Problem 1. Consider the following probabilistic game: There are four doors (Q, R, S, T). Behind each door is a device which displays ± 1 randomly according to the probability $P(Q = \pm 1, R = \pm 1, S = \pm 1, T = \pm 1)$. Alice and Bob are on the same team. Alice has to choose either Q and R, and then Bob has to choose either S and T. When the numbers match, they get $+1$ point; when the numbers do not match, they get -1 point. However, when they open Q and T, it's an exception. When the numbers (do not) match, they get -1 $(+1)$.

1.1 Let's assume Alice and Bob open the doors completely randomly. When all numbers are $+1$ with probability 1, what is the expectation value of the point they get?

Solution. Let $\mathbf{E}$ be the expectation value of the number of points. In this case, the numbers behind the two doors will always match. So

$$\mathbf{E} = \frac{QS + RS + RT - QT}{4} = \frac{1 + 1 + 1 - 1}{4} = \frac{1}{2}.$$

1.2 As it turns out, irrespective of how hard you fine tune the probability $P(Q = \pm 1, R = \pm 1, S = \pm 1, T = \pm 1)$, the expectation value of the point Alice and Bob get cannot exceed a certain value Max:

$$\frac{\mathbf{E}(QS) + \mathbf{E}(RS) + \mathbf{E}(RT) - \mathbf{E}(QT)}{4} \leq \text{Max}.$$

Here, $\mathbf{E}(QS)$, etc. is the expectation value of the point when Alice opens Q and Bob opens S. This is a Bell inequality. Determine Max.

Hint: For a given realization of the numbers $Q = \pm 1$, $R = \pm 1$, $S = \pm 1$, $T = \pm 1$, which occurs with probability $P(Q, R, S, T)$, note that $QS + RS + RT - QT = (Q + R)S + (R - Q)T$, where one of $\{(R + Q), (R - Q)\}$ is 2 and the other 0.

Solution. In addition to the information provided in the hint, both S and T must be ± 1. This means the only possibilities for the number of points earned are

$$\frac{(Q + R)S + (R - Q)T}{4} = \begin{cases} \dfrac{(0)(-1) + (2)(1)}{4} = \dfrac{1}{2}, \\ \dfrac{(0)(1) + (2)(-1)}{4} = -\dfrac{1}{2}. \end{cases}$$

Thus,

$$\text{Max} = \frac{1}{2}.$$

1.3 Frustrated by the upper bound set by the Bell inequality, Bob decides to cheat. He now changes the value of T after Alice chooses Q or R. Assume Q, R, S are set to be $+1$ with probability 1. To make the expectation value of the point they get equal to $+1$, what values should Bob set after Alice chooses Q or R?

Solution. If Alice chooses R, Bob should set $T = 1$. If Alice chooses Q, Bob should set $T = -1$. This way,

$$\frac{\mathbf{E}(QS) + \mathbf{E}(RS) + \mathbf{E}(RT) - \mathbf{E}(QT)}{4} = \frac{1 + 1 + 1 + 1}{4} = 1.$$

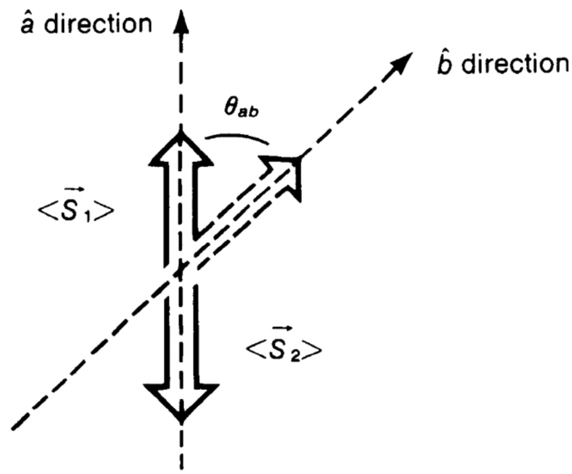

Figure 1: Evaluation of $P(\hat{\mathbf{a}}+;\hat{\mathbf{b}}+)$. Figure 3.9 in Sakurai.

1.4 Now consider a quantum mechanical version of the game. There are quantum states of two spin-1/2 degrees of freedom shared by Alice and Bob. Alice can measure the z component or x components of the first spin $\mathbf{S}^A$. (This corresponds to $Q = \pm 1$ or $R = \pm 1$.) Bob can measure the $-(z + x)$ component or the $(z - x)$ component of the second spin $\mathbf{S}^B$. (This corresponds to $S = \pm 1$ or $T = \pm 1$.)

More specifically, Alice and Bob share the quantum state

$$|\psi\rangle = \frac{|{\uparrow_z}\rangle \otimes |{\downarrow_z}\rangle - |{\downarrow_z}\rangle \otimes |{\uparrow_z}\rangle}{\sqrt{2}}.$$

The operators to be measured are

$$Q = S_z^A, \qquad R = S_x^A, \qquad S = -\frac{S_z^B + S_x^B}{\sqrt{2}}, \qquad T = \frac{S_z^B - S_x^B}{\sqrt{2}}.$$

Let us consider the case when Alice measures Q and Bob measures T. Calculate the probability $P(Q, T)$ for Alice and Bob getting the measurement outcomes $(Q, T) = (\pm 1, \pm 1)$.

Solution. From Sakurai (3.9.11), the probability of measuring $\mathbf{S} \cdot \hat{\mathbf{a}}$ and $\mathbf{S} \cdot \hat{\mathbf{b}}$ to both be positive is

$$P(\hat{\mathbf{a}}+;\hat{\mathbf{b}}+) = \frac{1}{2}\sin^2\left(\frac{\theta_{ab}}{2}\right),$$

where θ_{ab} is the angle between the $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$ directions. For the other combinations, we may generalize this expression using Fig. 3.9 in Sakurai, reproduced here as Fig. 1.

This gives us

$$P(\hat{\mathbf{a}}-;\hat{\mathbf{b}}-) = \frac{1}{2}\sin^2\left(\frac{\theta_{ab}}{2}\right) = P(\hat{\mathbf{a}}+;\hat{\mathbf{b}}+), \tag{1}$$

$$P(\hat{\mathbf{a}}+;\hat{\mathbf{b}}-) = \frac{1}{2}\sin^2\left(\frac{\theta_{ab}+\pi}{2}\right) = \frac{1}{2}\cos^2\left(\frac{\theta_{ab}}{2}\right) = P(\hat{\mathbf{a}}+;\hat{\mathbf{b}}-). \tag{2}$$

For Q and T, $\theta_{ab} = \pi/4$. So we have

$$P(Q = \pm 1, T = \pm 1) = \frac{1}{2}\sin^2\left(\frac{\pi}{8}\right) = \frac{1}{2}\left(\frac{\sqrt{2-\sqrt{2}}}{2}\right)^2 = \frac{1}{2}\frac{2-\sqrt{2}}{4} = \frac{2-\sqrt{2}}{8} \approx 0.073,$$

$$P(Q = \pm 1, T = \mp 1) = \frac{1}{2}\cos^2\left(\frac{\pi}{8}\right) = \frac{1}{2}\left(\frac{\sqrt{2+\sqrt{2}}}{2}\right)^2 = \frac{1}{2}\frac{2+\sqrt{2}}{4} = \frac{2+\sqrt{2}}{8} \approx 0.427.$$

1.5 Similarly, consider the case when Alice measures R and Bob measures T. Calculate the probability $P(R,T)$ for Alice and Bob getting the measurement outcomes $(R,T) = (\pm 1, \pm 1)$.

Solution. We can apply (1) and (2) for R and T, where $\theta_{ab} = 3\pi/4$. This yields

$$P(R = \pm 1, T = \pm 1) = \frac{1}{2}\sin^2\left(\frac{3\pi}{8}\right) = \frac{1}{2}\left(\frac{\sqrt{2+\sqrt{2}}}{2}\right)^2 = \frac{1}{2}\frac{2+\sqrt{2}}{4} = \frac{2+\sqrt{2}}{8} \approx 0.427,$$

$$P(R = \pm 1, T = \mp 1) = \frac{1}{2}\cos^2\left(\frac{3\pi}{8}\right) = \frac{1}{2}\left(\frac{\sqrt{2-\sqrt{2}}}{2}\right)^2 = \frac{1}{2}\frac{2-\sqrt{2}}{4} = \frac{2-\sqrt{2}}{8} \approx 0.073.$$

1.6 Compute the expectation values $\mathbf{E}(QS)$, $\mathbf{E}(RS)$, $\mathbf{E}(QT)$, and $\mathbf{E}(RT)$. Compute

$$\frac{\mathbf{E}(QS) + \mathbf{E}(RS) + \mathbf{E}(RT) - \mathbf{E}(QT)}{4}.$$

Solution. We need to find the probabilities of obtaining $(Q,S) = (\pm 1, \pm 1)$ and $(R,S) = (\pm 1, \pm 1)$. For Q and S, $\theta_{ab} = 3\pi/4$, so another application of (1) and (2) yields

$$P(Q = \pm 1, S = \pm 1) = P(R = \pm 1, T = \pm 1), \qquad P(Q = \pm 1, S = \mp 1) = P(R = \pm 1, T = \mp 1).$$

For R and S, $\theta_{ab} = 5\pi/4$, so

$$P(R = \pm 1, S = \pm 1) = \frac{1}{2}\sin^2\left(\frac{5\pi}{8}\right) = \frac{1}{2}\left(\frac{\sqrt{2+\sqrt{2}}}{2}\right)^2 = \frac{1}{2}\frac{2+\sqrt{2}}{4} = \frac{2+\sqrt{2}}{8} \approx 0.427,$$

$$P(R = \pm 1, S = \mp 1) = \frac{1}{2}\cos^2\left(\frac{5\pi}{8}\right) = \frac{1}{2}\left(\frac{\sqrt{2-\sqrt{2}}}{2}\right)^2 = \frac{1}{2}\frac{2-\sqrt{2}}{4} = \frac{2-\sqrt{2}}{8} \approx 0.073.$$

The expectation value of a random variable X is defined

$$E(X) = \sum_i p_i x_i,$$

where x_i are all of the possible values of X, and p_i the probabilities associated with each. Then

$$\mathbf{E}(QS) = 2P(Q = \pm 1, S = \pm 1) - 2P(Q = \pm 1, S = \mp 1) = \frac{2+\sqrt{2}}{4} - \frac{2-\sqrt{2}}{4} = \frac{\sqrt{2}}{2},$$

$$\mathbf{E}(RS) = 2P(R = \pm 1, S = \pm 1) - 2P(R = \pm 1, S = \mp 1) = \frac{2+\sqrt{2}}{4} - \frac{2-\sqrt{2}}{4} = \frac{\sqrt{2}}{2},$$

$$\mathbf{E}(RT) = 2P(R = \pm 1, T = \pm 1) - 2P(R = \pm 1, T = \mp 1) = \frac{2+\sqrt{2}}{4} - \frac{2-\sqrt{2}}{4} = \frac{\sqrt{2}}{2},$$

$$\mathbf{E}(QT) = 2P(Q = \pm 1, T = \pm 1) - 2P(Q = \pm 1, T = \mp 1) = \frac{2-\sqrt{2}}{4} - \frac{2+\sqrt{2}}{4} = -\frac{\sqrt{2}}{2}.$$

Finally,

$$\frac{\mathbf{E}(QS) + \mathbf{E}(RS) + \mathbf{E}(RT) - \mathbf{E}(QT)}{4} = \frac{1}{4}\left(\frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2}\right) = \frac{\sqrt{2}}{2},$$

which is greater than Max, thereby violating Bell's inequality.

Problem 2. Consider a quantum particle with mass m moving in the presence of the square well potential

$$V(r) = \begin{cases} -V_0 & r \leq a, \\ 0 & r > a. \end{cases}$$

2.1 Writing the wave function in polar coordinates as $\psi(\mathbf{r}) = R_l(r)\,Y_{lm}(\theta,\phi)$, write down the Schrödinger equation obeyed by R_l.

Solution. From (A.5.1) in Sakurai, the full Schrödinger equation is

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi_E}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi_E}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi_E}{\partial\phi^2}\right] + V(r)\,\psi_E = E\psi_E,$$

where the angular part of ψ_E satisfies (A.5.4),

$$-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]Y_{lm} = l(l+1)Y_{lm}.$$

Then the equivalent one-dimensional Schrödinger equation is the equation immediately following (A.5.8),

$$-\frac{\hbar^2}{2m}\frac{d^2u_E}{dr^2} + \left[V(r) + \frac{l(l+1)\hbar^2}{2mr^2}\right]u_E = Eu_E, \tag{3}$$

where $u_E(r) = rR_l(r)$. In terms of R_l,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}(rR_l) + \left[V(r) + \frac{l(l+1)\hbar^2}{2mr^2}\right]rR_l = ErR_l.$$

or

$$\left\{\frac{\hbar^2}{2m}\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{l(l+1)}{r^2}\right] + V(r)\right\}R_l(r) = E_l\,R_l(r).$$

From (7.7.1), the effective potential at low energies for the lth partial wave is

$$V_{\text{eff}} = V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2},$$

so the Schrödinger equation can be rewritten as

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + V_{\text{eff}}\right]R_l(r) = E_l\,R_l(r).$$

2.2 When V_0 is a certain value, there is one bound state for the s wave ($l=0$). The bound state energy ε is small ($0 < |\varepsilon| \ll V_0$). Obtain the range of the depth of the well V_0 ($? \leq V_0 < ?$). Also, calculate for the bound state the probability for the particle to exist outside of the well.

Solution. Inside the well, R_l are given by (A.5.16),

$$R_l(r) = \text{constant } j_l(\alpha r),$$

where α is defined in Eq. (A.5.17),

$$\alpha = \sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}},$$

and the spherical Bessel functions j_l are given by (A.5.12),

$$j_l(\rho) = \sqrt{\frac{\pi}{2\rho}} J_{l+1/2}(\rho).$$

For the s wave, the relevant Bessel function is given by (A.5.12),

$$j_0(\rho) = \frac{\sin\rho}{\rho}. \tag{4}$$

But for $l - 0$, V_{eff} reduces to $V(r)$, so (3) reduces to the one-dimensional problem for u_E,

$$-\frac{\hbar^2}{2m}\frac{d^2 u_E}{dr^2} + V(r)u_E = Eu_E.$$

The bound-state solutions are given by (A.2.6),

$$u_E \sim \begin{cases} e^{-\kappa r} & \text{for } r > a, \\ \cos kr \quad \text{(even parity)} & \text{for } r < a, \\ \sin kr \quad \text{(odd parity)} & \text{for } r < a, \end{cases} \tag{5}$$

where k and κ are defined by (A.2.7),

$$k = \sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}}, \qquad \kappa = \sqrt{\frac{2m|E|}{\hbar^2}}.$$

So we see that $\alpha = k$, and thus we are interested in the odd-parity solutions to the one-dimensional problem.

For the one-dimensional problem, the allowed values of bound-state energy,

$$E = -\frac{\hbar^2\kappa^2}{2m},$$

can be found by solving (A.2.8),

$$ka \tan ka = \kappa a \quad \text{(even parity)}, \qquad ka \cot ka = -\kappa a \quad \text{(odd parity)},$$

where κ and k are related by (A.2.9),

$$\frac{2mV_0 a^2}{\hbar^2} = (k^2 + \kappa^2)a^2.$$

We are interested in the odd parity solutions, so we want to solve

$$ka \cot ka = -\kappa a. \tag{6}$$

For the right side, we can write

$$-\kappa a = -\sqrt{\frac{2mV_0 a^2}{\hbar^2} - k^2 a^2} \equiv -\sqrt{z^2 - (ka)^2}, \tag{7}$$

where we have defined z.

Now we can solve the equation graphically. Note that ka is positive definite. This means that (6) has its first ka axis intercept at $ka = \pi/2$, where the slope is negative. Note also that $-\kappa a$ given by (7) is an equation for one quarter of an ellipse in quadrant IV, so it is not defined above the ka axis. Therefore it is not possible for

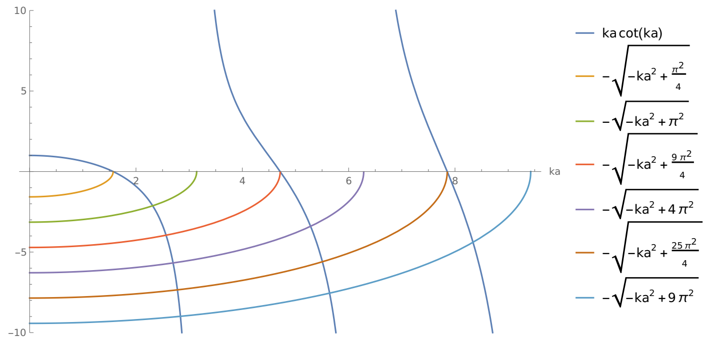

Figure 2: Plot demonstrating single bound state solutions to (6) in the range $\pi/2 < z < 3\pi/2$, where z is defined in (7).

the two graphs to intersect for $z < \pi/2$. For $z > 3\pi/2$, the graphs intersect more than once, meaning there is more than one bound state. In Fig. 2, this is illustrated with κa for $z = n\pi/2$ with $n = 1, 2, 3, \ldots$.

Finally, we have the restriction

$$\frac{\pi}{2} \leq \sqrt{\frac{2mV_0a^2}{\hbar^2}} < \frac{3\pi}{2} \qquad \Longrightarrow \qquad \frac{\pi^2\hbar^2}{8ma^2} \leq V_0 < \frac{9\pi^2\hbar^2}{8ma^2}. \tag{8}$$

For the probability for a particle in the bound state to exist outside the well, we impose the normalization condition

$$1 = \langle\psi|\psi\rangle = \int \psi_0^2(\mathbf{r})\, d^3x = \int R_0^2(r)\, Y_{00}(\theta,\phi)\, d^3x = \int_0^\infty R_0^2(r)\, r^2\, dr\,,$$

since Y_{lm} are normalized. From (5), we know

$$R_0(r) = \begin{cases} -\dfrac{e^{-\kappa r}}{\kappa r} & r > a, \\ \dfrac{\sin kr}{kr} & r < a, \end{cases}$$

so the normalization condition becomes

$$1 = \frac{1}{k^2}\int_0^a \sin^2 kr\, dr + \frac{1}{\kappa^2}\int_a^\infty e^{-2\kappa r}\, dr \equiv A + B,$$

where we have defined A and B. The probability for the particle to exist outside the well is then

$$P(r > a) = \frac{B}{A+B}.$$

Note that

$$A = \frac{1}{k^2}\int_0^a \sin^2 kr\, dr = \frac{1}{2k^2}\int_0^a (1 - \cos 2kr)\, dr = \frac{1}{2k^2}\left[r - \frac{\sin 2kr}{2k}\right]_0^a = \frac{2ka - \sin 2ka}{4k^3},$$

$$B = \frac{1}{\kappa^2}\int_a^\infty e^{-2\kappa r}\, dr = \frac{1}{\kappa^2}\left[-\frac{e^{-2\kappa r}}{2\kappa}\right]_a^\infty = \frac{e^{-2\kappa a}}{2\kappa^3},$$

and that

$$A + B = \frac{2k\kappa^3 a - \kappa^3 \sin 2ka + 2k^3 e^{-2\kappa a}}{4\kappa^3 k^3}.$$

Then the probability is

$$P(r > a) = \frac{e^{-2\kappa a}}{2\kappa^3} \frac{4\kappa^3 k^3}{2k\kappa^3 a - \kappa^3 \sin 2ka + 2k^3 e^{-2\kappa a}} = \frac{k^3 e^{-2\kappa a}}{k\kappa^3 a - \kappa^3 \sin ka \cos ka + k^3 e^{-2\kappa a}}.$$

Equating the two cases of R_0 at the boundary, we obtain

$$-\frac{e^{\kappa a}}{\kappa a} = \frac{\sin ka}{ka} \qquad \Longrightarrow \qquad k^2 e^{-2\kappa a} = \kappa^2 \sin^2 ka,$$

and we can write the probability entirely in terms of trigonometric functions of ka:

$$P(r > a) = \frac{k\kappa^2 \sin^2 ka}{k\kappa^3 a - \kappa^3 \sin ka \cos ka + k\kappa^2 \sin^2 ka} = \frac{k \sin^2 ka}{k\kappa a + k \sin^2 ka - \kappa \sin ka \cos ka}.$$

2.3 Consider the scattering problem by the well. For each l, for large enough r, when $R_l(r)$ is given by

$$R_l(r) \sim A_l \frac{\sin(kr - l\pi/2 + \delta_l)}{r}, \tag{9}$$

δ_l is called the scattering phase shift. For the value of V_0 within the range you obtained in the above problem, when the energy of the incident wave is $E = 9V_0/16$, calculate $\tan \delta_0$ (where δ_0 is the scattering phase shift for the s wave).

Solution. Now we will use the notation

$$k' = \sqrt{\frac{2m(V_0 + E)}{\hbar^2}}, \qquad\qquad k = \sqrt{\frac{2mE}{\hbar^2}}, \tag{10}$$

where $E > 0$ and the definition of k' comes from Sakurai (7.7.7),

$$E + V_0 = \frac{\hbar^2 k'^2}{2m},$$

where we have changed the sign of V_0 to match the notation used here.

We need to match (9) with the solution for $r < a$ at the boundary. In the new notation, the s wave solution for $r < a$ is

$$R_0(r) = B_0 \frac{\sin k'r}{k'r}. \tag{11}$$

Matching (11) and (9) for $l = 0$ at $r = a$, we obtain

$$A_0 \frac{\sin(ka + \delta_0)}{a} = B_0 \frac{\sin k'a}{k'a} \qquad \Longrightarrow \qquad \sin(ka + \delta_0) = \frac{B_0}{k' A_0} \sin k'a. \tag{12}$$

We also need to match the first derivative at the boundary. Differentiating (12), we find

$$\cos(ka + \delta_0) = \frac{B_0}{k A_0} \cos k'a. \tag{13}$$

Then, dividing (12) by (13) gives us

$$\tan(ka + \delta_0) = \frac{k}{k'} \tan k'a.$$

Using the tangent addition formula

$$\tan(a + b) = \frac{\tan a + \tan b}{1 - \tan a \tan b},$$

we get

$$\begin{aligned}
\frac{\tan ka + \tan\delta_0}{1 - \tan ka \tan\delta_0} &= \frac{k}{k'}\tan k'a \\
\tan ka + \tan\delta_0 &= \frac{k}{k'}\tan k'a - \frac{k}{k'}\tan k'a \tan ka \tan\delta_0 \\
\tan\delta_0\left(1 + \frac{k}{k'}\tan k'a \tan ka\right) &= \frac{k}{k'}\tan k'a - \tan ka \\
\tan\delta_0 &= \frac{k\tan k'a - k'\tan ka}{k' + k\tan k'a \tan ka}. \qquad (14)
\end{aligned}$$

When the energy of the incident wave is $E = 9V_0/16$,

$$k' = \sqrt{\frac{25mV_0}{8\hbar^2}}, \qquad k = \sqrt{\frac{9mV_0}{8\hbar^2}}, \qquad \frac{k}{k'} = \frac{3}{5}.$$

Using the range of V_0 given by (8), we obtain the ranges

$$\frac{5\pi}{8a} \le k' < \frac{15\pi}{8a} \qquad \frac{3\pi}{8a} \le k < \frac{9\pi}{8a}.$$

Substituting these into (21), the lower bounds give

$$\begin{aligned}
\tan\delta_0 &= \frac{3\tan(5\pi/8) - 5\tan(3\pi/8)}{5 + 3\tan(5\pi/8)\tan(3\pi/8)} = \frac{-3(1+\sqrt{2}) - 5(1+\sqrt{2})}{5 - 3(1+\sqrt{2})(1+\sqrt{2})} = \frac{8(1+\sqrt{2})}{3(3+2\sqrt{2}) - 5} = \frac{4+4\sqrt{2}}{2+3\sqrt{2}}\frac{2-3\sqrt{2}}{2-3\sqrt{2}} \\
&= \frac{4\sqrt{2}+16}{14} = \frac{\sqrt{8}+8}{7},
\end{aligned}$$

and the upper bounds give

$$\begin{aligned}
\tan\delta_0 &= \frac{3\tan(15\pi/8) - 5\tan(9\pi/8)}{5 + 3\tan(15\pi/8)\tan(9\pi/8)} = \frac{3(1-\sqrt{2}) + 5(1-\sqrt{2})}{5 - 3(1-\sqrt{2})(1-\sqrt{2})} = \frac{8(1-\sqrt{2})}{5 - 3(3-2\sqrt{2})} = \frac{4-4\sqrt{2}}{3\sqrt{2}-2}\frac{2+3\sqrt{2}}{2+3\sqrt{2}} \\
&= \frac{4\sqrt{2}-16}{14} = \frac{\sqrt{8}-8}{7}.
\end{aligned}$$

So we have the range

$$\frac{\sqrt{8}-8}{7} < \tan\delta_0 < \frac{\sqrt{8}+8}{7}.$$

2.4 Now consider the S matrix, $S \equiv e^{2i\delta_0} = e^{i\delta_0}/e^{-i\delta_0}$. Compare the condition on s wave bound state energies and the zero of the denominator of S. Explain their relation.

Solution. S has a pole on the imaginary axis when

$$0 = \mathrm{Re}[e^{-i\delta_0}] = \mathrm{Re}[\cos\delta_0 - i\sin\delta_0] = \cos\delta_0 \quad \Longrightarrow \quad \delta_0 = n\pi + \frac{\pi}{2}, \quad n = 0, 1, 2, \ldots.$$

This is similar to the condition we saw for bound state energies in 2.2. As displayed in Fig. 2, the $(n+1)$th bound state appears when $z = n\pi + \pi/2$. From the definition of z in (7), there are $(n+1)$ possible bound states when

$$\sqrt{\frac{2mV_0a^2}{\hbar^2}} > n\pi + \frac{\pi}{2}, \quad n = 0, 1, 2, \ldots,$$

which gives a relationship between V_0, the depth of the potential well, and the δ_0 corresponding to the poles of S. As we increase the depth of the potential well, we move along the imaginary axis, and an additional bound state appears for every pole we cross.

Problem 3. Consider a three dimensional potential

$$V(r) = \frac{\hbar^2\gamma}{2m}\delta(r-a).$$

The s wave Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\chi_0(r)}{dr^2} + \frac{\hbar^2\gamma}{2m}\delta(r-a)\,\chi_0(r) = E\,\chi_0(r).$$

The s wave function must be regular (zero) at $r=0$. At $r=a$, it is continuous, but its derivative can jump.

3.1 Calculate the s wave scattering phase shift $\delta_0(k)$, where k is related to E as $E = \hbar^2k^2/2m$.

Solution. Sakurai (7.7.2) gives the integral equation for the partial wave,

$$\frac{e^{i\delta_l}\sin\delta_l}{k} = -\frac{2m}{\hbar^2}\int_0^\infty j_l(kr)\,V(r)\,A_l(k;r)\,r^2\,dr\,. \tag{15}$$

This is given in the statement of Problem 8.b in Sakurai, as is

$$A_l(r) = j_l(kr) - \frac{2imk}{\hbar^2}\int_0^\infty j_l(kr_<)\,h_l^{(1)}(kr_>)\,V(r')\,A_l(k;r')\,r'^2\,dr'\,, \tag{16}$$

where $h_l^{(1)}$ are the spherical Hankel functions, defined by (A.5.18),

$$h_l^{(1)}(\rho) = j_l(\rho) + in_l(\rho), \tag{17}$$

where $r_<$ is the smaller of r and r', and $r_>$ the larger. Also, n_l are the spherical Neumann functions, given by (A.5.12),

$$n_l(\rho) = (-1)^{l+1}\sqrt{\frac{\pi}{2\rho}}J_{-l-1/2}(\rho).$$

For $r<a$, (16) becomes

$$A_l(k;r) = j_l(kr) - \frac{2imk}{\hbar^2}\int_0^\infty j_l(kr)\,h_l^{(1)}(kr')\,\frac{\hbar^2\gamma}{2m}\delta(r'-a)\,A_l(k;r')\,r'^2\,dr' = j_l(kr) - ika^2\gamma j_l(kr)\,h_l^{(1)}(ka)\,A_l(k;a),$$

and for $r>a$,

$$A_l(k;r) = j_l(kr) - \frac{2imk}{\hbar^2}\int_0^\infty j_l(kr')\,h_l^{(1)}(kr)\,\frac{\hbar^2\gamma}{2m}\delta(r'-a)\,A_l(k;r')\,r'^2\,dr' = j_l(kr) - ika^2\gamma j_l(ka)\,h_l^{(1)}(kr)\,A_l(k;a).$$

At $r=a$, both equations become

$$A_l(k;a) = j_l(ka) - ika^2\gamma h_l^{(1)}(ka)\,j_l(ka)\,A_l(k;a) \quad\implies\quad A_l(k;a) = \frac{j_l(ka)}{1+ika^2\gamma\,j_l(ka)\,h_l^{(1)}(ka)}.$$

Using this result, (15) gives us

$$\frac{e^{i\delta_l}\sin\delta_l}{k} = -\frac{2m}{\hbar^2}\int_0^\infty j_l(kr)\,\frac{\hbar^2\gamma}{2m}\delta(r-a)\,A_l(k;r)\,r^2\,dr = -a^2\gamma\,j_l(ka)\,A_l(k;a) = -\frac{a^2\gamma\,j_l^2(ka)}{1+ika^2\gamma\,j_l(ka)\,h_l^{(1)}(ka)},$$

or

$$e^{i\delta_l}\sin\delta_l = -\frac{ka^2\gamma\, j_l^2(ka)}{1 + ika^2\gamma\, j_l(ka)\, h_l^{(1)}(ka)}. \tag{18}$$

According to Gottfried Ch. 15 (5) we can apply (17) to find

$$\tan\delta_l = -\frac{ka^2\gamma\, j_l^2(ka)}{1 - ka^2\gamma\, j_l(ka)\, n_l(ka)}.$$

For the s wave, the relevant j_0 is given by (4), and from (A.5.12),

$$n_0(\rho) = -\frac{\cos\rho}{\rho}. \tag{19}$$

Then

$$\tan\delta_0 = -\frac{ka^2\gamma\, j_0^2(ka)}{1 - ka^2\gamma\, j_0(ka)\, n_0(ka)} = -\frac{ka^2\gamma\, \sin^2 ka/(ka)^2}{1 + ka^2\gamma \sin ka \cos ka/(ka)^2} = -\frac{\gamma\, \sin^2 ka}{k + \gamma \sin ka \cos ka} \tag{20}$$

and so we have found

$$\delta_0(k) = \tan^{-1}\!\left(-\frac{\gamma\, \sin^2 ka}{k + \gamma \sin ka \cos ka}\right). \tag{21}$$

3.2 When $\gamma \gg k$, $1/a$ and when $\sin ka$ is not small, discuss the behavior of the scattering phase shift.

Solution. In the limit $\gamma \gg k$, (21) becomes

$$\delta_0 \to \tan^{-1}\!\left(-\frac{\gamma\, \sin^2 ka}{\gamma \sin ka \cos ka}\right) = \tan^{-1}(-\cot ka) = \tan^{-1}[\cot(-ka)] = -ka.$$

This is the same as the hard sphere result discussed in Sec. 7.6 of Sakurai and given in (7.6.44). When the delta function potential's strength γ becomes very large compared to the energy $E = \hbar^2 k^2/2m$ of an incoming particle (coming from outside), the particle will not be able to penetrate the shell. This physical situation is just like the particle scattering off the surface of an infinitely hard sphere, so it makes sense that the phase shift is the same in both situations.

3.3 Obtain the condition to have resonant states and calculate the energy of the resonant states.

Solution. From the discussion in Sec. 7.8 of Sakurai, at a resonance where $k = k^*$ we must have

$$\cot[\delta_l(k^*)] = 0, \qquad \left.\frac{d\cot\delta_l}{dk}\right|_{k^*} < 0. \tag{22}$$

From (20),

$$\cot\delta_0 = -\frac{k + \gamma \sin ka \cos ka}{\gamma\, \sin^2 ka} = 0 \qquad \Longrightarrow \qquad -\frac{k}{\gamma} = \sin ka \cos ka = \frac{\sin(2ka)}{2}.$$

Rearranging this, we obtain

$$\sin(2ka) = -\frac{2ka}{\gamma a}, \tag{23}$$

which we may solve graphically. As shown in Fig. 3, (23) has roots near $ka = n\pi/2$ for $n = 0, 1, 2, \ldots \lessapprox 2\gamma$. As γ increases, they become closer to $n\pi/2$.

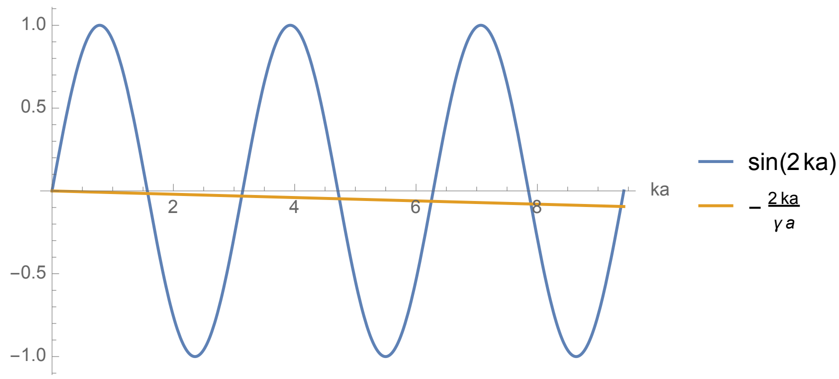

Figure 3: Plot demonstrating roots of (23). The roots at $n\pi$ $(n = 0, 1, 2, \ldots)$ correspond to resonances.

We must determine which roots fulfill the second condition in (22). Note that

$$\begin{aligned}\frac{d\cot\delta_0}{dk} &= -\frac{d}{dk}\left(\frac{k}{\gamma}\csc^2 ka + \cot ka\right) = -\left[\frac{\csc^2 ka}{\gamma}\frac{dk}{dk} + \frac{k}{\gamma}\frac{d}{dk}\left(\csc^2 ka\right) + \frac{d}{dk}\left(\cot ka\right)\right] \\ &= -\frac{\csc^2 ka}{\gamma} + \frac{2ka}{\gamma}\cot ka\csc^2 ka + a\csc^2 ka = \frac{a\gamma - 1 + 2ka\cot ka}{\gamma\sin^2 ka}. \end{aligned} \tag{24}$$

For $k^* = n\pi/2$ with n odd,

$$\left.\frac{d\cot\delta_0}{dk}\right|_{k^*} = \frac{a\gamma - 1}{\gamma} \sim a \not< 0,$$

since (23) has no solutions if $a\gamma < 1$, $a\gamma$ being positive definite. For n even, applying L'Hospital's rule gives us

$$\lim_{k\to k^*}\frac{d\cot\delta_0}{dk} = \lim_{k\to k^*}\frac{\cot ka - ka\csc^2 ka}{\gamma\sin ka\cos ka} = -\infty < 0,$$

since $\csc^2 ka$ blows up faster than $\cot ka$. So we have $ka \approx n\pi$ for $n = 0, 1, 2, \ldots \lessapprox \gamma$.

In the limit $\gamma \gg k$, we may approximate the offset of the resonances from the x axis as $-1/\gamma a$. Then the condition for resonance is

$$k_n \approx \frac{n\pi}{a}\left(1 - \frac{1}{\gamma a}\right), \quad n = 0, 1, 2, \ldots \lessapprox \gamma,$$

and the energies of the resonant states are

$$E_n \approx \frac{n^2\pi^2\hbar^2}{2ma^2}\left(1 - \frac{2}{\gamma R}\right), \quad n = 0, 1, 2, \ldots \lessapprox \gamma,$$

where we have dropped terms of $\mathcal{O}\big(\gamma^{-2}\big)$.

3.4 Calculate the width Γ of the resonance. Discuss its behavior when γ is big.

Solution. Sakurai (7.8.8) relates the width to the phase shift:

$$\left.\frac{d(\cot\delta_l)}{dE}\right|_{E=E_r} \equiv -\frac{2}{\Gamma}.$$

Applying (24),

$$\frac{d(\cot\delta_0)}{dE} = \frac{d(\cot\delta_0)}{dk}\frac{dk}{dE} = \frac{d(\cot\delta_0)}{dk}\frac{d}{dE}\left(\sqrt{\frac{2mE}{\hbar^2}}\right) = \sqrt{\frac{m}{2\hbar^2 E}}\frac{a\gamma - 1 + 2ka\cot ka}{\gamma\sin^2 ka} = \frac{m}{\hbar^2 k}\frac{a\gamma - 1 + 2ka\cot ka}{\gamma\sin^2 ka}.$$

Taking the limit that γ is reasonably large, we have

$$\sin ka = \sin\left(n\pi - \frac{n\pi}{\gamma a}\right) = \sin n\pi \cos\left(\frac{n\pi}{\gamma a}\right) - \cos n\pi \sin\left(\frac{n\pi}{\gamma a}\right) \approx (-1)^{n+1}\frac{n\pi}{\gamma a},$$
$$\cos ka = \sin\left(n\pi - \frac{n\pi}{\gamma a}\right) = \cos n\pi \cos\left(\frac{n\pi}{\gamma a}\right) + \sin n\pi \sin\left(\frac{n\pi}{\gamma a}\right) \approx (-1)^{n},$$

where we have dropped terms of $\mathcal{O}(\gamma^{-2})$. Then taking $\gamma \gg k$ and $k \approx n\pi/a$, and discarding large terms that will end up in the denominator of Γ,

$$\left.\frac{d(\cot\delta_l)}{dE}\right|_{E=E_n} = \frac{m}{\hbar^2 k}\left(\frac{a\gamma/k - 1/k}{\gamma/k} + \frac{2a\cos ka}{(\gamma/k)\sin ka}\right)\frac{1}{\sin^2 ka} \approx \frac{ma}{\hbar^2 k}\left(1 + \frac{2\cos ka}{\gamma \sin ka}\right)\frac{1}{\sin^2 ka}$$
$$\approx \frac{2ma}{\hbar^2 k\gamma}\frac{\cos ka}{\sin^3 ka} \approx \frac{2ma^2}{n\pi\hbar^2}\frac{(-1)^n}{(-1)^{3n+3}}\left(\frac{\gamma a}{n\pi}\right)^3 = -\frac{2ma^5\gamma^3}{n^4\pi^4\hbar^2},$$

so we obtain

$$\Gamma_n \approx \frac{n^4\pi^4\hbar^2}{ma^5\gamma^3}.$$

Inspecting the above, clearly $\Gamma \to 0$ quickly when γ is very large. This makes sense because the potential shell becomes impenetrable in the limit $\gamma \to \infty$, when a particle bound inside the shell is unable to escape. The lifetime of the bound state—which is proportional to Γ^{-1}—is infinite in this limit, hence $\Gamma \to 0$.

3.5 When the velocity of the incident wave is small, obtain the scattering cross section.

Solution. Sakurai (7.6.18) gives an expression for the total cross section,

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l.$$

In the low-energy limit, corresponding to low velocity of the incident wave, we need only consider s wave scattering. The total cross section becomes

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sin^2\delta_0.$$

From (4) and (17)–(19), according to Gottfried Ch. 15 (24) we can write

$$\sin^2\delta_0 = \frac{\gamma^2\sin^4 ka}{[k - \gamma\sin ka\cos ka]^2 + \gamma^2\sin^4 ka}.$$

Taking the limit $k \to 0$,

$$\sin^2\delta_0 \to \frac{\gamma^2(ka)^4}{[k-\gamma ka]^2 + \gamma^2(ka)^4} = \frac{\gamma^2(ka)^4}{k^2 - 2\gamma k^2 a - \gamma^2 k^2 a^2 + \gamma^2 k^4 a^4} = \frac{\gamma^2 k^2 a^4}{1 - 2\gamma a + \gamma^2 a^2 + \gamma^2 k^2 a^4}$$
$$\approx \frac{\gamma^2 k^2 a^4}{1 - 2\gamma a + \gamma^2 a^2} = \frac{k^2 a^4 \gamma^2}{(1-\gamma a)^2},$$

so

$$\sigma_{\text{tot}} = \frac{4\pi a^4\gamma^2}{(1-\gamma a)^2}.$$

I consulted Sakurai's *Modern Quantum Mechanics*, Merzbacher's *Quantum Mechanics*, Gottfried's *Quantum Mechanics Volume I: Fundamentals*, Napolitano's solutions to the problems in Sakurai, the MIT OpenCourseWare notes on Introduction to Applied Nuclear Physics, Masatsugu Sei Suzuki's notes on phase shift analysis, and Wolfram MathWorld while writing these solutions.