PHY 530
STEEM Refresher course 2
Plane waves and density of states

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UMR 9006

STEEM Refresher 2

1. From the potential well to free particles

2. (Tutorial) Tunnel effect - derivation

3. Tunnel effect - applications

4. Density of state - concepts

5. (Tutorial) Density of state - calculations

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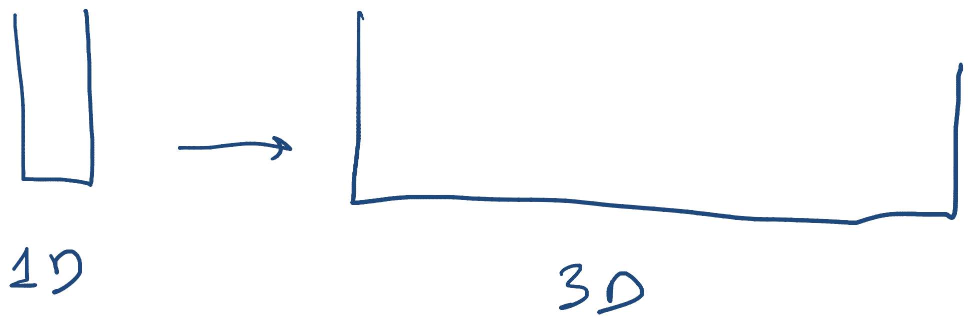
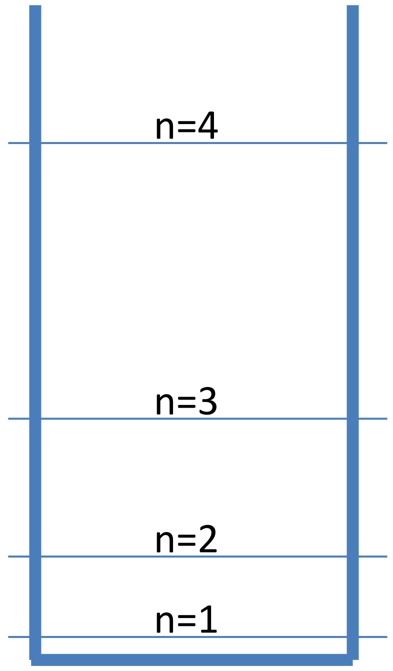


From 1D to 3D

In 1D : $\hat{H} = -\frac{\hbar^2}{2m}\partial_x^2$

$$\left.\begin{array}{l}\hat{H}\psi_n(x) = E_n\psi_n(x)\\ \psi(0) = \psi(L) = 0\end{array}\right\} \quad \psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$$

$$E_n = \frac{\pi^2\hbar^2}{2mL^2}\times n^2$$



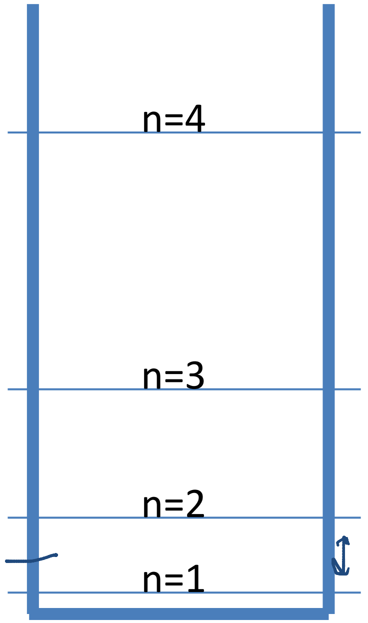
In 3D : $\hat{H} = -\frac{\hbar^2}{2m}\left(\partial_x^2 + \partial_y^2 + \partial_z^2\right)$ $\qquad \hat{H}\psi(\vec{r}) = E\psi(\vec{r})$

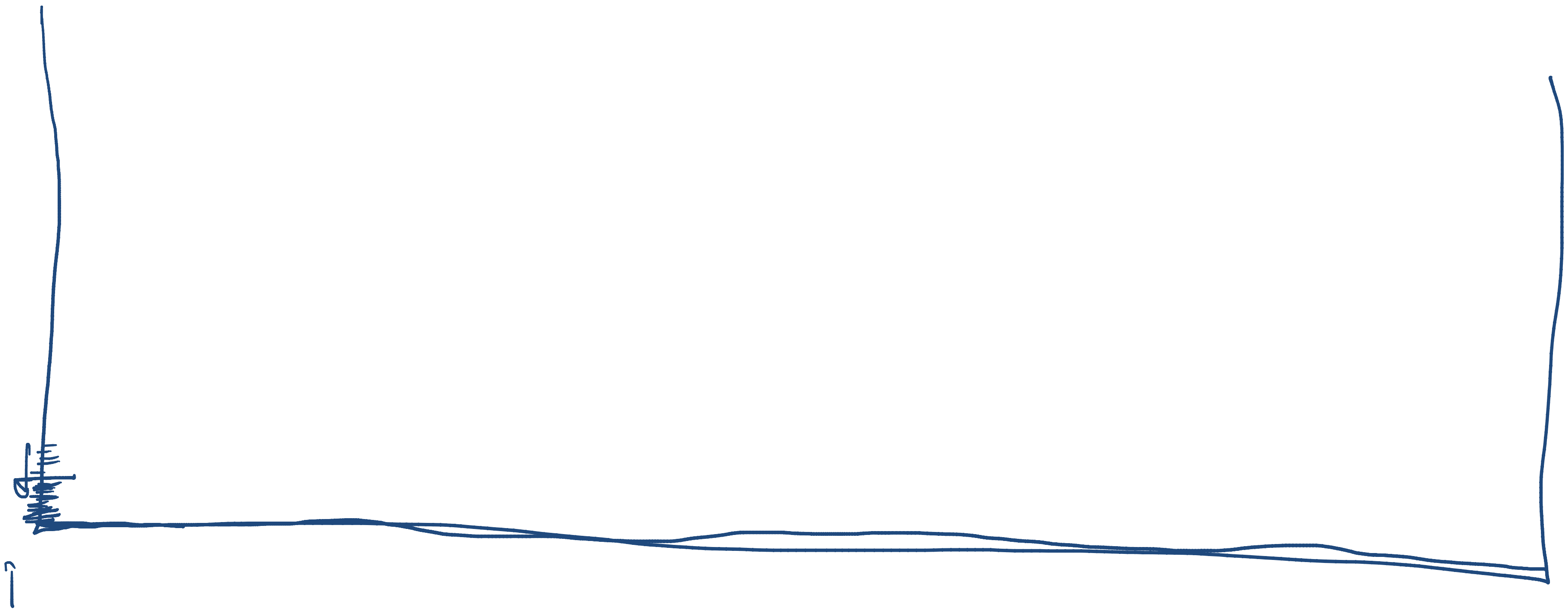
$$\psi(0) = \psi(L\vec{e_x}) = \psi(L\vec{e_y}) = \psi(L\vec{e_z}) = 0$$

eigenstate $\psi(\vec{r}) = \sqrt{\frac{8}{L^3}}\sin\left(\frac{\pi n_x}{L}x\right)\sin\left(\frac{\pi n_y}{L}y\right)\sin\left(\frac{\pi n_z}{L}z\right) \quad (n_x, n_y, n_z)$

eigen value. $E(n_x, n_y, n_z) = \frac{\pi^2\hbar^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$

Pushing the walls





Possible energies :

$$E_n = \frac{\pi^2 \hbar^2}{2m} \frac{n^2}{L^2}$$

$$L \to \infty$$

For any value of E, we can find n such that $E_n \simeq E$

Free particles – eigen states

Big 3D box

Free Hamiltonian eigen state :

$$H\psi = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi = E\psi$$

Boudary conditions

$$\psi(L) = 0 \qquad \psi(0) = 0$$

Wavefunction :

$$\psi(\mathbf{r}) = \sqrt{\frac{8}{L^3}}\sin\left(\frac{\pi n_x}{L}x\right)\sin\left(\frac{\pi n_y}{L}y\right)\sin\left(\frac{\pi n_z}{L}z\right)$$

Corresponding energy:

$$E_n = (n_x^2+n_y^2+n_z^2)\times\frac{\pi^2\hbar^2}{2mL^2}$$

(≈ continuous)

Big 3D box + pacman

Free Hamiltonian eigen state :

$$H\psi = \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi = E\psi$$

Boudary conditions

$$\psi(0) = \psi(L)$$

Wavefunction :

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{L^3}}e^{i\frac{2\pi n_x}{L}x}\,e^{i\frac{2\pi n_y}{L}y}\,e^{i\frac{2\pi n_z}{L}z}$$

Corresponding energy:

$$E_n = (n_x^2+n_y^2+n_z^2)\times\frac{4\pi^2\hbar^2}{2mL^2}$$

Free particles & plane waves

Free Hamiltonian eigen state:

$$H\psi = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi = E\psi$$

Wavefunction :

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{L^3}} e^{i\frac{2\pi n_x}{L}x}\, e^{i\frac{2\pi n_y}{L}y}\, e^{i\frac{2\pi n_z}{L}z}$$

$$= \frac{1}{\sqrt{L^3}} e^{i\mathbf{k}.\mathbf{r}} \quad \text{with} \quad \boxed{\mathbf{k} = \frac{2\pi}{\underset{\to +\infty}{L}}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}}$$

Energy

$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} \qquad k^2 = \frac{4\pi^2}{L^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$$= p^2/2m$$

Momentum eigen state:

$$\hat{\mathbf{p}}\psi = -i\hbar\nabla\psi = \underbrace{\hbar\mathbf{k}}_{\text{momentum}}\psi$$

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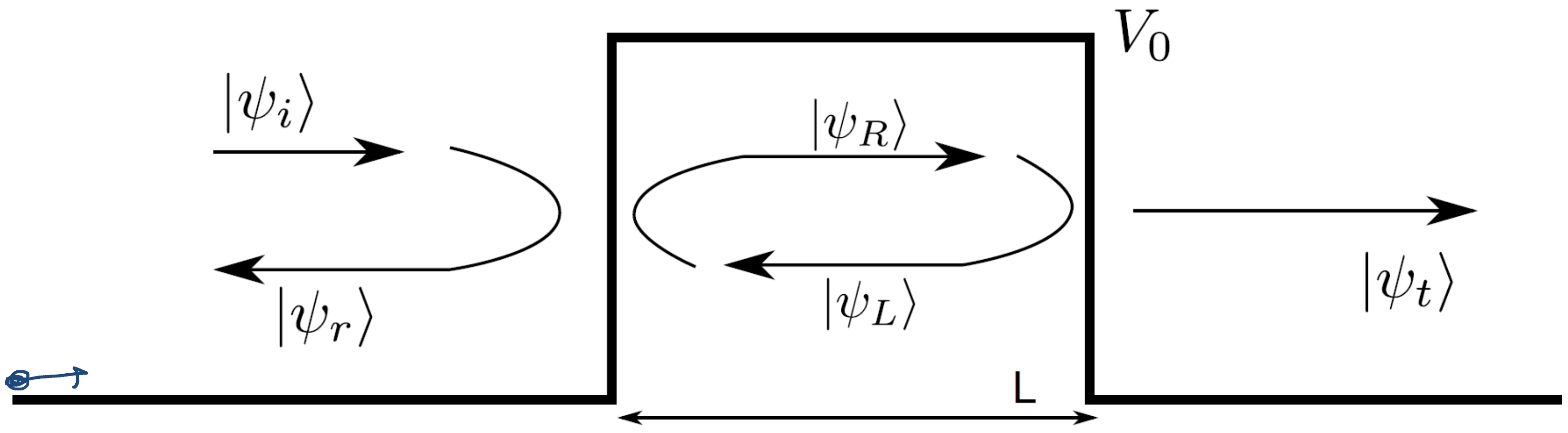
Problem statement



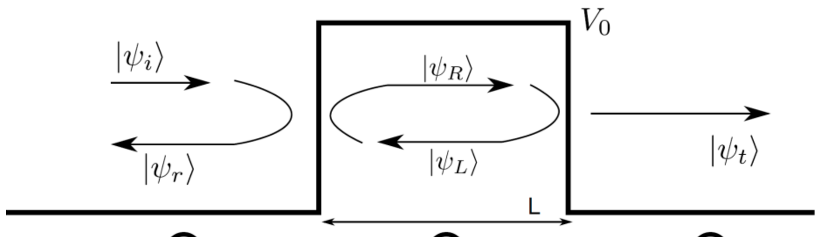
$E_c < V_0$
↳ can't pass

E_c

$E_c > V_0$
↳ pass the barrier

First case: E>V0

$$\psi(x) = \begin{cases} A_i \exp(ikx) + A_r \exp(-ikx) & \text{in region 1} \\ A_R \exp(ik'x) + A_L \exp(-ik'x) & \text{in region 2} \\ A_t \exp(ikx) & \text{in region 3} \end{cases}$$



$V_0 = 0$ $\quad V_0$ $\quad V = 0$

eigenstates

$\hat{H}\Psi = E\Psi$

$H_{①} = -\frac{\hbar^2}{2m}\partial_x^2 + 0 \qquad H_{②} = -\frac{\hbar^2}{2m}\partial_x^2 + V_0 \qquad H_{③} = H_{①}$

in ① and ③

$$-\frac{\hbar^2}{2m}\partial_x^2 \psi = -\frac{\hbar^2}{2m}\left(A_i (ik)^2 e^{ikx} + A_r (-ik)^2 e^{-ikx}\right)$$

$$= \frac{\hbar^2 k^2}{2m}\left(A_i e^{ikx} + A_r e^{-ikx}\right) = \frac{\hbar^2 k^2}{2m}\psi$$ eigenfunction indeed with $E = \frac{\hbar^2 k^2}{2m}$

in ② $\left(-\frac{\hbar^2}{2m}\partial_x^2 + V_0\right)\psi = \left(\frac{\hbar^2 k'^2}{2m} + V_0\right)\psi$ eigenfunction of $H_{②}$ with $E = \frac{\hbar^2 k'^2}{2m} + V_0 \rightarrow k' = \frac{1}{\hbar}\sqrt{\underbrace{(E-V_0)}_{>0}2m}$

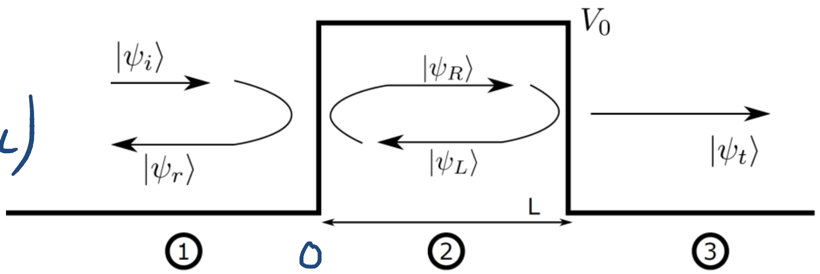
First case: E>V0

$$\Psi(0^-)=\Psi(0^+) \to A_i + A_r = A_R + A_L$$

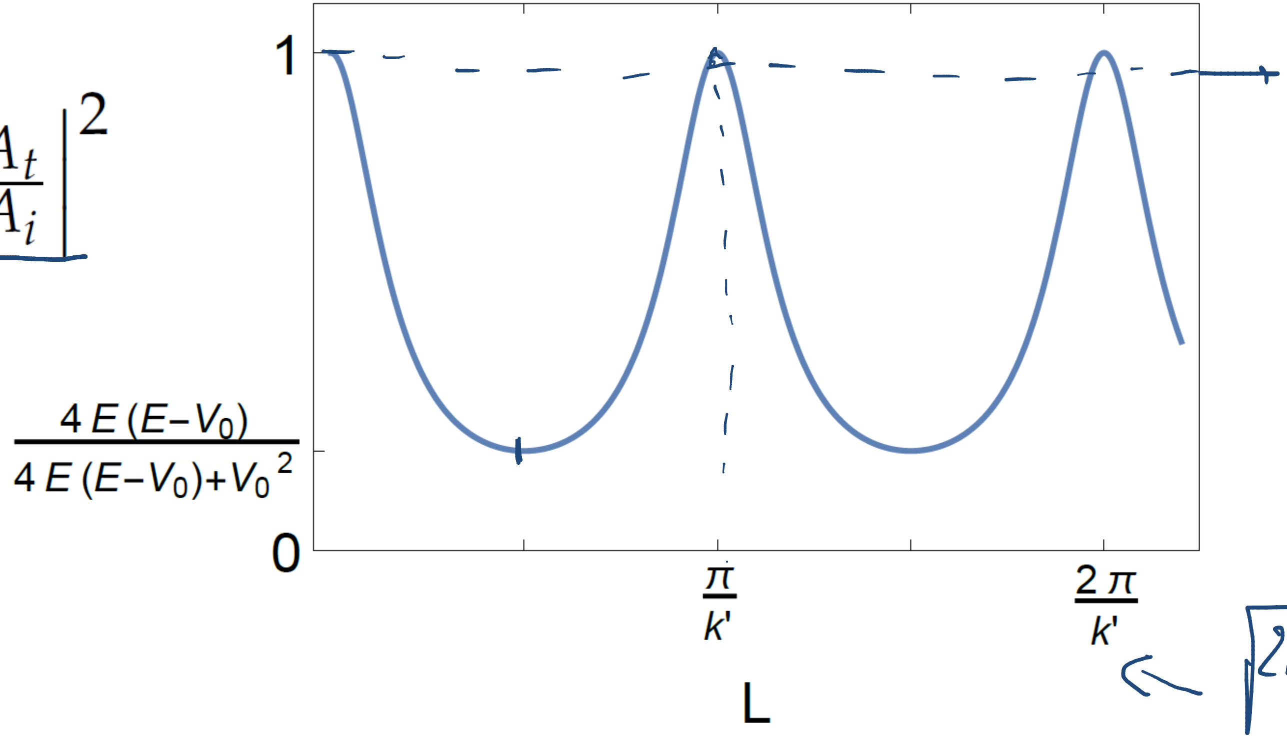
$$\Psi(L^-)=\Psi(L^+) \to A_R e^{ik'L} + A_L e^{-ik'L} = A_t e^{ikL}$$

$$\partial_x\Psi(0^-)=\partial_x\Psi(0^+) \to ik(A_i-A_r) = ik'(A_R-A_L)$$

$$\partial_x\Psi(L^-)=\partial_x\Psi(L^+) \to$$



$$\underline{T = \left|\frac{A_t}{A_i}\right|^2}$$

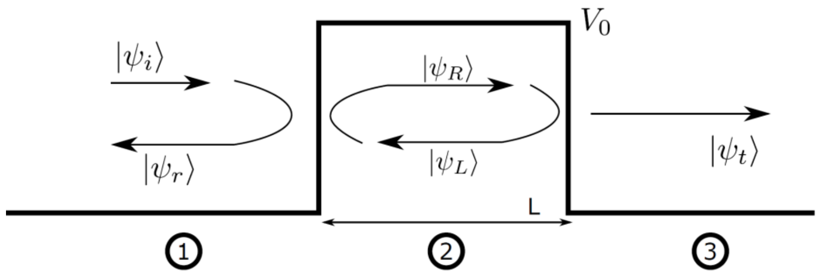


classical

$$k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

First case: E<V0

$$\psi(x) = \begin{cases} A_i \exp(-ikx) + A_r \exp(ikx) & \text{in region 1} \\ A_R \exp(-k''x) + A_L \exp(k''x) & \text{in region 2} \\ A_t \exp(-ikx) & \text{in region 3} \end{cases}$$



$V_0 > E$

in region 2: eigenstate $H_{(2)}\psi_{(2)} \overset{?}{=} E\psi_{(2)}$

$$= \left(-\frac{\hbar^2\partial_x^2}{2m} + V_0\right)\psi = \overbrace{\left(\frac{\hbar^2 k''^2}{2m} + V_0\right)}^{E}\psi$$

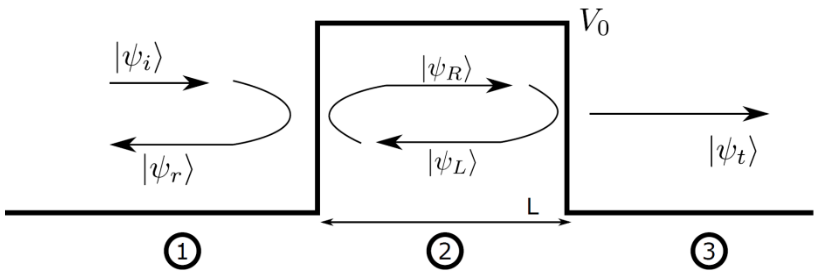
$$k''^2 = \frac{2m}{\hbar^2}\underbrace{(E - V_0)}_{<0} \rightarrow k'' = \pm i\sqrt{\frac{2m}{\hbar^2}\underbrace{(V_0 - E)}_{>0}}$$

ψ is evanescent in region 2.

First case: E<V0

$\psi(0^-) = \psi(0^+)$ $\qquad$ $\partial_x \psi(0^-) = \partial_x \psi(0^+)$

$\psi(L^-) = \psi(L^+)$ $\qquad$ $\partial_x \psi(L^-) = \partial_x \psi(L^+)$



$$\boxed{T = \left|\frac{A_t}{A_i}\right|^2} \simeq 16\,\frac{E\times(V_0 - E)}{V_0^2}\,\exp\left(-\frac{\sqrt{8m\,(V_0 - E)}}{\hbar}L\right) > 0$$

$T_{\text{classical}} = 0$

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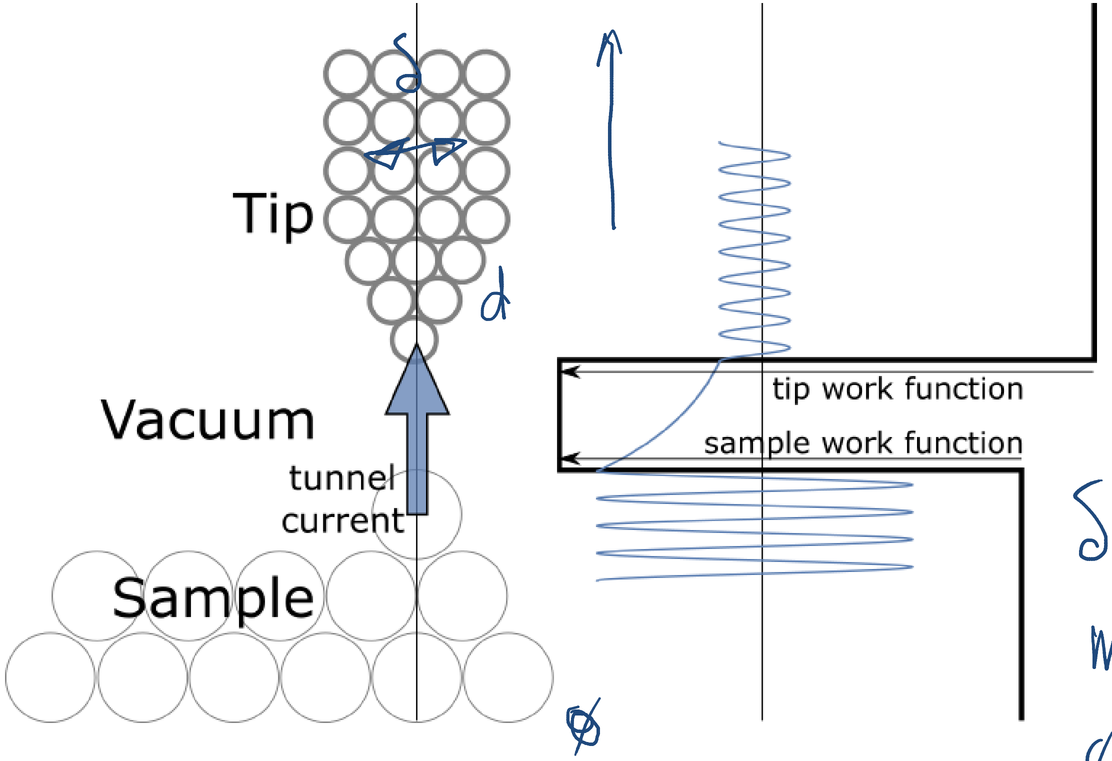
Scanning tunnelling micropscope



$$T \propto \exp\left(-\frac{\sqrt{8m\,\overbrace{(V_0 - E)}^{V_0 \sim \phi}}}{\hbar} L\right)$$

Current variation as the distance changes by the size of 1 single atom

$$\frac{I(d+\delta)}{I(d)} = \frac{T(d+\delta)}{T(d)}$$

$$= \frac{\exp\left(-\frac{\sqrt{8m\phi}}{\hbar}(\cancel{d} + \delta)\right)}{\exp\left(\cancel{-\frac{\sqrt{8m\phi}}{\hbar}d}\right)}$$

$$= \exp\left(-\frac{\sqrt{8m\phi}}{\hbar}\delta\right) \sim 0{,}1$$

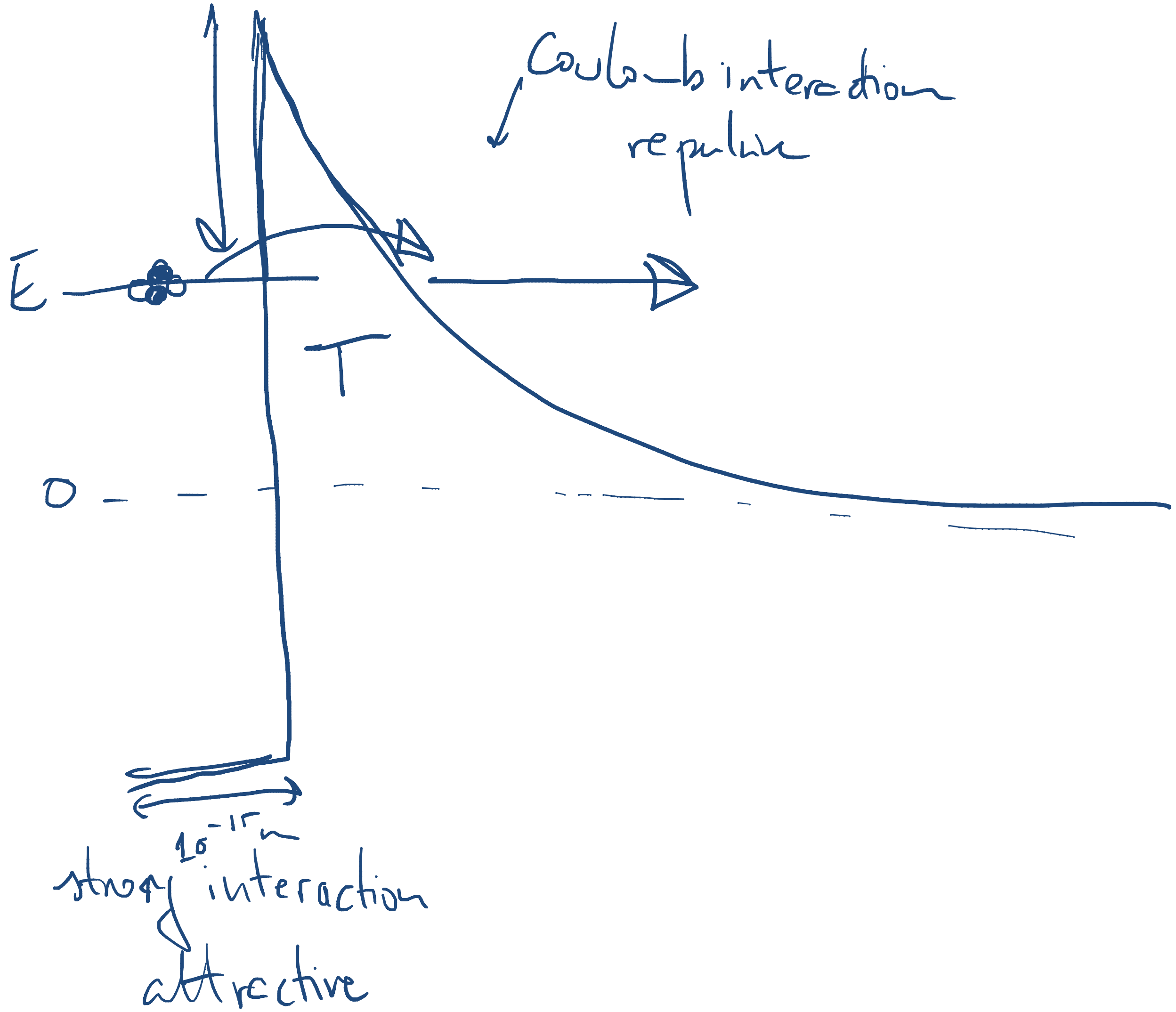
$\delta = 10^{-10}$ m

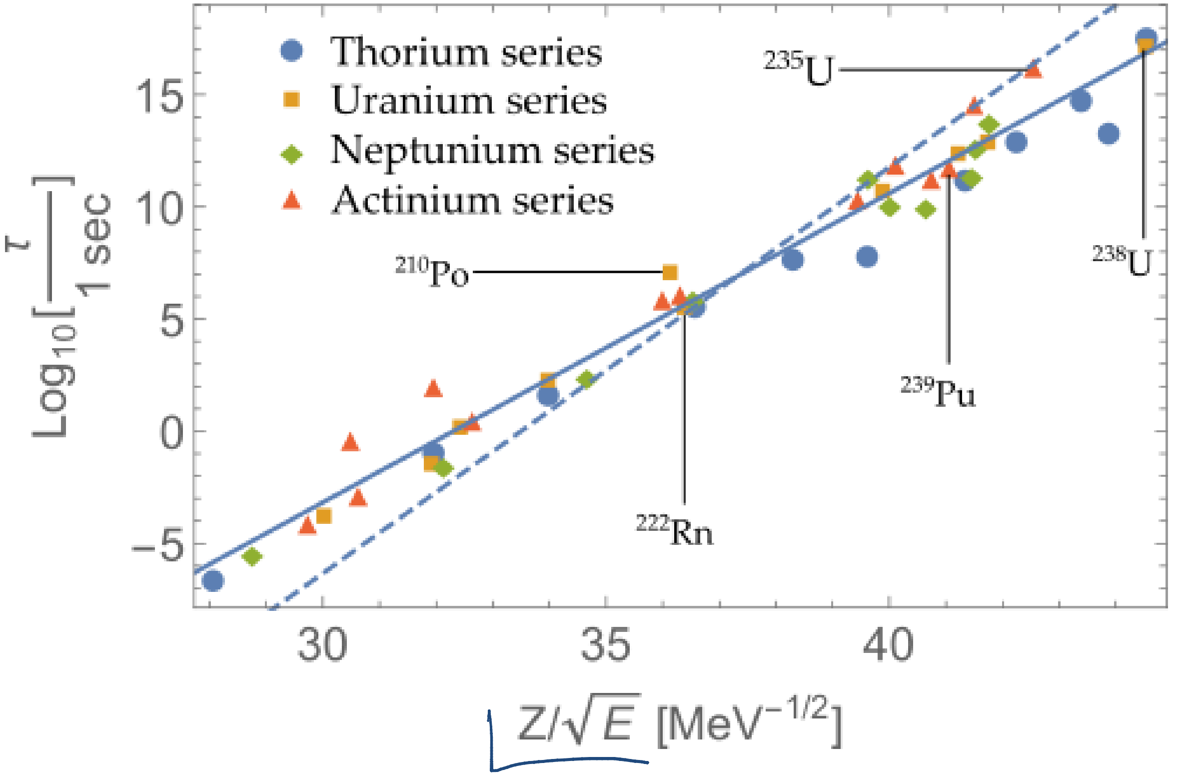
$m = 10^{-30}$ kg

$\phi \sim 5$ eV

$\hbar = 10^{-34}$ J.s

Alpha decay





Geiger and Nuttal law (1911)

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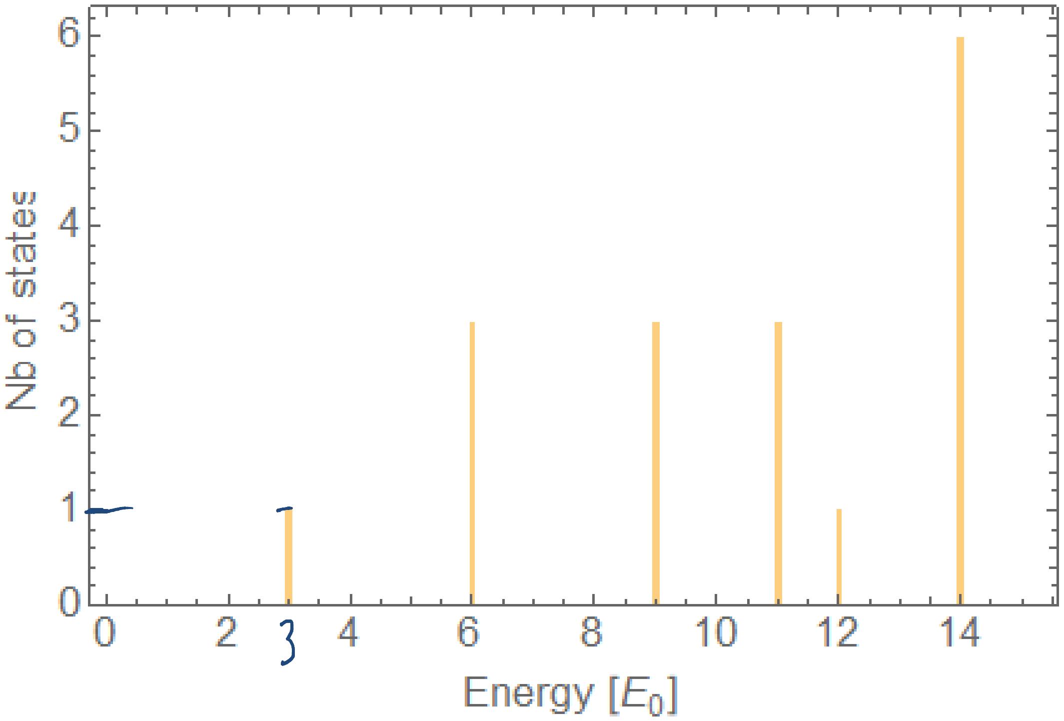
How many states with a given energy E ?

Potential well

$$E = (n_x^2 + n_y^2 + n_z^2)E_0$$

(n_x, n_y, n_z)

Discrete



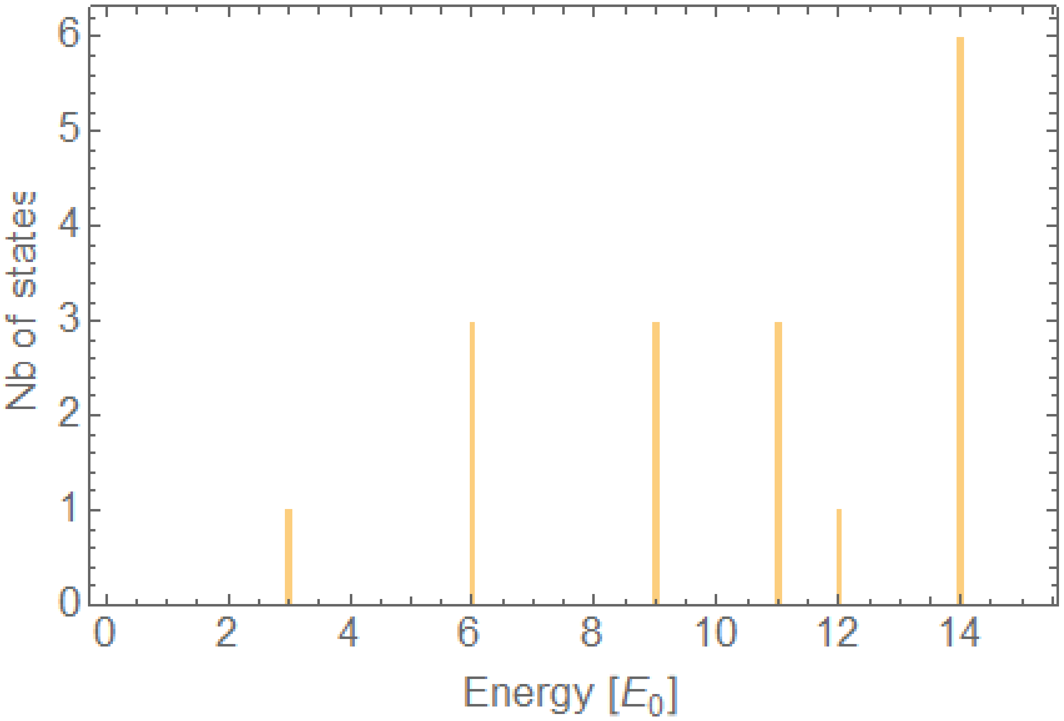
n_x	n_y	n_z	Energy	# states
1	1	1	$3E_0$	1
2	1	1	$6E_0$	3
1	2	1	$6E_0$	
1	1	2	$6E_0$	
2	2	1	$9E_0$	3
2	1	2		
1	2	2		
2	2	2	$12E_0$	1
1	1	3	$11E_0$	3
1	3	1		
3	1	1		

How many states with a given energy E ?

Potential well

$$E = (n_x^2 + n_y^2 + n_z^2)E_0$$

Discrete



Free particles

$$\boxed{E = \frac{\hbar^2 k^2}{2m}} \quad \text{with} \quad \mathbf{k} = \frac{2\pi}{L}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$$

Continuous

$L \to +\infty$

How many states with energy between E and E+dE?

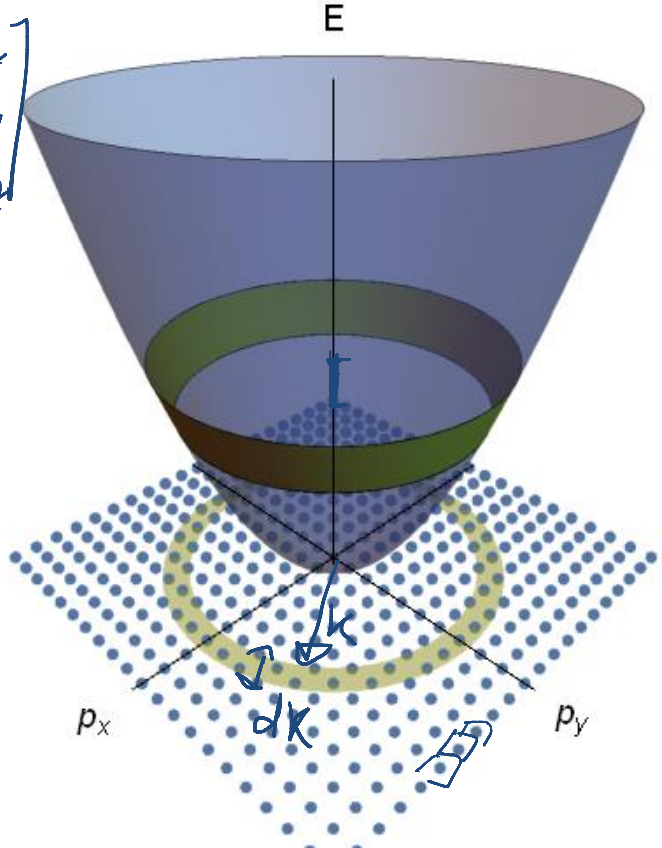
$$= \rho(E)dE$$

Density of state

Density of states

$$E = \frac{\hbar^2 k^2}{2m} \quad \text{with} \quad \mathbf{k} = \frac{2\pi}{L}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$$

$$\vec{p} = \hbar\vec{k} = \frac{2\pi\hbar}{L}\begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix}$$



How many states with energy between E and E+dE?

$$= \rho(E)dE$$

How many states with wave-vector between k and k+dk?

$$E = \frac{\hbar^2 k^2}{2m} \qquad (E + dE) = \frac{\hbar^2 (k+dk)^2}{2m}$$

Which "volume" does this represent ?

$$dV = V(k+dk) - V(k)$$
$$= 4\pi k^2 dk$$

How many states are located in this "volume" ?

$$dV / \left(\frac{2\pi}{L}\right)^3$$

$2\pi\hbar$

$$\rho(E)dE = dV / \left(\frac{2\pi}{L}\right)^3$$

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Density of states in 3D

$\boxed{E = \frac{\hbar^2 k^2}{2m}}$ with $\mathbf{k} = \frac{2\pi}{L}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$

How many states with energy between E and E+dE?

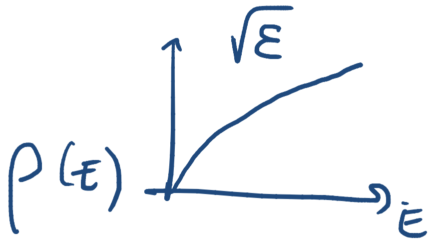
$E \quad (E + dE) = \rho(E)dE$

How many states with wave-vector between k and k+dk?

$$E = \frac{\hbar^2 k^2}{2m} \rightarrow dE = \frac{\hbar^2 2k\,dk}{2m} \rightarrow dk = \frac{m}{k\hbar^2} dE$$

Which "volume" does this represent ? $dV = V(k+dk) - V(k) = \underline{4\pi k^2 dk}$

How many states are located in this "volume" ? $dV / \left(\frac{2\pi}{L}\right)^3$



$$\rho(E)dE = dV / \left(\frac{2\pi}{L}\right)^3 = \frac{4\pi k^2}{(2\pi)^3} dk\, L^3 = \frac{L^3 4\pi \cancel{k^2}}{(2\pi)^3} \frac{m}{\cancel{k}\hbar^2} dE = \left[\frac{L}{2\pi}\right]^3 \frac{4\pi m}{\hbar^2} \sqrt{\frac{2mE}{\hbar^2}}\, dE$$

Density of states in 2D

$$E = \frac{\hbar^2 k^2}{2m} \quad \text{with} \quad \mathbf{k} = \frac{2\pi}{L}\begin{pmatrix} n_x \\ n_y \end{pmatrix}$$

How many states with energy between E and E+dE?

$$= \rho(E)dE$$

How many states with wave-vector between k and k+dk?

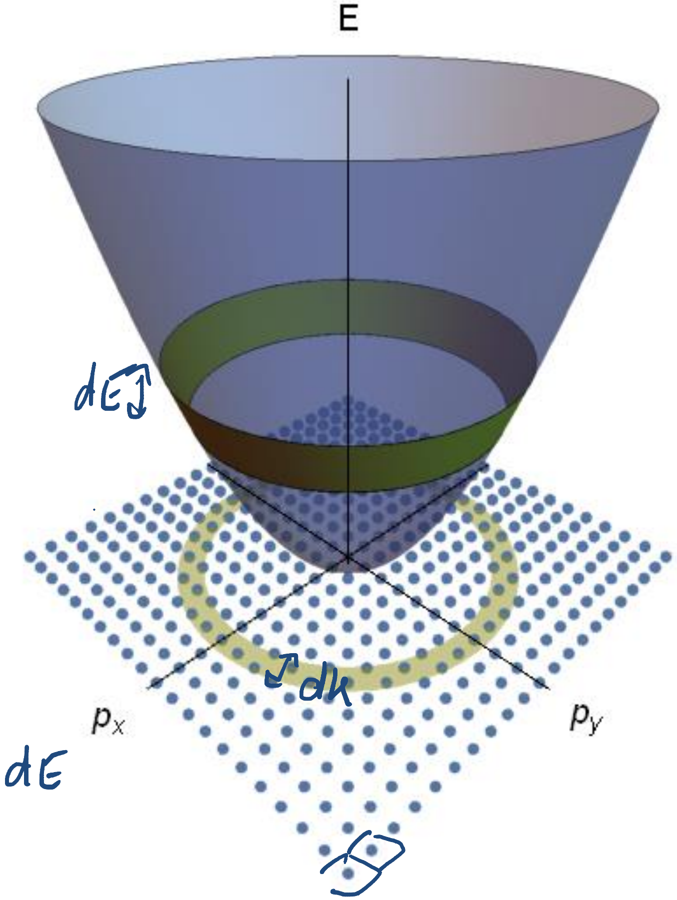
$$E = \frac{\hbar^2 k^2}{2m} \rightarrow dE = \frac{\hbar^2 k\,dk}{m} \rightarrow dk = \frac{m}{\hbar^2 k} dE$$

Which "volume" does this represent ?

$$dV = V(k+dk) - V(k) = 2\pi k dk = \pi(k+dk)^2 - \pi k^2$$

How many states are located in this "volume" ? $dV/\left(\frac{2\pi}{L}\right)^2$ $\rho_{2D}(E)$

$$\rho(E)dE = dV/\left(\frac{2\pi}{L}\right)^2 = 2\pi \cancel{k} \frac{m}{\hbar^2 \cancel{k}} dE \left[\frac{L}{2\pi}\right]^2 = \left[\frac{L}{2\pi}\right]^2 \frac{2\pi m}{\hbar^2} dE$$



Density of states in 1D

$$\boxed{E = \frac{\hbar^2 k^2}{2m}} \quad \text{with} \quad \boxed{\mathbf{k} = \frac{2\pi}{L} n_x}$$

How many states with energy between E and E+dE?

$$= \rho(E)dE$$

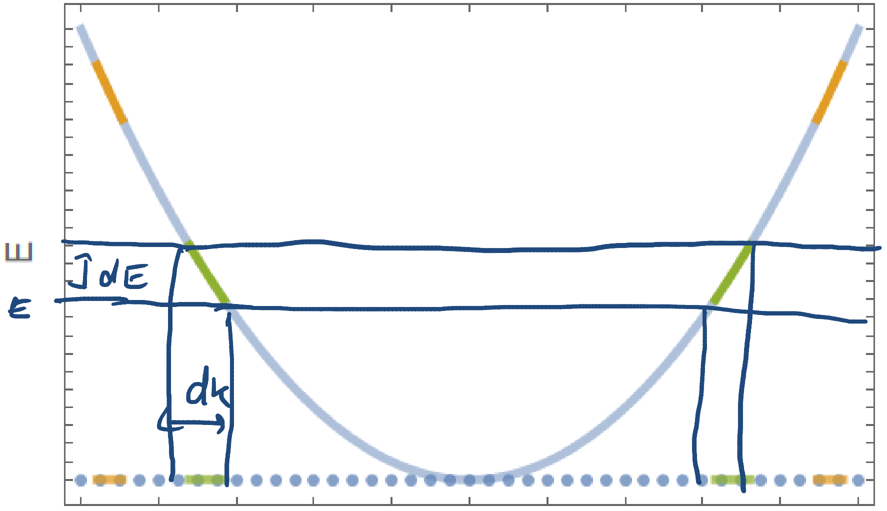
How many states with wave-vector between k and k+dk?

$$E = \frac{\hbar^2 k^2}{2m} \rightarrow dE = \frac{\hbar^2 k\, dk}{m} \rightarrow dk = \frac{m}{\hbar^2 k} dE$$

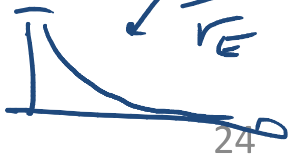
Which "volume" does this represent ?

$$dV = V(k + dk) - V(k) \quad = \underline{\underline{2}} \times dk$$

How many states are located in this "volume" ? $dV / \left(\frac{2\pi}{L}\right)$



$$\rho(E)dE = dV / \left(\frac{2\pi}{L}\right) = \frac{L}{2\pi} \frac{2m}{\hbar^2 k} dE = \boxed{\frac{L}{2\pi} \frac{2m}{\hbar^2} \sqrt{\frac{\hbar^2}{2mE}} dE} \rightarrow \rho_{1D}(E)$$



$\swarrow \frac{1}{\sqrt{E}}$

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6. **Take home message**

STEEM Refresher 2 – Take home message

- Wavefunction : $\psi(\mathbf{r}) = \frac{1}{\sqrt{L^3}} e^{i\mathbf{k}.\mathbf{r}}$

  Momentum eigen state: $\hat{\mathbf{p}}\psi = \underline{\hbar\mathbf{k}}\psi$

  with $\mathbf{k} = \frac{2\pi}{L}\begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}$

  ↳ L → +∞ ~ continuous

  Free Hamiltonian eigen state: $\hat{H}\psi = \underbrace{\frac{\hbar^2 k^2}{2m}}_{\frac{p^2}{2m}}\psi$

- Quantum particle facing a barrier :

  Can be reflected even if E > V0

  Can be transmitted even if E < V0 (tunnel effect)

- How many states with energy between E and E+dE? $= \underline{\rho(E)}dE$

  $1/\sqrt{E}$

  $\sqrt{E}$

  Depends on E=f(k) and 1D, 2D, 3D

  E^0