Quantum Mechanics: Interesting Problems

Bloch's Theorem and allowable states

Marko Brnović

Problem 1

Griffiths 5.26

Suppose we use delta function wells, instead of spikes (i.e. switch the sign of α in Equation 5.64). Analyze this case, constructing the analog to Figure 5.5. This requires no new calculation, for the positive energy solutions (except that β is now negative; use $\beta = -1.5$ for the graph), but you do need to work out the negative energy solutions (let $\kappa \equiv \sqrt{-2mE}/\hbar$ and $z \equiv -\kappa a$, for $E < 0$); your graph will now extend to negative z). How many states are there in the first allowed band?

Solution

If we have wells instead of spikes, the potential function will take form:

$$V = -\alpha \sum_{j=0}^{N-1} \delta(x - ja). \tag{1}$$

For $\alpha > 0$. Knowing this, we can analogously extract the solution to the problem with spikes (equation (5.71)), since the only thing that changes is $\alpha \longrightarrow -\alpha$:

$$\cos(qa) = \cos(ka) - \frac{m\alpha}{\hbar^2 k} \sin(ka) \tag{2}$$

For $k = \sqrt{2mE}/\hbar$. If we let $z = ka$ and $\beta = \frac{m\alpha a}{\hbar^2}$, this becomes:

$$\cos\left(\frac{qz}{k}\right) = \cos(z) - \beta \frac{\sin z}{z} = f(z) \tag{3}$$

The left side of the equality above is clearly bounded in the domain $[-1, 1]$. Hence, the right side must be bounded too. To visualise for which values of z the equality is true, it may be more useful to observe the graph for $\beta = 1.5$ (figure 1):

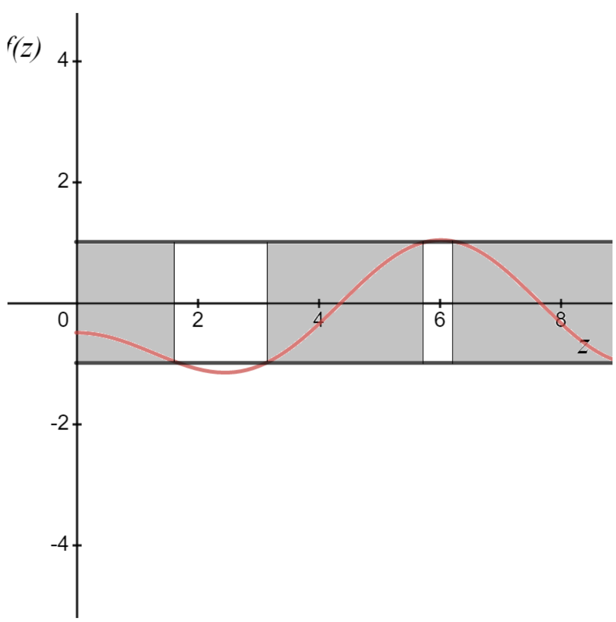

Figure 1: Plot of $f(z)$ against z for $\beta = -1.5$

Here, note that the allowed 'bands' are shown in grey, to distinguish them from the rest of the graph (red line is $f(z)$). Notably, since β is only 50% greater than the maximum of $f(z)$ for $\beta = 0$, this graph admits relatively plenty solutions from the beginning.

It is also to be noted here that the energies are taken to be positive in this part of Griffiths's examples. To account for negative solutions, let $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$ for $E < 0$. Since the equation between the wells still takes the same form, it holds that:

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{2mE}{\hbar^2}\psi \implies \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \kappa^2\psi \tag{4}$$

Since $\kappa > 0$, the solutions take form:

$$\psi(x) = Ae^{\kappa x} + Be^{-\kappa x} \tag{5}$$

We can use Bloch's theorem here, since it still holds that $|\psi(x)|^2$ is periodic at a distance a. In particular, we impose:

$$\psi(x + Na) = \psi(x)e^{iNqa} \tag{6}$$

And we can use the limit:

$$\lim_{N\to\infty} \psi(x + Na) = \psi(x) \tag{7}$$

To deduce that $e^{iNqa} = 1$, and in particular:

$$q = \frac{2\pi n}{Na} \quad \text{for } n \in \mathbb{N} \text{ and } n < N. \tag{8}$$

We then invoke Bloch's theorem for our specific wavefunction in the first potential-free region, and its neighbouring wavefunction to the left ($-a \leq x \leq 0$):

$$Ae^{\kappa(x+a)} + Be^{-\kappa(x+a)} = e^{iqa}\left(Ae^{\kappa x} + Be^{-\kappa x}\right) \tag{9}$$

Since it is continuous at $x = 0$, it holds that:

$$e^{-iqa}\left(Ae^{\kappa a} + Be^{-\kappa a}\right) = A + B \implies A\left(e^{-iqa}e^{\kappa a} - 1\right) = B\left(1 - e^{-iqa}e^{-\kappa a}\right) \tag{10}$$

We also examine the discontinuity of the derivatives at $x = 0$:

$$\left.\frac{\mathrm{d}\psi_{x\geq 0}}{\mathrm{d}x}\right|_{x=0} = \kappa A - \kappa B \tag{11}$$

$$\left.\frac{\mathrm{d}\psi_{x\leq 0}}{\mathrm{d}x}\right|_{x=0} = e^{-iqa}\left(\kappa Ae^{\kappa a} - \kappa Be^{-\kappa a}\right) \tag{12}$$

It holds that:

$$\left.\frac{\mathrm{d}\psi_{x\geq 0}}{\mathrm{d}x}\right|_{x=0} - \left.\frac{\mathrm{d}\psi_{x\leq 0}}{\mathrm{d}x}\right|_{x=0} = \frac{2m\alpha}{\hbar^2}\psi_{x\geq 0}|_{x=0} \tag{13}$$

Which implies

$$\kappa A - \kappa B - \kappa e^{-iqa}Ae^{\kappa a} + \kappa e^{-iqa}Be^{-\kappa a} = \frac{2m\alpha}{\hbar^2}(A + B) \tag{14}$$

$$\implies A\left(1 - \frac{2m\alpha}{\kappa\hbar^2} - e^{-iqa}e^{\kappa a}\right) = B\left(\frac{2m\alpha}{\kappa\hbar^2} + 1 - e^{-iqa}e^{-\kappa a}\right) \tag{15}$$

Combining (10) and (14) for non-zero A we get:

$$\frac{e^{-iqa}e^{\kappa a} - 1}{1 - e^{-iqa}e^{-\kappa a}} = \frac{1 - \frac{2m\alpha}{\kappa\hbar^2} - e^{-iqa}e^{\kappa a}}{\frac{2m\alpha}{\kappa\hbar^2} + 1 - e^{-iqa}e^{-\kappa a}} \tag{16}$$

After cross-multiplying and cancelling common terms, (15) simplifies to:

$$\frac{2m\alpha}{\kappa\hbar^2}e^{-iqa}\left(e^{ka}-e^{-ka}\right)+2e^{-iqa}\left(e^{ka}+e^{-ka}\right)=2+2e^{-2iqa} \tag{17}$$

Multiplying both sides by e^{iqa} and noticing that $e^{ka}-e^{-ka}=2\sinh(ka)$ and $e^{ka}+e^{-ka}=2\cosh(ka)$, this reduces to:

$$\frac{4m\alpha}{\kappa\hbar^2}\sinh(ka)+4\cosh(ka)=2(e^{iqa}+e^{-iqa})=4\cos(qa) \tag{18}$$

Or more succintly, letting $z=-\kappa a$ (representative of negative solutions) and $\beta=\frac{m\alpha a}{\hbar^2}$ as before:

$$\cos\left(\frac{zq}{k}\right)=\cosh(z)-\beta\frac{\sinh(z)}{z}=g(z) \tag{19}$$

Notice here that both $\cos\left(\frac{zq}{k}\right)$ and $\cosh(z)$ are the same as for $z=\kappa a$ whereas $\sinh(z)$ changes sign. Also, note that I chose $\beta>0$ since I defined $\alpha>0$. To visualise the allowed bands of energy for $\beta=1.5$, observe figure 2.

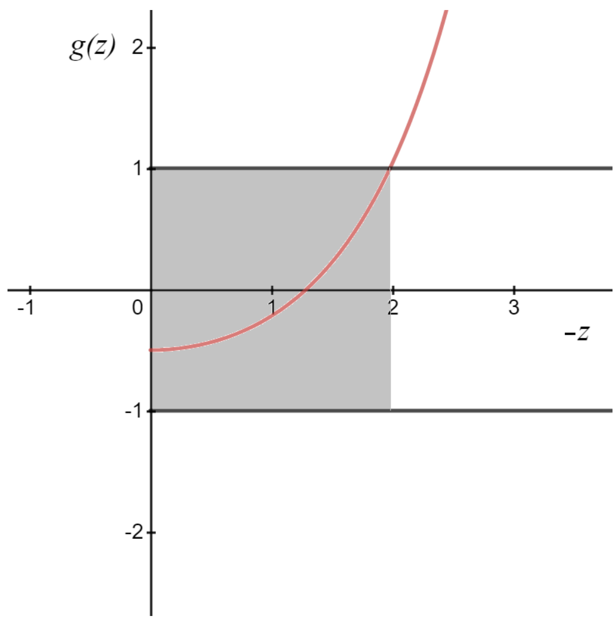

Figure 2: Plot of $g(z)$ against $-z$ for $\beta=1.5$

Here, $g(z)$ is drawn in red and the energetically 'allowed' regions are in grey for the same reasons as specified earlier.

In fact, if one takes into account the fact that in the first case $z=ka$ and in the second $z=-ka$, it is possible to draw a graph combining them together, for positive and negative z's. Here, $z=ka$ and $\beta=1.5$. For the final graph (which is clearly a superposition of the previous two, where $H(z)=f(z)+g(z)$), refer to figure 3.
To answer the question about the number of states, we need a reminder that the 'regions' of allowed energies we were talking about are actually really dense lines since N is a relatively large number. Each intersection of the line with $H(z)$ represents an admittable state. In particular, each of those states satisfy:

$$q=\frac{2\pi n}{Na}\text{ for }n\in\mathbb{N}\text{ and }n<N. \tag{20}$$

Since there are N possible values of q, we can count exactly N states for the first band.

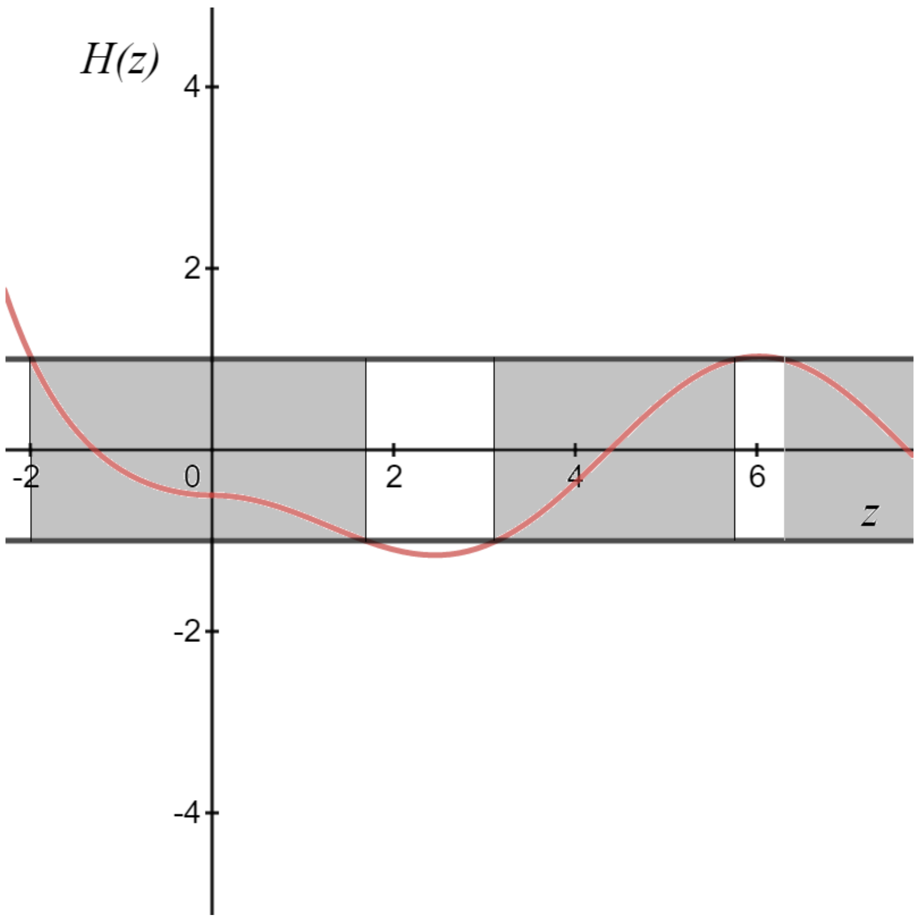

Figure 3: Plot of $H(z)$ against z for $\beta = 1.5$

Problem 2

Griffiths 5.36

We can extend the theory of a free electron gas (Section 5.3.1) to the relativistic domain by replacing the classical kinetic energy, $E = p^2/2m$, with the relativistic formula, $E = \sqrt{p^2c^2 + m^2c^4} - mc^2$. Momentum is related to the wavevector in the usual way: $\mathbf{p} = \hbar\mathbf{k}$. In particular, in the *extreme* relativistic limit, $E \approx pc = \hbar ck$.

a) Replace $\hbar^2k^2/2m$ in Equation 5.55 by the ultra-relativistic expression, $\hbar ck$, and calculate E_{tot} in this regime.
b) Repeat parts (a) and (b) of Problem 5.35 for the ultra-relativistic electron gas. Notice that in this case there is no stable minimum, regardless of R; if the total energy is positive, degeneracy forces exceed gravitational forces, and the star will expand, whereas if the total is negative, gravitational forces win out, and the star will collapse. Find the critical number of nucleons, N_c, such that gravitational collapse occurs for $N > N_c$. This is called the **Chandrasekhar limit**. *Answer*: 2.04×10^{57}. What is the corresponding stellar mass (give your answer as a multiple of the sun's mass). Stars heavier than this will not form white dwarfs, but collapse further, becoming (if conditions are right) neutron stars.
c) At extremely high density, **inverse beta decay**, $e^- + p^+ \longrightarrow n + \nu$, converts virtually all of the protons and electrons into neutrons (liberating neutrinos, which carry off energy, in the process). Eventually neutron degeneracy pressure stabilizes the collapse, just as electron degeneracy does for the white dwarf (see Problem 5.35). Calculate the radius of a neutron star with the mass of the sun. Also calculate the (neutron) Fermi energy, and compare it to the rest energy of a neutron. Is it reasonable to treat a neutron star nonrelativistically?

Solution

Part a

Modifying equation 5.55 we get:

$$\mathrm{d}E = \hbar ck\frac{V}{\pi^2}k^2\mathrm{d}k \implies \int_0^{E_{tot}} \mathrm{d}E = \frac{V\hbar c}{\pi^2}\int_0^{k_F} k^3\mathrm{d}k \tag{21}$$

Solving this integral we get the energy explicitly:

$$E_{tot} = \frac{V\hbar c {k_F}^4}{4\pi^2} \tag{22}$$

Since $k = \left(\frac{3Nq\pi^2}{V}\right)^{1/3}$, we cn write E_{tot} in terms of V:

$$E_{tot}(V) = \boxed{\frac{\hbar c\left(3Nq\pi^2\right)^{4/3}}{4\pi^2}V^{-1/3}} \tag{23}$$

Part b

Expressing E in terms of R is possible once one notes that $V = \frac{4}{3}\pi R^3$. Plugging this into (23) we get:

$$E_{tot}(R) = \frac{\hbar c\left(3Nq\pi^2\right)^{4/3}}{4\pi^2}\left(\frac{3}{4\pi R^3}\right)^{1/3} = \boxed{\frac{\hbar c}{3R\pi}\left(\frac{9qN\pi}{4}\right)^{4/3}} \tag{24}$$

So notably, $E_{tot} \propto \frac{1}{R}$. To account for the gravitational potential part, we can construct a sphere with a standard potential $-G\frac{m}{r}$. To enlarge this sphere's mass by dm and its radius by dr, work dW is done:

$$\mathrm{d}W = -G\frac{m\mathrm{d}m}{r} \tag{25}$$

Since we can assume uniformity of the ultrarelativistic gaseuos sphere, it holds that $m = \frac{4}{3}\rho r^3\pi$ which also implies $\mathrm{d}m = 4\rho r^2\pi\mathrm{d}r$. Thus (25) becomes:

$$\mathrm{d}W = -G\frac{\frac{4}{3}\rho r^3\pi 4\rho r^2\pi\mathrm{d}r}{r} = -G\frac{16\rho^2\pi^2}{3}r^4\mathrm{d}r \tag{26}$$

Since our sphere is 'built' from $r = 0$ to $r = R$, we can put (26) in a definite integral form:

$$W = -G\frac{16\rho^2\pi^2}{3}\int_0^R r^4\mathrm{d}r = -G\frac{16\rho^2\pi^2R^5}{15} \tag{27}$$

Since $\rho = \frac{3NM}{4R^3\pi}$, where M is the mass of one nucleon and N is the number of nucleons, (27) becomes:

$$W = -G\frac{16\left(\frac{3NM}{4R^3\pi}\right)^2\pi^2R^5}{15} = -\frac{3GN^2M^2}{5}\frac{1}{R} \tag{28}$$

The total energy is then:

$$E_{tot} = \frac{\hbar c}{3R\pi}\left(\frac{9qN\pi}{4}\right)^{4/3} - \frac{3GN^2M^2}{5}\frac{1}{R} \tag{29}$$

It is evident that $E_{tot} = 0$ at $N = N_c$. Thus:

$$\frac{3G{N_c}^2M^2}{5} = \frac{\hbar c}{3\pi}\left(\frac{9qN\pi}{4}\right)^{4/3} \implies N_c = \left(\frac{9q\pi}{4}\right)^2\left(\frac{5\hbar c}{9GM^2}\right)^{3/2} \tag{30}$$

Or more compactly:

$$N_c = \frac{15q^2}{16M^3}\sqrt{\frac{5\pi\hbar^3c^3}{G^3}} \tag{31}$$

Using $q = 1/2$, $M{\approx}1.67 \times 10^{-27}$ kg (average mass of one nucleon), $h{\approx}6.626 \times 10^{-34}$ Js, $c{\approx}3 \times 10^8$ m/s and $G{\approx}6.67 \times 10^{-11}$ Nm^{2}kg^{-2}, one gets:

$$N_c \approx 2.06 \times 10^{57} \tag{32}$$

The ratio of the two masses is given by:

$$\frac{M_c}{M_s} = \frac{N_cM}{M_s} \tag{33}$$

Where $M_s \approx 2 \times 10^{30}$ kg is the solar mass. Plugging in numbers, one gets:

$$\frac{M_c}{M_s}{\approx}1.72 \tag{34}$$

So it is about 1.72 the solar mass, and hence the solar number of nucleons.

Part c

Since both of our terms of energy are inverse related to R, we cannot compute it from the energy relation using the ultra-relativistic model. To answer this question, we need to refer to question 5.35 and the non-relativistic consideration. If, instead of $\hbar ck$ we wrote $\frac{\hbar^2k^2}{2m}$ in (21), we would get Griffiths's total degeneracy energy ith q instead of d (eq. 5.56 in the book):

$$E_1 = \frac{\hbar^2\left(3\pi^2Nq\right)^{5/3}}{10\pi^2m}V^{-2/3} \tag{35}$$

And if we use $V = \frac{4}{3}R^3\pi$, we get:

$$\frac{2\hbar^2}{15mR^2\pi}\left(\frac{9\pi Nq}{4}\right)^{5/3}. \tag{36}$$

Using the gravitational addition from (28), the total energy can be expressed (noting that we used m=M here, to stay consistent with notation):

$$E_{tot} = \frac{2\hbar^2}{15MR^2\pi}\left(\frac{9\pi Nq}{4}\right)^{5/3} - \frac{3GN^2M^2}{5}\frac{1}{R} \tag{37}$$

The radius of the neutron star can thus be calculated using the condition

$$\left.\frac{\mathrm{d}E}{\mathrm{d}R}\right|_{R_n} = 0 \tag{38}$$

$$\implies \frac{4\hbar^2}{15MR^3\pi}\left(\frac{9\pi Nq}{4}\right)^{5/3} = \frac{3GN^2M^2}{5}\frac{1}{R^2} \implies R = \frac{4\hbar^2}{9GN^2M^3\pi}\left(\frac{9\pi Nq}{4}\right)^{5/3} \tag{39}$$

If we use the constants specified above, alongside $q = 1$, $N = N_c\frac{M_s}{M_C}$ we get:

$$R{\approx}12420 \text{ m} = \boxed{12.42 \text{ km}} \tag{40}$$

The Fermi energy can be calculated using equation 5.54 from Griffiths:

$$E_f = \frac{\hbar^2}{2m}\left(\frac{3Nq\pi^2}{V}\right)^{2/3} \tag{41}$$

Using $V = \frac{4}{3}R^3\pi$, and $m = M$ one gets here:

$$E_f = \frac{\hbar^2}{2MR^2}\left(\frac{9Nq\pi}{4}\right)^{2/3} \tag{42}$$

Using the appropriate constants, we can calculate:

$$E_f \approx 9.934 \times 10^{-12} \text{ J} \tag{43}$$

The rest energy of a neutron is calculated as follows:

$$E_n = Mc^2 \approx 1.67 \times 10^{-27} \text{ kg} \cdot \left(3 \times 10^8 \text{ m/s}\right)^2 \approx 1.5 \times 10^{-10} \text{ J} \tag{44}$$

Comparing the two, we get:

$$\frac{E_f}{E_n} \approx 0.0661 \ll 1 \tag{45}$$

Thus, E_f is still negligible. No need for relativistic consideration.

Problem 3

Griffiths 7.1

Suppose we put a delta-function bump in the center of the infinite square well:

$$H' = \alpha\delta(x - a/2)$$

where α is a constant.

a) Find the first-order correction for the allowed energies. Explain why the energies are not perturbed for even n.
b) Find the first three nonzero terms in the expansion (Equation 7.13) of the correction to the ground state, ψ_1^1.

Solution

Part a

According to equation 7.9 in Griffiths:

$$E_n^1 = \langle\psi_n^0|H'|\psi_n^9\rangle = \frac{2\alpha}{a}\int_0^a \sin^2\left(\frac{n\pi}{a}x\right)\delta(x - \frac{a}{2})\mathrm{d}x \tag{46}$$

Due to the properties of the δ function, this integral is easily calculated:

$$E_n^1 = \frac{2\alpha}{a}\sin^2\left(\frac{n\pi}{2}\right) = \boxed{\begin{cases}\frac{2\alpha}{a} & n \text{ odd}\\ 0 & n \text{ even}\end{cases}} \tag{47}$$

Hence, it is clear from (47) that if n is even, each of the consecutive perturbations of energy, E_n^i for $i \in \mathbb{N}$ is exactly 0, since the wavefunction is always 0 at $x = \frac{a}{2}$.

Part b

Equation 7.13 states that the correction to the ground state following a perturbation H' could be calculated as follows:

$$\psi_n^1 = \sum_{m\neq n}\frac{\langle\psi_m^0|H'|\psi_n^0\rangle}{E_n^0 - E_m^0}\psi_m^0 \tag{48}$$

In our case, $n = 1$, so equation (48) simplifies to:

$$\psi_1^1 = \sum_{m=2}\frac{\langle\psi_m^0|H'|\psi_1^0\rangle}{E_1^0 - E_m^0}\psi_m^0 \tag{49}$$

To begin with:

$$\langle\psi_m^0|H'|\psi_1^0\rangle = \frac{2\alpha}{a}\int_{-\infty}^{\infty}\sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{\pi}{a}x\right)\delta(x - \frac{a}{2})\mathrm{d}x = \frac{2\alpha}{a}\sin\left(\frac{m\pi}{2}\right) \tag{50}$$

To find E_k^0 for any $k \in \mathbb{N}$, we can use the identity:

$$\hat{H}\psi_k^0 = E_k^0\psi_k^0 \implies E_k^0 = -\frac{\hbar^2}{2m\psi_k^0}\frac{\partial^2\psi_k^0}{\partial x^2} \tag{51}$$

This is a well known result:

$$E_k^0 = \frac{k^2\pi^2\hbar^2}{2ma^2} \tag{52}$$

Concretely, when (50) and (52) are input into equation (49) we get:

$$\psi_1^1 = \sum_{m \text{ odd}, m\geq 3} \frac{4ma\alpha(-1)^{\frac{m-1}{2}}}{\pi^2\hbar^2\left(1-m^2\right)}\psi_m^0 \tag{53}$$

In fact, since m is odd and larger than 2, we can write it as $m = 2k+1$ for any $k \in \mathbb{N}$. Then, (54) becomes:

$$\psi_1^1 = \frac{ma\alpha}{\pi^2\hbar^2}\sum_{k=1} \frac{(-1)^{k+1}}{k\,(k+1)}\psi_{2k+1}^0 \tag{54}$$

We can calculate first three non-zero terms of the series:

$$\psi_1^1 = \frac{ma\alpha}{\pi^2\hbar^2}\left(\frac{1}{2}\psi_3^0 - \frac{1}{6}\psi_5^0 + \frac{1}{12}\psi_7^0 + \dots\right) \tag{55}$$

Noting that $\psi_k^0 = \sqrt{\frac{2}{a}}\sin\left(\frac{k\pi}{a}x\right)$, (55) becomes:

$$\psi_1^1 \approx \boxed{\frac{m\alpha}{\pi^2\hbar^2}\sqrt{\frac{a}{2}}\left(\sin\left(\frac{3\pi}{a}x\right) - \frac{1}{3}\sin\left(\frac{5\pi}{a}x\right) + \frac{1}{6}\sin\left(\frac{7\pi}{a}x\right)\right)} \tag{56}$$

In fact, in functional form, equation (54) becomes:

$$\psi_1^1 = \frac{m\alpha}{\pi^2\hbar^2}\sqrt{2a}\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k\,(k+1)}\sin\left(\frac{(2k+1)\pi}{a}x\right) \text{ for } 0 < x < a \tag{57}$$

Using the fact that we know both ψ_1^0 and ψ_1^1, we can combine them and form a first order approximation of ψ_1 (red function on figure 4). The graph of this function clearly has a spike at $x = a/2$, as it should since there is a δ function at that position. A function of ψ_1^0 was superimposed onto the graph for comparison, and it is drawn in blue.

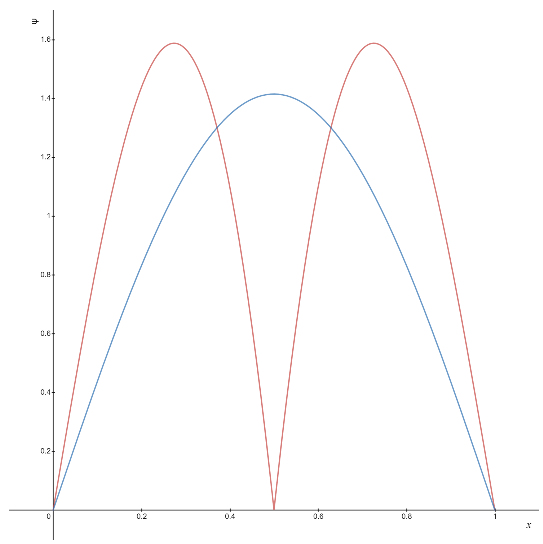

Figure 4: Graph of $\psi_1^0 + \psi_1^1$ (red) and ψ_1^0 (blue) versus x for $\frac{m\alpha}{\pi^2\hbar^2} = 1$ and $a = 1$

Problem 4

Griffiths 7.5

a) Find the second-order correction to the energies $\left(E_n^2\right)$ for the potential in Problem 7.1. Comment: You can sum the series explicitly, obtaining $-2m(\alpha/\pi\hbar n)^2$ for odd n.

Solution

Part a

Using Griffiths formula 7.15:

$$E_n^2 = \sum_{m\neq n} \frac{\left|\langle\psi_m^0|H'|\psi_n^0\rangle\right|^2}{E_n^0 - E_m^0} \tag{58}$$

Firstly we determine the numerator:

$$\langle\psi_m^0|H'|\psi_n^0\rangle = \frac{2\alpha}{a}\int_{-\infty}^{\infty} \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)\delta\left(x=\frac{a}{2}\right)\mathrm{d}x \tag{59}$$

Due to the properties of the delta function:

$$\langle\psi_m^0|H'|\psi_n^0\rangle = \frac{2\alpha}{a}\sin\left(\frac{m\pi}{2}\right)\sin\left(\frac{n\pi}{2}\right) = \frac{2\alpha}{a}(-1)^{\frac{m-1}{2}}(-1)^{\frac{n-1}{2}} \tag{60}$$

(60) is non-zero iff both m and n are odd. If so, then it could take values $-\frac{2\alpha}{a}$ or $\frac{2\alpha}{a}$. Then,

$$\left|\langle\psi_m^0|H'|\psi_n^0\rangle\right|^2 = \frac{4\alpha^2}{a^2} \tag{61}$$

If both m and n are odd. From equation (52):

$$E_n^0 - E_m^0 = \frac{\hbar^2\pi^2}{2ma^2}\left(n^2 - m^2\right) \tag{62}$$

Hence, (58) reduces to:

$$E_n^2 = \frac{8m\alpha^2}{\hbar^2\pi^2}\sum_{m,n\ \mathrm{odd} m\neq n}\frac{1}{(n^2-m^2)} \tag{63}$$

This series can be calculated as an infinite sum of infinite sums. Namely,

$$\frac{8m\alpha^2}{\hbar^2\pi^2}\sum_{m,n\ \mathrm{odd},m\neq n}\frac{1}{(n^2-m^2)} = \frac{8m\alpha^2}{\hbar^2\pi^2}\sum_{m\ \mathrm{odd},m\neq 1}\frac{1}{(1-m^2)} + \frac{8m\alpha^2}{\hbar^2\pi^2}\sum_{m\ \mathrm{odd},m\neq 3}\frac{1}{(9-m^2)} + \dots \tag{64}$$

For a fixed n:

$$\sum_{m\ \mathrm{odd},m\neq n}\frac{1}{(n^2-m^2)} = \frac{1}{2n}\sum_{m\ \mathrm{odd},m\neq n}\left(\frac{1}{n+m} - \frac{1}{m-n}\right) \tag{65}$$

This is a well-known telescoping series which can be calculated by noting the following, if $n = 2k+1$ and $m = 2p+1$ where $k,p\in\mathbb{N}$, and k is fixed and can take value 0:

$$\sum_{k\neq p}\left(\frac{1}{2(k+p+1)} - \frac{1}{2(p-k)}\right) = \frac{1}{2}\left(\frac{1}{k+1} + \frac{1}{k+2} + \frac{1}{k+3} + \dots + \frac{1}{k} - \frac{1}{1-k} - \frac{1}{2-k} - \dots\right) \tag{66}$$

Since this is a general formula, it does not contain the constraint of omitting the sum where $k = p$. We have to take care of that. So we do some clever guessing. We notice that as k increases, the total sum decreases, and in particular, suppose it is true for $k = r$ that:

$$\sum_{p \neq r} \left(\frac{1}{2(r+p+1)} - \frac{1}{2(p-r)} \right) = -\frac{1}{2(2r+1)} \tag{67}$$

Checking for $k = r + 1$:

$$\sum_{p \neq r+1} \left(\frac{1}{2(r+p+2)} - \frac{1}{2(p-r-1)} \right) = \frac{1}{2} \left(\frac{1}{r+2} + \frac{1}{r+3} + \frac{1}{r+4} + \cdots + \frac{1}{r+1} + \frac{1}{r} - \frac{1}{1-r} - \dots \right) \tag{68}$$

Due to the fact we are leaving out the term where $p = r + 1$, and including the term where $p = r$ it holds:

$$\sum_{p \neq r+1} \left(\frac{1}{2(r+p+2)} - \frac{1}{2(p-r-1)} \right) = \sum_{p \neq r} \left(\frac{1}{2(r+p+1)} - \frac{1}{2(p-r)} \right) + \frac{1}{2} \left(\frac{1}{2r+1} - \frac{1}{2r+3} \right) \tag{69}$$

Combining (67) and (69) we obtain:

$$\sum_{p \neq r+1} \left(\frac{1}{2(r+p+2)} - \frac{1}{2(p-r-1)} \right) = -\frac{1}{2(2r+3)} = -\frac{1}{2((2r+1)+1)} \tag{70}$$

Which is to say, if (67) hold for $k = r$, it then holds for $k = r + 1$ as well. (67)is true for $r = 0$ since:

$$\frac{1}{2} \left(\frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \cdots - 1 - \frac{1}{2} - \frac{1}{3} - \dots \right) = -\frac{1}{2} \tag{71}$$

So it is true for all $k \in \mathbb{N}_0$. It then holds for (65) that, for fixed n, where $n = 2k + 1$:

$$\sum_{m \text{ odd}, m \neq n} \frac{1}{(n^2 - m^2)} = \frac{1}{2n} \left(-\frac{1}{2(2k+1)} \right) = -\frac{1}{4n^2} \tag{72}$$

Putting this result back into (63), one obtains:

$$E_n^2 = \boxed{-\frac{2m\alpha^2}{\hbar^2 \pi^2 n^2}} \tag{73}$$

In fact, another interesting result occurs when trying to sum second-order corrections to the energy as n tends to infinity. Namely,

$$\sum_{n=1}^{\infty} E_n^2 = -\frac{m\alpha^2}{3\hbar^2} \tag{74}$$

Which is probably just a curiosity.

Problem 5

A particle of mass m moves in one dimension in a harmonic oscillator potential. The particle is perturbed by an additional weak anharmonic potential, $H_0 = \lambda \sin(kx)$. What are the first order corrections to the energy and wavefunction of the ground state?

Hint 1: $e^x = \sum_{j=0}^{\infty} \frac{x^j}{j!}$
Hint 2: $e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-[\hat{A},\hat{B}]/2}$, where $\hat{A}$ and $\hat{B}$ are operators.

Solution

According to Griffiths equation 7.9:

$$E_1^1 = \langle \psi_1^0 | H' | \psi_1^0 \rangle \tag{75}$$

And according to Griffiths 2.60:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \tag{76}$$

Combining the previous two equations, we obtain:

$$E_1^1 = \lambda \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar}x^2} \sin(kx) \mathrm{d}x \tag{77}$$

According to WolframAlpha, the integral above is exactly 0, hence:

$$E_1^1 = 0 \tag{78}$$

However, this is not the case with the first-order correction to the wavefunction of the ground state. Namely:

$$\psi_1^1 = \sum_{m \neq 1} \frac{\langle \psi_m^0 | H' | \psi_1^0 \rangle}{E_1^0 - E_m^0} \psi_m^0 \tag{79}$$

If we write $\sin(kx) = \frac{e^{ikx} - e^{-ikx}}{2i}$, we can write the inner product from (79) as:

$$\langle \psi_m^0 | H' | \psi_1^0 \rangle = \langle \psi_m^0 | \lambda \frac{e^{ikx} - e^{-ikx}}{2i} | \psi_1^0 \rangle = \frac{\lambda}{2i} \langle \psi_m^0 | \left(e^{ikx} - e^{-ikx}\right) | \psi_1^0 \rangle = \frac{\lambda}{2i} \left(\langle \psi_m^0 | e^{ikx} | \psi_1^0 \rangle - \langle \psi_m^0 | e^{-ikx} | \psi_1^0 \rangle \right) \tag{80}$$

Using the fact that

$$x = \hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a}_+ + \hat{a}_-\right) \tag{81}$$

Where

$$\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}} \left(\mp \hat{p} + m\omega x\right) \tag{82}$$

Hence, according to hint 2, noting that $[\hat{a}_-, \hat{a}_+] = 1$ we can write e^{ikx} as

$$e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_-} e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+} e^{\frac{k^2\hbar}{4m\omega}} \tag{83}$$

And e^{-ikx} as

$$e^{-ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_-} e^{-ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+} e^{\frac{k^2\hbar}{4m\omega}} \tag{84}$$

Then, we use Hint 1 to expand (83) and (84):

$$e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_-} = \sum_{j=0}^{\infty} \frac{\left(ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_-\right)^j}{j!} = 1 + ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_- - k^2 \frac{\hbar}{4m\omega}\hat{a}_-^2 - \dots \tag{85}$$

$$e^{ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+} = 1 + ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+ - k^2\frac{\hbar}{4m\omega}\hat{a}_+^2 - \dots \tag{86}$$

Similarly:

$$e^{-ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_-} = 1 - ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_- - k^2\frac{\hbar}{4m\omega}\hat{a}_-^2 + \dots \tag{87}$$

$$e^{-ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+} = 1 - ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+ - k^2\frac{\hbar}{4m\omega}\hat{a}_+^2 + \dots \tag{88}$$

Then, we notice:

$$\langle\psi_m^0|e^{ikx}|\psi_1^0\rangle = e^{\frac{k^2\hbar}{4m\omega}}\langle\psi_m^0|\left(1 + ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_- - k^2\frac{\hbar}{4m\omega}\hat{a}_-^2 - \dots\right)\left(1 + ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+ - k^2\frac{\hbar}{4m\omega}\hat{a}_+^2 - \dots\right)|\psi_1^0\rangle \tag{89}$$

Similarly:

$$\langle\psi_m^0|e^{-ikx}|\psi_1^0\rangle = e^{\frac{k^2\hbar}{4m\omega}}\langle\psi_m^0|\left(1 - ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_- - k^2\frac{\hbar}{4m\omega}\hat{a}_-^2 + \dots\right)\left(1 - ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+ - k^2\frac{\hbar}{4m\omega}\hat{a}_+^2 + \dots\right)|\psi_1^0\rangle \tag{90}$$

Let us observe the case $m = 2$. Due to orthogonality of eigenstates, (89) will reduce to:

$$\langle\psi_2^0|e^{ikx}|\psi_1^0\rangle = e^{\frac{k^2\hbar}{4m\omega}}\langle\psi_2^0|\left(ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+ - i\sqrt{\frac{\hbar}{2m\omega}}\frac{k^3\hbar}{4m\omega}\hat{a}_-\hat{a}_+^2 + \dots\right)|\psi_1^0\rangle \tag{91}$$

$$\langle\psi_2^0|e^{-ikx}|\psi_1^0\rangle = e^{\frac{k^2\hbar}{4m\omega}}\langle\psi_2^0|\left(-ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+ - i\sqrt{\frac{\hbar}{2m\omega}}\frac{k^3\hbar}{4m\omega}\hat{a}_-\hat{a}_+^2 + \dots\right)|\psi_1^0\rangle \tag{92}$$

For a simpler view, set $u = ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_-$ and $v = ik\sqrt{\frac{\hbar}{2m\omega}}\hat{a}_+$. Then (89) and (90) become:

$$\langle\psi_m^0|e^{ikx}|\psi_1^0\rangle = e^{\frac{k^2\hbar}{4m\omega}}\langle\psi_m^0|\left(1 + u + \frac{u^2}{2!} + \dots\right)\left(1 + v + \frac{v^2}{2!} + \dots\right)|\psi_1^0\rangle \tag{93}$$

$$\langle\psi_m^0|e^{-ikx}|\psi_1^0\rangle = e^{\frac{k^2\hbar}{4m\omega}}\langle\psi_m^0|\left(1 - u + \frac{u^2}{2!} - \dots\right)\left(1 - v + \frac{v^2}{2!} - \dots\right)|\psi_1^0\rangle \tag{94}$$

Then:

$$\langle\psi_2^0|e^{ikx}|\psi_1^0\rangle = e^{\frac{k^2\hbar}{4m\omega}}\langle\psi_m^0|\left(v + \frac{uv^2}{2!} + \frac{u^2v^3}{2!3!} + \dots\right)|\psi_1^0\rangle \tag{95}$$

$$\langle\psi_2^0|e^{-ikx}|\psi_1^0\rangle = e^{\frac{k^2\hbar}{4m\omega}}\langle\psi_m^0|\left(-v - \frac{uv^2}{2!} - \frac{u^2v^3}{2!3!}\dots\right)|\psi_1^0\rangle \tag{96}$$

And

$$\langle\psi_2^0|e^{ikx}|\psi_1^0\rangle - \langle\psi_2^0|e^{-ikx}|\psi_1^0\rangle = 2e^{\frac{k^2\hbar}{4m\omega}}\langle\psi_m^0|\left(v + \frac{uv^2}{2!} + \frac{u^2v^3}{2!3!} + \dots\right)|\psi_1^0\rangle \tag{97}$$

Note that each operator u^kv^{k+1} raises $k+1$ times, and lowers k times so the overall raise is just 1. Then all inner products are non-zero. In particular, for $m = 2$:

$$\langle\psi_2^0|e^{ikx}|\psi_1^0\rangle - \langle\psi_2^0|e^{-ikx}|\psi_1^0\rangle = 2e^{\frac{k^2\hbar}{4m\omega}}\left(\sqrt{2}ik\sqrt{\frac{\hbar}{2m\omega}} + \frac{3\sqrt{2}}{2!}\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^3 + \frac{3\cdot4\cdot\sqrt{2}}{2!3!}\left(ik\sqrt{\frac{\hbar}{2m\omega}}\right)^5 + \dots\right) \tag{98}$$

Or

$$\langle\psi_2^0|e^{ikx}|\psi_1^0\rangle - \langle\psi_2^0|e^{-ikx}|\psi_1^0\rangle = 2\sqrt{2}ie^{\frac{k^2\hbar}{4m\omega}}\left(k\sqrt{\frac{\hbar}{2m\omega}} - \frac{3}{2!}\left(k\sqrt{\frac{\hbar}{2m\omega}}\right)^3 + \frac{3\cdot4}{2!3!}\left(k\sqrt{\frac{\hbar}{2m\omega}}\right)^5 + \dots\right) \tag{99}$$

Problem 5 continued on next page. . .

So

$$\langle\psi_2^0|e^{ikx}|\psi_1^0\rangle - \langle\psi_2^0|e^{-ikx}|\psi_1^0\rangle = \sqrt{2}ie^{\frac{k^2\hbar}{4m\omega}}\sum_{n=0}^{\infty}(-1)^n\frac{(n+2)}{n!}\left(k\sqrt{\frac{\hbar}{2m\omega}}\right)^{2n+1} \tag{100}$$

Which gives us a hint on how the difference of 'even' inner products will behave. The actual formula requires clever guessing and noticing patterns (or induction, if you will). For full generality, for even coefficients $2m$:

$$\langle\psi_{2m}^0|e^{ikx}|\psi_1^0\rangle - \langle\psi_{2m}^0|e^{-ikx}|\psi_1^0\rangle = \frac{2}{\sqrt{(2m)!}}ie^{\frac{k^2\hbar}{4m\omega}}\sum_{n=m-1}^{\infty}(-1)^n\frac{(n+2m)}{n!}\left(k\sqrt{\frac{\hbar}{2m\omega}}\right)^{2n+1} \tag{101}$$

Where $m \in \mathbb{N}$

Notice the ambiguity in (101), the dimensionless term in the brackets that holds the position of a variable in this series also has m inside it, that stands for mass. In fact, if we write

$$x = k\sqrt{\frac{\hbar}{2m\omega}} \tag{102}$$

Then, (101) becomes:

$$\langle\psi_{2m}^0|e^{ikx}|\psi_1^0\rangle - \langle\psi_{2m}^0|e^{-ikx}|\psi_1^0\rangle = \frac{2}{\sqrt{(2m)!}}ie^{x^2}\sum_{n=m-1}^{\infty}(-1)^n\frac{(n+2m)}{n!}x^{2n+1} \tag{103}$$

And we avoid the ambiguity. Then, we know that:

$$E_1^1 - E_m^1 = \frac{\hbar\omega}{2} - \left(m+\frac{1}{2}\right)\hbar\omega = -m\hbar\omega \tag{104}$$

Thus (79) for even m becomes:

$$\psi_1^1 = \boxed{-\frac{\lambda}{\hbar\omega}e^{x^2}\sum_{m=1}\frac{\sum_{n=m-1}^{\infty}(-1)^n\frac{(n+2m)}{n!}x^{2n+1}}{2m\sqrt{(2m)!}}\psi_{2m}^0} \tag{105}$$

Where

$$x = k\sqrt{\frac{\hbar}{2m\omega}} \tag{106}$$

For odd m, it is clear from (89) an (90) that all terms cancel, and in general:

$$\langle\psi_{2m+1}^0|\sin(kx)|\psi_1^0\rangle = 0 \tag{107}$$

So (105) is the only solution, since there is no contribution for odd perturbations.