# Homework 8

## Problem 1

From page 154 of Griffiths, we have

```
In[•]:= R32[r_] := 4 a^(-3/2) (r/a)^2 Exp[-r/(3 a)]/(81 Sqrt[30])
        R31[r_] := 8 a^(-3/2) (r/a) (1 - r/(6 a)) Exp[-r/(3 a)]/(27 Sqrt[6])
```

The integral is then given by

```
In[•]:= Integrate[r^3 R32[r] × R31[r], {r, 0, ∞}] (* No need to conjugate as R_32 (r) is real *)
```

Out[•]=

$$-\frac{9\sqrt{5}\,a}{2} \quad \text{if } \mathrm{Re}[a] > 0$$

The spherical harmonics $Y_{lm}$ are incorporated in Mathematica. The matrix element of $\cos[\theta]$ is:

```
In[•]:= Integrate[ Conjugate@SphericalHarmonicY[2, 1, θ, ϕ]
          SphericalHarmonicY[1, 1, θ, ϕ] Sin[θ] Cos[θ], {θ, 0, Pi}, {ϕ, 0, 2 Pi}]
        Integrate[ Conjugate@SphericalHarmonicY[2, -1, θ, ϕ]
          SphericalHarmonicY[1, -1, θ, ϕ] Sin[θ] Cos[θ], {θ, 0, Pi}, {ϕ, 0, 2 Pi}]
```

Out[•]=

$$\frac{1}{\sqrt{5}}$$

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$$\frac{1}{\sqrt{5}}$$

# Problem 2

## (a)

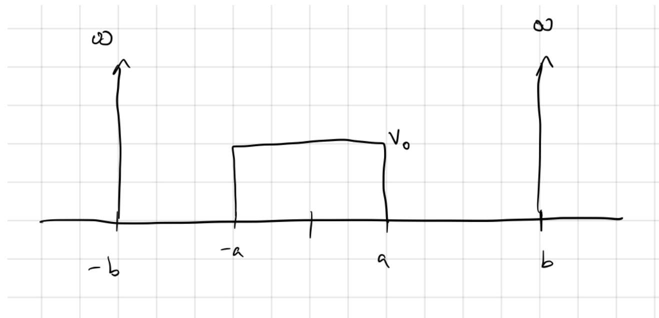



Figure 1: Sketch of $V(x)$

The sketch for $V(x)$ is shown in figure 1. The potential $V(x)$ is symmetric, which implies that the eigenstates are either symmetric or anti-symmetric[1]. Therefore, the solutions to the Shcrodinger equation are of the form

$$\psi_{\pm}(x) = \begin{cases} \psi_1(-x), & 0 \leq x < a \\ \pm\psi_1(x), & -a \leq x < 0 \\ \psi_2(x), & a \leq x < b \\ \pm\psi_2(-x), & -b < x < -a \\ 0, & |x| \geq b \end{cases} . \tag{1}$$

For symmetric functions, we need $d\psi/\psi x|_{x=0} = 0$ (otherwise $\psi(x)$ wouldn't be symmetric). For anti-symmetric functions we need $\psi(0) = -\psi(0) \implies \psi(0) = 0$. Since the solution for positive $x$ determines the solution for negative $x$, we can solve the problem in the interval $[0, b]$ and use the boundary conditions $\psi'(x = 0) = 0$ or $\psi(x = 0) = 0$ to find the symmetric and anti-symmetric solutions respectively. Note that we are changing the information from the potential on the negative side by the boundary conditions at $x = 0$.

## (b)

The Shcrodinger equation is

$$H = -\frac{\hbar^2}{2m}\partial_x^2 + V(x). \tag{2}$$

Let's write the solution as

$$\psi(x) = \begin{cases} Ae^{qx} + Be^{-qx}, & x < a \\ Ce^{ikx} + De^{-ikx}, & a < x < b. \end{cases} \tag{3}$$

Applying $H$ to both wavegunctions, we obtain

$$H\psi(x) = \begin{cases} \left(-\frac{\hbar^2 q^2}{2m} + V_0\right)\left(Ae^{qx} + Be^{-qx}\right) \\ \frac{\hbar^2 k^2}{2m}\left(Ce^{ikx} + De^{-ikx}\right) \end{cases} \tag{4}$$

Since $H\psi(x) = E\psi(x)$, the energy should be the same whether we are in $x < a$ or $a < x$. This implies

$$-\frac{\hbar^2 q^2}{2m} + V_0 = \frac{\hbar^2 k^2}{2m} \implies \boxed{(qa)^2 + (ka)^2 = \frac{2mV_0 a^2}{\hbar^2}}. \tag{5}$$

[1] One easy way to see this is that if $P$ is the parity (inversion) operator ($P\hat{x}P^{-1} = -\hat{x}$), then $PHP^{-1} = H$ (the Hamiltonian is symmetric under inversion). Then, the eigenstates $\psi$ can be written as eigenstates of $P$: $P\psi = \lambda\psi$. Since applying the parity operator twice should return the same wavefunction, we have $P^2\psi = \lambda^2\psi \implies \lambda = \pm 1$. Which means the eigenstates are either symmetric ($\lambda = 1$) or anti-symmetric ($\lambda = -1$).

For both symmetric and anti-symmetric states, the boundary condition at $x = b$ implies

$$\psi(x = b) = 0 = Ce^{ikb} + De^{-ikb} \implies D = -Ce^{2ikb}, \tag{6}$$

which means

$$\psi(a < x < b) \propto e^{ikx} - e^{-ik(x-2b)} = e^{ikb}\left[e^{ik(x-b)} - e^{-ik(x-b)}\right] = 2ie^{ikb}\sin(k(x-b)). \tag{7}$$

Then, we have

$$\psi(x) = \begin{cases} Ae^{qx} + Be^{-qx}, & x < a \\ 2ie^{ikb}\sin(k(x-b)), & a < x < b. \end{cases} \tag{8}$$

Above, we have set $C = 1$ (which we can do as long as we normalize our wavefunction at the end). For the symmetric states, we have $\psi'(x = 0) = 0$, that is,

$$\psi'(x = 0) = q(A - B) = 0 \implies A = B. \tag{9}$$

The above implies $\psi(x) = 2A\cosh(qx)$ for $x < a$. Since the wavefunctions have to match at $x = a$, we have

$$2A\cosh(qa) = 2ie^{ikb}\sin(k(a-b)) \tag{10}$$

The derivative $\psi'(x)$ should also be the same at $x = a$. We obtain

$$2Aq\sinh(qa) = 2ie^{ikb}k\cos(k(a-b)) \tag{11}$$

Diving the last equation by the previous one, we obtain

$$\boxed{qa\tanh(qa) = -\frac{ka}{\tan[k(b-a)]}} \tag{12}$$

(we have added a factor of $1/a$ on both sides and used the fact that the tangent is an anti-symmetric function) for the symmetric case. For the anti-symmetric function, we have

$$\psi(x) = 0 = A + B \implies A = -B. \tag{13}$$

Then, we have

$$\psi(x) = \begin{cases} 2A\sinh(qx) & x < a \\ 2ie^{ikb}\sin[k(x-b)] & a < x < b \end{cases} \tag{14}$$

From the boundary conditions for $\psi(a)$ and $\psi'(a)$, we obtain the equations

$$2A\sinh(qa) = 2ie^{ikb}\sin[k(a-b)], \tag{15}$$

$$2Aq\cosh D(qa) = 2ie^{ikb}k\cos[k(a-b)]. \tag{16}$$

Dividing the first one by the second one we get

$$\boxed{\frac{\tanh(qa)}{qa} = -\frac{\tan[k(b-a)]}{ka}}. \tag{17}$$

# Problem 2 (continuation)

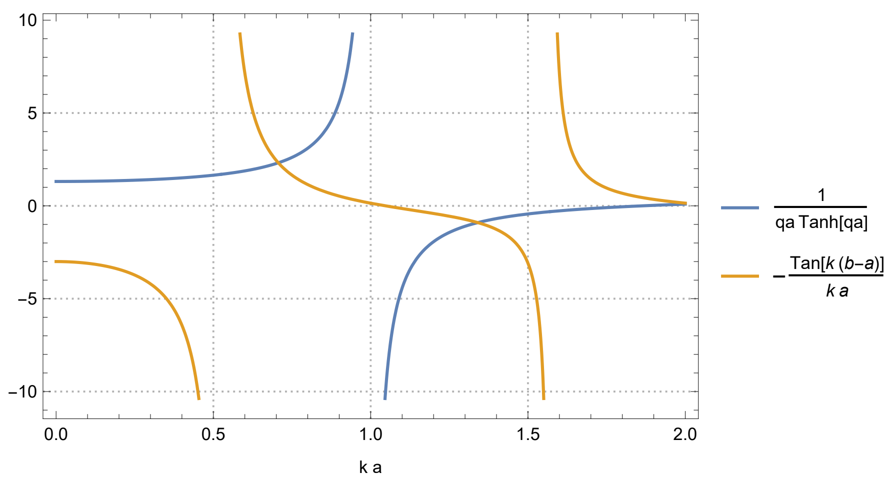
(c) Let’s find the solutions.

In[62]:=
```
a = 1;
b = 4 a;
q[k_] := Sqrt[1 - k^2]; (* Since the energy is ∝ k^2,
let's plot everything with respect to k*)
```

- Symmetric case

In[72]:=
```
Plot[{1/(Tanh[q[k] a] q[k] a), -Tan[k (b - a)]/(k a)},
 {k, 0, 2}, PlotLegends → {"1/(qa Tanh[qa])", "-Tan[k (b - a)]/(k a)"},
 PlotTheme → "Detailed", FrameLabel → {"k a"}]
```

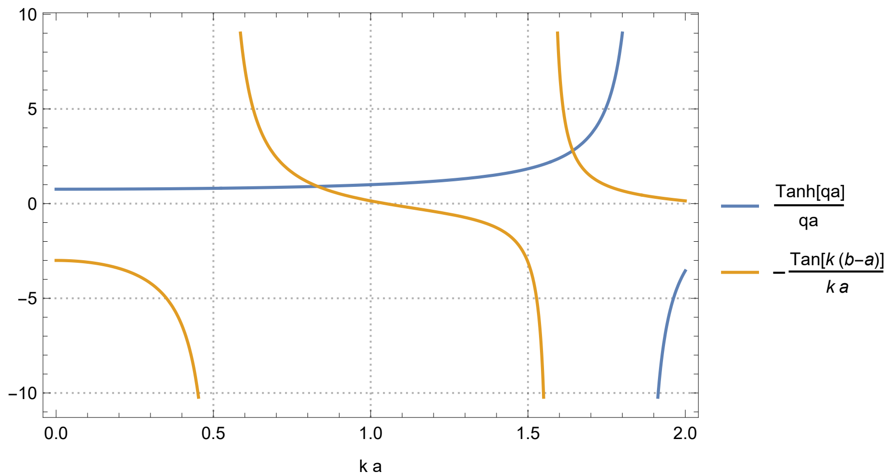
Out[72]=




- Anti-symmetric case

In[71]:= 
```
Plot[{Tanh[q[k] a]/(q[k] a), -Tan[k (b - a)]/(k a)},
  {k, 0, 2}, PlotLegends → {"Tanh[qa]/qa", "-Tan[k (b - a)]/(k a)"},
  PlotTheme → "Detailed", FrameLabel → {"k a"}]
```

Out[71]=




(d) The energy is $\propto (\text{k}\,a)^2$. We can see that there is a solution at an earlier k for the symmetric case, which means that the lowest-energy solution is symmetric. This is consistent with our physical intuition that the ground state wavefunction does not have nodes.

In[67]:=