tilde{V}_1(\vec{q})}{\partial q} = i \frac{m}{2\pi\hbar q} \vec{\sigma} \cdot (\vec{q} \times \vec{k}) \frac{\partial \tilde{V}_1(\vec{q})}{\partial q} \stackrel{(4)}{=} -i \frac{m}{2\pi\hbar q} \vec{\sigma} \cdot (\vec{k}' \times \vec{k}) \frac{\partial \tilde{V}_1(\vec{q})}{\partial q}, \end{aligned} \quad (22)$$

where in equality (1) I switched to index notation, in equality (2) I used $\hat{p}_k|\vec{k}\rangle = \hbar k_k|\vec{k}\rangle$, in equality (3) I used $\partial q/\partial q_j = q_j/q$, and in equality (4) I used $\vec{q} = \vec{k} - \vec{k}'$ and $\vec{k} \times \vec{k} = 0$.

If you lack of experience with index notation, the math we did in Eq. (22) may look intimidating. Below presented a brief introduction to this notation. Note that this notation is vastly used in advanced courses of general relativity and quantum field theory so it is very recommended that you master this notation at this stage.

Let us write explicitly the dot product of two vectors \vec{A} and \vec{B} :

$$\vec{A} \cdot \vec{B} = A_1 B_1 + A_2 B_2 + A_3 B_3 = \sum_{i=1}^3 A_i B_i \equiv A_i B_i, \quad (23)$$

where in the last step I omitted the \sum sign from the expression. This is called *Einstein summation convention*. It is very convenient notation, especially when you have many summations over many different indices and you don't want to write that annoying \sum sign for each summation. Within this convention, whenever you see a repeated index (i in the last example) this means that this index is summed up. For example, $A_i B_j$ means no summation (as there is no repeated index here) but $A_i B_j \delta_{ij} = A_i B_i$ does! Here there were two repeated indices (also called "dummy" indices): j (which the summation over it caused it to "turn" into i because of the Kronecker's delta δ_{ij}) and i . What happens if more than 2 dummy indices appear in the expression? Well, in this case this means that there is something wrong with your math — you should never end up with expressions that contain more than 2 dummy indices! Often students do this mistake because they forget to assign different letters to different terms. For example, I would write $(\vec{A} \cdot \vec{B})^2 = (\vec{A} \cdot \vec{B})(\vec{A} \cdot \vec{B}) = A_i B_i A_j B_j$ (and *not* $A_i B_i A_i B_i$).

An important indexed object you should be familiar with is the Levi-Civita symbol,

$$\epsilon_{ijk} = \begin{cases} +1 & ijk \text{ is an even permutation of } (123) \\ -1 & ijk \text{ is an odd permutation of } (123) \\ 0 & \text{otherwise} \end{cases}. \quad (24)$$

An even/odd permutation means that the permutation differs from the original order by an even/odd number of swaps of adjacent indices. Even permutations include (123), (231) and (312), while odd permutations include (213), (132) and (321). If two or more indices are the same (such as (122), (313) etc) then $\epsilon_{ijk} = 0$. The Levi-Civita symbol is important because it allows us to write cross product of the vectors \vec{A} and \vec{B} with index notation.

$$\vec{C} = \vec{A} \times \vec{B} \implies C_i = \epsilon_{ijk} A_j B_k. \quad (25)$$

A useful identity to remember that involves double Levi-Civita symbols is (try to explain to yourself why this is true!)

$$\epsilon_{ijk} \epsilon_{ilm} = \delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl}. \quad (26)$$

For example, you can easily prove to yourself that $\vec{A} \times (\vec{B} \times \vec{C}) = \vec{B}(\vec{A} \cdot \vec{C}) - \vec{C}(\vec{A} \cdot \vec{B})$ using the above identity.

Combining Eq. (18), (19), and (22), we get

$$f_k(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \left[\tilde{V}_0(\vec{q}) + i\hbar\vec{\sigma} \cdot (\vec{k}' \times \vec{k}) \frac{1}{q} \frac{\partial \tilde{V}_1(\vec{q})}{\partial q} \right]. \quad (27)$$

Next, we calculate

$$\tilde{V}_1(\vec{q}) = \frac{4\pi}{q} \int_0^\infty r \sin(qr) V_1(r) dr = \frac{4\pi\hbar}{qm^2c^2} \int_0^\infty \sin(qr) \frac{\partial V_0}{\partial r} dr = -\frac{4\pi\hbar}{m^2c^2} \int_0^\infty \cos(qr) V_0(r) dr, \quad (28)$$

where the last equality is due to integration by parts. We don't really need to calculate this integral (which actually diverges because $V_0(r) \xrightarrow{r \rightarrow 0} \infty$) but only its derivative with respect to q .

$$\frac{\partial \tilde{V}_1(\vec{q})}{\partial q} = \frac{4\pi\hbar}{m^2c^2} \int_0^\infty r \sin(qr) V_0(r) dr = \frac{\hbar q}{m^2c^2} \tilde{V}_0(\vec{q}), \quad (29)$$

where in the last step we identified $\tilde{V}_0(\vec{q})$ from Eq. (20). Plugging Eq. (29) in Eq. (27) yields

$$\boxed{f_k(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \tilde{V}_0(\vec{q}) \left(\hat{1} + i\hbar^2\vec{\sigma} \cdot \frac{\vec{k}' \times \vec{k}}{m^2c^2} \right) = f_0 \left(\hat{1} + i\hbar^2\vec{\sigma} \cdot \frac{\vec{k}' \times \vec{k}}{m^2c^2} \right)}. \quad (30)$$

Thus we see that the spin-orbit interaction adds a small correction to the scattering amplitude. If the deflection angle is small then $\vec{k}' \approx \vec{k}$ and the correction term vanishes. Even for a 90° deflection the numerator is proportional to $(\hbar k)^2 = p^2 = (mv)^2$ but the denominator is proportional to $(mc)^2$.

Question 3

In the Born approximation, obtain the scattering amplitude for the scattering of a particle with mass m and charge Q by a weak constant magnetic field $\vec{B}(\vec{r})$. Show that the result is gauge invariant.

Solution

The Hamiltonian for a charged particle in a magnetic field is

$$\hat{H} = \frac{\left(\hat{p} - \frac{Q}{c}\hat{A}\right)^2}{2m}, \quad (31)$$

where \vec{A} is the vector potential for the magnetic field (recall: $\vec{B} = \vec{\nabla} \times \vec{A}$).

Note: Where the Hamiltonian of Eq. (31) comes from? One of Hamilton's equations tell us that

$$v_i = \frac{dx_i}{dt} = \frac{\partial H}{\partial p_i} = \frac{p_i - \frac{Q}{c}A_i}{m} \implies p_i = mv_i + \frac{Q}{c}A_i. \quad (32)$$

The second Hamilton equation is

$$m \frac{dv_i}{dt} \stackrel{(1)}{=} \frac{dp_i}{dt} = -\frac{\partial H}{\partial x_i} = \frac{Q}{c} \frac{p_j - \frac{Q}{c}A_j}{m} \frac{\partial A_j}{\partial x_i} \stackrel{(2)}{=} \frac{Q}{c} v_j \frac{\partial A_j}{\partial x_i}, \quad (33)$$

where equalities (1),(2) holds because of Eq. (32) and the assumption of constant magnetic field (so the vector potential \vec{A} is constant in time).

Now we know that the RHS of Eq. (33) has to be $\frac{Q}{c}\vec{v} \times \vec{B}$ as this is the expression for Lorentz force with constant magnetic field. Therefore, let us calculate

$$\left(\vec{v} \times \vec{B}\right)_i = \epsilon_{ijk} v_j B_k \stackrel{(3)}{=} \epsilon_{ijk} v_j \epsilon_{klm} \partial_l A_m \stackrel{(4)}{=} v_j \partial_l A_m (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) = v_j \partial_i A_j - v_j \partial_j A_i \quad (34)$$

where in equality (3) we used the index notation form for $\vec{B} = \vec{\nabla} \times \vec{A}$ and in equality (4) we used Eq. (26). Notice that the last term in Eq. (34) vanishes because

$$v_j \partial_j A_i = \frac{dx_j}{dt} \frac{\partial A_i}{\partial x_j} = \frac{dA_i}{dt} = 0, \quad (35)$$

where the last equality is due to the assumption of constant magnetic field. Thus, we conclude

$$m \frac{d\vec{v}}{dt} = \frac{Q}{c} \vec{v} \times \vec{B}. \quad (36)$$

This is the exact equation of motion for a particle in constant magnetic field so the Hamiltonian of Eq. (31) must be right. I encourage you to do the same calculation for a time-dependent magnetic field (hint: remember that in that case there is also an induced electric field).

We can infer the potential from the Hamiltonian¹:

$$\hat{V} = -\frac{Q}{2mc} \left(\hat{A} \cdot \hat{p} + \hat{p} \cdot \hat{A} \right) + \mathcal{O}(\hat{A}^2). \quad (37)$$

In the remaining parts of the calculation we neglect the $\mathcal{O}(A^2)$ term under the assumption of weak magnetic field. In the Born approximation the scattering amplitude is given by

$$f_k(\theta, \phi) = -\frac{mL^3}{2\pi\hbar^2} \langle \vec{k}' | \hat{V} | \vec{k} \rangle = \frac{QL^3}{4\pi\hbar c} (\vec{k} + \vec{k}') \cdot \langle \vec{k}' | \hat{A} | \vec{k} \rangle, \quad (38)$$

where we used $\hat{p} | \vec{k} \rangle = \hbar \vec{k} | \vec{k} \rangle$. The object $\langle \vec{k}' | \hat{A} | \vec{k} \rangle$ is in fact

$$\begin{aligned} \langle \vec{k}' | \hat{A} | \vec{k} \rangle &= \int \int d^3r d^3r' \langle \vec{k}' | \vec{r}' \rangle \langle \vec{r}' | \hat{A} | \vec{r} \rangle \langle \vec{r} | \vec{k} \rangle = \frac{1}{L^3} \int \int d^3r d^3r' e^{i(\vec{k} \cdot \vec{r} - \vec{k}' \cdot \vec{r}')} \vec{A}(\vec{r}) \delta^3(\vec{r} - \vec{r}') \\ &= \frac{1}{L^3} \int d^3r e^{i\vec{q} \cdot \vec{r}} \vec{A}(\vec{r}) = \frac{1}{L^3} \vec{A}(\vec{q}), \end{aligned} \quad (39)$$

and therefore

$$\boxed{f_k(\theta, \phi) = \frac{Q}{4\pi\hbar c} (\vec{k} + \vec{k}') \cdot \vec{A}(\vec{q})}. \quad (40)$$

In order to see that this result is indeed gauge invariant we apply a gauge transformation on \vec{A} ,

$$\vec{A}(\vec{r}) \rightarrow \vec{A}'(\vec{r}) = \vec{A}(\vec{r}) + \vec{\nabla} f(\vec{r}), \quad (41)$$

where $f(\vec{r})$ is any arbitrary function. In Fourier space, this transformation corresponds to

$$\vec{A}(\vec{q}) \rightarrow \vec{A}'(\vec{q}) = \vec{A}(\vec{q}) + i\vec{q} \tilde{f}(\vec{q}), \quad (42)$$

and so the scattering amplitude transforms according to

$$f_k(\theta, \phi) \rightarrow f'_k(\theta, \phi) = f_k(\theta, \phi) + i\tilde{f}(\vec{q}) \frac{Q}{4\pi\hbar c} (\vec{k} + \vec{k}') \cdot \vec{q}, \quad (43)$$

but

$$(\vec{k} + \vec{k}') \cdot \vec{q} = (\vec{k} + \vec{k}') \cdot (\vec{k} - \vec{k}') = k^2 - k'^2 = 0, \quad (44)$$

where the last equality is due to energy conservation ($E' = E = \hbar^2 k^2 / 2m$). Thus, the scattering amplitude is indeed gauge invariant as it should be (since it is a measurable quantity).

¹Note that $\hat{A} \cdot \hat{p} \neq \hat{p} \cdot \hat{A}$ since \hat{A} and \hat{p} do not commute with each other!