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

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

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

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

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

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

Thus the conditions for $x = L$ are

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

The determinant of this system is given by

$$\Delta = \kappa\cos(kL) - k\sin(kL). \tag{5}$$

We this obtain the equation

$$\tan kL = \frac{\kappa}{k}. \tag{6}$$

We can parametrize this equation by setting

$$\frac{\kappa}{k} = \tan\theta, \qquad \tan\theta \ge 0. \tag{7}$$

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

$$k = q\left|\cos\theta\right|, \qquad \kappa = q\left|\sin\theta\right|, \tag{8}$$

and

$$\tan kL = \tan\theta, \tag{9}$$

i.e.,

$$\frac{\theta}{qL} = \left|\cos\theta\right|, \qquad \text{for } \tan\theta \geq 0. \tag{10}$$

Case $(-)$**:** We set

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

Thus we obtain the equations

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

The determinant of this system reads

$$\Delta = -\left(\kappa\sin kL + k\cos kL\right). \tag{13}$$

We this obtain

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

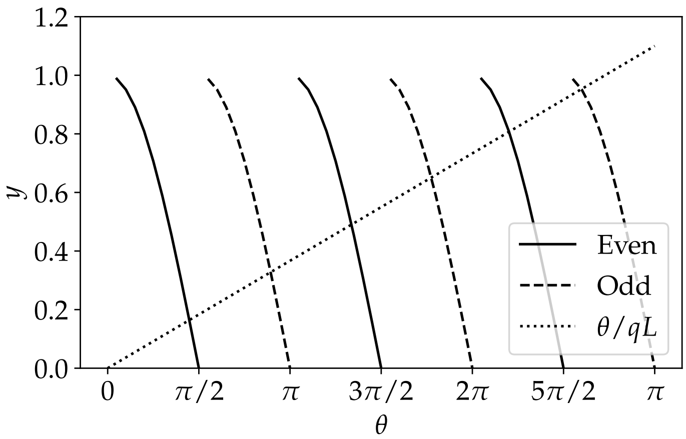
Thus we obtain the equation, for $\tan\theta \leq 0$,

$$k = \left|\sin\theta\right|, \qquad \kappa = \left|\cos\theta\right|, \tag{15}$$

leading to

$$\frac{\theta}{qL} = \left|\sin\theta\right|, \qquad \text{for } \tan\theta \leq 0. \tag{16}$$

Thus for $n\pi/2 \leq qL < (n+1)\pi/2$ we have $(n+1)$ bound states, alternatively even and odd. The figure shows the geometrical construction for $qL = 3\pi/1.1$.



2 Square well between walls (Problem 26)

Problem

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

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

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

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

We obtain the equations

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

The determinant reads

$$\Delta = \kappa \cos ka \, \cosh \kappa(L-a) - k \sin ka \, \sinh \kappa(L-a). \tag{20}$$

Thus we obtain the equation

$$k \tan ka = \kappa \coth \kappa(L-a). \tag{21}$$

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

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

We obtain the equations

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

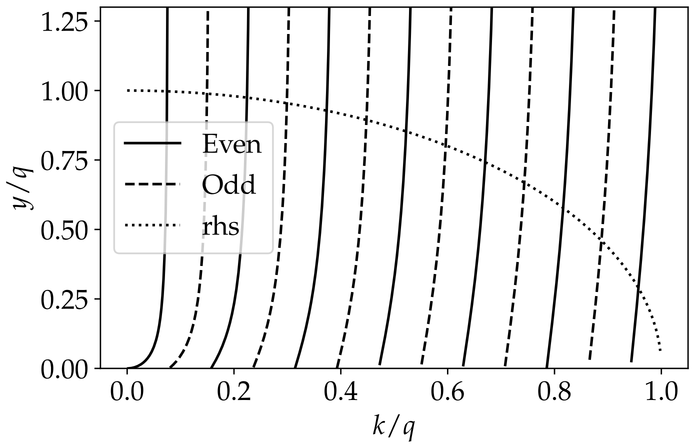
The determinant reads

$$\Delta = \kappa \sin ka \, \cosh \kappa(L-a) - k \cos ka \, \sinh \kappa(L-a). \tag{24}$$

Thus we obtain the equation

$$-k \cot ka = \kappa \coth \kappa(L-a). \tag{25}$$

The figure shows the construction for $a = 20$ and $L = 100$.



"Free" states: $E > 0$

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

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

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

We obtain the conditions

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

The determinant reads

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

Thus we obtain the equation

$$k \tan ka = K \cot K(L-a). \tag{29}$$

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

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

The continuity conditions read

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

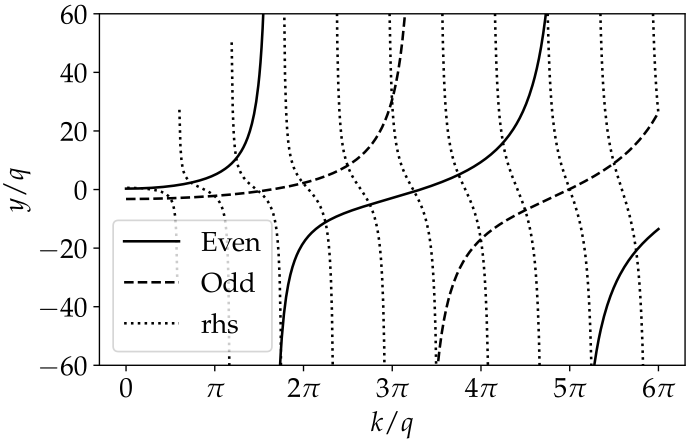
The determinant is given by

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

This leads to the equation

$$-k \cot ka = K \cot K(L-a). \tag{33}$$

For $L \gg a$, and $Ka \gg 1$, there is exactly one even and one odd solution in each KL interval of width π. The figure shows the costruction for $a = 0.3$ and $L = 2$.



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

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

We have likewise

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

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

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

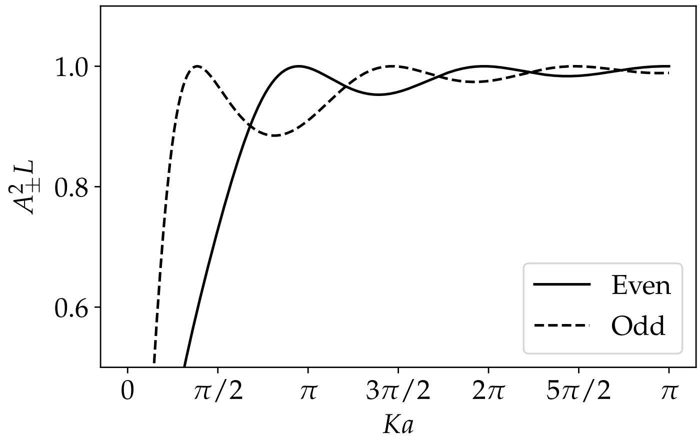
$$\frac{1}{A_-^2 L} \approx \sin^2 ka + \frac{k^2}{K^2}\cos^2 ka. \tag{37}$$

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

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

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

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



3 Virtual levels (Problem 27)

The potential $V(x)$ is given by

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

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

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

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

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

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

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

This implies

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

Therefore

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

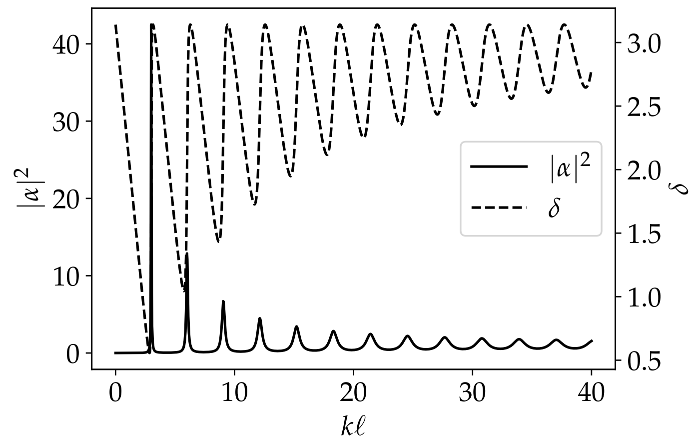
When $k^2 \ll \Omega$, these levels lie very close to the values of k for which $\sin(k\ell) = 0$. The dependence of $\alpha(k)$ on k smoothens out as k increases. The phase shift of the wavefunction upon crossing ℓ is given by $\delta = \phi(k) - k\ell$. It satisfies the relation

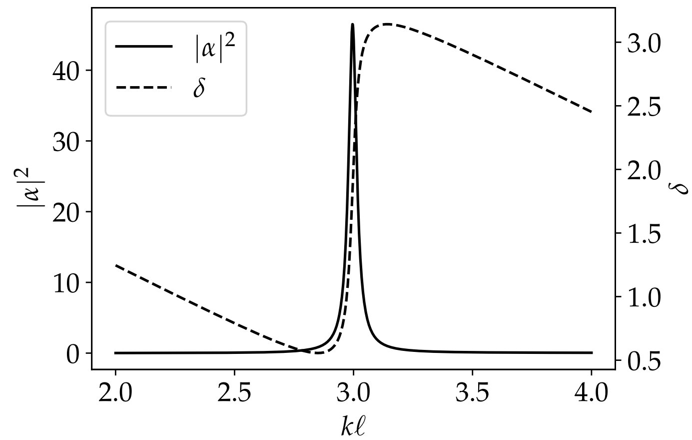
$$\tan\delta = -\frac{\Omega}{k}\frac{\sin^2(k\ell)}{1 + (\Omega/2k)\sin(2k\ell)}. \tag{46}$$

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

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

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:

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

determine the energy bands for this potential.

Solution

Let us consider the fundamental solutions

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

Let $u(x)$ be given by

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

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

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

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

This implies

$$\mathrm{e}^{\mathrm{i}\kappa a}(A_+ + A_-) = \left(A_+ \mathrm{e}^{\mathrm{i}ka} + A_- \mathrm{e}^{-\mathrm{i}ka}\right); \tag{53}$$

$$\mathrm{i}k\, \mathrm{e}^{\mathrm{i}\kappa a}\,(A_+ - A_-) = \mathrm{i}k\left(A_+ \mathrm{e}^{\mathrm{i}ka} - A_- \mathrm{e}^{-\mathrm{i}ka}\right) + 2\Omega(A_+ \mathrm{e}^{\mathrm{i}ka} + A_- \mathrm{e}^{-\mathrm{i}ka}). \tag{54}$$

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

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

This equation allows for real values of κ provided

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

Thus the edges of the bands are given by the condition

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

Case $(+1)$**:** We have

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

and

$$\sin ka = 2\sin\frac{ka}{2}\cos\frac{ka}{2}. \tag{59}$$

Thus we obtain

$$\sin\frac{ka}{2} = 0, \qquad \text{or} \qquad \frac{\Omega}{k} = \tan\frac{ka}{2}. \tag{60}$$

The conditions correspond respectively to

$$\frac{ka}{2} = m\pi, \qquad \text{and} \qquad \frac{k}{\Omega} = \cot\frac{ka}{2}. \tag{61}$$

Case (-1)**:** We have

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

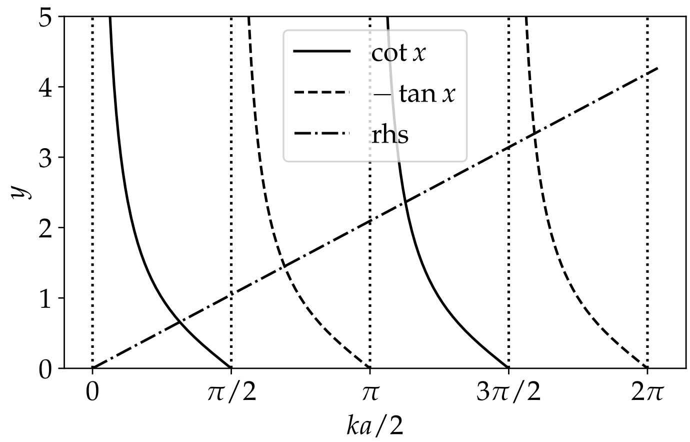
and therefore

$$\cos\frac{ka}{2} = 0, \qquad \text{or} \qquad \frac{\Omega}{k} = -\cot\frac{ka}{2}. \tag{63}$$

The conditions correspond respectively to

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

This allows to solve the equation graphically.



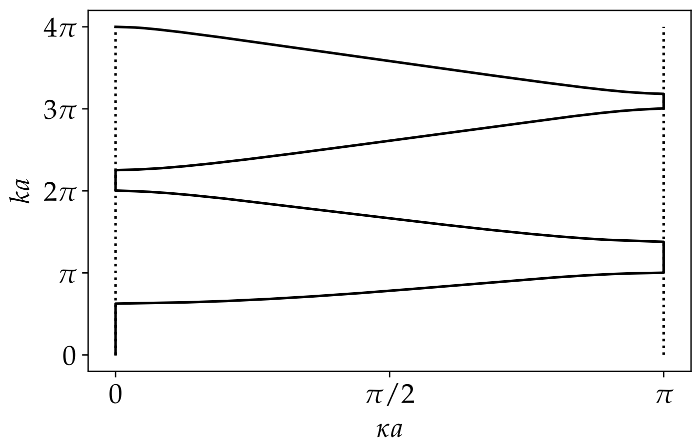
The spectrum can be obtained by expressing k as a function of the quasi-momentum κ. We have indeed

$$E = \frac{\hbar^2 k^2}{2m}, \tag{65}$$

where

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

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

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

where

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

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

$$\psi_k(x) = \begin{cases} a\,\mathrm{e}^{\mathrm{i}kx} + b\,\mathrm{e}^{-\mathrm{i}kx}, & \text{for } 0 \le x \le \ell; \\ \alpha\,\mathrm{e}^{\kappa(x-\ell)} + \beta\,\mathrm{e}^{-\kappa(x-\ell)}, & \text{for } \ell \le x \le \ell + L. \end{cases} \tag{69}$$

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

$$\kappa = \sqrt{\Omega^2 - k^2}. \tag{70}$$

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

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = \mathsf{T} \cdot \begin{pmatrix} a \\ b \end{pmatrix}, \tag{71}$$

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:

$$\mathsf{T} = \mathsf{A}_0^{-1} \cdot \mathsf{B} \cdot \mathsf{B}_0^{-1} \cdot \mathsf{A}, \tag{72}$$

where

$$\mathsf{A} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k\ell}, & \mathrm{e}^{-\mathrm{i}k\ell} \\ \mathrm{i}k\,\mathrm{e}^{\mathrm{i}k\ell}, & -\mathrm{i}k\,\mathrm{e}^{-\mathrm{i}k\ell} \end{pmatrix}; \tag{73}$$

$$\mathsf{A}_0 = \begin{pmatrix} 1, & 1 \\ \mathrm{i}k, & -\mathrm{i}k \end{pmatrix}; \tag{74}$$

$$\mathsf{B} = \begin{pmatrix} \mathrm{e}^{\kappa L}, & \mathrm{e}^{-\kappa L} \\ \kappa\,\mathrm{e}^{\kappa L}, & -\kappa\,\mathrm{e}^{-\kappa L} \end{pmatrix}; \tag{75}$$

$$\mathsf{B}_0 = \begin{pmatrix} 1, & 1 \\ \kappa, & -\kappa \end{pmatrix}. \tag{76}$$

We obtain therefore

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

with

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

One can check that

$$\det \mathsf{T} = 1; \tag{79}$$

$$\mathrm{Tr}\,\mathsf{T} = \frac{1}{k\kappa}\left[2k\kappa\cos(k\ell)\cosh(\kappa L) + (\kappa^2-k^2)\sin(k\ell)\sinh(\kappa L)\right]. \tag{80}$$

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

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

We are looking for the eigenvalues $\lambda_\pm$ of T that satisfy

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

where K (the quasi-momentum) is real. Since $\det \mathsf{T} = 1$, 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 $\mathrm{Tr}\,\mathsf{T}$ satisfies the inequality

$$|\mathrm{Tr}\,\mathsf{T}| \leq 2. \quad (83)$$

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

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

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

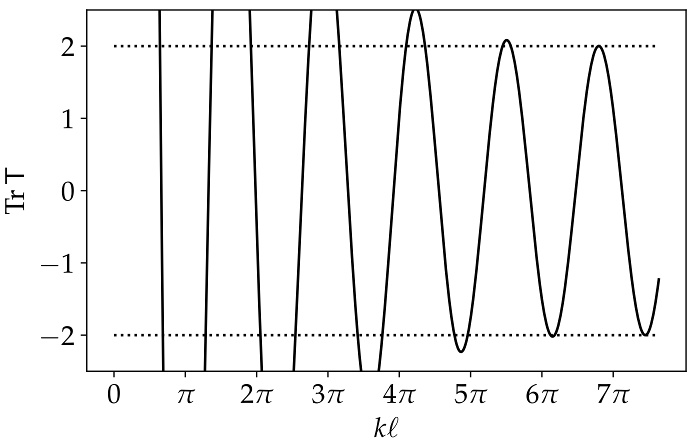
$$\mathrm{Tr}\,\mathsf{T} \approx \frac{1}{k}\left(2k\cos(k\ell)\cosh(\Omega L) + \Omega\sin(k\ell)\sinh(\Omega L)\right). \quad (85)$$

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

$$\mathrm{Tr}\,\mathsf{T} \approx \frac{1}{k}\left(2k\cos(k\ell) + \Omega^2 L\sin(k\ell)\right), \quad (86)$$

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 $\mathrm{Tr}\,\mathsf{T} \approx 2(\cos^2(k\ell) - \sin^2(k\ell)) = 2\cos(2k\ell)$, and the forbidden bands appear close to the values of k such that $2k\ell = (2n+1)\pi/2$.



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