HW #1 Solutions (221B)

1) Lippmann and Schwinger grow thin

Taking the x representation and inserting a complete set of x' eigenstates, the Lippmann-Schwinger equation reads

$$\psi(x) = \phi(x) + \int dx' \langle x| \frac{1}{E - H_0 + i\epsilon} |x'\rangle V(x')\psi(x'),$$

with notation as in the lecture notes. Following the notes we insert a complete set of momentum eigenstates to find

$$\psi(x) = \phi(x) + \int dx' V(x')\psi(x') \int \frac{dp}{2\pi\hbar} \frac{e^{ip(x-x')/\hbar}}{E - \frac{p^2}{2m} + i\epsilon}.$$

Considering now the dp integral, the denominator factors so that

$$\int \frac{dp}{2\pi\hbar} \frac{e^{ip(x-x')/\hbar}}{E - \frac{p^2}{2m} + i\epsilon} = \int \frac{dp}{2\pi\hbar} \frac{-2me^{ip(x-x')/\hbar}}{(p - \sqrt{2mE} - i\epsilon)(p + \sqrt{2mE} + i\epsilon)},$$

where ϵ stands for any positive infinitessimal and the signs on the ϵ terms in the right hand equation are chosen to reproduce $+i\epsilon$ in the left hand equation. The dp integral can be performed by a contour integration. When $(x-x') > 0$ we can close the contour in the upper half plane, picking up the pole at $p = \sqrt{2mE} + i\epsilon$; when $(x - x') < 0$ we must close the contour in the lower half plane, picking up the pole at $p = -\sqrt{2mE} - i\epsilon$. Taking $2\pi i$ times the residue at the appropriate poles and calling $E = \hbar^2 k^2/2m$,

$$\int \frac{dp}{2\pi\hbar} \frac{e^{ip(x-x')/\hbar}}{E - \frac{p^2}{2m} + i\epsilon} = \left\{ \begin{array}{ll} \frac{-im}{\hbar^2 k} e^{ik(x-x')}, & (x - x') > 0 \\ \frac{-im}{\hbar^2 k} e^{-ik(x-x')}, & (x - x') < 0 \end{array} \right\} = \frac{-im}{\hbar^2 k} e^{ik|x-x'|}.$$

The Lippmann-Schwinger equation in one dimension is therefore

$$\psi(x) = \frac{e^{ikx}}{\sqrt{2\pi\hbar}} + \frac{-im}{\hbar^2 k} \int dx' e^{ik|x-x'|} V(x')\psi(x').$$

We can check that

$$G(x, x') = \frac{-im}{\hbar^2 k} e^{ik|x-x'|}$$

is indeed a Green's function for the free Schrodinger operator:

$$\left(\frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)G(x, x') = \delta(x - x').$$

Using $|x - x'| = (x - x')\theta(x - x') - (x - x')\theta(x - x')$, $\frac{d}{dx}\theta(x) = \delta(x)$ we compute

$$\begin{aligned} \tfrac{d}{dx} e^{ik|x-x'|} &= ik\, e^{ik|x-x'|}[\theta(x - x') + (x - x')\delta(x - x') - \theta(x' - x) + (x - x')\delta(x' - x)] \\ &= ik\, e^{ik|x-x'|}[\theta(x - x') - \theta(x' - x)]; \end{aligned}$$

$$\begin{aligned} \tfrac{d^2}{dx^2} e^{ik|x-x'|} &= -k^2 e^{ik|x-x'|}[\theta(x - x') - \theta(x' - x)]^2 + ik\, e^{ik|x-x'|}[\delta(x - x') + \delta(x' - x)] \\ &= -k^2 e^{ik|x-x'|} + 2ik\, \delta(x - x'). \end{aligned}$$

So that $G(x, x')$ is indeed the desired function.

2) Far from home

At asymptotic distances from the region of significant potential, $r := |x| \gg a$, we can expand in the exponential,

$$|x - x'| = \sqrt{(x - x')^2} = |x|\sqrt{1 - 2\frac{xx'}{|x|^2} + \frac{|x'|^2}{|x|^2}} \approx |x|(1 - \frac{xx'}{|x|^2}) = r - \frac{xx'}{r}.$$

Then

$$\psi(x) = \frac{e^{ikx}}{\sqrt{2\pi\hbar}} + \frac{-im}{\hbar^2 k} \int dx' e^{ikr - i\frac{kx}{r}x'} V(x')\psi(x') = \frac{1}{\sqrt{2\pi\hbar}}(e^{ikx} + f(k', k)e^{ikr})$$

is of the desired form, where

$$k' = \tfrac{kx}{r} = \pm k \quad \text{and} \quad f(k', k) = -\tfrac{2\pi i m}{\hbar k}\langle \hbar k'|V|\psi\rangle.$$

3) Playing with tigers

a)

Inserting the potential $V(x) = \gamma\delta(x)$ into the Lippmann-Schwinger equation from problem (1) and integrating over the delta-function,

$$\psi(x) = \frac{e^{ikx}}{\sqrt{2\pi\hbar}} + \frac{-im\gamma}{\hbar^2 k} e^{ik|x|}\psi(0).$$

Evaluating this equation at $x = 0$ gives an expression which we can solve for $\psi(0)$,

$$\psi(0) = \frac{1}{\sqrt{2\pi\hbar}} + \frac{-im\gamma}{\hbar^2 k} e^{ik|x|}\psi(0) \Rightarrow \psi(0) = \frac{1}{\sqrt{2\pi\hbar}} \frac{\hbar^2 k}{\hbar^2 k + im\gamma},$$

so that

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}(e^{ikx} - e^{ikr}\frac{im\gamma}{\hbar^2 k + im\gamma}).$$

b)

In the regions $x > 0$, $x < 0$, the potential vanishes and $\psi(x)$ is just a sum of same-energy plane waves which clearly satisfies the free Schrodinger equation. At $x = 0$ there is a delta-function, which instructs us to check that the Schrodinger equation holds under an integral sign:

$$\lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + \gamma\delta(x)\psi \stackrel{?}{=} \frac{\hbar^2 k^2}{2m}\psi.$$

In fact the equality holds since

$$\begin{aligned} \lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} -\tfrac{\hbar^2}{2m}\tfrac{d^2}{dx^2}\psi + \gamma\delta(x)\psi &= \lim_{\epsilon\to 0} -\tfrac{\hbar^2}{2m}(\psi'(\epsilon)-\psi'(-\epsilon)) + \gamma\psi(0) \\ &= -\tfrac{\hbar^2}{2m}\tfrac{2km\gamma}{\hbar^2 k + im\gamma} + \gamma\tfrac{\hbar^2 k}{\hbar^2 k + im\gamma} = 0, \end{aligned}$$

and also

$$\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} \frac{\hbar^2 k^2}{2m}\psi(x) = 0.$$

Alternatively, you can just differentiate carefully as in the solution to problem (1). Such derivatives are well-defined as part of the mathematical theory of 'distributions.' Distributions are defined as continuous functionals on the space of suitably well-defined 'test functions' (usually taken to be infinitely differentiable functions which are zero everywhere but a compact subspace of R^{n}). $\theta(x)$, $\delta(x)$, 1, are all examples of such distributions which are defined with an integral. I.e. for a test function f,

$$\theta[f] := \textstyle\int_{-\infty}^{\infty} dx f(x)\,\theta(x) := \int_0^{\infty} f(x),$$

$$\delta[f] := \textstyle\int_{-\infty}^{\infty} dx f(x)\,\delta(x) := f(0),$$

$$1[f] := \textstyle\int_{-\infty}^{\infty} dx f(x)\,1 = \int_{-\infty}^{\infty} dx f(x).$$

Distributions are infinitely differentiable, differentiation being defined in analogy with integration by parts. That is, for a distribution T, $\frac{d}{dx}T[f] := T[-\frac{d}{dx}f]$. It is easy to check from the above definitions that this gives $\frac{d}{dx}\theta = \delta$.

A rigorous formulation of distributions isn't too relevant to physics, because objects like delta-functions only appear in physics as idealized limits of more respectible functions, e.g. gaussians. So we might as well add funny math to our funny physics when we make these idealizations. But if you ever do see an expression with delta functions in it, know that it's best hope of being defined involves integration. That said, our above use of delta functions in scattering problems is not well-defined, because complex exponentials (plane waves) are not integrable and so fail to qualify as well-defined test functions. This is why we have to resort to the somewhat awkward prescription of integrating over $(-\epsilon, \epsilon)$ and taking the limit $\epsilon \to 0$. On true test functions, an equation involving distributions is said to hold when it holds under an integral over all R^{n}.

c)

As we discussed in section, it is generally true that a scattering amplitude has poles at energies of any 'relevant' bound states. A pole at a real energy E corresponds to true bound state, while a pole at complex E corresponds to a metastable bound state which can appear as a resonance in a scattering experiment. One way to think about this latter phenomenon is to look at equation (26) in the first lecture notes which describes the time-dependent solution for scattering of a wave packet. For $\vec{q}$ sufficiently near $\vec{k}$, the $d\vec{q}$ integral will pick up a pole in $f(\vec{q}', \vec{q})$ and give a contribution to ψ with time dependence $\sim e^{-iEt/\hbar}$, which for $E = E_r - i\Gamma/2$ will decay in time as $e^{-\Gamma t/2\hbar}$. At small times there is a high probability to find the particle trapped near the source of potential, but at long times this configuration becomes unlikely and the particle escapes to infinity.

In this problem the pole in $f(k', k)$ is at $k = -im\gamma/\hbar^2$, which corresponds to the real energy $E = -m\gamma^2/2\hbar^2$. So we know there exists a stable bound state of that energy. In our derivation of the Lippmann-Schwinger equation, the only place we assume $E > 0$, i.e. a scattering state, is when we add the incoming plane wave $\phi(x)$ to the right hand side to satisfy our boundary conditions. We can do this because a continuum state by definition can have any energy > 0; in particular we can always find a free solution $\phi(x)$ which has the same energy as our scattering state $\psi(x)$. This does not work for bound states which have discrete energies < 0. But if we leave out $\phi(x)$ and fix different boundary conditions, our derivation of the Lippmann-Schwinger equation holds for bound states too. That is, we can read off the bound-state wavefunction from our solution to part (a):

$$\psi_{bound}(x) \sim e^{ikr}$$

will be a bound-state solution when we plug in $k = -im\gamma/\hbar^2$. Boundary conditions for a bound state are that the wavefunction decays at both infinities, which this clearly does for $\gamma < 0$. Normalizing,

$$\psi_{bound} = \sqrt{\frac{-m\gamma}{\hbar^2}} e^{m\gamma r/\hbar^2}.$$

It is easy to check that

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} e^{m\gamma r/\hbar^2} + \gamma\delta(x) e^{m\gamma r/\hbar^2} = \frac{-m\gamma^2}{2\hbar^2} e^{m\gamma r/\hbar^2}.$$

d)

Plugging $V(\vec{x}) = \gamma\delta(\vec{x})$ into the 3-d Lippmann-Schwinger equation gives

$$\psi(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{k}\vec{x}} - \frac{2m}{\hbar^2}\frac{e^{ik|\vec{x}|}}{4\pi|\vec{x}|}\gamma\psi(0).$$

To avoid singularity at the origin we require $\psi(0) = 0$, but then the scattering term vanishes, and we are left with the free plane wave

$$\psi(x) = \begin{cases} \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{k}\vec{x}}, & x \neq 0 \\ 0, & x = 0 \end{cases},$$

the singularity in the potential allowing the discontinuous wavefunction. I made an argument on email that this is a solution to the Schrodinger equation, and I contrived a bad explation for the consistency of the Lippmann-Schwinger equation at the origin. Professor Murayama explains that the consistency instead follows from the relation $\frac{0}{0} = 1$. Or rather, it is possible to arrange that

$$-\frac{2m}{\hbar^2}\frac{e^{ik|\vec{x}|}}{4\pi|\vec{x}|}\gamma\psi(0) = -\frac{1}{(2\pi\hbar)^{3/2}} \quad \text{as } |\vec{x}| \to 0.$$

This is at least a logical possibility, and I think justification must rely on solving the problem for, say, a spherically symmetric square well and taking the limit as the square well approaches a delta-function. Then we can compute

$$-\frac{2m}{\hbar^2}\int d\vec{x}'\,\frac{e^{ik|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|}V(\vec{x}')\psi(\vec{x}')$$

and convince ourselves that in the limit $V(\vec{x}) \to \delta(\vec{x})$ this integral does tend to the appropriate value (0 for $|\vec{x}| \neq 0$, $1/(2\pi\hbar)^{3/2}$ for $|\vec{x}| = 0$). The square well problem can be solved exactly using a partial wave expansion, and we can come back to this when we cover partial waves if there is large demand, but the computation is a little tedious which is a lot more than the significance of this point.

One thing we should do when we come to partial waves is to look at the phase shifts for the square well potential to convince ourselves that the scattering amplitude vanishes as the square well becomes a delta-function. Explicitly, we want to study

$$V = \begin{cases} -V_0, & |\vec{x}| \leq a \\ 0, & |\vec{x}| > a \end{cases}.$$

in the limit $V_0 \to \infty$, $a \to 0$, $V_0 a^3$ fixed. I had hoped to demonstrate this with the Born approximation, but in my initial calculation I was taking the wrong limit, and in fact the Born approximation to the scattering amplitude does not vanish:

$$\begin{aligned} f(\vec{k}', \vec{k}) &= -\tfrac{(2\pi\hbar)^3}{4\pi}\tfrac{2m}{\hbar^2}\langle\hbar\vec{k}'|V|\hbar\vec{k}\rangle \\ &= -\tfrac{m}{2\pi\hbar^2}\int d\vec{x}\, e^{i\vec{q}\cdot\vec{x}}V \\ &= \tfrac{2mV_0}{i\hbar^2 q^2}(-a\cos qa + \tfrac{1}{q}\sin qa), \end{aligned}$$

where $\vec{q} = \vec{k} - \vec{k}'$ is the momentum transfer. In the limit

$$\begin{aligned} \tfrac{d\sigma}{d\Omega} = |f|^2 &= \tfrac{4m^2}{\hbar^4 q^4}| - V_0 a\cos qa + \tfrac{V_0}{q}\sin qa|^2 \\ &\approx \tfrac{4m^2}{\hbar^4 q^4}| - V_0 a(1 - \tfrac{q^2 a^2}{2}) + \tfrac{V_0}{q}(qa - \tfrac{q^3 a^3}{6}) + \mathrm{O}(V_0 a^5)|^2 \\ &\to \tfrac{4m^2 V_0^2 a^6}{9\hbar^4}, \end{aligned}$$

which is clearly non-zero.

This seeming contradiction arises because the Born approximation itself fails in the limit, the validity criterion

$$(\text{const})\, V_0 a^2 \ll 1$$

breaking down for sufficiently small a since V_0 diverges as a^{-3}. We need to treat the square well exactly (or at least in a better approximation scheme) to see that the scattering amplitude vanishes as the square well becomes a delta-function.

The lesson here is that playing with delta functions is a little bit like walking through Tilden park oblivious of the tigers hiding in the chapparal. Most of the time we're fine, but it can be dangerous, and if we want to verify our math with physical understanding we should treat delta functions as limits of more sociable functions. Even then these tigers may turn out to be dragons in tigers' clothing, because the limits themselves may make the physics ill-defined.