Advanced Quantum Mechanics SS 2024

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Sheet 05: Collision theory in Born approximation (to be handed in by 03.07.2024)

1 Fourier Transform and Riemann-Lebesgue lemma

Consider the Fourier transform of an integrable function, f, in one dimension

$$\hat{f}(k) \equiv \int_{-\infty}^{\infty} dx \, f(x) \, e^{ikx},\tag{1}$$

than, the Riemann-Lebesgue lemma states that

$$\lim_{k \to \pm \infty} \hat{f}(k) = 0.$$
⁽²⁾

- 1. Give a qualitative explanation of the lemma.
- 2. Prove the lemma. *Hint*: use the shift $x \to x + \frac{\pi}{k}$.
- 3. Can you replace the integrable function f with something for which the lemma does not work?
- 4. Consider a function g(u) on the interval (-1, 1) and assume that the function and all its derivatives vanish at in $u = \pm 1$. This function has the properties we required for the detector acceptance function that we have seen in class, $g(\theta, \phi)$. Prove that, in the limit $k \to \pm \infty$, $\hat{g}(k) = \int_{-1}^{1} g(u) e^{iku}$ vanishes faster than $\frac{1}{k^n}$ for any integer n.

The Riemann-Lebesgue lemma can be generalised in more than one dimension.

1.1 Warm-up

Compute the Fourier transform and verify the lemma for the following functions

- a) $V_0 \theta(x-a)\theta(b-x)$
- b) $\theta(x)e^{-x}$
- c) $e^{-|x|}$
- d) e^{-x^2}

e) the ground state of Hydrogen, $\psi_{(1,0,0)}(\vec{x})$. Choose \vec{k} parallel to the quantization axis,

where θ is the Heaviside step function, that is: $\theta(x) = 0$ for x < 0 and $\theta(x) = 1$ for x > 0.

We have seen in class that the Born approximation of a scattering cross section requires the computation of Fourier transforms of scattering potential.



1.2 Three dimensional potentials

Compute the Fourier transform of the following interaction potentials in three dimension (here $r = |\vec{x}|$)

- a) potential well $V(\vec{x}) = -V_0 \theta(R-r)$
- b) a gaussian potential $V(\vec{x}) = V_0 e^{-r^2/a^2}$
- c) Yukawa potential $V_0 \frac{e^{-\mu r}}{r}$
- d) Obtain the transform of the Coulomb potential as a limit of the Yukawa case.

Very often we deal with spherically symmetric potential. As a last exercise, prove that the Fourier transform for a spherically symmetric function $f(\vec{x}) = f(r)$ can be written as

$$\frac{4\pi}{k} \int_0^\infty dr \, rf(r) \sin kr. \tag{3}$$

2 Elastic scattering off a potential well

Consider an incoming particle with mass m and momentum \vec{k} and a potential well

$$V(\vec{x}) = V_0 \,\theta(R - r). \tag{4}$$

- 1. Using the result from the previous exercise, compute the elastic scattering amplitude in Born approximation.
- 2. Show that, for small $kR \ll 1$, the scattering amplitude does not depend on the emission angle at leading order in kR. Compute also the first non trivial correction in power of kR. What can be said about the sign of the amplitude in this limit?
- 3. Suppose now kR is not small. What can be said now about the sign of the amplitude as a function of the scattering angle?

3 Elastic scattering off a Yukawa like potential, Rutherford formula and gaussian potential

Consider the same setup as in the previous excercise, but change our potential and consider a Yukawa potential of the form

$$V(\vec{x}) = V_0 b \, \frac{e^{-r/b}}{r}.$$
(5)

1. Compute the differential cross section, $d\sigma_y/d\Omega$, in Born approximation as a function of the scattering angle θ and of the potential parameters V_0 and b.

2. Replace

$$V_0 b \to \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0}$$

and take the limit $b \to 0$. You should recover the result for the differential cross section, $d\sigma_C/d\Omega$, for a charged light particle, with charge Z_1 , scattered off a heavy charged particle, with charge Z_2 , through a Coloumb potential. This result describes, for example, what happens when protons beams at low energy are elastically scattered by heavy nuclei (Rutherford diffusion).

Consider now a different potential again,

$$V_q(\vec{x}) = \hat{V}_0 e^{-r^2/a^2}.$$
(6)

- 3. Compute the differential cross section, $d\sigma_g/d\Omega$, in Born approximation as a function of the scattering angle θ and of the potential parameters V_0 and a.
- 4. Consider $d\sigma_y/d\Omega$ and $d\sigma_g/d\Omega$ and tune the parameters V_0 , \hat{V}_0 , b and a in such a way that the cross section and its first derivative in θ , are the same in the two cases in the forward limit $\theta = 0$. After the match, compare the two cross section for very low momentum and very high momentum. Can you give an explanation of the differences in the two regimes?

4 Photoelectric effect

In this exercise we compute the cross section for the inelastic process

$$\gamma + (\text{atom}) \longrightarrow (\text{atom})^+ + e^-$$
 (7)

known as photoelectric effect. The energy of the incoming photon is $E_{\gamma} = \hbar \omega$, $epsilon_{\lambda}$ its polarization vector, the binding energy of the electron to the atom is E_B and the mass of the electron is m. Assume the initial state of the electron can be described by the ground state wave function of an Hydrogen-like system, $\psi_{(1,0,0)}$, with atomic charge Z. Use, as final state for the electron, a free wave normalised in a box of side L.

- 1. Using Fermi golden rule, write down the general formula for the rate $\Gamma_{i \to f}$ of this process. Write explicitly the matrix element between initial and final state, $\langle f | V | i \rangle$ using minimal coupling to an external electromagnetic potential for the operator V. Do **not** apply dipole approximation.
- 2. Adding a proper flux term, compute the differential cross section for the process, $d\sigma/d\Omega$. Work in a regime in which $|E_B| \ll p_e^2/2m \ll mc^2$. Do not specify any polarization state for the photon at this stage. *Hint*: at some point you have compute the Fourier transform of the Hydrogen ground state. Use the results from one of the previous exercises. Also, observe that the final state is an eigenstate of the momentum operator, which should appear as $\vec{p} \cdot \vec{\epsilon}_{\lambda}$ in your expressions.
- 3. Suppose the photon is incoming with momentum along the quantization axis \hat{z} . Take as polarization states two vectors parallel to \hat{x} and \hat{y} , respectively. Average the cross section over the polarizations of the incoming photon and express it a function of the angle, θ , between the momentum of the electron and \hat{z} .

The correct result for the cross section is

$$\frac{d\sigma}{d\Omega} = 2\sqrt{2}Z^7 \alpha^8 \left(\frac{a_0}{Z}\right)^2 \left(\frac{p^2}{2m^2 c^2}\right)^{-7/2} \frac{(\sin\theta)^2}{(1 - v_e/c\,\cos\theta)^4},\tag{8}$$

where v_e is the velocity of the electron.

5 The total cross section and the Optical theorem

We have seen how to relate the elastic cross section for an incoming particle beam off a potential V through the formula

$$d\sigma(\theta,\phi) = |f(\vec{k},\vec{k}')|^2 \, d\Omega,\tag{9}$$

where \vec{k} is the momentum of the incoming particle, θ and ϕ parametrize direction of the scattered outgoing particle, which has momentum $\vec{k'}$, and f is called scattering amplitude. The scattering amplitude can be written as

$$f(\vec{k},\vec{k}') = -\frac{mL^3}{2\pi\hbar^2} \langle \vec{k}' | V | \psi^+ \rangle = -\frac{mL^3}{2\pi\hbar^2} \langle \vec{k}' | T | \vec{k} \rangle$$
(10)

where the operator T is defined through the relation $T|\vec{k}\rangle = V|\psi^+\rangle$ and the system is normalized in a box of side L. The Lippmann-Schwinger formalism gives us the following expression for T

$$T = V + V \frac{1}{E - H_0 + i\epsilon} V + \dots = V \sum_{n \ge 0} \left(\frac{1}{E - H_0 + i\epsilon} V \right)^n \tag{11}$$

Assume the potential is local $\langle \vec{x}|V|\vec{x}'\rangle = V(\vec{x})\delta(\vec{x}-\vec{x}')$. Finally, we also proved a useful relation that relates the imaginary part of the forward scattering amplitude to the total cross section, known as optical theorem. It reads,

$$\operatorname{Im} f(\vec{k}, \vec{k}) = \frac{k}{4\pi} \sigma_{tot}.$$
(12)

5.1 total cross section through direct integration in Born approximation

- 1. Write down the expression the scattering amplitude $f(\vec{k}, \vec{k}')$ at first order in the expansion of (11), that is $T \approx V$. Write also an expression for the differential cross section. This is called first order Born approximation.
- 2. Consider the averaged cross section $\langle \sigma_{tot} \rangle = \frac{1}{4\pi} \int d\Omega d\Omega' \frac{d\sigma}{d\Omega}$, where the integration $d\Omega$ refers to the final state solid angle, while $d\Omega'$ refers to the direction of the incoming beam. Prove that

$$\langle \sigma_{tot} \rangle = \frac{m^2}{4\pi\hbar^4} \int d_x^3 d^3 x' V(\vec{x}) V(\vec{x}') 4 \left(\frac{\sin(k \mid \vec{x} - \vec{x}' \mid)}{k \mid \vec{x} - \vec{x}' \mid} \right)^2 \tag{13}$$

3. Consider now an isotropic potential, $V(\vec{x}) = V(|\vec{x}|)$ and argue why the result from the previous point is now the exact total cross section (in Born approximation), $\langle \sigma_{tot} \rangle = \sigma_{tot}$.

5.2 total cross section through the optical theorem

In the second part of the exercise you need to prove the same result using optical theorem.

- 4. Argue why, for a symmetric potential $V(\vec{x}) = V(-\vec{x})$, the first order Born approximation is not a good enough approximation to use the optical theorem. In particular, prove the scattering amplitude is real, so that through the optical theorem the total cross section is zero.
- 5. Consider the second order Born approximation, that is keep the first correction in (11) and write down an expression for $f(\vec{k}, \vec{k}')$ at this order. Remember the definition and the expression for the advanced green function

$$G_{+}(\vec{x}, \vec{x}') = \langle \vec{x}' | \frac{1}{E - H_{0} + i\epsilon} | \vec{x} \rangle = -\frac{1}{4\pi} \frac{e^{ik|\vec{x} - \vec{x}'|}}{|\vec{x} - \vec{x}'|}.$$
 (14)

- 6. Compute $\text{Im}\langle f(\vec{k},\vec{k})\rangle = \frac{1}{4\pi} \int d\Omega \,\text{Im}f(\vec{k},\vec{k})$, averaging over the incoming beam direction. Assume isotropic potential and argue again why $\text{Im}\langle f(\vec{k},\vec{k})\rangle = \text{Im}f(\vec{k},\vec{k})$. Relate your result to the total cross section. You should get the same result as in the previous case.
- 7. Can you explain the different perturbative order that we had to consider in the two approaches to get the same result?

6 Appendix

The spherical harmonics, $Y_{l,m}(\theta, \phi)$, are defined in terms of the associated Legendre polynomials, P_l^m , as

$$Y_{l,m}(\theta,\phi) = C_{l,m} e^{im\phi} P_l^{(m)}(\cos\theta), \qquad (15)$$

where $C_{l,m}$ and P_l^m are real. For m = 0,

$$Y_{l,0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l^{(0)}(\cos\theta),$$
(16)

$$P_l^{(0)}(u) = (-1)^l \frac{1}{2^l l!} \left(\frac{d}{du}\right)^l (1-u^2)^l \tag{17}$$

In the case of the Hydrogen-like atom, the first radial functions are:

$$R_{10}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} \exp\left(-Zr/a_0\right),$$

$$R_{20}(r) = 2\left(\frac{Z}{2a_0}\right)^{3/2} \left(1 - \frac{Zr}{2a_0}\right) \exp\left(-Zr/2a_0\right),$$

$$R_{21}(r) = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{a_0} \exp\left(-Zr/2a_0\right).$$
(18)