Density of state for metal superlattice

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I encounter this topic when I read the Ph.D. Thesis of Jeremiah. Here we discuss the density of states for the metal superlattice.

1. 3D density of states for the quantum box with side L.

The wavefunction for the 3D system is given by the plane wave

$$\psi(\boldsymbol{r}) = \exp(ik \cdot r) .$$

Schrödinger equation.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r}) = \varepsilon\psi(\boldsymbol{r})$$

leading to the energy dispersion

$$\varepsilon = \varepsilon_k = \frac{\hbar^2}{2m}\boldsymbol{k}^2$$

Form the periodic boundary condition

$$\psi(x+L, y, z) = \psi(x, y, z), \qquad \psi(x, y+L, z) = \psi(x, y, z),$$

$$\psi(x, y, z+L) = \psi(x, y, z)$$

we have

$$\exp(ik_x L) = 1, \qquad k_x = \frac{2\pi}{L}n_x \qquad (n_x : \text{integer})$$

$$\exp(ik_y L) = 1, \qquad k_y = \frac{2\pi}{L}n_y \qquad (n_y : \text{integer})$$

$$\exp(ik_z L) = 1, \qquad k_z = \frac{2\pi}{L}n_z \qquad (n_y : \text{integer})$$

The density of states

$$D(\varepsilon)d\varepsilon = 2\frac{1}{(\frac{2\pi}{L})^3}4\pi k^2 dk = \frac{L^3}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\sqrt{\varepsilon}d\varepsilon$$

or

$$D_{3D}(\varepsilon) = \frac{L^3}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\sqrt{\varepsilon}$$

where the factor 2 comes from spin 1/2 (Pauli exclusion principle), and the energy is discrete and can be expressed as

$$\varepsilon = \frac{\hbar^2}{2m}(\frac{2\pi}{L})^2(n_x^{\ 2} + n_y^{\ 2} + n_z^{\ 2})$$

where $n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots$. When $L \to \infty$, the energy becomes continuous.

2. Density of state for the 2D system

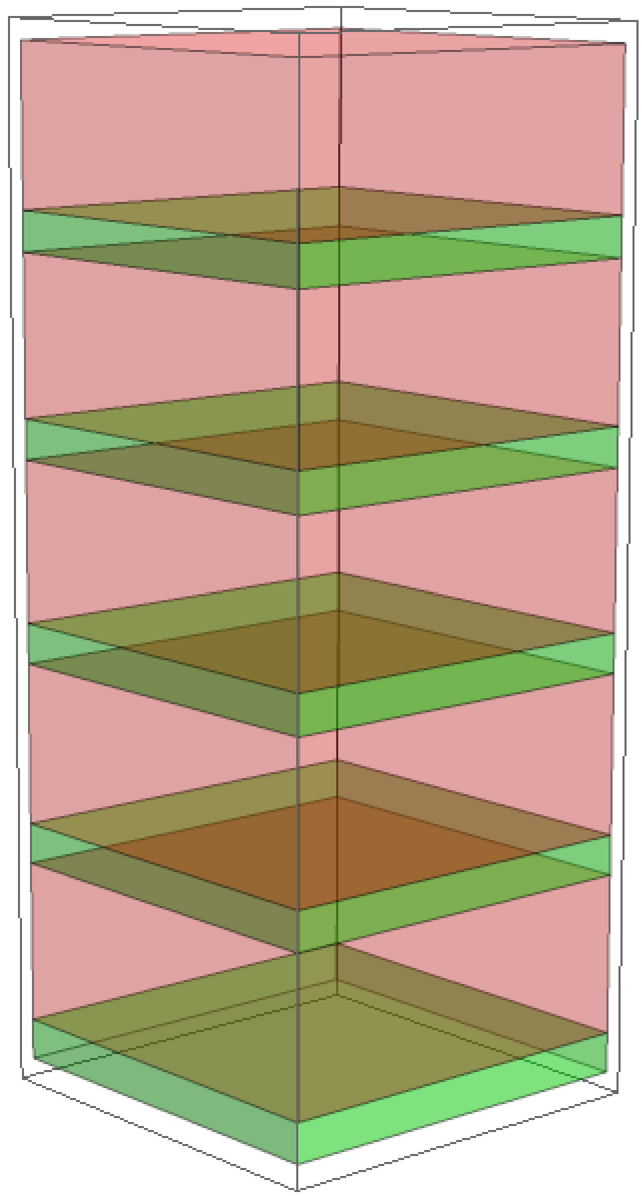


Fig. 2D metal superlattice; where the 2D metal layers (denoted by green) is periodically stacked along the *z* axis, with the periodicity *d*.

The wavefunction for the 2D system van be expressed by

$$\psi(x, y, z) = \exp[i(k_x x + k_y y)]Z(z)$$

The substitution of the wavefunction into the Schrödinger equation yields

$$-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})\psi(\boldsymbol{r})=\varepsilon\psi(\boldsymbol{r})$$

or

$$(-k_x{}^2-k_y{}^2)\exp[i(k_x x+k_y y)]Z(z)+\exp[i(k_x x+k_y y)]Z''(z)$$
$$=-\frac{2m}{\hbar^2}\varepsilon\exp[i(k_x x+k_y y)]Z(z)$$

This equation is simplified as

$$(-k_x{}^2-k_y{}^2)Z(z)+Z''(z)=-\frac{2m}{\hbar^2}\varepsilon Z(z)=-\boldsymbol{k}^2 Z(z)$$

or

$$Z''(z)+k_z{}^2 Z(z)=0\,,\qquad\qquad Z(z)=\sqrt{\frac{2}{d}}\sin(k_z z)=\sqrt{\frac{2}{d}}\sin(\frac{n_z\pi}{d}z)$$

where

$$\boldsymbol{k}^2=k_x{}^2+k_y{}^2+k_z{}^2$$

Form the periodic boundary condition

$$\psi(x+L,y,z)=\psi(x,y,z)\,,\qquad \psi(x,y+L,z)=\psi(x,y,z)\,,$$

$$\psi(x,y,z=d)=\psi(x,y,z=0)=0$$

we get the wavevector

$$\boldsymbol{k}^2=k_x{}^2+k_y{}^2+k_z{}^2$$

with

$$k_x=\frac{2\pi}{L}n_x\,,\qquad k_y=\frac{2\pi}{L}n_y\,,\qquad k_z=\frac{\pi}{d}n_z$$

where $d << L$ and $\sin(k_z d) = 0$. Note that n_z is positive integer, while n_x and n_y are integers. We note that the energy can be expressed as

$$\varepsilon = \frac{\hbar^2}{2m}[(\frac{2\pi}{L})^2(n_x{}^2 + n_y{}^2) + (\frac{\pi}{d})^2 n_z{}^2]$$
$$= \frac{\hbar^2}{2m}[(k_x{}^2 + k_y{}^2) + (\frac{\pi}{d})^2 n_z{}^2]$$

or

$$\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2 = \frac{\hbar^2}{2m}(k_x{}^2 + k_y{}^2) = \frac{\hbar^2}{2m}k_\perp{}^2$$

or

$$\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2 = \frac{\hbar^2}{2m}(k_x{}^2 + k_y{}^2) = \frac{\hbar^2}{2m}k_\perp{}^2$$

where

$$k_\perp{}^2 = k_x{}^2 + k_y{}^2$$

We note that

$$k_\perp = \sqrt{\frac{2m}{\hbar^2}}\sqrt{\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2}\,\Theta[\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]$$

where $\Theta(x)$ is a step function; $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$. The density of states is given by

$$D_\perp(\varepsilon)d\varepsilon = 2\frac{n_z}{(\frac{2\pi}{L})^2}2\pi k_\perp dk_\perp = \frac{L^2}{\pi}n_z k_\perp dk_\perp$$

Note that

$$k_{\perp}dk_{\perp}=\sqrt{\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2}\Theta[\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]\{\frac{1}{2}\frac{\Theta[\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]}{\sqrt{\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2}}$$

$$+\sqrt{\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2}\delta[\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]\}\frac{2m}{\hbar^2}d\varepsilon$$

$$=\frac{1}{2}\Theta[\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]\frac{2m}{\hbar^2}d\varepsilon+[\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]$$

$$\times\delta[\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]\Theta[\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]\frac{2m}{\hbar^2}d\varepsilon$$

$$=\frac{1}{2}\Theta[\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]\frac{2m}{\hbar^2}d\varepsilon$$

Thus we have the density of states as

$$D_{2D}(\varepsilon)=\frac{L^2}{\pi}\frac{m}{\hbar^2}n_z\Theta[\varepsilon-\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]$$

where

$$D_{2D}(\varepsilon=\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2)=\frac{L^2}{\pi}(\frac{m}{\hbar^2})n_z$$

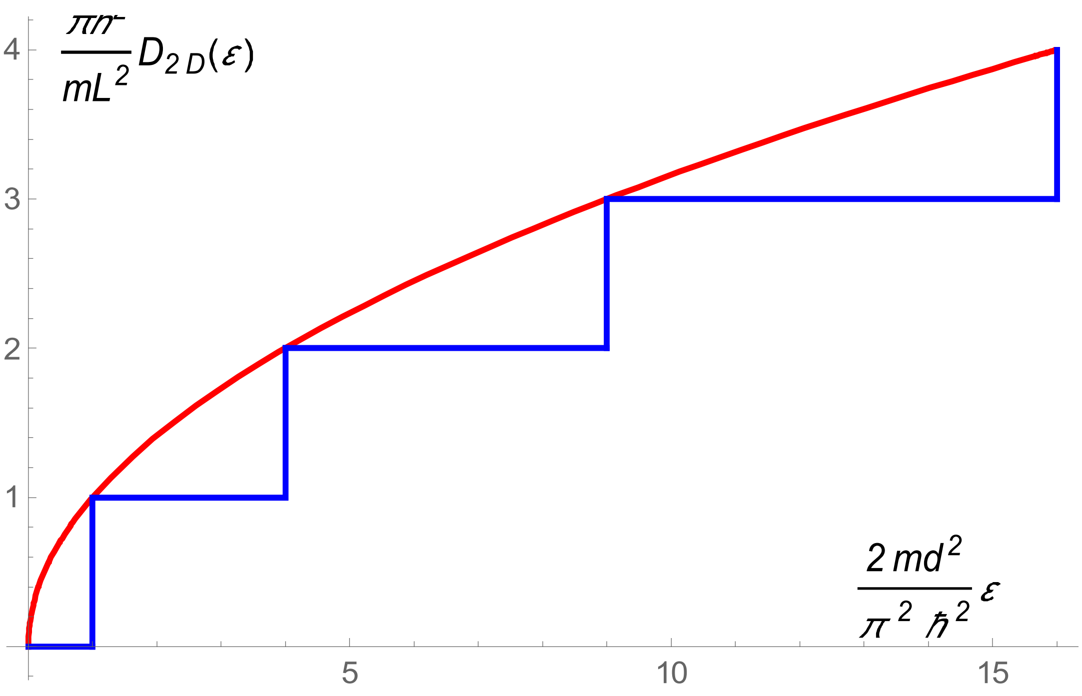


Fig. Density of states for the 2D superlattice where the 2D metal layers are stacked periodically along the z axis with the periodicity d. The red line denote the density of states for the 3D system with sides L. $\frac{d}{L}D_{3D}(\varepsilon)$.

Noting that

$$D_{3D}[\varepsilon = \frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2] = \frac{L^3}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\sqrt{\frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2} = \frac{L^3}{\pi}\frac{m}{\hbar^2}\frac{1}{d}n_z$$

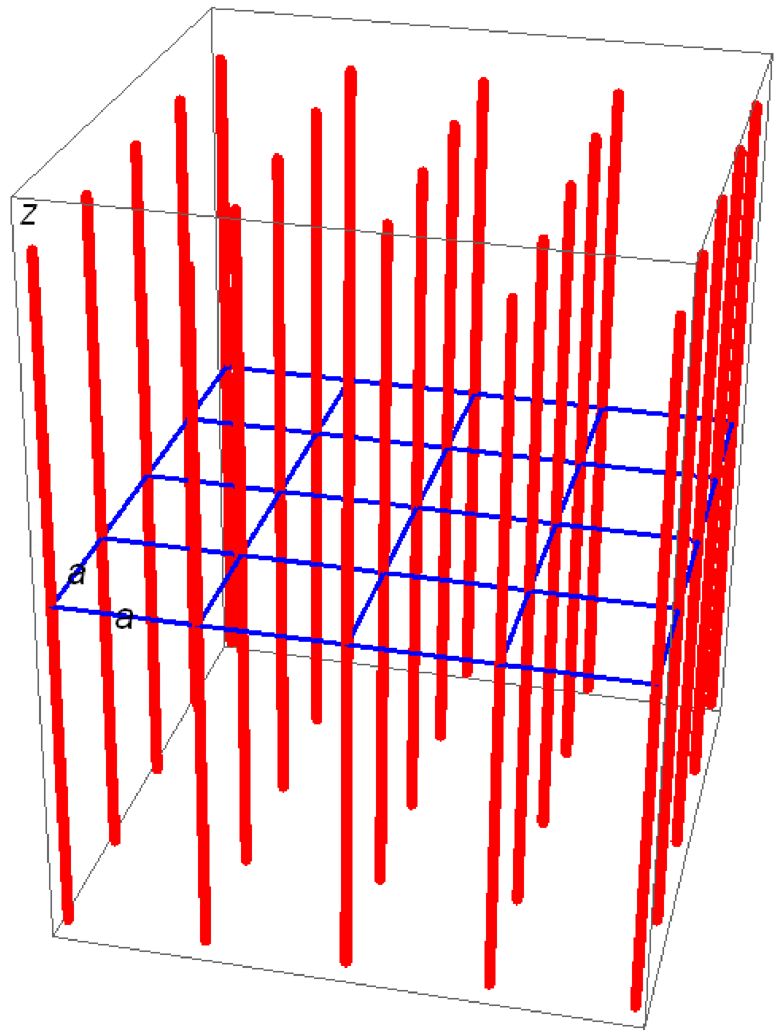
we have

$$\frac{D_{2D}(\varepsilon = \frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2)}{D_{3D}[\varepsilon = \frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]} = \frac{\frac{L^2}{\pi}(\frac{m}{\hbar^2})n_z}{\frac{L^3}{\pi}\frac{m}{\hbar^2}\frac{1}{d}n_z} = \frac{d}{L}$$

The final form of the density of states for the 2D system

$$D_{2D}(\varepsilon, n_z) = \frac{d}{L}[D_{3D}(\varepsilon = \frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2)]\,\Theta[\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{d})^2 n_z{}^2]$$

3. Density of states for the 1D system



$$\psi(x,y,z) = \exp i(k_z z)X(x)Y(y) \qquad \text{(separation variable)}$$

with the boundary condition

$$\psi(x=a,y,z) = \psi(x=0,y,z) = 0, \qquad \psi(x,y=a,z) = \psi(x,y=0,z) = 0,$$

$$\psi(x,y,z+L) = \psi(x,y,z)$$

The wavenumber k_z is given by

$$k_z = \frac{2\pi}{L}n_z$$

The substitution of the wavefunction into the Schrödinger equation yields

$$-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})\psi(\boldsymbol{r})=\varepsilon\psi(\boldsymbol{r})$$

or

$$-k_z{}^2\exp[i(k_z z)X(x)Y(y)+\exp[i(k_z z)](X''(x)Y(z)+X(x)Y''(z)$$
$$=-\frac{2m}{\hbar^2}\varepsilon\exp i(k_z z)X(x)Y(y)$$

This equation is simplified as

$$-k_z{}^2X(x)Y(y)+(X''(x)Y(z)+X(x)Y''(z)=-\frac{2m}{\hbar^2}\varepsilon X(x)Y(y)$$

or

$$-k_z{}^2+\frac{X''(x)}{X(x)}+\frac{Y''(z)}{Y(y)}=-\frac{2m}{\hbar^2}\varepsilon$$

or

$$X''(x)+k_x{}^2X(x)=0,\qquad X(x)=\sqrt{\frac{2}{a}}\sin(k_x z)=\sqrt{\frac{2}{a}}\sin(\frac{n_x\pi}{a}x)$$

$$Y''(y)+k_y{}^2Y(y)=0,\qquad Y(y)=\sqrt{\frac{2}{a}}\sin(k_y y)=\sqrt{\frac{2}{a}}\sin(\frac{n_y\pi}{a}y)$$

with

$$k_x=\frac{n_x\pi}{a},\qquad k_y=\frac{n_y\pi}{a}\qquad (n_x,n_y\text{; positive integers})$$

Then we get the dispersion relation

$$\varepsilon=\frac{\hbar^2}{2m}(k_x{}^2+k_y{}^2+k_z{}^2)$$

or

$$k_z = (\frac{2m}{\hbar^2})^{1/2}\sqrt{\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2(n_x{}^2 + n_y{}^2)}\Theta[\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2(n_x{}^2 + n_y{}^2)]$$

$$= (\frac{2m}{\hbar^2})^{1/2}\sqrt{\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2}\Theta[\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2]$$

where

$$n_\perp{}^2 = n_x{}^2 + n_y{}^2$$

The density of states is

$$D_{1D}(\varepsilon)d\varepsilon = 2\cdot 2\frac{\pi n_\perp{}^2}{(\frac{2\pi}{L})}\frac{dk_z}{d\varepsilon}d\varepsilon$$

$$= Ln_\perp{}^2(\frac{2m}{\hbar^2})^{1/2}\frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2}}\Theta[\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2]$$

since

$$\frac{dk_z}{d\varepsilon} = (\frac{2m}{\hbar^2})^{1/2}[\sqrt{\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2}\delta[\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2]$$

$$+ (\frac{2m}{\hbar^2})^{1/2}\{\frac{1}{2\sqrt{\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2}}\Theta[\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2]\}$$

$$= \frac{1}{2}(\frac{2m}{\hbar^2})^{1/2}\frac{1}{\sqrt{\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2}}\Theta[\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_\perp{}^2]$$

Then the density of states is

$$D_{1D}(\varepsilon) = Ln_{\perp}{}^{2}(\frac{2m}{\hbar^2})^{1/2} \frac{\Theta[\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_{\perp}{}^{2}]}{\sqrt{\varepsilon - \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 n_{\perp}{}^{2}}}$$

$$= \frac{aL}{\pi} n_{\perp}{}^{2}(\frac{2m}{\hbar^2}) \frac{\Theta[x - n_{\perp}{}^{2}]}{\sqrt{x - n_{\perp}{}^{2}}}$$

where

$$x = \frac{2m}{\hbar^2}(\frac{a}{\pi})^2 \varepsilon$$

Note that the density of states for the 1 D system is given by

$$D_{1D}{}^{(0)}(\varepsilon)d\varepsilon = 2 \cdot 2 \frac{1}{(\frac{2\pi}{L})} \frac{dk_z}{d\varepsilon} d\varepsilon$$

$$= \frac{L}{\pi}(\frac{2m}{\hbar^2})^{1/2} \frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon}} \Theta[\varepsilon]$$

for the energy dispersion for the 1D system (not a super lattice)

$$D_{1D}{}^{(0)}(\varepsilon) = \frac{L}{\pi}(\frac{2m}{\hbar^2})^{1/2} \frac{1}{\sqrt{\varepsilon}} \Theta[\varepsilon]$$

$$= \frac{L}{\pi}(\frac{2m}{\hbar^2})^{1/2} \frac{(\frac{2m}{\hbar^2})^{1/2} \frac{a}{\pi}}{\sqrt{x}} \Theta[x]$$

$$= \frac{aL}{\pi^2}(\frac{2m}{\hbar^2}) \frac{1}{\sqrt{x}} \Theta[x]$$

$$= D_{1D}{}^{(0)}(x)$$

When $x = n_{\perp}{}^{2}$, we have

$$D_{1D}{}^{(0)}(x = n_{\perp}{}^{2}) = \frac{aL}{\pi^2}(\frac{2m}{\hbar^2}) \frac{1}{n_{\perp}}$$

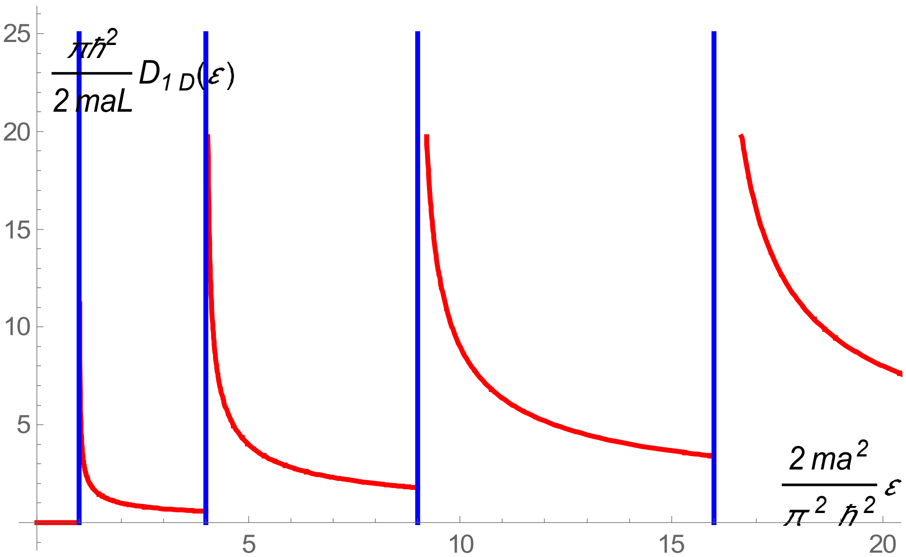
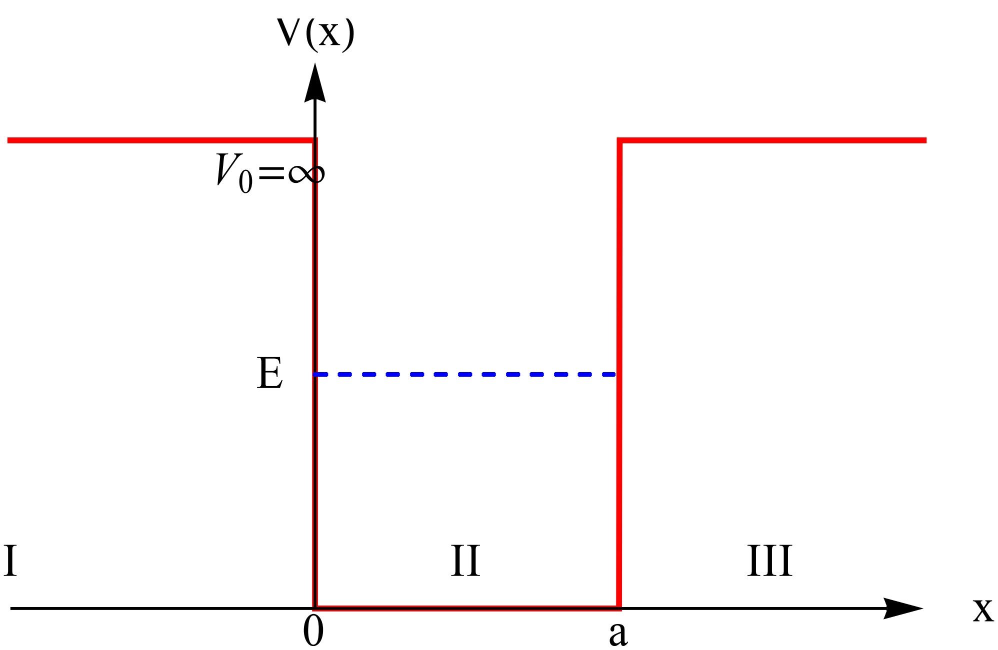


Fig. Density of states for the 1D superlattice.

APPENDIX Quantum box

1. 1D one-dimensional well potential



$$\hat{H} = \frac{\hat{p}^2}{2m}$$

$$H\varphi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) = E\varphi(x) = \frac{\hbar^2 k^2}{2m}\varphi(x)$$

The solution of this equation is

$$\varphi(x) = A\sin(kx) + B\cos(kx)$$

where

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

Using the boundary condition:

$$\varphi(x = 0) = \varphi(x = a) = 0$$

we have

$B = 0$ and $A \neq 0$.

$$\sin(ka) = 0$$

$$ka = n\pi \quad (n = 1, 2, \ldots)$$

Note that $n = 0$ is not included in our solution because the corresponding wave function becomes zero. The wave function is given by

$$\varphi_n(x) = \langle x|\varphi_n\rangle = A_n \sin(\frac{n\pi x}{a}) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})$$

with

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$$

((**Normalization**))

$$1 = \int_0^a A_n^{\ 2}\sin^2(\frac{n\pi x}{a})dx = \frac{a}{2}A_n^{\ 2}$$

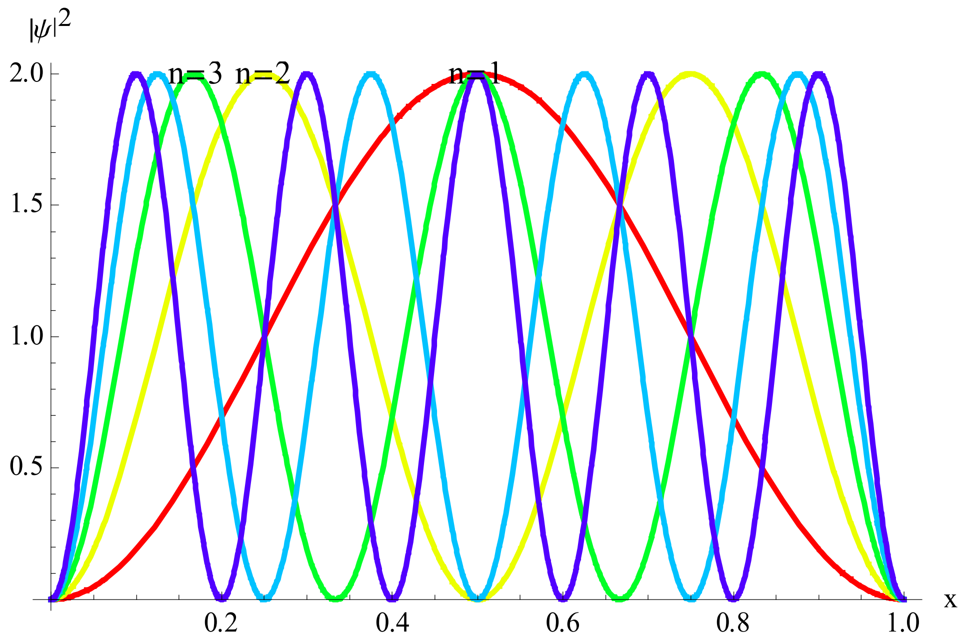


Fig. Plot of $|\varphi_n(x)|^2$ with $a = 1$, as a function of x. $n = 1$ (red), 2 (yellow), 3 (green), 4 (blue), and 5 (dark blue). There are n peaks for the state $|n\rangle$.