Delta potential well F2016

Problem 6: Delta function in a 1-D well(10 pts)

A particle of mass m is placed in an attractive 1-D delta function potential

$$V(x) = -\hbar^2 \lambda \delta(x)/m$$

with positive λ. The particle and the potential are located in an infinite box with walls at x=$\pm$ $a/2$ (i.e $V(a/2) = V(-a/2) = \infty$)

a) Determine the condition on the parameters for which the system will have exactly one bound state with negative energy eigenvalue E and give its wave function (4 pts).

b) For the same system, determine the energy eigenvalues and eigenvectors for states with positive E. (3 pts)

c) If the coefficient $\lambda < 0$, explain in detail how your results change for parts a) and b) (3 pts)

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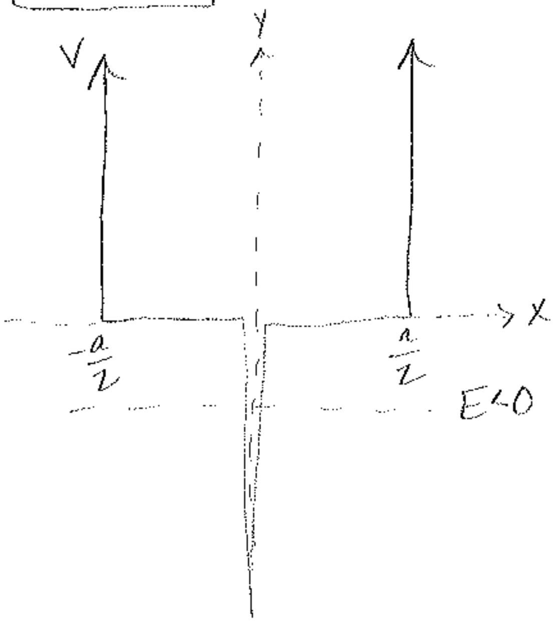
Part (a)



In general, the Schrödinger equation tells us

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right]\psi = E\psi.$$

For the regions $-\frac{a}{2}<x<0$ and $0<x<\frac{a}{2}$, this becomes

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi.$$

If we let

$$k = \frac{\sqrt{-2mE}}{\hbar}$$

Since $E<0$, this becomes

$$\frac{d^2\psi}{dx^2} = k^2\psi.$$

The general solution in each region is

$$\psi_-(x) = Ae^{kx} + Be^{-kx}, \quad -\frac{a}{2}<x<0$$

$$\psi_+(x) = Ce^{kx} + De^{-kx}, \quad 0<x<\frac{a}{2}.$$

Now we want to apply our boundary conditions to simplify this function.

We know that we must have $\psi(x)=0$ at $x=\pm\frac{a}{2}$ since $V=0$ for $|x|<\frac{a}{2}$. So

$$\psi_-\left(-\frac{a}{2}\right) = 0 = Ae^{-\frac{ka}{2}} + Be^{\frac{ka}{2}}$$
$$\psi_+\left(\frac{a}{2}\right) = 0 = Ce^{\frac{ka}{2}} + De^{-\frac{ka}{2}},$$

which implies

$$B = -Ae^{-ka}$$
$$D = -Ce^{ka}.$$

So we are left with

$$\psi_-(x) = Ae^{kx} - Ae^{-k(x+a)}$$
$$\psi_+(x) = Ce^{kx} - Ce^{-k(x-a)}.$$

Now we want to relate A and C. At $x=0$, we know that the wave-function must be continuous. So

$$\psi_-(0) = \psi_+(0)$$
$$A - Ae^{-ka} = C - Ce^{ka}$$
$$A(1-e^{-ka}) = C(1-e^{ka})$$
$$C = A\,\frac{1-e^{-ka}}{1-e^{ka}}$$

and our wavefunction becomes

$$\psi_-(x) = Ae^{kx} - Ae^{-k(x+a)}$$
$$\psi_+(x) = A\,\frac{1-e^{-ka}}{1-e^{ka}}\left(e^{kx} - e^{-k(x-a)}\right)$$

Now, we know that the derivative of ψ is not continuous at $x=0$ since our potential is infinite there. So we want to integrate Schrödinger's equation over a small ε-neighborhood around $x=0$. Then

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2\psi}{dx^2}\,dx - \frac{\hbar^2\lambda}{m}\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)\,dx = E\int_{-\varepsilon}^{\varepsilon}\psi(x)\,dx$$

$$-\frac{\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{-\varepsilon}^{\varepsilon} - \frac{\hbar^2\lambda}{m}\psi(0) = E\int_{-\varepsilon}^{\varepsilon}\psi(x)\,dx$$

Now let $\varepsilon\to 0$. This gives us zero for the right-hand side since $\psi(x)$ is continuous at $x=0$. However, our derivative is not continuous, so we must take the limit as $\varepsilon\to 0^-$ (left) and $\varepsilon\to 0^+$ (right) for the appropriate region. So we have

$$-\frac{\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{\varepsilon\to 0}^{\varepsilon\to 0} = -\frac{\hbar^2}{2m}\left[\frac{d\psi_+}{dx}\Big|_{\varepsilon\to 0^+} - \frac{d\psi_-}{dx}\Big|_{\varepsilon\to 0^-}\right].$$

We know

$$\frac{d\psi_+}{dx} = A\,\frac{1-e^{-ka}}{1-e^{ka}}\left(ke^{kx}+ke^{-k(x-a)}\right)$$

$$\frac{d\psi_-}{dx} = Ake^{kx} + Ake^{-k(x+a)},$$

So

$$\frac{d\psi_+}{dx}\Big|_{\varepsilon\to 0^+} = Ak\,\frac{1-e^{-ka}}{1-e^{ka}}\left(1+e^{ka}\right)$$

$$\frac{d\psi_-}{dx}\Big|_{\varepsilon\to 0^-} = Ak\left(1+e^{-ka}\right)$$

and so

$$\frac{-\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{-\varepsilon\to 0}^{\varepsilon\to 0} = \frac{-\hbar^2}{2m}\left[Ak\,\frac{1-e^{-ka}}{1-e^{ka}}\left(1+e^{ka}\right) - Ak\left(1+e^{-ka}\right)\right]$$

$$= \frac{-\hbar^2}{2m}kA\left[\frac{1-e^{-ka}}{1-e^{ka}}\left(1+e^{ka}\right) - \left(1+e^{-ka}\right)\right].$$

Then we have

$$\frac{-\hbar^2}{2m}kA\left[\frac{1-e^{-ka}}{1-e^{ka}}\left(1+e^{ka}\right) - \left(1+e^{-ka}\right)\right] - \frac{\hbar^2\lambda}{m}A\left(1-e^{-ka}\right) = 0$$

$$\frac{-\cancel{\hbar^2}}{\cancel{2m}}k\cancel{A}\left[\frac{\left(1-e^{-ka}\right)\left(1+e^{ka}\right)}{1-e^{ka}} - \left(1+e^{-ka}\right)\right] = \frac{\cancel{\hbar^2}\lambda}{\cancel{m}}\cancel{A}\left(1-e^{-ka}\right)$$

$$k\left[\frac{\left(1-e^{-ka}\right)\left(1+e^{ka}\right)}{\left(1-e^{ka}\right)\left(1-e^{-ka}\right)} - \frac{\left(1+e^{-ka}\right)}{\left(1-e^{-ka}\right)}\right] = -2\lambda$$

$$k\left[\frac{\left(1-e^{-ka}\right)\left(1+e^{ka}\right)}{\left(1-e^{ka}\right)\left(1-e^{-ka}\right)} - \frac{\left(1+e^{-ka}\right)\left(1-e^{ka}\right)}{\left(1-e^{ka}\right)\left(1-e^{-ka}\right)}\right] = -2\lambda$$

$$k\left[\frac{\cancel{1}+e^{ka}-e^{-ka}-\cancel{1} - \left(\cancel{1}-e^{ka}+e^{-ka}-\cancel{1}\right)}{\left(1-e^{ka}\right)\left(1-e^{-ka}\right)}\right] = -2\lambda$$

$$k\left[\frac{2e^{ka}-2e^{-ka}}{\left(1-e^{ka}\right)\left(1-e^{-ka}\right)}\right] = -2\lambda$$

$$k\left[\frac{2\left(e^{ka}-e^{-ka}\right)}{\left(1-e^{ka}\right)\left(1-e^{-ka}\right)}\right] = -2\lambda$$

$$k\left[\frac{2(1+e^{ka})(1-e^{-ka})}{(1-e^{ka})(1-e^{-ka})}\right]=-2\lambda$$

$$k\left[\frac{-2(1+e^{ka})}{(e^{ka}-1)}\right]=-2\lambda$$

$$k\,\frac{1+e^{ka}}{e^{ka}-1}=\lambda$$

$$k\,\frac{1+e^{ka}}{e^{ka}-1}\cdot\frac{e^{-ka/2}}{e^{-ka/2}}=\lambda$$

$$k\left[\frac{e^{-ka/2}+e^{ka/2}}{e^{ka/2}-e^{-ka/2}}\right]=\lambda$$

But

$$2\sinh(x)=e^{x}-e^{-x}$$
$$2\cosh(x)=e^{x}+e^{-x},$$

so we have

$$k\left[\frac{2\cosh(ka/2)}{2\sinh(ka/2)}\right]=\lambda,$$

which simplifies to the transcendental equation

$$\boxed{k=\lambda\tanh\left(\frac{ka}{2}\right)},$$

where $k=\frac{\sqrt{-2mE}}{\hbar}$.

Now we want to determine the condition such that we have a single bound state, other than $k=0$. In order for $y=k$ and $y=\lambda \tanh\left(\frac{ka}{2}\right)$ to intersect at another point other than $k=0$, we know that the slope of our hyperbolic function, at $k=0$, must be greater than the slope of our line at $k=0$. So

$$\frac{d}{dk}\left(\lambda \tanh\left(\frac{ka}{2}\right)\right) > \frac{d}{dk}(k)$$

$$\lambda \frac{d}{dk}\left(\tanh\left(\frac{ka}{2}\right)\right) > 1$$

$$\lambda \operatorname{sech}^2\left(\frac{ka}{2}\right)\cdot \frac{a}{2}\Big|_{k=0} > 1$$

$$a\cdot \operatorname{sech}^2(0) > \frac{2}{\lambda}$$

$$a \frac{1}{\cosh^2(0)} > \frac{2}{\lambda}$$

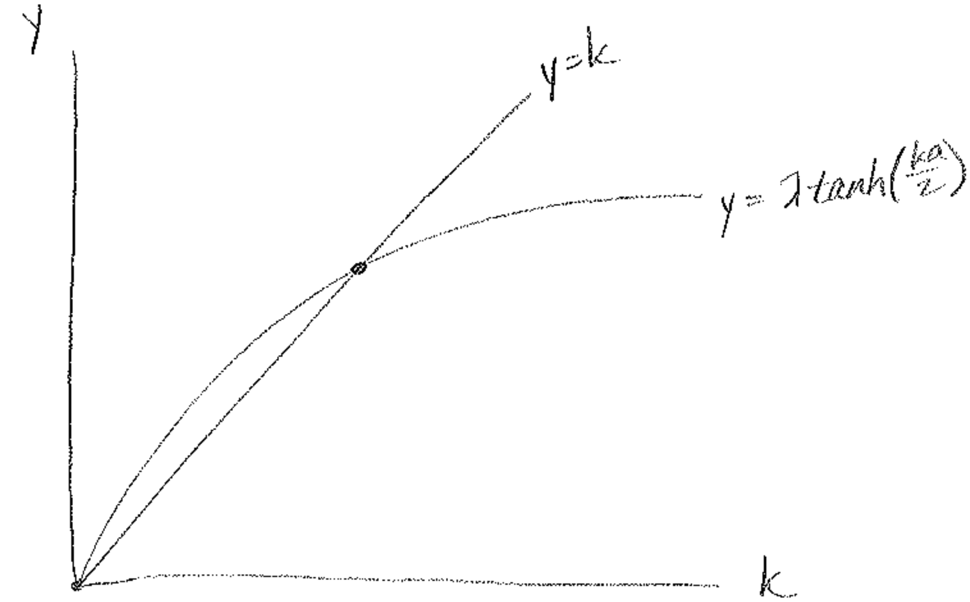
but

$$\cosh(0) = \frac{e^{(0)}+e^{(0)}}{2} = 1,$$

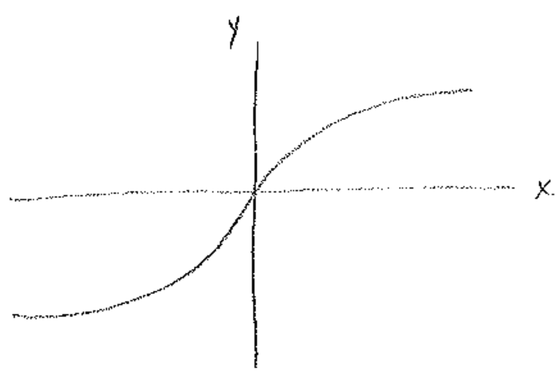
So our condition is that

$$\boxed{a > \frac{2}{\lambda}}$$

If this condition is met, then we have something like this:



Hyperbolic tangent:



Normalizing the wavefunction...

$$2\int_{-a/2}^{0} |\psi_-(x)|^2 \, dx = 1$$

Get

$$A = \left(\frac{k}{1 - e^{-2ka} - 2kae^{-ka}} \right)^{1/2}.$$

Part (b)

We still divide the well into two regions. For $-\frac{a}{2} < x < 0$ and $0 < x < \frac{a}{2}$, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi.$$

Let

$$k = \frac{\sqrt{2mE}}{\hbar}$$

since $E > 0$. Then our equation becomes

$$\frac{d^2\psi}{dx^2} = -k^2\psi.$$

The general solution in each region is

$$\psi_-(x) = A\sin(kx) + B\cos(kx), \quad -\frac{a}{2} < x < 0$$

$$\psi_+(x) = D\sin(kx) + F\cos(kx), \quad 0 < x < \frac{a}{2}$$

Since our potential is symmetric about the origin, we know that $\psi(x)$ can be either even or odd. The parity operator tells us that for even functions,

$$\psi(-x) = \psi(x)$$

and for odd functions,

$$\psi(-x) = -\psi(x).$$

Consider some $x > 0$. Then in the case of odd solutions, we have

$$\psi(-x) = \psi_-(-x) = -\psi(x) = -\psi_+(x),$$

or

$$\psi_-(-x) = -\psi_+(x).$$

So

$$\psi_-(-x) = A\sin(-kx) + B\cos(-kx) = -D\sin(kx) - F\cos(kx)$$

$$-A\sin(kx) + B\cos(kx) = -D\sin(kx) - F\cos(kx),$$

which implies

$$-A = -D$$
$$D = A$$

and

$$B = -F$$
$$F = -B.$$

So our odd wavefunction is given by

$$\psi_-(x) = A\sin(kx) + B\cos(kx) \quad , \quad -\frac{a}{2} < x < 0$$
$$\psi_+(x) = A\sin(kx) - B\cos(kx). \quad , \quad 0 < x < \frac{a}{2}$$

In the case of even solutions, we have

$$\psi(-x) = \psi_-(-x) = \psi(x) = \psi_+(x)$$

or

$$\psi_-(-x) = \psi_+(x).$$

So

$$\psi_-(-x) = A\sin(-kx) + B\cos(-kx) = D\sin(kx) + F\cos(kx)$$
$$-A\sin(kx) + B\cos(kx) = D\sin(kx) + F\cos(kx),$$

which implies

$$D = -A$$

and

$$F = B.$$

Then our even wave-function is given by

$$\psi_-(x) = A\sin(kx) + B\cos(kx)$$
$$\psi_+(x) = -A\sin(kx) + B\cos(kx).$$

Now we want to apply our boundary conditions.

We must have

$$\psi\left(-\frac{a}{2}\right)=0 \quad \text{and} \quad \psi\left(\frac{a}{2}\right)=0.$$

For the odd wavefunction, we have

$$\psi\left(-\frac{a}{2}\right)=\psi_-\left(-\frac{a}{2}\right)=A\sin\left(-\frac{ka}{2}\right)+B\cos\left(-\frac{ka}{2}\right)=0$$

$$-A\sin\left(\frac{ka}{2}\right)=-B\cos\left(\frac{ka}{2}\right)$$

$$B=A\tan\left(\frac{ka}{2}\right).$$

For the even wavefunction, we have the same result. We must also have continuity at $x=0$. For the odd wavefunction, we have

$$\psi_-(0)=\psi_+(0)$$

$$A\sin(0)+B\cos(0)=A\sin(0)-B\cos(0)$$

$$B=-B,$$

which implies $B=0$. Then we must have

$$A\tan\left(\frac{ka}{2}\right)=0.$$

The only nontrivial result tells us

$$\tan\left(\frac{ka}{2}\right)=\frac{\sin\left(\frac{ka}{2}\right)}{\cos\left(\frac{ka}{2}\right)}=0$$

or

$$\sin\left(\frac{ka}{2}\right)=0.$$

This holds true when

$$\frac{ka}{2} = n\pi$$

$$k = \frac{2n\pi}{a}.$$

But

$$k = \frac{\sqrt{2mE}}{\hbar},$$

so

$$\frac{\sqrt{2mE}}{\hbar} = \frac{2n\pi}{a}$$

$$\frac{2mE}{\hbar^2} = \frac{4n^2\pi^2}{a^2}$$

$$\boxed{E = \frac{2n^2\pi^2\hbar^2}{ma^2}}$$

for the odd wavefunction. Now we want to normalize our odd wavefunction. We have

$$\psi_-(x) = A\sin\left(\frac{2n\pi x}{a}\right), \quad -\frac{a}{2} < x < 0$$

$$\psi_+(x) = A\sin\left(\frac{2n\pi x}{a}\right), \quad 0 < x < \frac{a}{2}.$$

We must have

$$\int |\psi(x)|^2 dx = 1.$$

So

$$A^2\int_{-\frac{a}{2}}^{0} \sin^2\left(\frac{2n\pi x}{a}\right)dx + A^2\int_{0}^{a/2} \sin^2\left(\frac{2n\pi x}{a}\right)dx = 1$$

$$A^2\int_{-\frac{a}{2}}^{a/2} \sin^2\left(\frac{2n\pi x}{a}\right)dx = 1$$

but

$$\sin^2(x) = \frac{1}{2}\left[1-\cos(2x)\right],$$

So

$$A^2\int_{-a/2}^{a/2} \frac{1}{2}\left[1-\cos\left(\frac{4n\pi x}{a}\right)\right]dx = 1$$

$$\frac{A^2}{2}\int_{-a/2}^{a/2} \left(1-\cos\left(\frac{4n\pi x}{a}\right)\right)dx = 1$$

$$\frac{A^2}{2}\left[x - \frac{a}{4n\pi}\sin\left(\frac{4n\pi x}{a}\right)\right]\Bigg|_{-a/2}^{a/2} = 1$$

$$\frac{A^2}{2}(a) = 1$$

$$A = \sqrt{\frac{2}{a}}$$

and our odd wave-function is

$$\boxed{\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{2n\pi x}{a}\right)}.$$

This solution essentially does not "see" the delta potential at $x=0$ since the wave-function has a node there.

Now we want to look at the even wavefunction. So

$$\psi_-(0) = \psi_+(0)$$

$$A\sin(0) + B\cos(0) = -A\sin(0) + B\cos(0)$$

$$B = B,$$

which doesn't tell us anything useful. Our next step is to integrate the Schrödinger equation about an ε-neighborhood surrounding $x = 0$. So

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2\psi}{dx^2} - \frac{\hbar^2\lambda}{m}\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi(x)dx = E\int_{-\varepsilon}^{\varepsilon}\psi(x)dx$$

$$-\frac{\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{-\varepsilon}^{\varepsilon} - \frac{\hbar^2\lambda}{m}\psi(0) = E\int_{-\varepsilon}^{\varepsilon}\psi(x)dx.$$

Now let $\varepsilon \to 0$. So

$$-\frac{\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{-\varepsilon\to 0}^{\varepsilon\to 0} = -\frac{\hbar^2}{2m}\left[\frac{d\psi_+}{dx} - \frac{d\psi_-}{dx}\right]\Big|_{\varepsilon\to 0}$$

$$= -\frac{\hbar^2}{2m}\Big[\big(-Ak\cos(kx) - Bk\sin(kx)\big) - \big(Ak\cos(kx) - Bk\sin(kx)\big)\Big]_{\varepsilon\to 0}$$

$$= -\frac{\hbar^2}{2m}\left[-Ak - Ak\right]$$

$$= \frac{\hbar^2 kA}{m}$$

and

$$\frac{\hbar^2 k}{m}A - \frac{\hbar^2\lambda}{m}(B) = 0$$

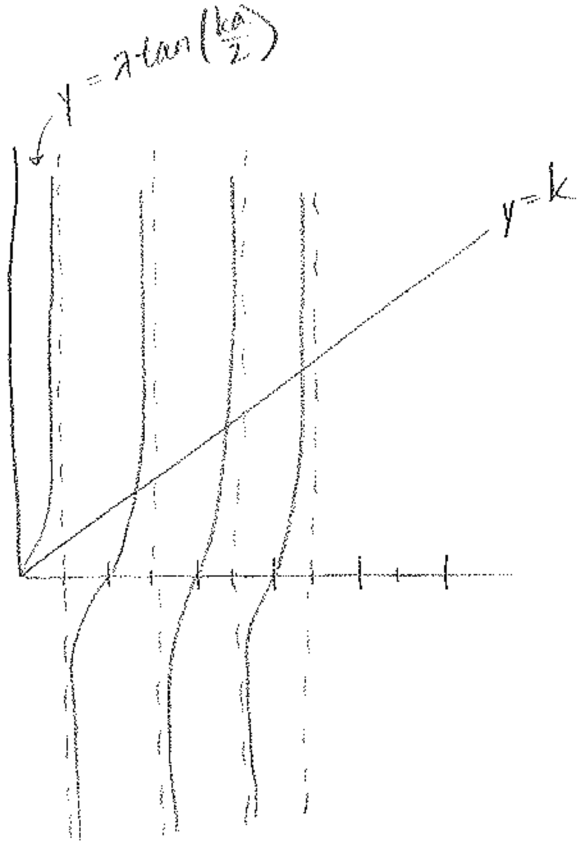
$$\frac{\cancel{\hbar^2} k}{\cancel{m}} \cancel{A} = \frac{\cancel{\hbar^2} \lambda}{\cancel{m}} \left(\cancel{A} \tan\left(\frac{ka}{2}\right) \right)$$

$$\boxed{k = \lambda \tan\left(\frac{ka}{2}\right)},$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}.$$

Plotting, we have



Then, clearly, we have more than one energy for which this equation is satisfied.

Part (c)

If $\lambda < 0$, the delta potential well becomes a potential barrier. Since the only time λ comes into the picture is when we take the ε-neighborhood around $x = 0$, the only thing that will change is the transcendental equation.

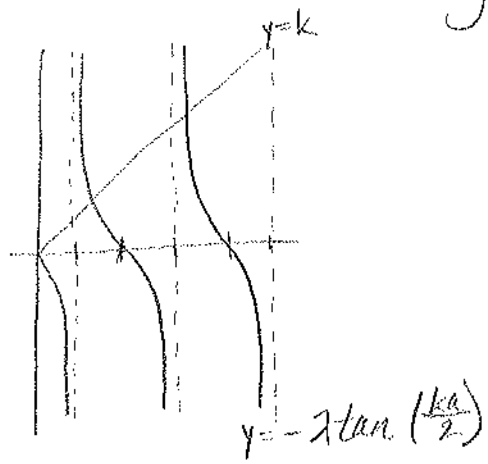
So from part (a), we get

$$k = -\lambda \tanh\left(\frac{ka}{2}\right).$$

There are no solutions other than $k=0$ for this equation. From part (b), we get

$$k = -\lambda \tan\left(\frac{ka}{2}\right).$$

In this case, there are solutions. Plotting, we see



This equation does not admit as low of a ground state as before, but the energies are shifted lower by comparison.