Exam 2014: solutions

Section S18 ADVANCED QUANTUM MECHANICS

1. A non-relativistic quantum particle of mass m and wavenumber k is incident from the negative x direction on the one-dimensional potential well $U(x) \leq 0$, where $U(x) \to 0$ for $x \to \pm\infty$.

Find the Green's function of a Schrödinger operator for a free particle with $E < 0$ obeying the equation

$$\left(\hat{H} - E\right) G(x, x') = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} G(x, x') - E\, G(x, x') = \delta(x - x')$$

with the boundary condition $G(x, x') \to 0$ as $|x - x'| \to \infty$. [4]

Using the Greens's function $G(x, x')$, show that the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + U(x)\,\psi(x) = E\,\psi(x)$$

for a particle in a potential $U(x)$ with $E < 0$ and wavefunction asymptotics $\psi(x) \to 0$ for $x \to \pm\infty$, corresponding to the bound states in the potential $U(x)$, can be written as an integral equation

$$\psi(x) = -\frac{m}{\kappa\hbar^2}\int_{-\infty}^{\infty} \mathrm{e}^{-\kappa|x-x'|} U(x')\psi(x')\,\mathrm{d}x',$$

where $\kappa = \sqrt{-2mE}/\hbar$.

Using the integral equation, find the normalized wavefunction and the energy of the bound state in the potential $U(x) = -q\delta(x)$, where $q > 0$. [7]

Show that for a free particle with $E = \hbar^2 k^2/2m > 0$ the Green's functions of the Schrödinger operator are given by

$$G^{\pm}(x, x') = \pm\frac{\mathrm{i}m}{k\hbar^2}\mathrm{e}^{\pm \mathrm{i}k|x-x'|}.$$

Explain why there are *two* Green's functions for $E > 0$, G^+ and G^-. [4]

Show that the wavefunction of a particle of mass m and wavenumber k incident from the negative x direction on the one-dimensional potential well $U(x)$ obeys the integral equation

$$\psi(x) = \mathrm{e}^{\mathrm{i}kx} - \int_{-\infty}^{\infty} G^+(x, x')\,U(x')\,\psi(x')\,\mathrm{d}x'.$$

Using this integral equation, find the transmission and reflection amplitudes $S(k)$ and $A(k)$, and the corresponding transmission and reflection probabilities $T(k)$ and $R(k)$, for the potential $U(x) = -q\delta(x)$, $q > 0$. Show that $T + R = 1$.

Find the poles (singularities) of the transmission amplitude $S(k)$ in the complex k-plane and show that they correspond to the bound state energies in the same potential. [10]

2. In the (first) Born approximation, the scattering amplitude for particles with energy $E = \hbar^2 k^2/2m$ is given by

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2} \int_0^\infty \frac{r' \sin qr'}{q} U(r')\,\mathrm{d}r',$$

where $q = 2k\sin(\theta/2)$ and θ is the scattering angle.

Show that the first Born approximation violates the Optical Theorem. Does this make the theory invalid? Explain.

Show that in the first Born approximation the total cross section $\sigma(E)$ in a generic central potential $U(r)$ obeys the inequality

$$\frac{\mathrm{d}}{\mathrm{d}E}[E\sigma(E)] \geq 0,$$

i.e. that the function $E\sigma(E)$ is a monotonically increasing function of energy in this approximation. [Hint: use $q = 2k\sin(\theta/2)$ as the integration variable.] [8]

In the first Born approximation compute the differential cross-section $\mathrm{d}\sigma/\mathrm{d}\Omega$ in the case of the Yukawa potential

$$U(r) = \frac{U_0 \mathrm{e}^{-\mu r}}{r}.$$

Show that in the limit $\mu \to 0$ with $U_0 = Z_1 Z_2 e^2$ and $\vec{p} = \hbar\vec{k}$, the cross section reduces to the classical Rutherford scattering cross-section. [6]

Show that the scattering length a_0 in the potential

$$U(r) = \begin{cases} -U_0, & r \leq L, \\ 0, & r > L \end{cases}$$

is given by

$$a_0 = L\left(1 - \frac{\tan\xi_0}{\xi_0}\right),$$

where $\xi_0^2 = 2mU_0L^2/\hbar^2$. [6]

Compute the total cross-section σ at zero energy. Explain what happens at $\xi_0 = \pi(n + 1/2)$, $n = 0, 1, \ldots$. [5]

3. A spinless relativistic particle of mass m and charge $e > 0$ in an external electromagnetic field Φ obeys the Klein–Gordon equation

$$\left[-\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - e\Phi\right)^2 - \hbar^2 c^2 \Delta + m^2 c^4\right]\psi = 0.$$

Consider a one-dimensional scattering problem for such a particle incident from the left on the potential of the form

$$\Phi(x) = \begin{cases} 0 & x < 0, \\ V_0 & x > 0. \end{cases}$$

Define the charge density ρ_e and the current density $\mathbf{j}_e = (j_e, 0, 0)$ by

$$\rho_e = \frac{\mathrm{i}e\hbar}{2mc^2}\left[\psi^*\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^*}{\partial t}\right] - \frac{e^2\Phi}{mc^2}|\psi|^2, \qquad j_e = \frac{e\hbar}{2m\mathrm{i}}\left[\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right].$$

Show that the Klein–Gordon equation implies that $\partial\rho_e/\partial t + \operatorname{div}\mathbf{j}_e = 0$. [2]

Show that the wavefunction $\psi(t, x) = \mathrm{e}^{-\mathrm{i}\varepsilon t/\hbar}u(x)$, where

$$u(x) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + A\mathrm{e}^{-\mathrm{i}kx} & x < 0, \\ S\mathrm{e}^{\mathrm{i}k'x} & x > 0 \end{cases}$$

is a solution of the Klein–Gordon equation. Find k^2 and k'^2 in terms of ε, m, eV_0. Consider k'^2 as a function of the potential strength V_0. Identify the three regions with definite sign of k'^2 and compute the group velocity of waves $v = \partial\varepsilon/\partial p$, where $p = \hbar k'$, for each of the three regions.

Show that in the region $eV_0 < \varepsilon - mc^2$ the charge density is positive for a particle of any mass, whereas in the region $eV_0 > \varepsilon + mc^2$ the charge density is negative. What is the charge density in the region $\varepsilon - mc^2 < eV_0 < \varepsilon + mc^2$?

For $k'^2 > 0$, compute the current densities for the incident, reflected and transmitted waves. By requiring that the group velocity is positive for $x > 0$, determine the sign of k' for $eV_0 < \varepsilon - mc^2$ and for $eV_0 > \varepsilon + mc^2$. [11]

Show that the reflection and transmission coefficients are given, correspondingly, by $R = |A|^2$, $T = (k'/k)|S|^2$. Use the Klein–Gordon equation to determine the continuity properties of the wavefunction and its first derivative at $x = 0$. Using the continuity properties, find the amplitudes A and S for $k'^2 > 0$ and show that the reflection and transmission coefficients are given by

$$R = \frac{(k - k')^2}{(k + k')^2}, \qquad T = \frac{4k^2}{(k + k')^2}\frac{k'}{k}.$$

[6]

Show that for $\varepsilon - mc^2 < eV_0 < \varepsilon + mc^2$ (i.e. for $k'^2 < 0$) $T = 0$ and $R = 1$ (total reflection). Show that for a weak potential $eV_0 < \varepsilon - mc^2$ one finds $0 < T < 1$ and $0 < R < 1$, $R + T = 1$, whereas for a strong potential $eV_0 > \varepsilon + mc^2$, surprisingly, $T < 0$ and $R > 1$. Explain this result. [6]

S18 Advanced Quantum Mechanics
2014
Solutions

Problem 1

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}G(x,x') - E\,G(x,x') = \delta(x-x')$$

$G(x,x') \to 0$ for $|x-x'| \to \infty$

$E < 0$

1 a) Solution for $x < x'$:

$$G(x,x') = A(x')\,e^{\varkappa(x-x')} + B(x')\,e^{-\varkappa(x-x')}$$

$\varkappa = \sqrt{2m|E|}/\hbar \quad > 0$

$x - x' \to -\infty$: should have $G \to 0$

$\Rightarrow B(x') = 0$

1 b) Solution for $x > x'$:

$$G(x,x') = C(x')\,e^{-\varkappa(x-x')}$$

c) At $x = x'$: G is contin. but G' is not ($\Rightarrow$ δ-function)

$\Rightarrow$ integrating the eq. from $x'-\varepsilon$ to $x'+\varepsilon$ get

$$\begin{cases} G'(x=x'+\varepsilon, x') - G'(x=x'-\varepsilon, x') = -\dfrac{2m}{\hbar^2} \\ G(x=x'+\varepsilon, x') = G(x=x'-\varepsilon, x') \end{cases}$$

$\Rightarrow A = C = m/\varkappa\hbar^2 \Rightarrow$

$$G(x,x') = \frac{m}{\varkappa\hbar^2} e^{-\varkappa|x-x'|}.$$

Solution of an inhomogeneous eq

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi - E\psi = f(x)$$

is

$$\psi(x) = A e^{-\varkappa x} + B e^{\varkappa x} + \int_{-\infty}^{\infty} G(x,x') f(x') dx'$$

With $f = -U(x)\psi(x)$ we get

$$\psi(x) = A e^{-\varkappa x} + B e^{\varkappa x} - \int_{-\infty}^{\infty} G(x,x') U(x') \psi(x') dx'$$

We are interested in $\psi \to 0$ for $|x| \to \infty$

$\Rightarrow$ $A, B = 0$ and thus for $E < 0$ states

$$\psi(x) = -\frac{m}{\varkappa \hbar^2} \int_{-\infty}^{\infty} e^{-\varkappa |x - x'|}\, U(x')\, \psi(x')\, dx',$$

i.e. the Schrödinger eq. is written as integral. eq.

For $U(x) = -q\,\delta(x)$, $q > 0$:

the integral eq. gives

$$\psi(x) = \frac{mq}{\varkappa \hbar^2}\, e^{-\varkappa |x|}\, \psi(0)$$

$$\Rightarrow \quad x = 0 \text{ gives: } \quad 1 = \frac{mq}{\varkappa \hbar^2} \quad \Rightarrow$$

$$-\frac{2mE}{\hbar^2} = \frac{m^2 q^2}{\hbar^4} \quad \Rightarrow \quad E = -\frac{mq^2}{2\hbar^2}.$$

Normalizing by $|\psi(x)|^2 = 1$:

$$1 = \psi^2(0) \left(\frac{mq}{\varkappa \hbar^2} \right)^2 \frac{1}{\varkappa} \quad \Rightarrow$$

$$\Rightarrow \psi(0) = \frac{\varkappa \hbar^2}{mq}\sqrt{\varkappa} \Rightarrow$$

1 $\psi(x) = \sqrt{\varkappa}\, e^{-\varkappa |x|}, \quad \varkappa = mq/\hbar^2.$

1 For a free particle with $E > 0$:

$\varkappa = \sqrt{-2mE}/\hbar = \pm i k$, where

$k = \sqrt{2mE}/\hbar > 0 \Rightarrow$

2 $$G^{\pm}(x, x') = \pm \frac{i m}{k \hbar^2} e^{\pm i k |x - x'|}$$

(or one can follow the steps of the derivation for $E < 0$).

1 Two Green's functions corresp. to 2 b. c. at $x \to \pm\infty$ $(e^{\pm ikx})$.

The integral eq. is

1 $$\psi(x) = A e^{ikx} + B e^{-ikx} - \int_{-\infty}^{\infty} G^{\pm}(x, x') U(x') \psi(x') dx'$$

For a particle incident from the negative x-dir. :

$x - x' < 0$ for $x \to -\infty$ but

$x - x' > 0$ for $x \to +\infty$.

At $x \to +\infty$ should only have waves $\sim e^{ikx}$ (no source at $+\infty$)

$\Rightarrow$ should choose $G^+(x, x')$.

Also, $A = 1$ (normaliz. to 1) and $B = 0$:

$$\psi(x) = e^{ikx} - \int_{-\infty}^{\infty} G^+(x,x')\, U(x')\, \psi(x')\, dx'.$$

Consider $U(x) = -q\,\delta(x)$, $q > 0$.

Then

$$\psi(x) = e^{ikx} + q\, G^+(x, 0)\, \psi(0) =$$

$$= e^{ikx} + \frac{iqm}{k\hbar^2}\, e^{ik|x|}\, \psi(0)$$

$\Rightarrow$

$$\Rightarrow \psi(0) = 1 + \frac{iqm}{k\hbar^2}\psi(0)$$

$$\psi(0) = \frac{1}{1 - \frac{iqm}{k\hbar^2}}.$$

$$x<0: \psi(x) = e^{ikx} + A e^{-ikx}$$

$$\Rightarrow A = \frac{i\lambda}{1-i\lambda}, \quad \lambda = \frac{qm}{k\hbar^2}$$

$$x>0: \psi(x) = \left(1 + \frac{i\lambda}{1-i\lambda}\right)e^{ikx} =$$

$$= \frac{1}{1-i\lambda}e^{ikx} = S(k)\, e^{ikx}$$

$$\Rightarrow S(k) = \frac{1}{1-i\lambda}.$$

$$T = |S|^2 = \frac{1}{1+\lambda^2}.$$

$$R = |A|^2 = \frac{\lambda^2}{1+\lambda^2}.$$

$$R + T = 1$$

$$S = \frac{1}{1 - \frac{iqm}{k\hbar^2}}$$

$\Rightarrow$ singul. (pole) at

$$\frac{iqm}{\hbar^2} = k \Rightarrow k^2 = -\frac{q^2m^2}{\hbar^4}$$

or $E = \frac{\hbar^2 k^2}{2m} = -\frac{mq^2}{2\hbar^2}$, i.e.

exactly the bound state energy.

<u>Note</u>: this material has been covered in lectures.

Problem 2

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2}\int_0^\infty \frac{r'\sin qr'}{q}\,U(r')\,dr'$$

$q = 2k\sin\theta/2$.

1 Optical Theorem: $\sigma_{tot}(E) = \frac{4\pi}{k}\,\mathrm{Im}\, f(0)$

1 In the first Born approx. the theorem is violated since $f^{(1)}(\theta)$ is real.

Born series has a small param. ($m|U_0|a^2/\hbar^2$ or $|U_0|a/\hbar v$, where U_0, a are characteristic parameters of the pot., v - velocity of inc. particles). Since $\sigma \sim |f|^2$, expansion of σ starts with a square of that

1 small param. => this can only be captured by the second Born approx. in f (and $\mathrm{Im}\, f$).

$$\sigma(E) = 2\pi \int |f(\theta)|^2 \sin\theta \, d\theta ,$$

1 $$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \frac{q^2}{4\sin^2 \theta/2}$$

$$f^{(1)}(\theta) = -\frac{2m}{q\hbar^2} \int_0^\infty r' \sin qr' \cdot U(r')\, dr'$$

2 $$\sigma(E) = 2\pi \int |f|^2 \frac{dq^2}{2k^2} \quad \left(\text{since } q = 2k \sin\frac{\theta}{2}\right)$$

$$\Rightarrow \sigma(E) = 2\pi\hbar^2 \int \frac{|f|^2 dq^2}{2 \cdot 2mE} \Rightarrow$$

1 $$\Rightarrow E\sigma(E) = \frac{\pi\hbar^2}{2m} \int_0^{8mE/\hbar^2} |f|^2 dq^2$$

The integral is a monotonically increasing function of E $\Rightarrow$

1 $$\frac{d}{dE}\left(E\sigma(E)\right) \geq 0 .$$

For the Yukawa pot. $U(r) = V_0 \frac{e^{-\mu r}}{r}$

one first computes $f =$

$$= -\frac{m}{2\pi\hbar^2}\int e^{-i\bar{q}\bar{r}}\,U(r)\,d^3x =$$

$$= \frac{im}{\hbar^2 q}\int_0^\infty U(r)\left[e^{iqr}-e^{-iqr}\right]r\,dr$$

$$d\sigma = |f|^2 d\Omega \Rightarrow$$

$$\sigma(E) = \frac{\pi\hbar^2}{2mE}\int_0^{8mE/\hbar^2} f^2(q)\,dq^2 \quad \text{as before.}$$

$$\Rightarrow f^{(1)} = -\frac{2mU_0}{\mu^2\hbar^2(1+q^2/\mu^2)} \quad \text{(direct calc.)}$$

$$\sigma(E) = 16\pi\left(\frac{mU_0}{\mu^2\hbar^2}\right)^2 \frac{1}{1+\frac{8mE}{\mu^2\hbar^2}}$$

$$d\sigma = \frac{4m^2U_0^2}{\hbar^4(q^2+\mu^2)^2}\,d\Omega$$

$q = 2k\sin\theta/2$

With $U_0 = Z_1 Z_2 e^2$ $\quad \vec{p} = \hbar\vec{k}$

we get in the limit $\mu \to 0$:

$$d\sigma = \frac{(Z_1 Z_2 m e^2)^2}{4p^4\sin^4\theta/2} \quad \text{(Rutherford).}$$

$$U(r) = \begin{cases} -U_0, & r < L \\ 0, & r > L \end{cases}$$

To find the scattering length, one needs to find a solution to the radial Schrödinger eq.

$$R'' + \frac{2}{r} R' + \left[k^2 - \frac{l(l+1)}{r^2} - \bar{U}(r)\right] R = 0$$

with $E = 0$ $(k = 0)$ and $l = 0$ and compare to the asymptotics

$$R_{l=0, E=0} \simeq 1 - \frac{a_0}{r}, \quad r \to \infty,$$

where a_0 is the scattering length.

Here $\bar{U} = \frac{2mU}{\hbar^2}$.

With $R = \varphi / r$ (and $k = 0$, $l = 0$) the eq. becomes

$$\varphi'' - U(r)\varphi = 0$$

whose solution in the above pot.

is ($R(r)$ must be regular at $r=0$):

1 $$\varphi = \begin{cases} A \sin \frac{\xi_0 r}{L}, & r < L, \\ r - a_0, & r > L, \end{cases}$$

where $\xi_0 = 2m U_0 L^2/\hbar^2$.

Continuity of φ, φ' at $r=L$ gives

1 $$\begin{cases} A \sin \xi_0 = L - a_0 \\ \frac{A\xi_0}{L} \cos \xi_0 = 1 \end{cases}$$

$$\Rightarrow \frac{\tan \xi_0}{\xi_0} = 1 - a_0/L \quad \text{or}$$

1 $$a_0 = L\left(1 - \frac{\tan \xi_0}{\xi_0}\right).$$

2 $\sigma = 4\pi a_0^2$ (at $E=0$).

When $\xi_0 = \pi(n + 1/2)$, the scatt. length and σ diverge (the condition

3 corr. to bound state formation).

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Problem 3

$$\frac{\partial \rho_e}{\partial t} + \operatorname{div} \vec{j}_e = \frac{\partial \rho_e}{\partial t} + \frac{\partial j_e}{\partial x} = 0$$

2 - direct calculation with ρ_e, j_e given.

For $e^{\pm ikx}$:

$$-k^2 = \frac{m^2c^4 - (\varepsilon - eV_0)^2}{(\hbar c)^2}$$

1 $x<0$: $k^2 = \dfrac{\varepsilon^2 - m^2c^4}{(\hbar c)^2} > 0$

$(\varepsilon = mc^2 + E)$

$x>0$: $e^{ik'x} \Rightarrow$

1 $$k'^2 = \frac{(\varepsilon - eV_0)^2 - m^2c^4}{(\hbar c)^2} \quad (*)$$

Considering k'^2 as function of V_0:

$k'^2 > 0$ | $k'^2 < 0$ | $k'^2 > 0$ $\longrightarrow$ eV_0

$\varepsilon - mc^2$ $\qquad$ $\varepsilon + mc^2$

The group velocity $v = \partial\varepsilon / \partial p =$

$= \partial\varepsilon / \partial k\hbar$: from eq (*)

$$v = \frac{\hbar k' c^2}{\varepsilon - eV_0}$$

$\Rightarrow$ for $eV_0 > \varepsilon + mc^2$ we have $\varepsilon - eV_0 < 0 \Rightarrow k' < 0$ to have $v > 0$ (transmitted waves with no source at $x \to +\infty$)

for $eV_0 < \varepsilon - mc^2$: $\varepsilon - eV_0 > 0$ and $k' > 0$

for $\varepsilon - mc^2 < eV_0 < \varepsilon + mc^2$: no waves as $k'^2 < 0$

Computing the charge density ρ_e:

$$\rho_e = \frac{e\mathcal{E}}{mc^2}|\psi|^2 - \frac{e^2 V_0}{mc^2}|\psi|^2 =$$

$$= \frac{e(\mathcal{E} - eV_0)}{mc^2}|\psi|^2 ;$$

$\rho_e > 0$ for $eV_0 < \varepsilon - mc^2$ since

$\varepsilon - eV_0 > mc^2 > 0$.

$\rho_e < 0$ for $eV_0 > \varepsilon + mc^2$.

For $\varepsilon - mc^2 < V_0 < \varepsilon + mc^2$ we have $\psi \sim e^{-\varkappa X}$, $\varkappa > 0$

$\Rightarrow \rho_e \sim e^{-2\varkappa X}$

Current densities (from definition of $\vec{J}$ and the form of $u(X)$ given):

$$j_{inc} = \frac{\hbar k}{m} \qquad j_{ref} = \frac{\hbar k}{m}|A|^2$$

1 $j_{tr} = \frac{\hbar k'}{m} \Rightarrow R = |A|^2 = \frac{j_{ref}}{j_{inc}},$

2 and $T = \frac{k'}{k} |S|^2 = \frac{j_{tr}}{j_{inc}}.$

1 At $x = 0$ $u(x)$ and $u'(x)$ are

contin. (no sing. in eq) $\Rightarrow$

2 $$\begin{cases} 1 + A = S \\ ik - Aik = ik'S \end{cases}$$

$$\Rightarrow A = \frac{k-k'}{k+k'}, \quad S = \frac{2k}{k+k'}.$$

1 $$\Rightarrow R = \left(\frac{k-k'}{k+k'}\right)^2, \quad T = \frac{4k^2}{(k+k')^2} \frac{k'}{k}.$$

1 For $k'^2 < 0$: $j_{tr} \sim e^{-2\varkappa x} \xrightarrow[x \to +\infty]{} 0$

2 $T = 0, \quad R = 1.$

The sign of k' is crucial:

for $eV_0 < \varepsilon - mc^2$ $T < 1$, $R < 1$

(the usual scattering as in the non-rel. case), but for $eV_0 > \varepsilon + mc^2$ $k' < 0$ and thus

$$R = \frac{(k + |k'|)^2}{(k - |k'|)^2} > 1$$

and $T < 0$ $(T + R = 1)$.

This is happening for $eV_0 > \varepsilon + mc^2 = 2mc^2 + E$ and can be interpreted as pair creation process by strong potential (antiparticles travel to $x \to +\infty$, particles - to $-\infty$ enhancing the reflected wave) or/and as a breakdown of one-particle interpret. of rel. wave eq.