$$\psi_k(x) = Ae^{iqx} + Be^{-iqx} = e^{ikx}u_k(x)$$

For x such that $x \neq na$, $U(x) = 0 \Rightarrow -\frac{\hbar^2}{2m}\psi'' = E\psi \Rightarrow$

(a) $$\boxed{E_k = \frac{\hbar^2 q^2}{2m}}$$

(b) $\psi_k(a) = e^{ika}\psi_k(0) \Rightarrow$

$$\boxed{A + B = Ae^{i(q-k)a} + Be^{-i(q+k)a}}$$

(c) Schrödinger eq. is

$$\left(E_k + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi_k(x) = \sum_n a U_0 \delta(x - na)\psi(x)$$

Integrate both sides between $-\delta$ and δ, δ very small:

$$\underbrace{E_k \int_{-\delta}^{\delta} dx\, \psi_k(x)}_{0} + \frac{\hbar^2}{2m}\left[\left(\frac{\partial\psi_k}{\partial x}\right)_{x=\delta} - \left.\frac{\partial\psi_k}{\partial x}\right|_{x=-\delta}\right] = aU_0\psi(0)$$

$$\left.\frac{\partial\psi_k}{\partial x}\right)_{x=\delta} = iq(A - B)$$

$$\left.\frac{\partial\psi_k}{\partial x}\right|_{x=-\delta} = e^{-ika}\left.\frac{\partial\psi_k}{\partial x}\right)_{x=a-\delta} = e^{-ika}\, iq\left(Ae^{iqa} - Be^{-iqa}\right)$$

and $\psi(0) = A + B$, so

$$\boxed{\frac{\hbar^2}{2m} iq\left[A - B - Ae^{i(q-k)a} + Be^{-i(q+k)a}\right] = aU_0(A + B)}$$

(d) So we have the system of eqs for A, B

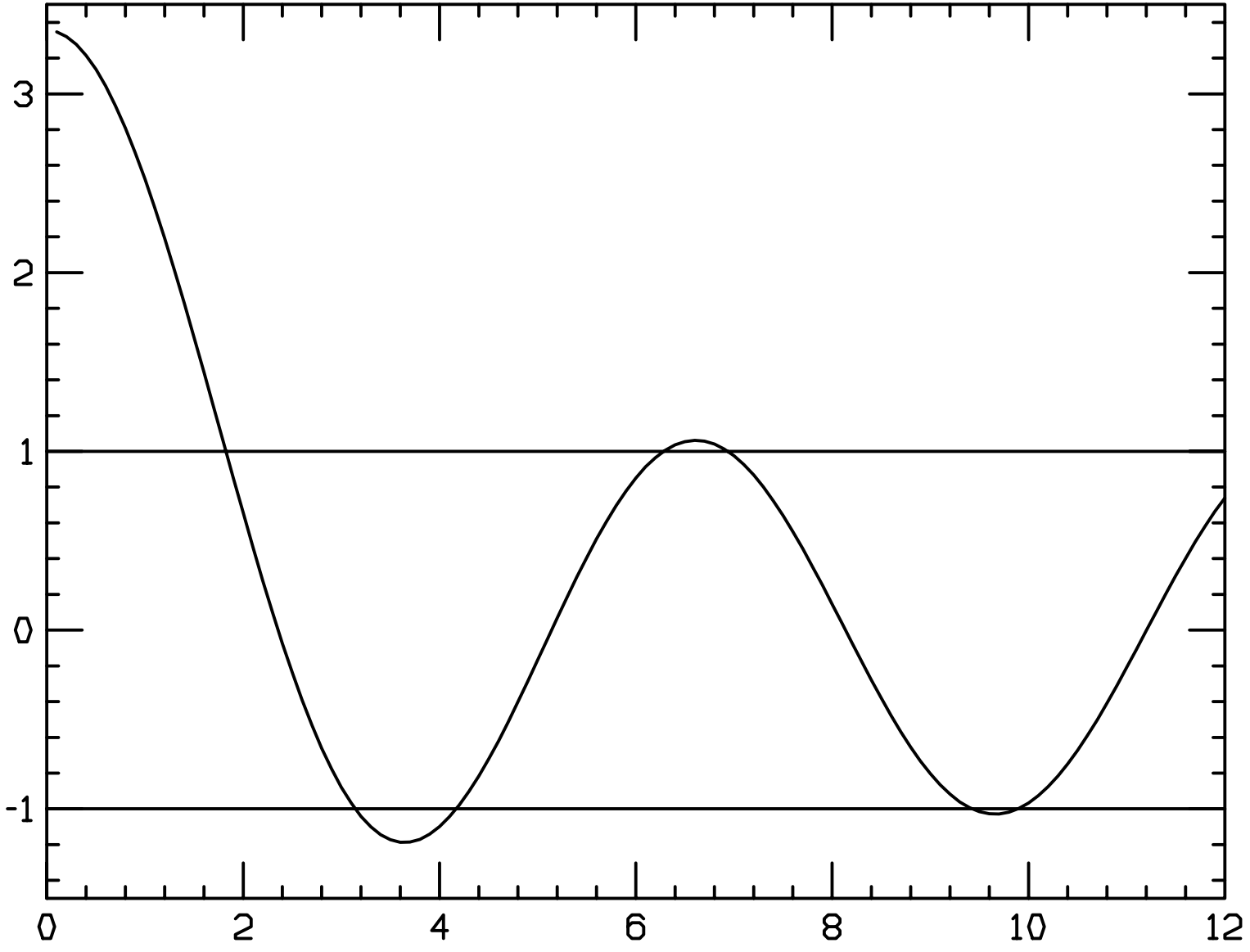
$$\left(1-e^{i(q-k)a}\right)A+\left(1+e^{-i(q+k)a}\right)B=0$$

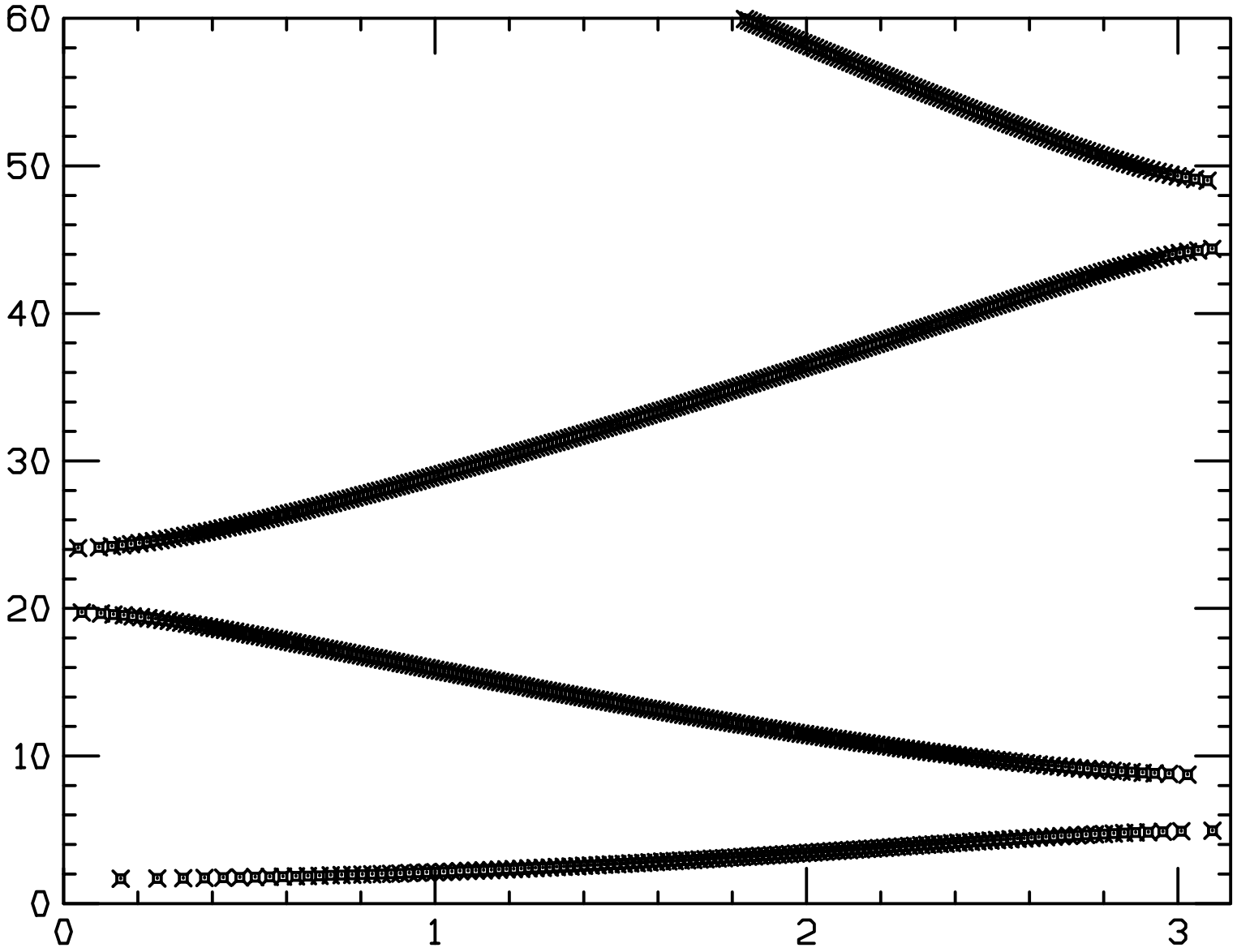
$$\left[\frac{\hbar^2}{2m}iq\left(1-e^{i(q-k)a}\right)-aU_0\right]A+\left[\frac{\hbar^2}{2m}iq\left(-1+e^{-i(k+q)a}\right)-aU_0\right]B=0$$

Set determinant = 0

Algebra .... yields

$$\boxed{\cos(ka)=\cos(qa)+\frac{ma}{\hbar^2 q}U_0\sin(qa)}$$


3
2
1
0
-1
0
2
4
6
8
10
12


60
50
40
30
20
10
0
0
1
2
3

(f) Give the numerical values of the bandwidth of the three lowest bands.
band 1: 3.26
band 2: 11.01
band 3: 20.29

(g) Give the numerical values of the energy gaps between the first and second, and between the second and third bands.
first gap: 3.81
second gap: 4.37

(h) Find numerical values of m*/m at the bottom and top of the first and second bands (m*=effective mass, m=bare mass).
bottom of band 1: 1.09
top of band 1: -0.26
bottom of band 2: 0.18
top of band 2: -0.073

The following charge densities are for:

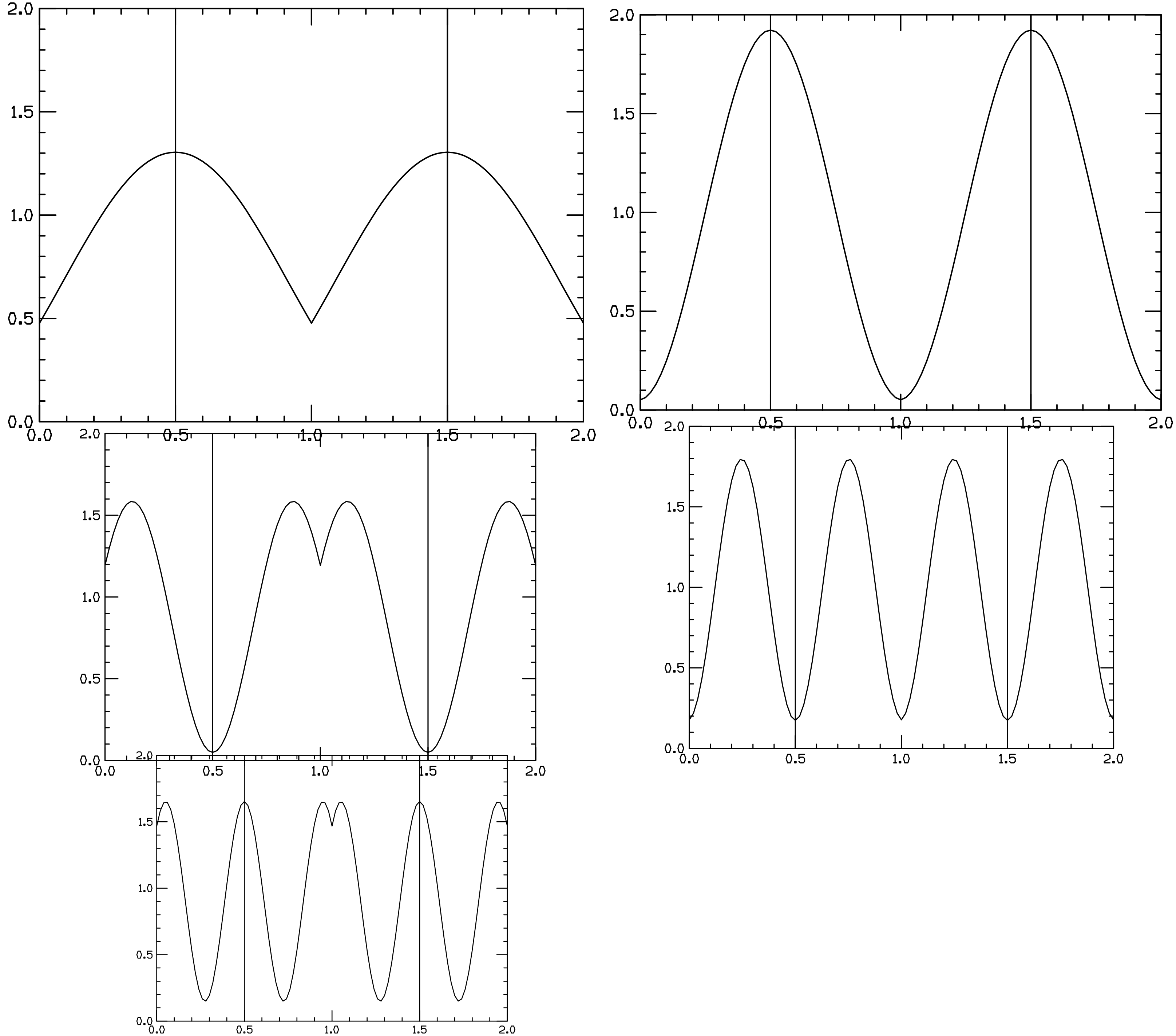
Bottom of band 1

Top of band 1

Bottom of band 2

Top of band 2

Bottom of band 3



0.0
0.5
1.0
1.5
2.0