Quantum Mechanics

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Lesson VII
March 26, 2019

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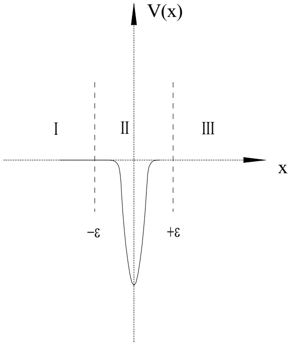
- A δ-function is infinitely high, infinitesimally narrow spike at $x = a$
- If $a = 0$ ☞ potential of form

$$V(x) = -\alpha\delta(x)$$

  α ☞ some constant of appropriate dimension
- Schrödinger equation for δ-function potentail well reads

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) - \alpha\delta(x)\psi(x) = E\psi(x)$$



- In region I and III Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x)$$

or

$$\frac{\partial^2}{\partial x^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x)$$

- It has a solution of the form $\psi(x) = Ae^{\lambda x}$
- Plugging this back into Schrödinger equation reveals that $\lambda = \pm ik$
- If $E < 0$ ☞ k is imaginary so we write

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{-\frac{2m|E|}{\hbar^2}} = i\kappa$$

and the solution becomes

$$\psi_I(x) = A\,e^{+\kappa x} + B\,e^{-\kappa x} \qquad x < 0$$

$$\psi_{III}(x) = Fe^{+\kappa x} + Ge^{-\kappa x} \qquad x > 0$$

- Region I: $E < 0$ ☞ solution blows up as $x \to -\infty$ unless $B = 0$
- Region III: $E > 0$ ☞ solution blows up as $x \to +\infty$ unless $F = 0$
- This means that solutions in regions I and III are:

$$\psi_I(x) = Ae^{+\kappa x} \qquad x < 0$$

$$\psi_{III}(x) = Ge^{-\kappa x} \qquad x > 0$$

- Recall ☞ wave function must be continuous
  to have meaning as a probability amplitude
- For δ-function potential where region II has no real width wave function in regions I and III must have same value at $x = 0$
- This requires that $A = G$ so solution to Schrödinger's equation is

$$\psi_I(x) = Ae^{\kappa x} \qquad x < 0$$

$$\psi_{III}(x) = Ae^{-\kappa x} \qquad x > 0$$

- Equivalently

$$\psi_{I,III}(x) = Ae^{-\kappa |x|}$$

- Second condition on wave function solution to Schrödinger eq.: first derivative of wave function must be continuous for piecewise-continuous potentials
- BUT ☞ δ-function potential is not piecewise continuous but infinite
- Look carefully at requirement imposed on first derivative of wave function by Schrödinger equation
- Integrate Schrödinger eq. with respect to x over small interval $\Delta\epsilon$

$$-\frac{\hbar}{2m}\int_{x_0-\epsilon}^{x_0+\epsilon}\frac{\partial^2\psi(x)}{\partial x^2}dx+\int_{x_0-\epsilon}^{x_0+\epsilon}V(x)\psi(x)dx=E\int_{x_0-\epsilon}^{x_0+\epsilon}\psi(x)dx$$

- If $\Delta\epsilon\to 0$ ☞ integral over wave function must go to zero because $\psi(x)$ is a continuous single-valued function
- Integral of $\psi''(x)$ is just $\psi'(x)$ so that we are left with

$$\lim_{\Delta\epsilon\to 0}\frac{\partial\psi(x)}{\partial x}\bigg|_{x_0-\epsilon}^{x_0+\epsilon}=\lim_{\Delta\epsilon\to 0}\frac{2m}{\hbar^2}\int_{x_0-\epsilon}^{x_0+\epsilon}V(x)\psi(x)dx$$

- Using definition of δ-function we evaluate integral

$$\lim_{\Delta\epsilon\to 0} \frac{\partial\psi(x)}{\partial x}\bigg|_{-\epsilon}^{+\epsilon} = \lim_{\Delta\epsilon\to 0} \frac{2m}{\hbar^2}\int_{-\epsilon}^{+\epsilon} -\alpha\delta(x)\psi(x)dx = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

which we rewrite as

$$\lim_{\Delta\epsilon\to 0}\left(\frac{\partial\psi(x)}{\partial x}\bigg|_{+\epsilon} - \frac{\partial\psi(x)}{\partial x}\bigg|_{-\epsilon}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0) = -\frac{2m\alpha}{\hbar^2}A$$

- Now ☞ first partial derivative is evaluated in region $x > 0$ while second partial is evaluated in region $x < 0$ giving

$$\lim_{\Delta\epsilon\to 0}\left(-\kappa A e^{-\kappa x}\big|_{+\epsilon} - (+\kappa A e^{+\kappa x})\big|_{-\epsilon}\right) = -\frac{2m\alpha}{\hbar^2}A$$

- Limit as $\epsilon \to 0$ fixes value of κ

$$\lim_{\Delta\epsilon\to 0}(-2\kappa A e^{-\kappa\epsilon}) = -2m\alpha\hbar^2 A$$

and therefore of energy E according to equation

$$\kappa = \frac{m\alpha}{\hbar^2} = \sqrt{\frac{2m|E|}{\hbar^2}}$$

- We see that there is only one allowed energy given by

$$E = -\frac{m^2\alpha^2}{\hbar^4}\,\frac{\hbar^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$$

α ☞ "depth" of δ-function potential

$$\int_{-\infty}^{0} A^2 e^{+2\kappa x} dx + \int_{0}^{+\infty} A^2 e^{-2\kappa x} dx = 1$$

$$\left.\frac{A^2 e^{+2\kappa x}}{+2\kappa}\right|_{-\infty}^{0} + \left.\frac{A^2 e^{-2\kappa x}}{-2\kappa}\right|_{0}^{+\infty} = 1$$

$$\frac{A^2}{\kappa} = 1 \Rightarrow A = \sqrt{\kappa}$$

- For δ-function potential ☞ we have only one eigenstate corresponding to energy $E < 0$ given by

$$\psi_E(x) = \sqrt{\kappa}\, e^{-\kappa|x|} \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$

- In region I and III the Schrödinger equation is again

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x)$$

or

$$\frac{\partial^2}{\partial x^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x)$$

- It has a solution of the form $\psi(x) = Ae^{\lambda x}$
- Plugging this back into Schrödinger equation reveals that $\lambda = \pm ik$
- If $E > 0$ ☞ k is real given by

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

and the solution becomes

$$\psi_I(x) = Ae^{+ikx} + Be^{-ikx} \qquad x < 0$$

$$\psi_{III}(x) = Fe^{+ikx} + Ge^{-ikx} \qquad x > 0$$

- Time-dependent have form of two traveling sinusoidal waves moving in opposite directions
- Assume particles originate in negative half-plane ☞ region $x < 0$
- Particles moving from left encounter δ-function potential at $x = 0$: will either continue moving in $+x$ direction (i.e., they are transmitted through the region of potential change) or will be reflected and move back in $-x$ direction
- If $x < 0$ we must allow for possibility of 2 opposite going waves but in region where $x > 0$ there is only one possibility ☞ wave moves only in $+x$ direction
- Based upon the initial conditions ☞ $G = 0$ and so

$$\psi_I(x) = A^{+ikx} + B^{-ikx} \qquad x < 0$$

$$\psi_{III}(x) = Fe^{+ikx} \qquad x > 0$$

- Since wave function must be continuous these two equations must be equal at $x = 0$ giving the condition

$$A + B = F$$

- Second condition on wave function solution to Schrödinger eq.: first derivative of wave function must be continuous for piecewise-continuous potentials
- BUT again ☞ potential is not piecewise continuous but infinite.
- As before ☞ we integrate Schrödinger eq. over small interval $\Delta\epsilon$

$$-\frac{\hbar}{2m}\int_{x_0-\epsilon}^{x_0+\epsilon}\frac{\partial^2\psi(x)}{\partial x^2}dx+\int_{x_0-\epsilon}^{x_0+\epsilon}V(x)\psi(x)dx=E\int_{x_0-\epsilon}^{x_0+\epsilon}\psi(x)dx$$

- If $\Delta\epsilon\to 0$ ☞ integral over wave function must go to zero because $\psi(x)$ is a continuous single-valued function
- Integral of $\psi''(x)$ is just $\psi'(x)$ so that we are left with

$$\lim_{\Delta\epsilon\to 0}\left.\frac{\partial\psi(x)}{\partial x}\right|_{x_0-\epsilon}^{x_0+\epsilon}=\lim_{\Delta\epsilon\to 0}\frac{2m}{\hbar^2}\int_{x_0-\epsilon}^{x_0+\epsilon}V(x)\psi(x)dx$$

- Using definition of δ-function we evaluate integral

$$\lim_{\Delta\epsilon\to 0} \frac{\partial\psi(x)}{\partial x}\bigg|_{-\epsilon}^{+\epsilon} = \lim_{\Delta\epsilon\to 0} \frac{2m}{\hbar^2}\int_{-\epsilon}^{+\epsilon} -\alpha\delta(x)\psi(x)dx = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

which we rewrite as

$$\lim_{\Delta\epsilon\to 0}\left(\frac{\partial\psi(x)}{\partial x}\bigg|_{+\epsilon} - \frac{\partial\psi(x)}{\partial x}\bigg|_{-\epsilon}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0) = -\frac{2m\alpha}{\hbar^2}(A+B)$$

- Now ☞ first partial derivative is evaluated in region $x > 0$ while second partial is evaluated in region $x < 0$ giving

$$\lim_{\Delta\epsilon\to 0}\left\{ikFe^{+ikx}\Big|_{+\epsilon} - \left[ikAe^{+ikx} + (-ik)Be^{-ikx}\right]\Big|_{-\epsilon}\right\} = -\frac{2m\alpha}{\hbar^2}(A+B)$$

- In the limit

$$\lim_{\Delta\epsilon\to 0} ik\left[(F+B)e^{+ik\epsilon} - Ae^{-ik\epsilon}\right] = -\frac{2m\alpha}{\hbar^2}(A+B)$$

this reduces to

$$F + B - A = \frac{i2m\alpha}{\hbar^2 k}(A+B) = 2i\beta(A+B) \quad \text{with} \quad \beta = \frac{m\alpha}{\hbar^2 k}$$

- Using condition on continuity of wave function $F = A + B$ this last equation reduces to $B = i\beta(A + B)$ or

$$B = \frac{i\beta}{1 - i\beta} A$$

- Since $F = A + B$ solving for F gives

$$F = \frac{1}{1 - i\beta} A$$

- Probability current density

$$j = -\frac{i\hbar}{2m}\left[\Psi^*(x,t)\frac{\partial}{\partial x}\Psi(x,t) - \Psi(x,t)\frac{\partial}{\partial x}\Psi^*(x,t)\right]$$

- It should be obvious that:
  amplitude A related to probability of measuring incoming particle
  amplitude B related to probability of measuring reflected particle
  and amplitude F to measuring transmitted particle

$$R \equiv \left|\frac{j_{\text{reflected}}}{j_{\text{incident}}}\right| \quad \text{and} \quad T \equiv \left|\frac{j_{\text{transmitted}}}{j_{\text{incident}}}\right|$$

- Solutions for δ-function potential are travelling plane waves

$$\Psi(x,t) = Ae^{i(kx-\omega t)}$$

- Probability current density for plane waves is

$$j = -\frac{i\hbar}{2m}\left[A^* e^{-i(kx-\omega t)}\frac{\partial}{\partial x}Ae^{i(kx-\omega t)} - Ae^{i(kx-\omega t}\frac{\partial}{\partial x}A^* e^{-i(kx-\omega t)}\right]$$

$$j = -\frac{i\hbar}{2m}\left[A^* e^{-i(kx-\omega t)} ikAe^{i(kx-\omega t)} - Ae^{i(kx-\omega t}(-ik)A^* e^{-i(kx-\omega t)}\right]$$

$$j = -\frac{i\hbar}{2m}\left[ik|A|^2 - (-ik)|A|^2\right]$$

$$j = -\frac{i\hbar}{2m}2ik|A|^2 = \frac{\hbar k}{m}|A|^2$$

- This has the form

  $j = \frac{p}{m}|A|^2 = u|A|^2$ where u ☞ velocity

  and will be positive or negative depending upon sign of k

- Incident probability current density

$$j_{\rm incident} = +\frac{\hbar k}{m}|A|^2$$

- Reflected probability current density

$$j_{\rm reflected} = -\frac{\hbar k}{m}|B|^2$$

- Transmitted probability current density

$$j_{\rm transmitted} = +\frac{\hbar k}{m}|F|^2$$

- Recall ☞ $\beta^2 = \frac{m^2\alpha^2}{\hbar^4 k^2} = \frac{m^2\alpha^2}{\hbar^4(2mE/\hbar^2)} = \frac{m\alpha^2}{2\hbar^2 E}$
- Reflection coefficient

$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2} = \frac{1}{1+1/\beta^2} = \frac{1}{1+2\hbar^2 E/(m\alpha^2)}$$

- Transmission coeffcient

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2} = \frac{1}{1+m\alpha^2/(2\hbar^2 E)}$$

- For δ-function potential barrier ☞ sign of potential is changed

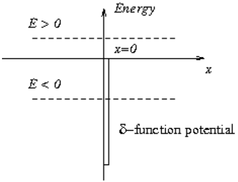
$$V(x) = +\alpha\delta(x)$$

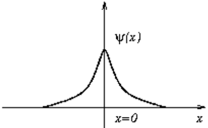
- $V(x)$ acts as infinitely narrow, infinitely tall potential barrier in otherwise constant potential background
- It should be obvious that there is no bound state solution for $E < 0$
- For $E > 0$ ☞ all we have to do to find solution for infinite barrier is change sign of α
- But reflection and transmission coefficients are function only of α^2 so that we obtain the same result as for the potential well
- This means that a quantum mechanical particle can penetrate a potential barrier of infinite height!

- Particularly interesting potentials having lot of practical relevances are double or multiple (periodic) square well potentials
- These potentials are often found in electronic arrangements in solids or molecules
- First ☞ consider attractive double δ-function potential

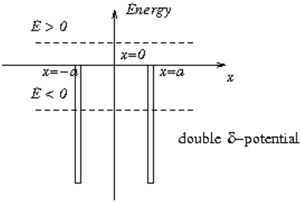
$$V(x) = -\alpha[\delta(x+a) + \delta(x-a)] \quad \text{with} \quad \alpha = \hbar^2/(ma)$$

- Interest is in $E < 0$ bound states





Bound state wave function
for δ–function potential



- Schrödinger equations are solved for wave functions in regions

$$\begin{cases} I: & x < a \\ II: & a \leq x \leq a \\ III: & x > a \end{cases}$$

- In all these regions we have same Schrödinger equation

$$\frac{d^2\psi}{dx^2} - \kappa^2\psi = 0 \quad \text{with} \quad \kappa^2 = -\frac{2mE}{\hbar^2}$$

- Solutions are (discarding those that blow up at $\pm\infty$):

$$\begin{aligned} x < -a \quad &: \quad \psi(x) = Ae^{\kappa x} \\ -a \leq x \leq a \quad &: \quad \psi(x) = Ce^{\kappa x} + De^{-\kappa x} \\ x > a \quad &: \quad \psi(x) = Fe^{-\kappa x} \end{aligned}$$

- Apply boundary conditions to evaluate unknown constants
  - Continuity of $\psi(x)$ at $x = -a$

$$Ae^{-\kappa a} = Ce^{-\kappa a} + De^{\kappa a}$$

  - Continuity of $\psi(x)$ at $x = a$

$$Fe^{-\kappa a} = Ce^{\kappa a} + De^{-\kappa a}$$

  - Discontonuity of $d\psi/dx$ at $x = -a$

$$\kappa(Ce^{-\kappa a} - De^{\kappa a}) - \kappa Ae^{-\kappa a} = -\frac{2m\alpha}{\hbar^2} Ae^{-\kappa a} = -\frac{2}{a} Ae^{-\kappa a}$$

  - Discontonuity of $d\psi/dx$ at $x = a$

$$-\kappa Fe^{-\kappa a} - \kappa(Ce^{-\kappa a} - De^{\kappa a}) = -\frac{2m\alpha}{\hbar^2} Fe^{-\kappa a} = -\frac{2}{a} Fe^{-\kappa a}$$

- Discontinuous boundary equations can be simplified as
  For $x = -a$ ☞ $Ae^{-\kappa a}(\kappa - 2/a) = \kappa(Ce^{-\kappa a} - De^{\kappa a})$
  For $x = a$ ☞ $Fe^{-\kappa a}(2/a - \kappa) = \kappa(Ce^{-\kappa a} - De^{\kappa a})$

- To determine allowed energies
  we solve boundary equations for C and D eliminating A and F

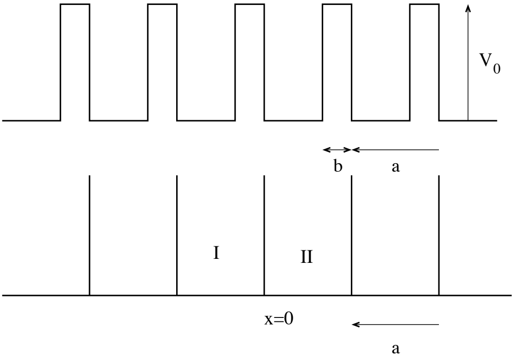
$$\left.\begin{array}{l} Ce^{-\kappa a} = De^{\kappa a}(\kappa a - 1) \\ De^{-\kappa a} = Ce^{\kappa a}(\kappa a - 1) \end{array}\right\} C^2 = D^2 \Rightarrow C = \pm D$$

- Not surprising ☞ because of symmetry of potential
  we have both even and odd parity solutions
  - Even parity $C = D$ ☞ $\psi(x) = C(e^{\kappa x} + e^{-\kappa x}) = C' \cosh(\kappa x)$
  - Odd parity $C = -D$ ☞ $\psi(x) = C(e^{\kappa x} - e^{-\kappa x}) = C' \sinh(\kappa x)$
- Solving for bound state(s) through transcendental equations
  - Even: $C = D$ ☞ $e^{-2\kappa a} = \kappa a - 1 \Rightarrow e^{-2y} = y - 1$
  - Odd: $C = -D$ ☞ $e^{-2\kappa a} = 1 - \kappa a \Rightarrow e^{-2y} = 1 - y$
- Only even bound state solution ☞ $y = \kappa a \approx 1.11$
- $y = \kappa a = 0$ leaves bound state wave function non normalizable
- For $\alpha > \hbar^2/ma$ we can get one odd parity bound state too
- For $\alpha = \hbar^2/(ma)$ ☞ double δ-function gives lower bound state E

$$E_s = -\frac{m\alpha^2}{2\hbar^2} = -\frac{\hbar^2}{2ma} \quad \text{and} \quad E_d = -(1.11)^2 \frac{\hbar^2}{2ma^2}$$

- Kronig-Penney model
  describes electron motion in periodic array of rectangular barriers
- Kronig-Penney-Dirac model ☞ special case of Kronig-Penney obtained by taking limit $b \to 0$ and $V_0 \to \infty$ but $U_0 \equiv V_0 b$ finite
- In this limit ☞ each rectangular barrier becomes a Dirac δ-function

$$U(x) = U_0 \sum_{n=-\infty}^{+\infty} \delta(x - na)$$



- Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\psi''(x) + U(x)\psi(x) = E\psi(x)$$

- Consider two segments: $\begin{cases} I & a < x < 0 \\ II & 0 < x < a \end{cases}$
- Since potential energy is equal to zero inside each segment wave functions are linear combinations of two plane waves

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$$

$$\psi_{II}(x) = Ce^{ikx} + De^{-ikx}$$

- Recall $k = \sqrt{2mE}/\hbar$
- Wave function must satisfy Bloch theorem ☞ $\psi(x+a) = e^{iqa}\psi(x)$
- Imposing symmetry condition for $0 \leq x \leq a$ we have

$$\psi_{II}(x) = e^{iqa}\psi_I(x-a)$$

$$Ce^{ikx} + De^{-ikx} = e^{iqa}\left(Ae^{ik(x-a)} + Be^{-ik(x-a)}\right)$$

- Since e^{ikx} and e^{-ikx} are linearly independent functions, the coefficients in front of the e^{ikx} terms must match

$$C = Ae^{iqa}e^{-ika} \quad \text{and} \quad D = e^{iqa}e^{ika}$$

  wave function ψ_{II} becomes

$$\psi_{II}(x) = e^{iqa}\left[Ae^{ik(x-a)} + Be^{-ik(x-a)}\right]$$

- Boundary conditions
  - wave function is continuos at $x = 0$

$$A + B = e^{iqa}\left[Ae^{ika} + Be^{-ika}\right]$$

  - discontinuity of wave function at $x = 0$ is obtained by integrating the Schrödinger equation over narrow interval $(-\epsilon, \epsilon)$ around $x = 0$

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\psi''(x)dx + U_0\int_{-\epsilon}^{+\epsilon}\delta(x)\psi(x)dx = E\int_{-\epsilon}^{+\epsilon}\psi(x)dx$$

    which gives

$$-\frac{\hbar^2}{2m}\left(\psi'_{II}(0) - \psi'_{I}(0)\right) + U_0\psi_I(0) = 0$$

- Derivatives

$$\psi_I'(0) = ik\left[Ae^{ikx} - Be^{-ikx}\right]\Big|_{x=0} = ik(A-B)$$

$$\psi_{II}'(0) = ike^{iqa}\left[Ae^{ik(x-a)} - Be^{-ik(x-a)}\right]\Big|_{x=0} = ike^{iqa}\left[Ae^{-ika} - Be^{ika}\right]$$

- Substituting derivatives back ☞ obtain 2×2 system for A and B

$$A\left(1 - e^{i(k-q)a}\right) + B\left(1 - e^{i(k+q)a}\right) = 0$$

$$A\left(e^{i(q-k)a} - 1 - \frac{2mU_0}{i\hbar k}\right) + B\left(-e^{i(k+q}a + 1 - \frac{2mU_0}{i\hbar k}\right) = 0$$

- Non-trivial solution ☞ determinant must equal zero

$$\left(1 - e^{i(q-k)a}\right)\left(-e^{i(q+k)a} + 1 - \frac{2mU_0}{i\hbar^2 k}\right) = \left(1 - e^{i(q+k)a}\right)\left(e^{i(q-k)a} - 1 - \frac{2mU_0}{i\hbar^2 k}\right)$$

- Opening brackets and simplifying yields

$$\cos(qa) = \cos(ka) + \frac{mU_0 a}{\hbar^2}\,\frac{\sin(ka)}{ka}$$

- $u = mU_0 a/\hbar$ ☞ dimensionless parameter of model "measuring" strength of periodic potential

- Transcendental equation

$$\cos(qa) = \cos(ka) + u\frac{\sin(ka)}{ka}$$

constrains allowed k values (and therefore E)
similar to quantized energies for bound states

- If $U_0 > 0$ ☞ maximum value of RHS reached at $ka = 0$

$$\lim_{ka \to 0} [\cos(ka) + u \sin(ka)/(ka)] = 1 + u > 0$$

- For larger $|ka|$ ☞ RHS decreases and oscillates
- LHS bounded by unity ☞ $-1 \leq \cos(qa) \leq 1$
- Solution in real numbers for k only possible within those intervals where magnitude of RHS is less than unity
- There are allowed bands of k and gap between those bands
- Appearence of energy bands separated by energy gaps is hallmark of periodic lattice potential system

Example

- $\cos(ka) + u\frac{\sin(ka)}{ka}$ ☞ $u = 10$
- Horizontal lines ☞ bounds on $\cos(qa)$