PHYS852 Quantum Mechanics II, Spring 2010
HOMEWORK ASSIGNMENT 11: Solutions

Topics covered: Scattering amplitude, differential cross-section, scattering probabilities.

1. [5 pts] Using only the definition, $G_0 = (E - H_0 + i\epsilon)^{-1}$, show that the free-space Green's function is the solution to

$$\left[E + \frac{\hbar^2}{2M}\nabla^2_{\vec{r}}\right] G_0(\vec{r}, \vec{r}') = \delta^3(\vec{r} - \vec{r}'). \tag{1}$$

The purpose of this problem is just to establish the equivalence between our operator-based approach, and the standard Green's function formalism encountered, e.g., in classical EM.
According to it's definition, we must have:

$$[E - H_0 + i\epsilon]G_0 = I. \tag{2}$$

Hitting from the left with $< \vec{r}|$ and from the right with $|\vec{r}'\rangle$ then gives:

$$\langle\vec{r}|[E - H_0 + i\epsilon]G_0|\vec{r}'\rangle = \langle\vec{r}|\vec{r}'\rangle. \tag{3}$$

Using $H_0 = \frac{1}{2M}P^2$ and taking $\epsilon \to 0$ then gives

$$\left[E + \frac{\hbar^2}{2M}\nabla^2_{\vec{r}}\right] G_0(\vec{r}, \vec{r}') = \delta^3(\vec{r} - \vec{r}'). \tag{4}$$

2. If we define the operator F via $f(\vec{k}', \vec{k}) = \langle \vec{k}' | F | \vec{k} \rangle$, then it follows that $F = -\frac{(2\pi)^2 M}{\hbar^2} T$, where T is the T-matrix operator. In principle, one would like to deduce the form of the potential V from scattering data.

First, derive an expression for the operator V in terms of the operators G_0 and T only.

In preparation for problem 11.4, use this expression for V to prove that the full Green's function, $G = (E - H_0 - V + i\epsilon)^{-1}$ is related to the background Green's function, G_0 via the simple relation:

$$G = G_0 + G_0 T G_0. \tag{5}$$

(Hint: don't forget that order matters in operator inversion $(AB)^{-1} = B^{-1}A^{-1}$.)

The relationship between T, V, and G_0 is

$$T = (1 - VG_0)^{-1} V. \tag{6}$$

Operating from the left with $(1 - VG_0)$ then gives

$$(1 - VG_0) T = V. \tag{7}$$

Multiply out the l.h.s. to get

$$T - VG_0 T = V \tag{8}$$

Putting all terms containing V on the r.h.s. gives

$$\begin{aligned} T &= V + VG_0 T \\ &= V(1 + G_0 T). \end{aligned} \tag{9}$$

Operate from the right with $(1 + G_0 T)^{-1}$ to find

$$V = T(1 + G_0 T)^{-1}. \tag{10}$$

Note that if you started from $T = V(1 - G_0 V)^{-1}$, you would arrive at the equivalent expression $V = (1 + TG_0)^{-1} T$.

The definition of the full Green's function is:

$$G = (E - H_0 - V + i\epsilon)^{-1} \tag{11}$$

Inserting the definition of G_0 and our expression for V then gives

$$G = (G_0^{-1} - T(1 + G_0 T)^{-1})^{-1}. \tag{12}$$

Using the fact that $G_0^{-1} G_0 = I$, we can then write this as

$$G = (G_0^{-1} - G_0^{-1} G_0 T(1 + G_0 T)^{-1})^{-1}. \tag{13}$$

Pulling the common factor G_0^{-1} out of the inverse via $(AB)^{-1} = B^{-1}A^{-1}$ gives

$$G = (1 - G_0 T(1 + G_0 T)^{-1})^{-1} G_0. \tag{14}$$

Using a similar trick for the $(1 + G_0 T)^{-1}$ term gives

$$\begin{aligned} G &= ((1 + G_0 T)(1 + G_0 T)^{-1} - G_0 T(1 + G_0 T)^{-1})^{-1} G_0 \\ &= (1 + G_0 T)(1 + G_0 T - G_0 T)^{-1} G_0 \\ &= (1 + G_0 T) G_0 \\ &= G_0 + G_0 T G_0. \end{aligned} \tag{15}$$

3. Consider a system described by H_0 that has no bound states, but has a continuum of states for $E > 0$. This means that

$$G_0(E) = \int_0^\infty dE' \frac{|E'^{(0)}\rangle\langle E'^{(0)}|}{E - E' + i\epsilon}, \tag{16}$$

where we have assumed that the bare states $|E^{(0)}\rangle$ are non-degenerate. Incorporating any degeneracy is accomplished by adding additional quantum numbers and summing/integrating over them.

Now consider a different system, described by $H = H_0 + V$, that in addition to a continuum of states for $E > 0$, may have a set of negative energy bound states, $\{E_n\}$, . In this case, it follows from the definition $G = (E - H + i\epsilon)^{-1}$, that

$$G = \sum_n \frac{|E_n\rangle\langle E_n|}{E - E_n + i\epsilon} + \int_0^\infty dE' \frac{|E'\rangle\langle E'|}{E - E' + i\epsilon}. \tag{17}$$

Show that for $E < 0$, as $\epsilon \to 0$, G remains finite unless E matches the energy of one of the bound states. Thus the negative energy singularities of a system's Green's function correspond to the energies of the bound states of the potential V. Show that the bound-state wavefunction is given by the formula

$$\psi_n(\vec{r}) = \sqrt{\langle \vec{r}| \lim_{E \to E_n} (E - E_n) G |\vec{r}\rangle}. \tag{18}$$

For $E < 0$ and $E_n < 0$, we see that for $\epsilon \to 0$,

$$\begin{aligned} G &= \sum_n \frac{|E_n\rangle\langle E_n|}{-|E| + |E_n|} + \int_0^\infty dE' \frac{|E'\rangle\langle E'|}{-|E| - |E|'} \\ &= -\sum_n \frac{|E_n\rangle\langle E_n|}{|E| - |E_n|} - \int_0^\infty dE' \frac{|E'\rangle\langle E'|}{|E| + |E'|}. \end{aligned} \tag{19}$$

This shows that the first terms blows up only if $E = E_n$, while the second term has no singularity.

Based on Eq. (17), we have

$$\begin{aligned} \lim_{E \to E_n} (E - E_n) G &= \lim_{E \to E_n} \left(\sum_{n'} \frac{E - E_n}{E - E_{n'}} |E_{n'}\rangle\langle E_{n'}| + \int_0^\infty \frac{E - E_n}{E - E'} |E'\rangle\langle E'| \right) \\ &= |E_n\rangle\langle E_n| \end{aligned} \tag{20}$$

Taking the diagonal matrix element with respect to coordinate then gives

$$\langle \vec{r}| \lim_{E \to E_n} (E - E_n) G |\vec{r}\rangle = |\langle \vec{r}|E_n\rangle|^2. \tag{21}$$

With $\psi_n(\vec{r}) := \langle \vec{r}|E_n\rangle$, which can also be chosen as real-valued, we arrive at the desired result:

$$\psi_n(\vec{r}) = \sqrt{\langle \vec{r}| \lim_{E \to E_n} (E - E_n) G |\vec{r}\rangle}. \tag{22}$$

4. Based on Eq. (2), it follows that if G_0 has no negative energy singularities, then the singularities in G must come from the T-matrix. Consider the case of a particle in one dimension with $H_0 = \frac{P^2}{2M}$ and $V = g\delta(X)$, where $g < 0$. Compute the T-matrix, and find it's negative energy singularity, then use Eq. (5) to find the bound-state wavefunction. Does this procedure give the true bound-state energy and wavefunction? Is it necessary to normalize the resulting state by hand, or is it automatically normalized?

Starting from $G = G_0 + G_0 T G_0$, we have

$$\begin{aligned} |\phi_n(x)|^2 &= \langle x| \lim_{E\to E_n} (E - E_n) G |x\rangle \\ &= \langle x| \lim_{E\to E_n} (E - E_n)(G_0 - G_0 T G_0)|x\rangle \\ &= \lim_{E\to E_n} (E - E_n)\langle x|G_0 T G_0|x\rangle \end{aligned} \tag{23}$$

where we obtain the last line due to the fact that G_0 is finite in the limit $E \to E_n < 0$, and $\langle x|$ is independent of E. Inserting the projector onto coordinate basis twice then gives,

$$|\phi_n(x)|^2 = \lim_{E\to E_n} (E - E_n) \int dx' dx''\, \langle x|G_0|x'\rangle T(x', x'')\langle x''|G_0|x\rangle. \tag{24}$$

From the lecture notes, Eq. (48), we have

$$T(x, x') = \frac{g\delta(x)\delta(x')}{1 + i\frac{gM}{\hbar^2 k}}, \tag{25}$$

which gives

$$\begin{aligned} |\phi_n(x)|^2 &= \lim_{E\to E_n} (E - E_n) \int dx' dx''\, G_0(x, x') \frac{g\delta(x)\delta(x')}{1 + i\frac{gM}{\hbar^2 k}} G_0(x'', x) \\ &= -|g| \lim_{E\to E_n} G_0(x, 0) G_0(0, x) \frac{E - E_n}{1 - i\frac{|g|M}{\hbar^2 k}} \\ &= -i\frac{\hbar^2}{M} \lim_{E\to E_n} k\, G_0(x, 0) G_0(0, x) \frac{E - E_n}{1 + ika} \end{aligned} \tag{26}$$

where we have introduced $a = \frac{\hbar^2}{M|g|}$. We see that the T-matrix has only one singularity at $k_b = \frac{i}{a}$, so that there is only a single bound-state at $E_b = \frac{\hbar^2 k_b^2}{2M} = -\frac{\hbar^2}{2Ma^2}$. With $E = \frac{\hbar^2 k^2}{2M}$, and

$$G_0(x, x') = -i\frac{M}{\hbar^2 k} e^{ik|x-x'|}, \tag{27}$$

Eq. (26) becomes

$$\begin{aligned} |\phi_b(x)|^2 &= \frac{i}{2a^2} \lim_{k\to\frac{i}{a}} \frac{e^{2ik|x|}}{k} \frac{1 + k^2 a^2}{1 - ika} \\ &= \frac{i}{2a^2} \lim_{k\to\frac{i}{a}} \frac{e^{2ik|x|}}{k}(1 - ika) \\ &= \frac{1}{a} e^{-2\frac{|x|}{a}} \end{aligned} \tag{28}$$

From which we find the bound-state wavefunction to be

$$\phi_b(x) = \frac{1}{\sqrt{a}} e^{-\frac{|x|}{a}}. \tag{29}$$

Checking the normalization, we find

$$\begin{aligned} \int_{-\infty}^{\infty} dx\, |\phi_b(x)|^2 &= \frac{1}{a} \int_{-\infty}^{\infty} dx\, e^{-2\frac{|x|}{a}} \\ &= \frac{2}{a} \int_{0}^{\infty} dx\, e^{-2\frac{x}{a}} \\ &= \int_{0}^{\infty} du e^{-u} \\ &= 1 \end{aligned} \tag{30}$$

So in fact, the procedure gives the properly normalized bound-state, so that it is not necessary to normalize it by hand.

5. Follow the same steps as in the previous problem, but for the three-dimensional Huang-Fermi pseudo-potential, defined by $\langle \vec{r}|V|\psi\rangle = g\delta^3(\vec{r})\frac{d}{dr}r\psi(r)$. Show that a single bound state exists only for the repulsive case $g > 0$, and find the bound-state energy and wavefunction.

From HW10.3b, the T-matrix for the Huang-Fermi pseudo-potential is

$$T = \frac{V_{HF}}{1 + ika} \tag{31}$$

where

$$a = \frac{Mg}{2\pi\hbar^2} \tag{32}$$

The singularity in the T-matrix occurs for $k = \frac{i}{a}$, corresponding to a binding energy of $E_b = -\frac{\hbar^2}{2Ma^2}$. Using

$$G_0(\vec{r}, \vec{r}') = -\frac{M}{2\pi\hbar^2}\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \tag{33}$$

the bound-state formula gives

$$\begin{aligned} |\psi_b(\vec{r})|^2 &= \lim_{k\to\frac{i}{a}} \frac{\hbar^2}{2M}\left(k^2 + \frac{1}{a^2}\right)\langle\vec{r}|G_0 T G_0|\vec{r}\rangle \\ &= \lim_{k\to\frac{i}{a}} \frac{\hbar^2 g}{2Ma^2} G_0(\vec{r}, 0)\frac{1 + k^2a^2}{1 + ika} G_0(0, \vec{r}) \\ &= \lim_{k\to\frac{i}{a}} \frac{Mg}{8\pi^2\hbar^2 a^2}(1 - ika)\frac{e^{-2r/a}}{r^2} \\ &= \frac{1}{2\pi a}\frac{e^{-2r/a}}{r^2} \end{aligned} \tag{34}$$

First, we note that this state is physical (i.e. normalizable) only for $a > 0$, which corresponds to $g > 0$. Checking normalization, we then have

$$\begin{aligned} \int d^3r\, |\psi_b(\vec{r})|^2 &= 4\pi\int_0^\infty r^2 dr\, \frac{e^{-2r/a}}{2\pi a r^2} \\ &= \frac{2}{a}\int_0^\infty dr\, e^{-2r/a} \\ &= \int_0^\infty du\, e^{-u} \\ &= 1 \end{aligned} \tag{35}$$