Problem Set 7

Due Tuesday April 9 at 11.00AM

Assigned Reading:

E&R 6_{all}
Li. 7_{1-9}, 8_1
Ga. 4_{all}, 6_{all}, 19_2
Sh. 1_6, 5_{all}, 11_{all}, 19_2

1. **(15 points) Mathematical Preliminaries: Facts about Unitary Operators**

   A *Unitary* operator U is an operator whose Adjoint is its inverse, ie

   $$U^\dagger U = \hat{\mathbb{1}} = U\,U^\dagger$$

   (a) Show that all eigenvalues λ_i of a Unitary operator are pure phases, $\lambda_j = e^{i\phi_j}$.

   (b) Can an operator be both Hermitian and Unitary?

   (c) Suppose M is a Hermitian operator. Show that e^{iM} is a Unitary operator.

   (d) Show that the product of two Unitary operators is also Unitary.

   (e) Suppose U is a Unitary operator, and v a state. Show that acting on v with U preserves the norm of v.

   (f) Recall our old friend the "Translate-by-L" operator which shifts the expectation value of the position by L,

   $$\hat{T}_L = e^{-L\frac{i}{\hbar}\hat{p}}\,, \qquad\qquad \hat{T}_L f(x) = f(x - L)\,.$$

   We can similarly define a "Boost by q" operator which shifts the expectation value of the momentum by q (*c.f.* problem 2 on Problem Set 6),

   $$\hat{B}_q = e^{+q\frac{i}{\hbar}\hat{x}}\,, \qquad\qquad \hat{B}_q f(x) = e^{i\frac{qx}{\hbar}} f(x)\,.$$

   Verify that $\hat{T}_L$ and $\hat{B}_q$ are both Unitary operators, and demonstrate that

   $$\hat{T}_L{}^\dagger = \hat{T}_{-L}\,, \qquad\qquad \hat{B}_q{}^\dagger = \hat{B}_{-q}\,.$$

2. **(20 points) Quantum Evolution is Unitary**

   The time evolution of a quantum state is dictated by the Schrödinger equation,

   $$i\hbar\, \partial_t \psi(x,t) = \hat{E}\, \psi(x,t)\,,$$

   where $\hat{E}$ is the energy operator. The meaning of the Schrödinger equation is this: given the state $\psi(x,0)$ at some moment in time $t = 0$, and given the operator $\hat{E}$, we can unambiguously determine the state at any later moment in time by directly integrating this differential equation. We can thus define an operator, $\hat{U}_t$, which maps any wavefunction at time 0 to its Schrödinger-evolved form at at time t,

   $$\hat{U}_t\, \psi(x,0) = \psi(x,t)\,.$$

   (a) Give a physical reason why $\hat{U}_t$ must be unitary,

   $$\hat{U}_t^\dagger \hat{U}_t = \hat{\mathbb{1}}\,.$$

   (b) Give a physical reason why $\hat{U}_t$ must satisfy a simple composition law,

   $$\hat{U}_{t_2} \hat{U}_{t_1} = \hat{U}_{t_1+t_2}\,.$$

   (c) Use the Schrödeinger equation to show that $\hat{U}_t$ satisfies the operator equation,

   $$\partial_t \hat{U}_t = -\frac{i}{\hbar} \hat{E}\, \hat{U}_t\,.$$

   (d) Find the most general solution to this differential equation which satisfies the above two properties.

   Aside: $\hat{U}_t$ is often called the "Evolution operator" or the "Propagator". In principle, we can always solve the Schrödinger equation by simply exponentiating $-\frac{i}{\hbar}t\hat{E}$; acting with the resulting $\hat{U}_t$ on a given wavefunction ψ then evolves ψ forward in time. However, exponentiating an operator is generally not a trivial thing to do. Nonetheless, we can often learn a lot about a system by studying the propagator and its properties.

   (e) As an example, identify $\hat{U}_t$ for the harmonic oscillator in terms of $\hat{N}$.

Aside: **Symmetries in Quantum Mechanics**

Let's pause to explore how symmetry transformations are realized in quantum mechanics. Consider a transformation, T, which leaves physical observables invariant when acting upon all elements in the system – for example, translation in space, translation in time, spatial rotations, etc. In QM, leaving physical observables invariant means preserving probabilities. T must thus be represented by an operator, $\hat{T}$, which satisfies,

$$\left| \langle \hat{T}\phi | \hat{T}\psi \rangle \right|^2 = |\langle \phi | \psi \rangle|^2 \quad \forall \phi, \psi$$

It is easy to check that any Unitary operator $\hat{U}$ with $\hat{U}^\dagger \hat{U} = \hat{\mathbb{1}}$ satisfies this condition:

$$\left| \langle \hat{U}\phi | \hat{U}\psi \rangle \right|^2 = \left| \langle \phi | \hat{U}^\dagger \hat{U}\psi \rangle \right|^2 = |\langle \phi | \psi \rangle|^2 \,,$$

and indeed all the symmetry transformations we have studied so far (time-translations, spatial-translations and momentum-boosts) have been represented by unitary operators ($\hat{U}_t$, $\hat{T}_L$ and $\hat{B}_q$, respectively).

Importantly, Unitary operators are not the only operators which satisfy our symmetry condition. Consider a so-called "anti-unitary operator", $\hat{A}$, which satisfies

$$\langle \hat{A}\phi | \hat{A}\psi \rangle = \langle \psi | \phi \rangle$$

It is easy to check that an anti-unitary operator satisfies the symmetry condition, too:

$$\left| \langle \hat{A}\phi | \hat{A}\psi \rangle \right|^2 = |\langle \psi | \phi \rangle|^2 = |\langle \phi | \psi \rangle|^2$$

It is also easy to check that any anti-unitary operator squares to a unitary operator:

$$\langle \hat{A}^2 \phi | \hat{A}^2 \psi \rangle = \langle \hat{A}\psi | \hat{A}\phi \rangle = \langle \phi | \psi \rangle$$

You can thus think of an anti-unitary operator as a sort of square-root of a unitary operator. Examples include the operator $\hat{\mathbb{T}}$ representing time-reversal, $t \to -t$, as discussed in lecture. Note that time-reversing twice is equivalent to doing nothing, so $\hat{\mathbb{T}}$ does indeed square to a unitary operator, if a trivial one: $\hat{\mathbb{T}}^2 = \hat{\mathbb{1}}$. Can you think of further examples of anti-unitary operators? What transformations do they realize?

The fact that every symmetry operation must be represented in quantum mechanics by a unitary or anti-unitary operator is known as "Wigner's Theorem", and has many important consequences which you will explore in greater detail in 8.05 and 8.06.

3. **(20 points) Getting a Sense for T.**

   (a) Consider the scattering of particles of mass m off a step of height V_o. Compute t, r, T and R for both $E > V_o$ and $E < V_o$. Sketch $T(E)$. How do your results differ when you scatter uphill versus downhill?

   (b) In lecture we derived the transmission probability T for a particle of mass m incident on a barrier of width L and height V_o. For $E < V_o$, T was given by

   $$T = \frac{1}{1 + \frac{V_o^2}{4E(V_o - E)} \sinh^2(\alpha L)} \, ,$$

   where $\alpha^2 = \frac{2m}{\hbar^2}(V_o - E)$, while for $E > V_o$ it was given by,

   $$T = \frac{1}{1 + \frac{V_o^2}{4E(E - V_o)} \sin^2(k_2 L)} \, ,$$

   where $k_2^2 = \frac{2m}{\hbar^2}(E - V_o)$ and $g_o^2 = \frac{2mL^2 V_o}{\hbar^2}$ measures the strength of the barrier.

   Sketch[1] T as a function of $\frac{E}{V_o}$ for a very wide barrier ($g_o = 20$), a medium barrier ($g_0 = 2$), and a thin barrier ($g_o = 0.2$). (Hint: it helps to express T in terms of dimensionless variables g_o and $\frac{E}{V_o}$.) What is the limit of the transmission probability as the energy approaches the barrier height ($E \to V_o$) in each case?

   (c) For a high, wide barrier, *i.e.* $g_o \gg 1$, how does T vary with L when $E < V_o$? Comment on the probability of a goldfish tunneling through the wall of its bowl.

   (d) As we saw in lecture, the transmission probability for a particle of mass m incident on a potential well of depth $-V_o$ is given by,

   $$T = \frac{1}{1 + \frac{V_o^2}{4E(E + V_o)} \sin^2(k_2 L)} \, ,$$

   where $k_2^2 = \frac{2m}{\hbar^2}(E + V_o)$. Show that you can derive this result from that of the barrier of height $+V_o$ by taking V_o negative and keeping track of resulting signs and factors of i. Why does this work? Again, sketch T as a function of E/V_o for a very wide well ($g_o = 20$), a medium well($g_0 = 2$), and a thin well ($g_o = 0.2$).

---

[1]You may use a program of your choice to generate the curves, but you should sketch them by hand in your solutions, indicating any values of particular importance.

(e) A hypothetical experimentalist friend of mine is conducting an experiment with a particularly interesting piece of wire which has a curious localized feature half way along its length. My friend, being a excellent quantum mechanic, decides to measure $T(E)$, the transmission amplitude for scattering a single electron with energy E (measured in eV, electron volts) past this feature. She eventually reports the following data:
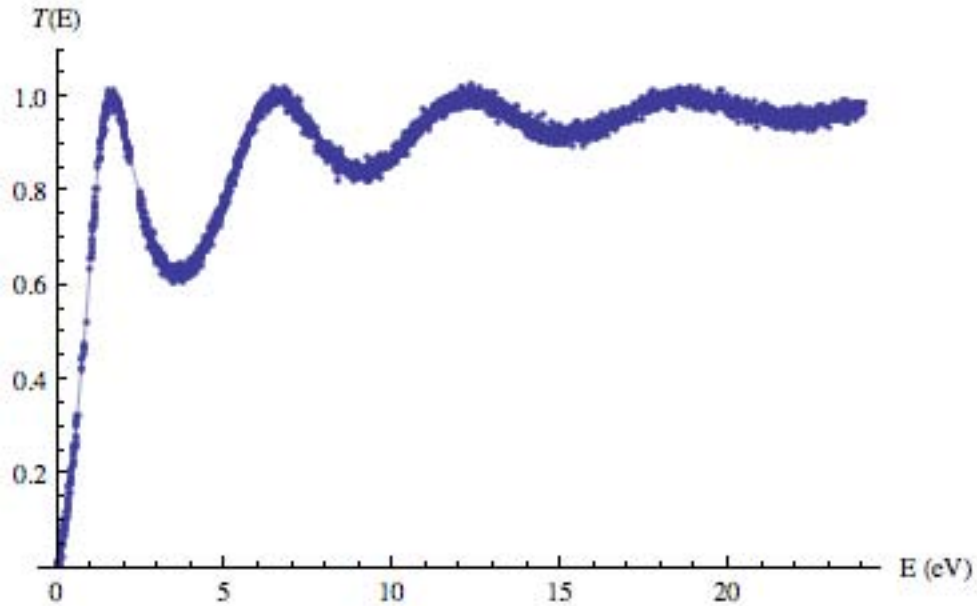
Use this data to come up with a numerically reasonable model potential describing the localized feature on the wire. Estimate a characteristic energy and width for the feature on the wire which is scattering these electrons. Sketch the resulting potential, indicating any important features.

4. **(20 points) Properties of the S-Matrix**

Consider a localized potential, $V(x)$, which vanishes outside some region (*e.g.* a finite square well, or a δ-function barrier, etc.). Outside this "interaction" region the potential is constant, so the energy eigenstates are simple plane-waves moving either toward or away from the interaction region, with direction and amplitudes given in the plot below. Note that the amplitudes A, B, C and D are *not* independent; precisely how these amplitudes are related to each other is determined by the potential.
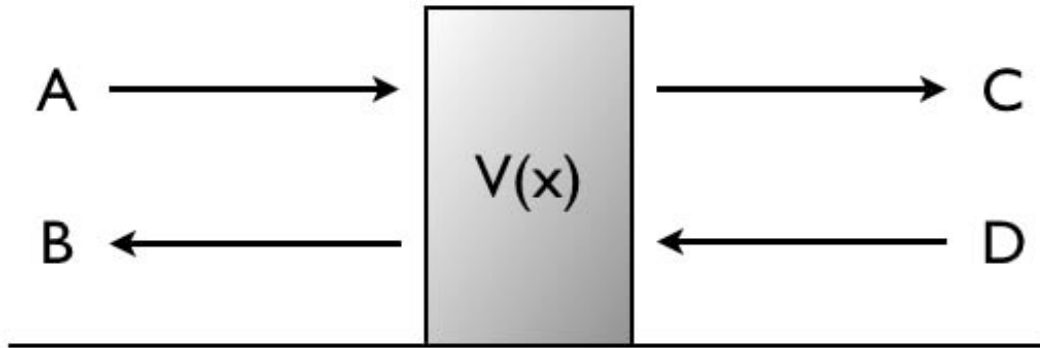
"Scattering" is the process of sending particles in toward the interaction region from far away, watching what comes flying back, and deducing the physics of the interaction region from the results (does it contain a finite well? a delta function? a manticore?). Explicitly, by sending in a known set of waves from far away (with amplitude A from the left and D from the right), then observing the outgoing waves leaving the interaction region (with scattered amplitudes B and C), we can *infer* the relations between A, B, C and D imposed by the potential, and thus infer the physics of the potential itself.

A convenient way to encode these relations is via the "Scattering matrix" or S-matrix, $\hat{S}(E)$, which relates incoming and outgoing waves at fixed energy E,

$$\phi_E^{out} = \hat{S}(E)\, \phi_E^{in} \, .$$

In our 1d localized potentials, the in-going waves have amplitudes A and D, while the out-going waves have amplitudes B and C, so $\hat{S}(E)$ is simply a 2×2 matrix acting as:

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix} \begin{bmatrix} A \\ D \end{bmatrix}, \qquad \hat{S}(E) = \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix}.$$

Note that we've suppressed the E-dependence of the components of $\hat{S}(E)$. Keep in mind, however, that these are non-trivial functions of the energy, E. As we'll see, the detailed E-dependence of these components encodes all of the physics of the system.

(a) Give a physical interpretation for $|r|^2$, $|t|^2$, $|\tilde{r}|^2$ and $|\tilde{t}|^2$ in terms of observable quantities. Design an experiment which measures $|t|^2$. Design another experiment which measures the *phase* of t.

(b) Physically, why must the S-matrix be a unitary matrix?

(c) Use Unitarity of $\hat{S}$ to show that,

$$|r|^2 + |t|^2 = 1, \qquad |\tilde{t}|^2 + |\tilde{r}|^2 = 1, \qquad r^*\tilde{t} + t^*\tilde{r} = 0.$$

The columns of $\hat{S}$ are thus orthogonal unit vectors. Physically, why must this be true?

(d) Show that Parity (symmetry of $V(x)$ under $x \to -x$) implies that $t = \tilde{t}$ and $r = \tilde{r}$, *i.e.* that scattering is identical whether from left or right.

(e) The *scattering phase* φ is defined as the phase of the transmission amplitude[2], $t = |t|e^{-i\varphi}$. Show that, for any symmetric potential, we must have that

$$r = \pm i|r|e^{-i\varphi}$$

(f) Discuss the physical meaning of the scattering phase φ, and illustrate this interpretation in terms of your experiments in part (a).

---

[2]You will find all sorts of conventions for how to define *the* scattering phase in the literature, differing *e.g.* by adding or subtracting π, by overall signs, etc. Of course, nothing physical depends on our choice of conventions – different conventions just make different equations look simple. But keep this in mind when you see the phrase "scattering phase" in the literature, and always check which conventions are being used!

5. **(25 points) Scattering off an Attractive δ-function Well**

Consider the scattering of particles of mass m off an attractive delta function potential of strength V_o located at the origin,

$$V(x) = -V_o\,\delta(x)\;,$$

with $V_o > 0$.

(a) Suppose a beam of particles is incident from the left with typical energy E. Calculate the fraction of particles in the incident beam that are reflected by this potential, i.e. find the reflection coefficient R. Write your answer in terms of E, m, V_o and any fundamental constants needed. Check if your result is reasonable in the limits $V_o \to 0$ for constant E, and $E \to 0$ for constant V_o.

(b) Compute the S-matrix for this system. Verify that it is Unitary.

(c) Find the scattering phase, φ, and sketch it as a function of E.

(d) Observe that $\hat{S}$ has a pole at an imaginary value of k corresponding to a negative value of E. Show that the corresponding energy is none other than the energy of the sole bound state of this potential.

(e) Explain, heuristically, why this last result must be true – why must S diverge precisely at the energy of every bound state of a potential?

Now consider a potential made up of two delta functions, as you studied in PSet 6 last week:

$$V(x) = -V_o\,\delta(x + L) - V_o\,\delta(x - L)\,.$$

where V_o is again positive.

(d) Compute the S-matrix for this system. Verify that it is Unitary.
   Hint: Derive the matching conditions by hand, but solve the resulting linear equations using Mathematica – it's faster and more reliable that doing the algebra by hand, and it's good to get used to Mathematica (or the symbolic algebra package of your choice).

(e) Again find the bound states from the S-matrix.

8.04 Quantum Physics I

Spring 2013