

Simple quantum systems

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Abstract

Solution of several problems of [1, Vol. I].

1 Finite square well (Problem 25)

Let us consider the potential $V(x)$ defined by

$$V(x) = \begin{cases} -\hbar^2 q^2 / 2m, & \text{for } |x| < L; \\ 0, & \text{otherwise.} \end{cases} \quad (1)$$

We are looking for normalizable solutions of the Schrödinger equation. Let us consider solutions which behave like $e^{-\kappa|x|}$ as $x \rightarrow \pm\infty$. We then have

$$E = -\frac{\hbar^2 \kappa^2}{2m}. \quad (2)$$

Since the potential is even, the eigenfunction will be either even (+) or odd (-). Even functions will be proportional to $\cos kx$ for $|x| < L$, where $k^2 = q^2 - \kappa^2$, and odd functions will be proportional to $\sin kx$. We must impose the continuity of the function and its derivative at $x = \pm L$. We have

Case (+): We set

$$\psi_+(x) = \begin{cases} A \cos kx, & \text{for } |x| \leq L; \\ A' e^{-\kappa(|x|-L)}, & \text{otherwise.} \end{cases} \quad (3)$$

Thus the conditions for $x = L$ are

$$\begin{aligned} 0 &= A \cos(kL) - A'; \\ 0 &= -kA \sin(kL) + \kappa A'. \end{aligned} \quad (4)$$

The determinant of this system is given by

$$\Delta = \kappa \cos(kL) - k \sin(kL). \quad (5)$$

We thus obtain the equation

$$\tan kL = \frac{\kappa}{k}. \quad (6)$$

We can parametrize this equation by setting

$$\frac{\kappa}{k} = \tan \theta, \quad \tan \theta \geq 0. \quad (7)$$

Then we have, when $\tan \theta \geq 0$,

$$k = q |\cos \theta|, \quad \kappa = q |\sin \theta|, \quad (8)$$

and

$$\tan kL = \tan \theta, \quad (9)$$

i.e.,

$$\frac{\theta}{qL} = |\cos \theta|, \quad \text{for } \tan \theta \geq 0. \quad (10)$$

Case (-): We set

$$\psi_-(x) = \begin{cases} A \sin kx, & \text{for } |x| \leq L; \\ A' \operatorname{sign} x e^{-\kappa(|x|-L)}, & \text{otherwise.} \end{cases} \quad (11)$$

Thus we obtain the equations

$$\begin{aligned} 0 &= A \sin kL - A' = 0; \\ 0 &= kA \cos kL + \kappa A'. \end{aligned} \quad (12)$$

The determinant of this system reads

$$\Delta = -(\kappa \sin kL + k \cos kL). \quad (13)$$

We thus obtain

$$\tan kL = -\frac{k}{\kappa} = -\frac{1}{\tan \theta} > 0. \quad (14)$$

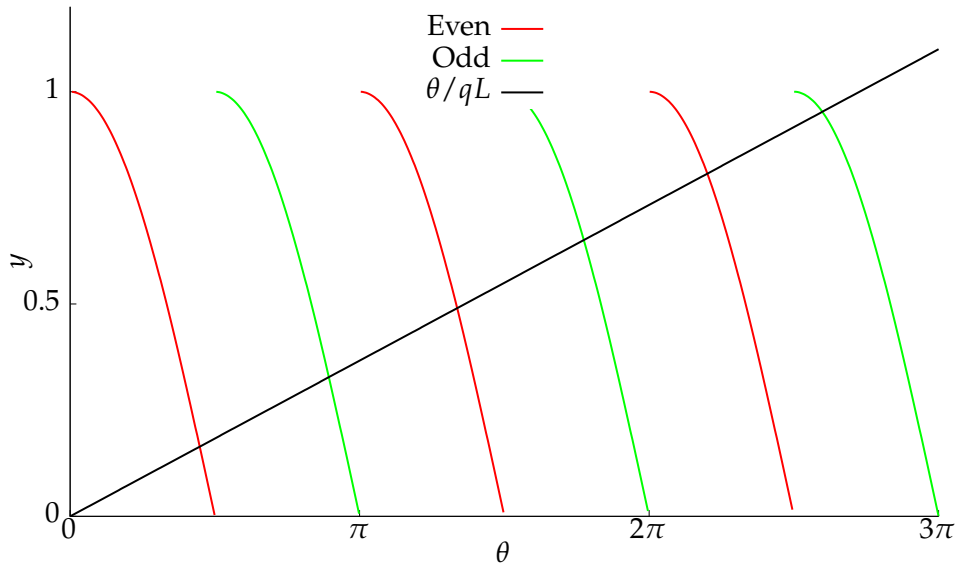
Thus we obtain the equation, for $\tan \theta \leq 0$,

$$k = |\sin \theta|, \quad \kappa = |\cos \theta|, \quad (15)$$

leading to

$$\frac{\theta}{qL} = |\sin \theta|, \quad \text{for } \tan \theta \leq 0. \quad (16)$$

Thus for $n\pi/2 \leq qL < (n+1)\pi/2$ we have $(n+1)$ bound states, alternatively even and odd.



2 Square well between walls (Problem 26)

Problem

Solve the Schrödinger equation for the potential $V(x)$ given by

$$V(x) = \begin{cases} -\frac{\hbar^2 q^2}{2m}, & \text{for } |x| \leq a; \\ 0, & \text{for } a < |x| \leq L; \\ +\infty, & \text{otherwise.} \end{cases} \quad (17)$$

Solution

“Bound” states: $E < 0$

We set $E = -\hbar^2 \kappa^2 / 2m$, $k^2 = q^2 - \kappa^2$.

Even states: Let $u_+(x)$ be defined by

$$u_+(x) = \begin{cases} A_+ \cos kx, & \text{for } |x| \leq a; \\ A'_+ \cos ka \sinh \kappa(L - x), & \text{for } a < x \leq L; \\ 0, & \text{otherwise.} \end{cases} \quad (18)$$

We obtain the equations

$$\begin{aligned} 0 &= A_+ - A'_+ \sinh \kappa(L - a); \\ 0 &= kA_+ \sin ka + \kappa A'_+ \cos ka \cosh \kappa(L - a). \end{aligned} \quad (19)$$

The determinant reads

$$\Delta = \kappa \cos ka \cosh \kappa(L - a) - k \sin ka \sinh \kappa(L - a). \quad (20)$$

Thus we obtain the equation

$$k \tan ka = \kappa \coth \kappa(L - a). \quad (21)$$

Odd states: Let $u_-(x)$ be defined by

$$u_-(x) = \begin{cases} A_+ \sin kx, & \text{for } |x| \leq a; \\ A'_+ \sin ka \sinh \kappa(L - x), & \text{for } a < x \leq L; \\ 0, & \text{otherwise.} \end{cases} \quad (22)$$

We obtain the equations

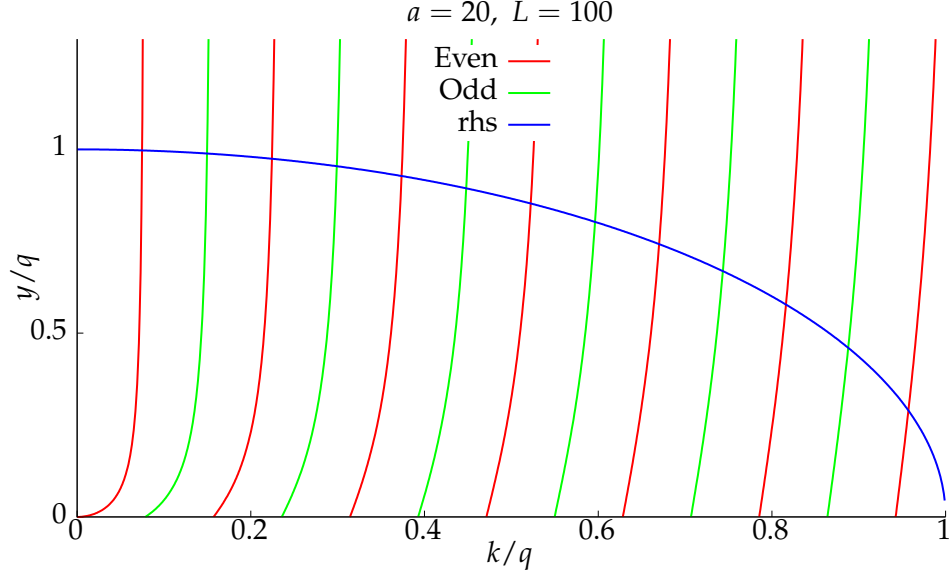
$$\begin{aligned} 0 &= A_+ - A'_+ \sinh \kappa(L - a); \\ 0 &= kA_+ \cos ka + \kappa A'_+ \sin ka \cosh \kappa(L - a). \end{aligned} \quad (23)$$

The determinant reads

$$\Delta = \kappa \sin ka \cosh \kappa(L - a) - k \cos ka \sinh \kappa(L - a). \quad (24)$$

Thus we obtain the equation

$$-k \cot ka = \kappa \coth \kappa(L - a). \quad (25)$$



“Free” states: $E > 0$

Set $E = \hbar^2 K^2 / 2m$, $k^2 = q^2 + K^2$.

Even states: Define $u_+(x)$ by

$$u_+(x) = \begin{cases} A_+ \cos kx, & \text{for } 0 < x \leq a; \\ A'_+ \cos ka \sin K(L - x), & \text{for } a < x \leq L; \\ u_+(x) = u_+(-x), & \text{for } 0 > x > -L; \\ 0, & \text{otherwise.} \end{cases} \quad (26)$$

We obtain the conditions

$$\begin{aligned} 0 &= A_+ - A'_+ \sin K(L - a); \\ 0 &= -kA_+ \sin ka + KA'_+ \cos ka \cos K(L - a). \end{aligned} \quad (27)$$

The determinant reads

$$\Delta = K \cos ka \cos K(L - a) - k \sin ka \sin K(L - a) = 0. \quad (28)$$

Thus we obtain the equation

$$k \tan ka = K \cot K(L - a). \quad (29)$$

Odd states: Define $u_-(x)$ by

$$u_-(x) = \begin{cases} A_- \sin kx, & \text{for } 0 \leq x \leq a; \\ A'_- \sin ka \sin K(L - x), & \text{for } a < x \leq L; \\ -u_-(-x), & \text{for } 0 > x > -L; \\ 0, & \text{otherwise.} \end{cases} \quad (30)$$

The continuity conditions read

$$\begin{aligned} 0 &= A_- - A'_- \sin K(L - a); \\ 0 &= kA_- \cos ka + KA'_- \sin ka \cos K(L - a). \end{aligned} \quad (31)$$

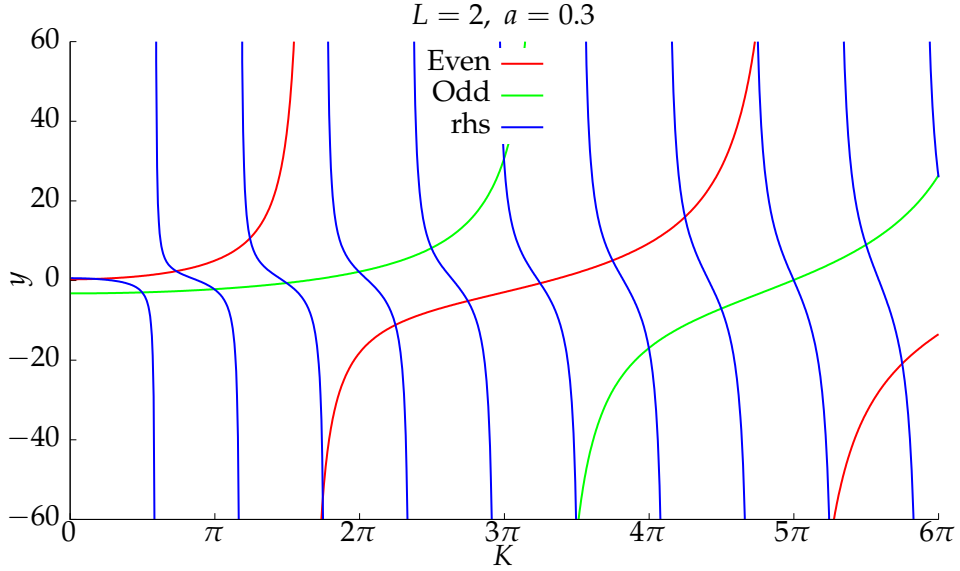
The determinant is given by

$$\Delta = K \sin ka \cos K(L - a) + k \cos ka \sin K(L - a). \quad (32)$$

This leads to the equation

$$-k \cot ka = K \cot K(L - a). \quad (33)$$

For $L \gg a$, and $Ka \gg 1$, there is exactly one even and one odd solution in each KL interval of width π .



Let us evaluate the normalization integral $\mathcal{N}_\pm = \int_{-L}^{+L} dx u_\pm^2(x)$. We have

$$\begin{aligned} \mathcal{N}_+ &= 2 \int_0^a dx \cos^2 kx + 2 \frac{\cos^2 ka}{\sin^2 K(L - a)} \int_a^L dx \sin^2 K(L - x) \\ &= \frac{1}{k} (ka + \sin ka \cos ka) - \frac{\cos^2 ka}{K} [\cot K(L - a) - K(L - a) (1 + \cot^2 K(L - a))] \\ &= \frac{1}{k} (ka + \sin ka \cos ka) - \frac{\cos^2 ka}{K} \left[\frac{k}{K} \tan ka - K(L - a) \left(1 + \frac{k^2}{K^2} \tan^2 ka \right) \right] \\ &= \frac{1}{k} \left[ka + \left(1 - \frac{k^2}{K^2} \sin ka \cos ka \right) \right] + (L - a) \left(\cos^2 ka + \frac{k^2}{K^2} \sin^2 ka \right). \end{aligned} \quad (34)$$

We have likewise

$$\mathcal{N}_- = \frac{1}{k} \left[ka - \left(1 - \frac{k^2}{K^2} \sin ka \cos ka \right) \right] + (L - a) \left(\sin^2 ka + \frac{k^2}{K^2} \cos^2 ka \right). \quad (35)$$

For large values of L , the amplitude of the wave function inside the hole is dominated by the last term. We obtain therefore

$$\frac{1}{A_+^2 L} \approx \cos^2 ka + \frac{k^2}{K^2} \sin^2 ka; \quad (36)$$

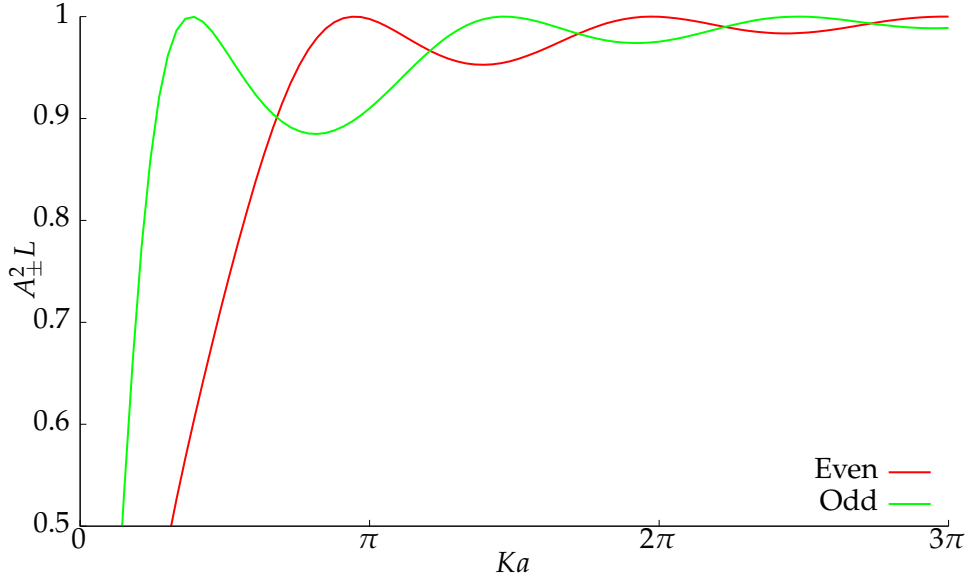
$$\frac{1}{A_-^2 L} \approx \sin^2 ka + \frac{k^2}{K^2} \cos^2 ka. \quad (37)$$

Notice that this amplitude reaches a maximum for $Ka = (2m + 1)\pi/2$ (even) and $Ka = m\pi$ (odd). These values correspond to the resonances. In the limit $KL \gg 1$, the amplitude of the wave function beyond the hole is given by

$$\lim_{L \rightarrow \infty} \frac{\sin^2 K(L - a)}{A_+^2 \cos^2 ka} = L; \quad \lim_{L \rightarrow \infty} \frac{\cos^2 K(L - a)}{A_+^2 \sin^2 ka} = L. \quad (38)$$

Thus we obtain, for $|x| > a$ and $KL \gg 1$,

$$u_{\pm}(x) = \pm \frac{1}{\sqrt{L}} \sin K(L - |x|). \quad (39)$$



3 Virtual levels (Problem 27)

The potential $V(x)$ is given by

$$V(x) = \begin{cases} +\infty, & \text{for } x < 0; \\ (\hbar^2 \Omega / 2m) \delta(x - \ell), & \text{for } x \geq 0. \end{cases} \quad (40)$$

We look for the wavefunctions $\psi_k(x)$ satisfying $\psi_k(x) = a \sin(kx)$ for $x \leq \ell$, and $a \cos(k(x - \ell)) + b \sin(k(x - \ell))$ for $x > \ell$. We obtain the conditions

$$\begin{aligned} a &= a \sin(k\ell); \\ b &= a [\cos(k\ell) + (\Omega/k) \sin(k\ell)]. \end{aligned} \quad (41)$$

These equations obviously admit solutions for all positive values of k . Let us set $a = -\sin \phi(k)$, $b = \cos \phi(k)$, so that $\psi_k(x) = \sin(k(x - \ell) - \phi)$ for $x > \ell$. We then have

$$\alpha = -\frac{\sin \phi(k)}{\sin(k\ell)} = \frac{\cos \phi(k)}{\cos(k\ell) + (\Omega/k) \sin(k\ell)}. \quad (42)$$

We obtain therefore the expression of $\phi(k)$:

$$-\cot \phi(k) = \cot(k\ell) + \frac{\Omega}{k}. \quad (43)$$

This implies

$$\sin^2 \phi(k) = \frac{1}{1 + \cot^2 \phi(k)} = \frac{\sin^2(k\ell)}{1 + (\Omega/k) \sin(2k\ell) + (\Omega/k)^2 \sin^2(k\ell)}. \quad (44)$$

Therefore

$$|\alpha(k)|^2 = \frac{1}{1 + (\Omega/k) \sin(2k\ell) + (\Omega/k)^2 \sin^2(k\ell)}. \quad (45)$$

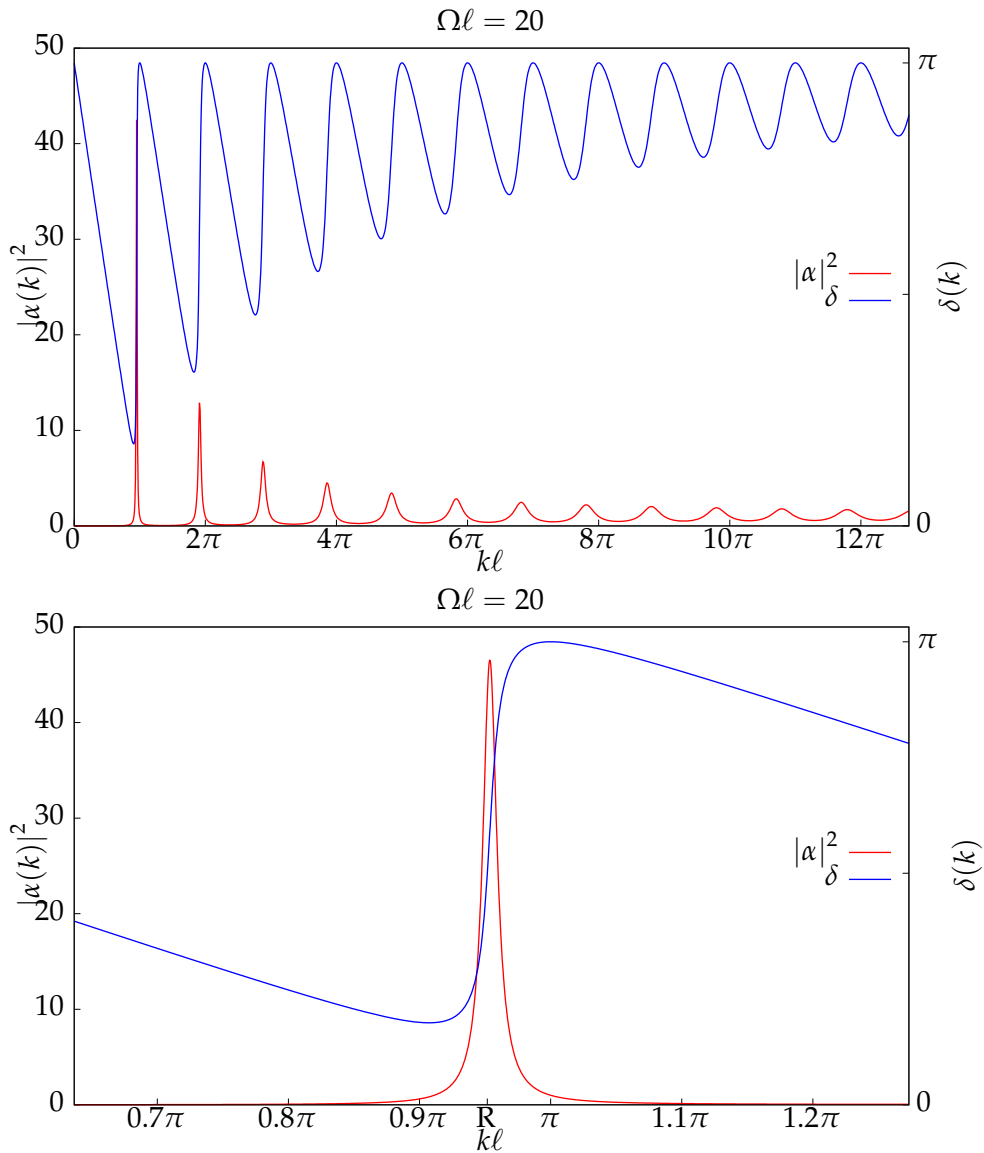
When $k^2 \ll \Omega$, these levels lie very close to the values of k for which $\sin(k\ell) = 0$. The dependence of $\alpha(k)$ on k smoothens out as k increases. The phase shift of the wavefunction upon crossing ℓ is given by $\delta = \phi(k) - k\ell$. It satisfies the relation

$$\tan \delta = -\frac{\Omega}{k} \frac{\sin^2(k\ell)}{1 + (\Omega/2k) \sin(2k\ell)}. \quad (46)$$

Note that when k is smaller than $\Omega/2$, the denominator on the rhs vanishes when

$$\sin(2k\ell) = -\frac{2k}{\Omega}. \quad (47)$$

This equation has solutions for $2k\ell$ close to $(2n + 1)\pi$ or to $2n\pi$. In the first case, the numerator is close to 1 and about constant. Then $\tan \delta$ goes through infinity, but the actual value of the wave function changes smoothly. In the second case there is a zero of $\tan \delta$ very close to the point in which it diverges. This means that the phase goes from, say, $\pi/2$ to π in a very short range of $k\ell$. Here I plot the amplitude $|\alpha(k)|^2$ on the left y axis and the phase shift δ on the right δ axis. In the plot I have redefined the determination of arctan in order to make it smooth. A second plot shows the behavior of $|\alpha|^2$ and δ close to the first resonance for $k\ell \approx \pi$. Note that δ goes through $\pi/2$ exactly at the resonance (marked with "R"). For larger values of k , δ makes only small ripples away from π .



4 Dirac comb (Problem 29)

Problem

Given a periodic potential formed by a sequence of Dirac functions with a distance a between them:

$$V(x) = \frac{\hbar^2}{m} \Omega \sum_{n=-\infty}^{+\infty} \delta(x - na), \quad (48)$$

determine the energy bands for this potential.

Solution

Let us consider the fundamental solutions

$$u_{\pm}(x) = e^{\pm ikx}. \quad (49)$$

Let $u(x)$ be given by

$$u(x) = \begin{cases} A_+ u_+(x) + A_- u_-(x), & \text{for } 0 < x < a; \\ e^{i\kappa a} (A_+ u_+(x-a) + A_- u_-(x-a)), & \text{for } a < x < 2a. \end{cases} \quad (50)$$

At $x = a$, we have the boundary conditions

$$\lim_{x \rightarrow a^+} u(x) = \lim_{x \rightarrow a^-} u(x); \quad (51)$$

$$\lim_{x \rightarrow a^+} u'(x) = \lim_{x \rightarrow a^-} u'(x) + 2\Omega u(a). \quad (52)$$

This implies

$$e^{i\kappa a} (A_+ + A_-) = (A_+ e^{i\kappa a} + A_- e^{-i\kappa a}); \quad (53)$$

$$i\kappa e^{i\kappa a} (A_+ - A_-) = i\kappa (A_+ e^{i\kappa a} - A_- e^{-i\kappa a}) + 2\Omega (A_+ e^{i\kappa a} + A_- e^{-i\kappa a}). \quad (54)$$

We need to find non-vanishing solution to this homogeneous system. This can only happen if the determinant vanishes. By evaluating the determinant we obtain the equation

$$\cos \kappa a = \cos ka + \frac{\Omega}{k} \sin ka. \quad (55)$$

This equation allows for real values of κ provided

$$\left| \cos ka + \frac{\Omega}{k} \sin ka \right| \leq 1. \quad (56)$$

Thus the edges of the bands are given by the condition

$$\cos ka + \frac{\Omega}{k} \sin ka = \pm 1. \quad (57)$$

Case (+1): We have

$$\frac{\Omega}{k} \sin ka = 1 - \cos ka = 2 \sin^2 \frac{ka}{2}, \quad (58)$$

and

$$\sin ka = 2 \sin \frac{ka}{2} \cos \frac{ka}{2}. \quad (59)$$

Thus we obtain

$$\sin \frac{ka}{2} = 0, \quad \text{or} \quad \frac{\Omega}{k} = \tan \frac{ka}{2}. \quad (60)$$

The conditions correspond respectively to

$$\frac{ka}{2} = m\pi, \quad \text{and} \quad \frac{k}{\Omega} = \cot \frac{ka}{2}. \quad (61)$$

Case (-1): We have

$$\frac{\Omega}{k} \sin ka = -(1 + \cos ka) = -2 \cos^2 \frac{ka}{2}, \quad (62)$$

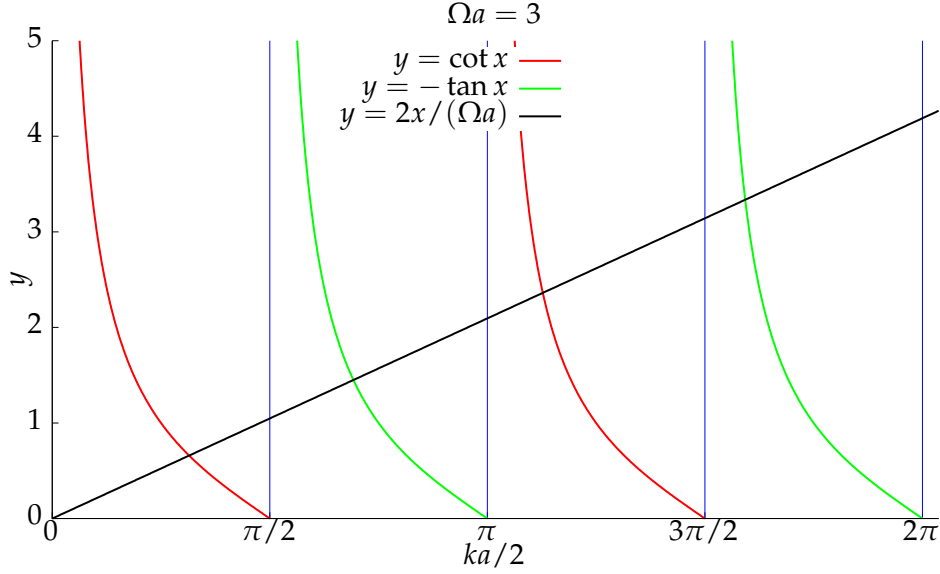
and therefore

$$\cos \frac{ka}{2} = 0, \quad \text{or} \quad \frac{\Omega}{k} = -\cot \frac{ka}{2}. \quad (63)$$

The conditions correspond respectively to

$$\frac{ka}{2} = (2m+1)\pi, \quad \text{and} \quad \frac{k}{\Omega} = -\tan \frac{ka}{2}. \quad (64)$$

This allows to solve the equation graphically.



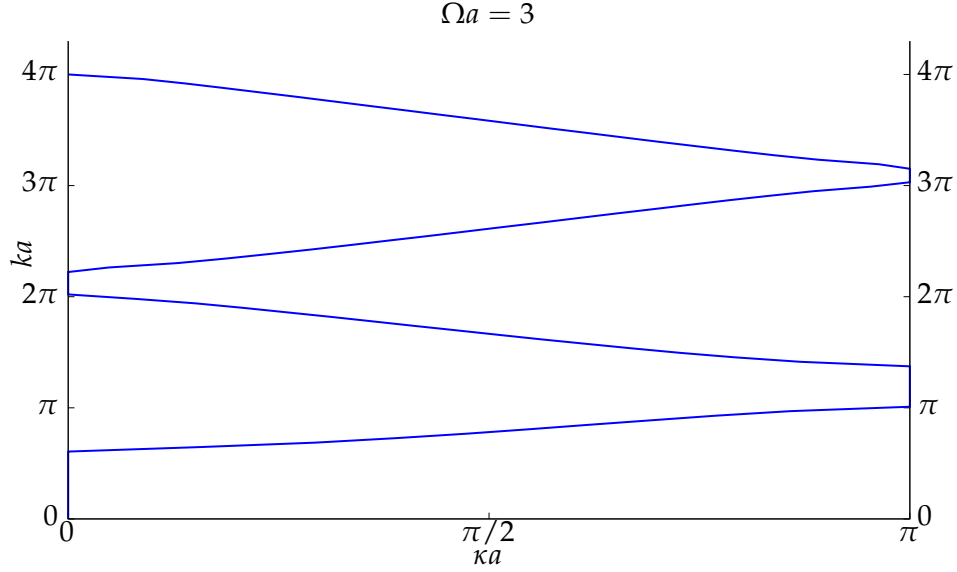
The spectrum can be obtained by expressing k as a function of the quasi-momentum κ . We have indeed

$$E = \frac{\hbar^2 k^2}{2m}, \quad (65)$$

where

$$\kappa a = \cos^{-1} \left(\cos ka + \frac{\Omega}{k} \sin ka \right). \quad (66)$$

Thus $\kappa a \in [0, \pi]$. We can plot κa as a function of k over the intervals in which the condition (57) is satisfied.



5 Periodic square barriers

We consider a periodic potential of period $\ell + L$, defined by

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq \xi \leq L; \\ (h^2/2m)\Omega^2, & \text{if } L \leq \xi \leq L + \ell; \end{cases} \quad (67)$$

where

$$\xi = (L + \ell) \left\lfloor \frac{x}{L + \ell} \right\rfloor, \quad (68)$$

where $\lfloor x \rfloor$ denotes the fractional part of x . We consider wavefunctions $\psi_k(x)$ that have the form

$$\psi_k(x) = \begin{cases} a e^{ikx} + b e^{-ikx}, & \text{for } 0 \leq x \leq \ell; \\ \alpha e^{\kappa(x-\ell)} + \beta e^{-\kappa(x-\ell)}, & \text{for } \ell \leq x \leq \ell + L. \end{cases} \quad (69)$$

Here κ is expressed as a function of k and Ω by

$$\kappa = \sqrt{\Omega^2 - k^2}. \quad (70)$$

It is imaginary when $k > \Omega$. In the region $(\ell + L) \leq x \leq (2\ell + L)$, the wave function will have the form $a' e^{ik(x-\ell-L)} + b' e^{-ik(x-\ell-L)}$, where (a', b') are related to (a, b) by

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = T \cdot \begin{pmatrix} a \\ b \end{pmatrix}, \quad (71)$$

where T is a certain matrix. By imposing the continuity of ψ_k and its first derivative at the discontinuities of V , we obtain the expression of T :

$$T = A_0^{-1} \cdot B \cdot B_0^{-1} \cdot A, \quad (72)$$

where

$$A = \begin{pmatrix} e^{ik\ell} & e^{-ik\ell} \\ ik e^{ik\ell} & -ik e^{-ik\ell} \end{pmatrix}; \quad (73)$$

$$A_0 = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix}; \quad (74)$$

$$B = \begin{pmatrix} e^{\kappa L} & e^{-\kappa L} \\ \kappa e^{\kappa L} & -\kappa e^{-\kappa L} \end{pmatrix}; \quad (75)$$

$$B_0 = \begin{pmatrix} 1 & 1 \\ \kappa & -\kappa \end{pmatrix}. \quad (76)$$

We obtain therefore

$$T = \frac{1}{2k\kappa} \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}, \quad (77)$$

with

$$\begin{aligned} T_{11} &= e^{ik\ell} [i(k^2 - \kappa^2) \sinh(\kappa L) + 2k\kappa \cosh(\kappa L)], \\ T_{12} &= -ie^{-ik\ell} (k^2 + \kappa^2) \sinh(\kappa L), \\ T_{21} &= ie^{ik\ell} (k^2 + \kappa^2) \sinh(\kappa L), \\ T_{22} &= e^{-ik\ell} [-i(k^2 - \kappa^2) \sinh(\kappa L) + 2k\kappa \cosh(\kappa L)]. \end{aligned} \quad (78)$$

One can check that

$$\det T = 1; \quad (79)$$

$$\text{Tr } T = \frac{1}{k\kappa} [2k\kappa \cos(k\ell) \cosh(\kappa L) + (\kappa^2 - k^2) \sin(k\ell) \sinh(\kappa L)]. \quad (80)$$

For $k > \Omega$, let us define $\kappa = \sqrt{k^2 - \Omega^2}$. We then obtain again $\det T = 1$ and

$$\text{Tr } T = \frac{1}{k\kappa} [2k\kappa \cos(k\ell) \cos(\kappa L) - (k^2 + \kappa^2) \sin(k\ell) \sin(\kappa L)]. \quad (81)$$

We are looking for the eigenvalues λ_{\pm} of T that satisfy

$$\lambda_{\pm} = e^{\pm K(L+\ell)}, \quad (82)$$

where K (the quasi-momentum) is real. Since $\det T = 1$, the eigenvalues can be either real (and then one will larger than one, and the other smaller than one, leading to a non-normalizable wavefunction) or complex, with modulus equal to one. This will obtain (and the wavefunction will be extended) if the discriminant of the secular equation of T is negative, i.e., if $\text{Tr } T$ satisfies the inequality

$$|\text{Tr } T| \leq 2. \quad (83)$$

Thus the band edges k^* are given by the conditions

$$\text{Tr } T(k^*) = \pm 2. \quad (84)$$

Deep in the wells, i.e., when $k \ll \Omega$, we can set $\kappa \approx \Omega$ and we obtain

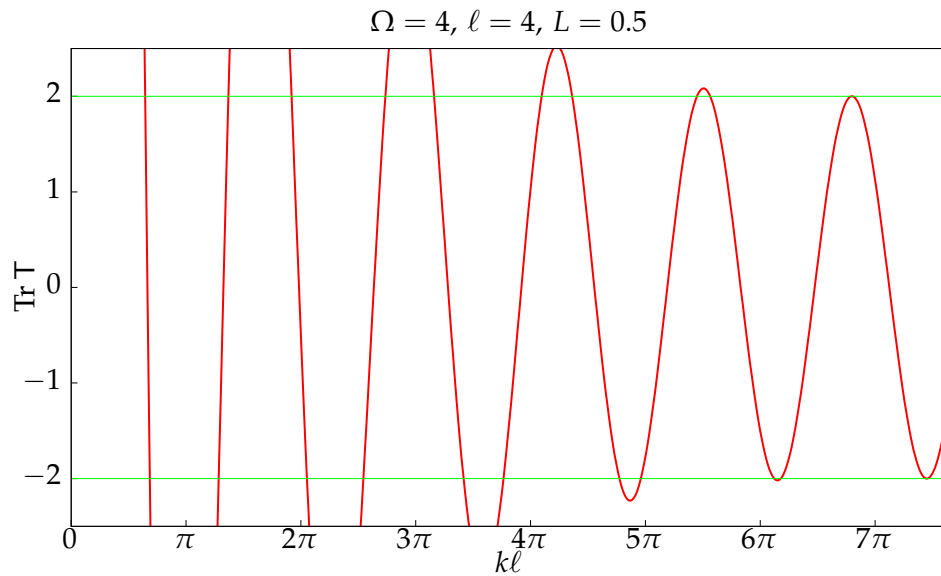
$$\text{Tr } T \approx \frac{1}{k} (2k \cos(k\ell) \cosh(\Omega L) + \Omega \sin(k\ell) \sinh(\Omega L)). \quad (85)$$

For $\Omega L \ll 1$ the right-hand side yields

$$\text{Tr } \mathbb{T} \approx \frac{1}{k} (2k \cos(k\ell) + \Omega^2 L \sin(k\ell)), \quad (86)$$

which compares with the result (57) obtained for the Dirac comb, taking into account the difference of notation.

For $k \gg \Omega$ we have $\kappa \approx k$, and therefore $\text{Tr } \mathbb{T} \approx 2(\cos^2(k\ell) - \sin^2(k\ell)) = 2 \cos(2k\ell)$, and the forbidden bands appear close to the values of k such that $2k\ell = (2n + 1)\pi/2$.



References

- [1] S. Flügge, *Practical Quantum Mechanics* (Berlin: Springer, 1974).