



i-PERC

電気通信大学

基礎電子工学CH-4

曾我部 東馬

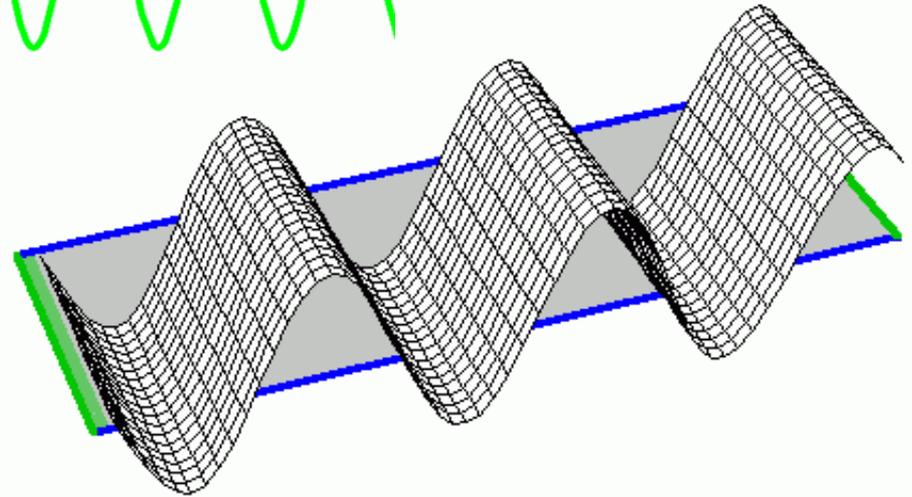
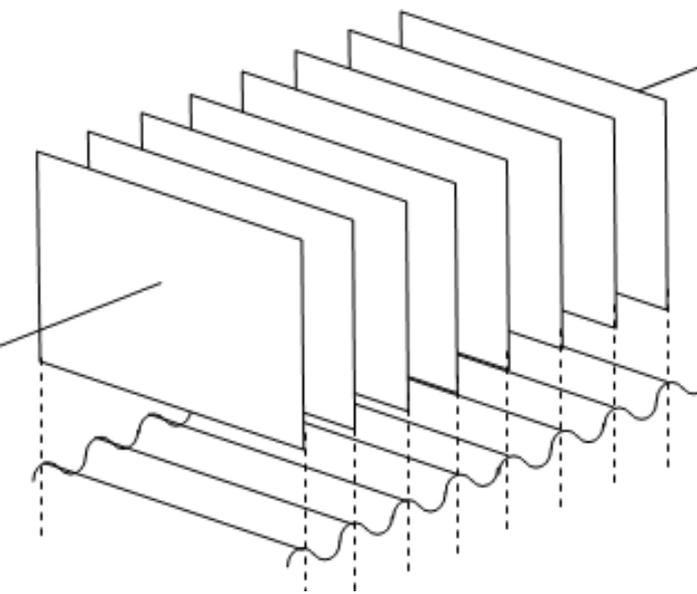
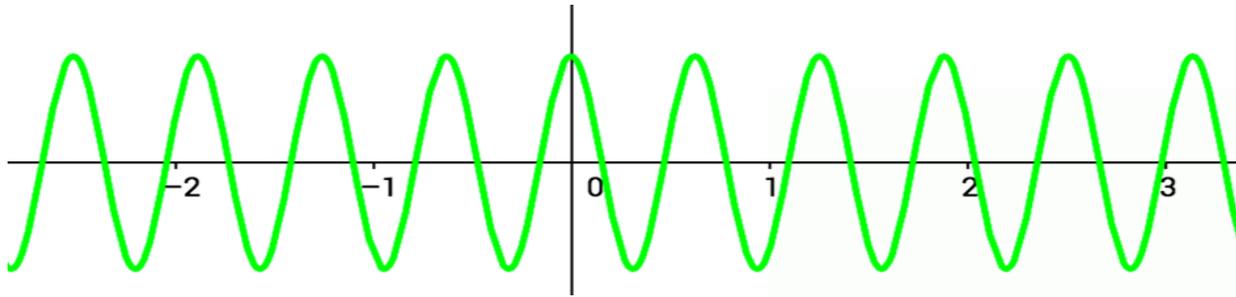
電気通信大学

i-パワードエネルギーシステム研究センター(i-PERC)

概要:



平面波という概念の導入：一次元から2, 3次元を拡張

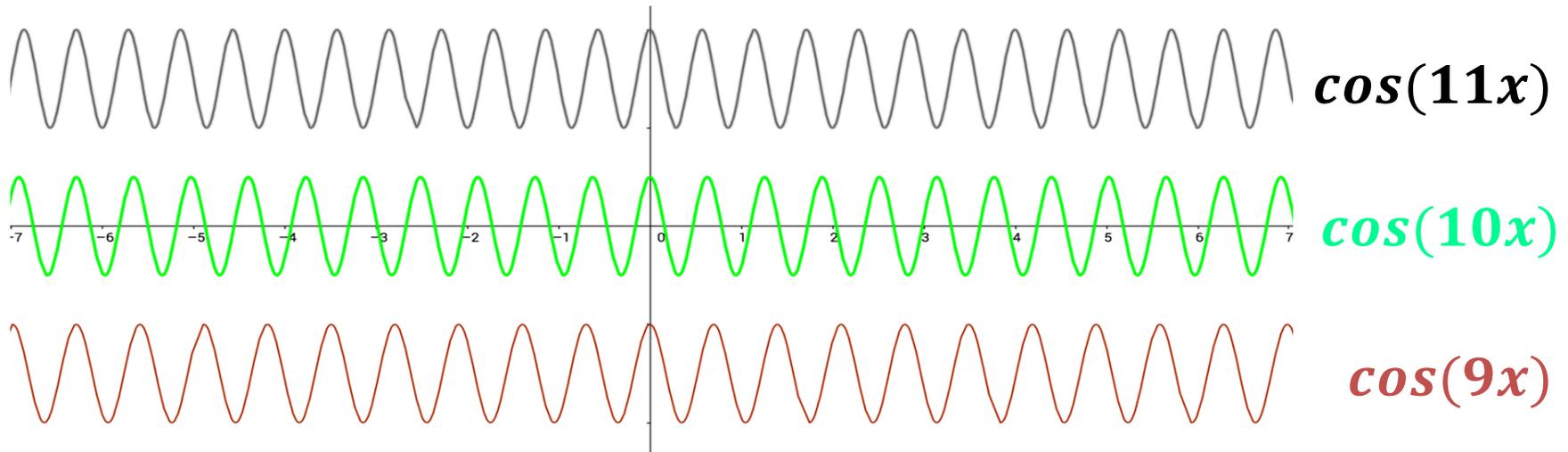


$$\Psi(x, t) = e^{i(\mathbf{k} \cdot \mathbf{x})}$$

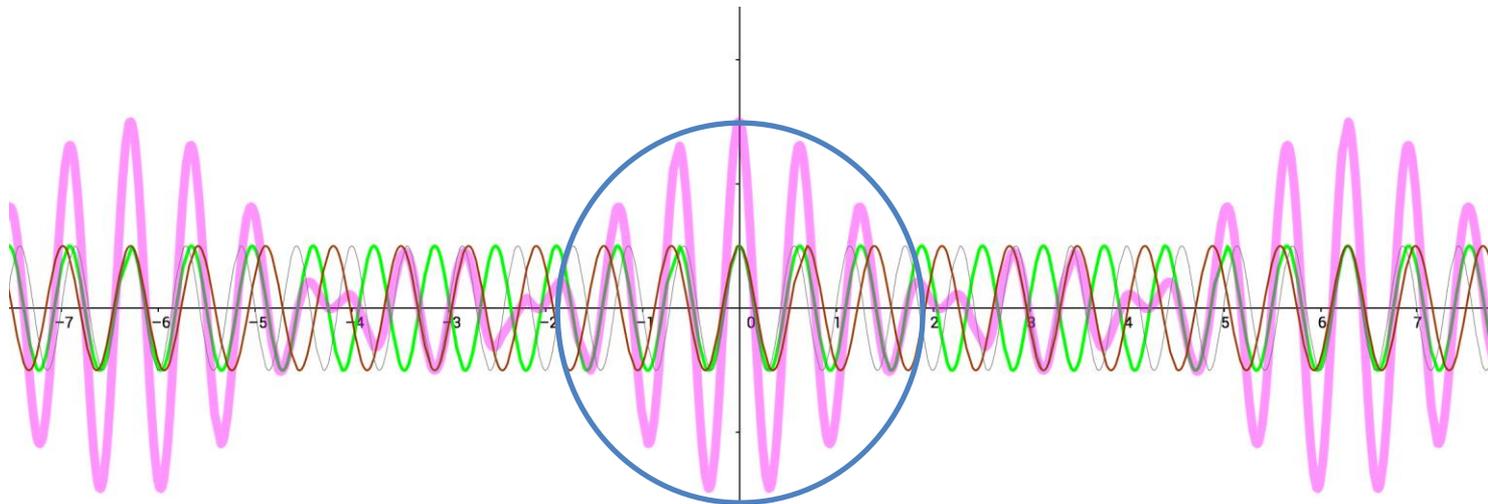
$$\mathbf{k} \cdot \mathbf{x} = \text{位相} = \text{定数}$$

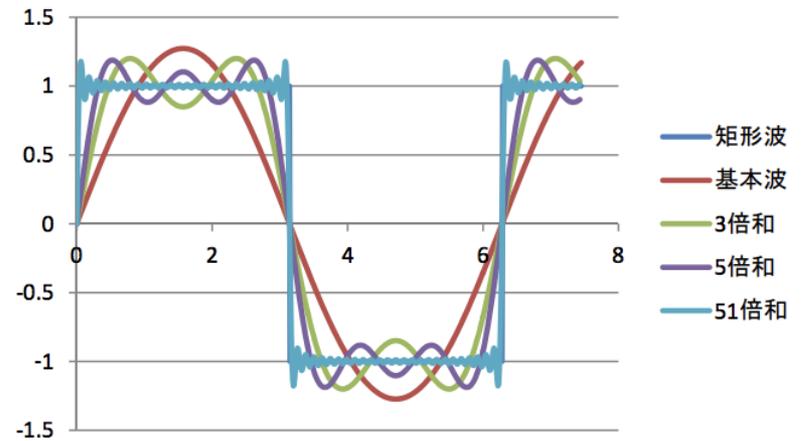
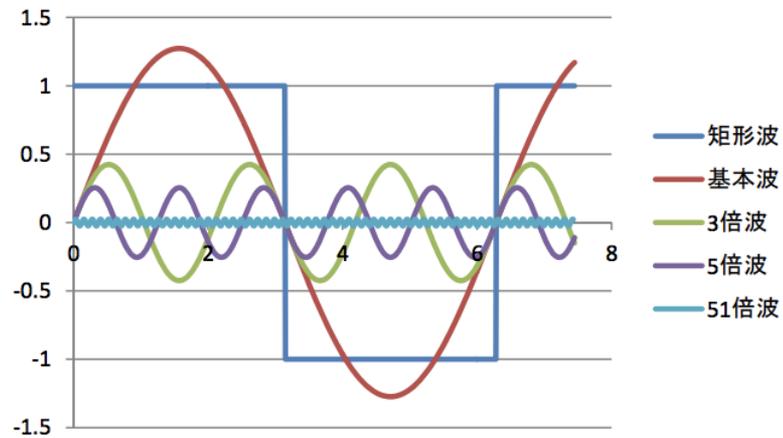
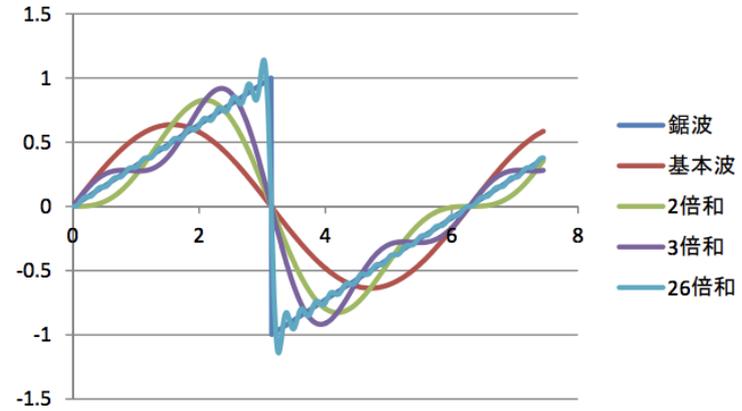
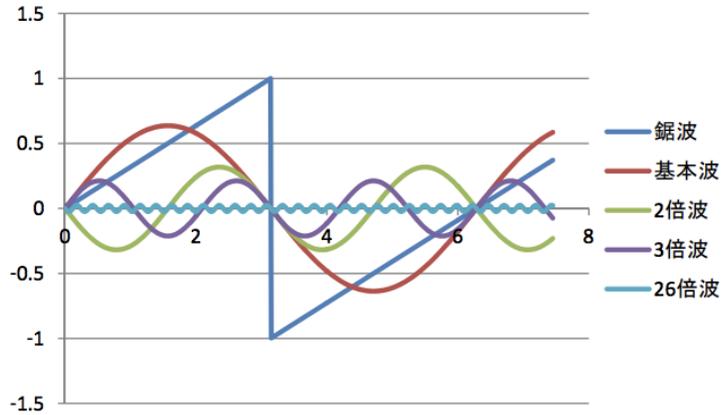
余弦波の等位相面が平面になっているので、平面波と呼んでいる

平面波の合成:

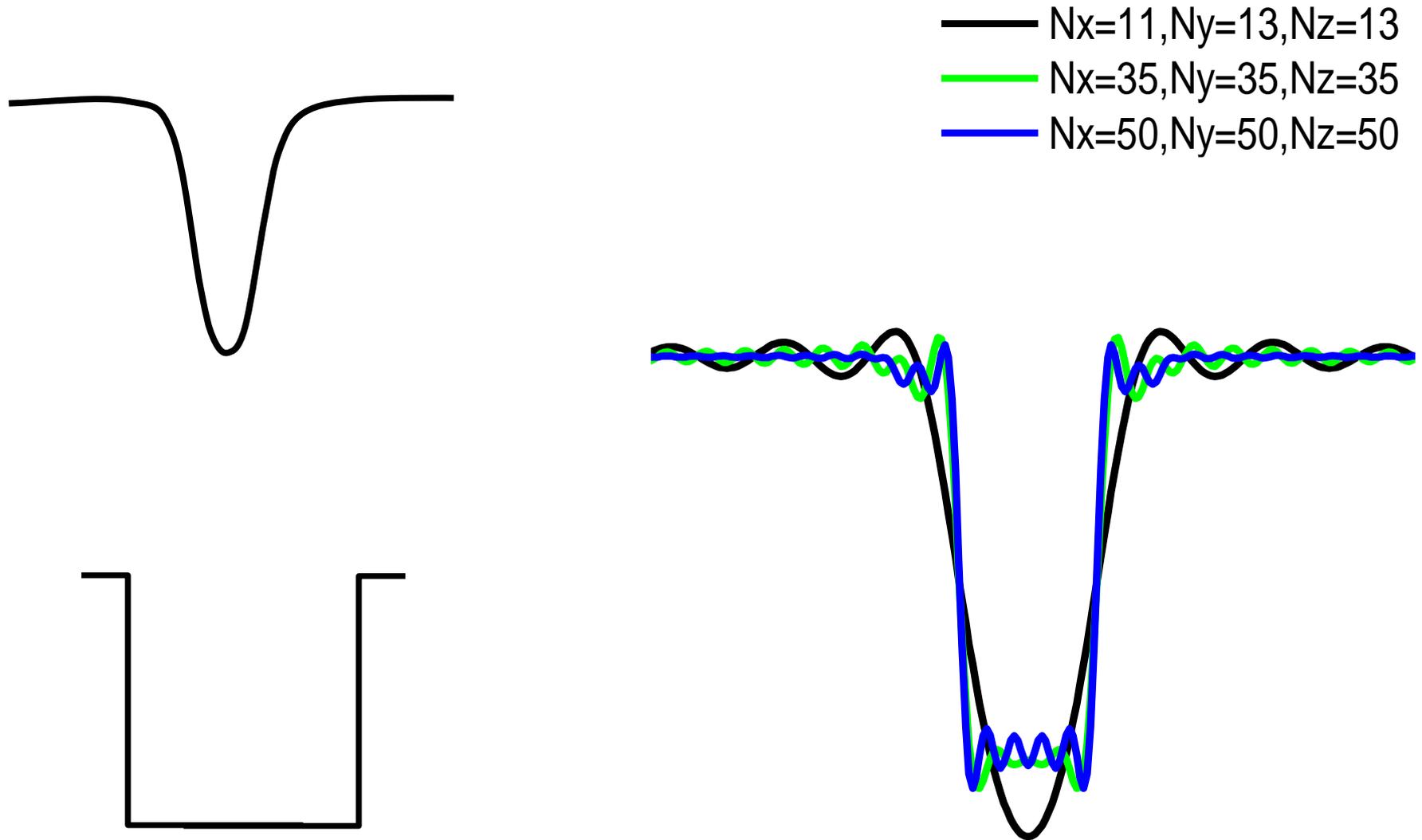


$$\cos(9x) + \cos(10x) + \cos(11x)$$





平面波の合成による任意形状のポテンシャルを作成する:



シュレーディンガー方程式を少し変形する

$$\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V) \Psi(x) = 0$$

$$\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + (E - V) \Psi(x) = 0$$

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

シュレーディンガー方程式を少し変形する

$$\frac{\partial^2 \Psi(x)}{\partial x^2} = -\frac{p^2}{\hbar^2} \Psi(x)$$

①

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

②

$$\left(\frac{p^2}{2m} + V\right)\Psi(x) = E\Psi(x)$$

$$H\Psi(x) = E\Psi(x)$$

波動関数の平面波基底近似

$$\Psi(x) = \sum_i c_i e^{ik_i x}$$

$$\left\{ \frac{p^2}{2m} + V(x) \right\} \Psi = E \Psi$$

$$\left\{ \frac{p^2}{2m} + V(x) \right\} \sum_i c_i e^{ik_i x} = E \sum_i c_i e^{ik_i x}$$

両側に $e^{-ik_j x}$ をかけて積分する

波動関数の平面波基底近似

$$e^{-ik_j x} \left\{ \frac{p^2}{2m^*} + V(x) \right\} \sum_i c_i e^{ik_i x} dx = e^{-ik_j x} E \sum_i c_i e^{ik_i x} dx$$

$$\int e^{-ik_j x} \left\{ \frac{p^2}{2m^*} + V(x) \right\} \sum_i c_i e^{ik_i x} dx = \int e^{-ik_j x} E \sum_i c_i e^{ik_i x} dx$$

$$\delta(k_i - k_j) = \frac{1}{2\pi} \int e^{ix(k_i - k_j)} dx$$

式の展開と計算:

$$\begin{aligned}
 \int e^{-ik_j x} \left\{ \frac{p^2}{2m} \right\} \sum_i c_i e^{ik_i x} dx &= \delta_{ij} \frac{\hbar^2 k_i^2}{2m} c_i \\
 &+ \\
 \int e^{-ik_j x} \{V(x)\} \sum_i c_i e^{ik_i x} dx &= \int V(x) e^{k_i - k_j} dx c_i \\
 &= \\
 \int e^{-ik_j x} E \sum_i c_i e^{ik_i x} dx &= E \delta_{ij} c_i
 \end{aligned}$$

行列計算における固有値と固有関数

$$\left\{ \frac{p^2}{2m} + V(x) \right\} \Psi = E \Psi$$

$$H_{ij} = \delta_{ij} \frac{\hbar^2 k_i^2}{2m} + \int V(x) e^{k_i - k_j} dx = E \delta_{ij}$$

(例: 4個の平面波を展開した場合: $H_{4,4}$)

$\frac{\hbar^2 k_1^2}{2m}$	$\int V(x) e^{k_1 - k_2} dx$	$\int V(x) e^{k_1 - k_3} dx$	$\int V(x) e^{k_1 - k_4} dx$
$\int V(x) e^{k_2 - k_1} dx$	$\frac{\hbar^2 k_2^2}{2m}$	$\int V(x) e^{k_2 - k_3} dx$	$\int V(x) e^{k_2 - k_4} dx$
$\int V(x) e^{k_3 - k_1} dx$	$\int V(x) e^{k_3 - k_2} dx$	$\frac{\hbar^2 k_3^2}{2m}$	$\int V(x) e^{k_3 - k_4} dx$
$\int V(x) e^{k_4 - k_1} dx$	$\int V(x) e^{k_4 - k_2} dx$	$\int V(x) e^{k_4 - k_3} dx$	$\frac{\hbar^2 k_4^2}{2m}$

=

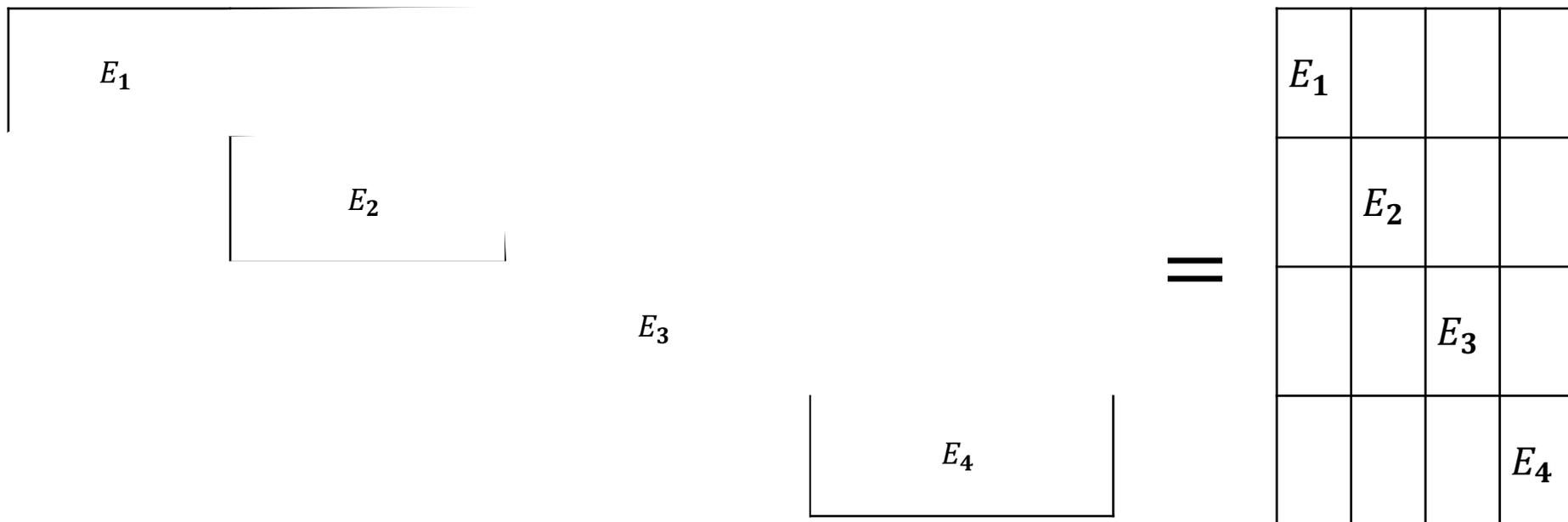
E_1			
	E_2		
		E_3	
			E_4

行列の対角化：固有値と固有関数

$$\left\{ \frac{p^2}{2m} + V(x) \right\} \Psi = E \Psi$$

$$H_{ij} = \delta_{ij} \frac{\hbar^2 k_i^2}{2m} + \int V(x) e^{k_i - k_j} dx = E \delta_{ij}$$

(例：4個の平面波を展開した場合： $H_{4,4}$)



行列計算における固有値と固有関数

$$\left\{ \frac{p^2}{2m} + V(x) \right\} \Psi = E \Psi$$

$$H_{ij} = \delta_{ij} \frac{\hbar^2 k_i^2}{2m} + \int V(x) e^{k_i - k_j} dx = E \delta_{ij}$$

(例: 4個の平面波を展開した場合: $H_{4,4}$)

$\frac{\hbar^2 k_1^2}{2m}$	$\int V(x) e^{k_1 - k_2} dx$	$\int V(x) e^{k_1 - k_3} dx$	$\int V(x) e^{k_1 - k_4} dx$
$\int V(x) e^{k_2 - k_1} dx$	$\frac{\hbar^2 k_2^2}{2m}$	$\int V(x) e^{k_2 - k_3} dx$	$\int V(x) e^{k_2 - k_4} dx$
$\int V(x) e^{k_3 - k_1} dx$	$\int V(x) e^{k_3 - k_2} dx$	$\frac{\hbar^2 k_3^2}{2m}$	$\int V(x) e^{k_3 - k_4} dx$
$\int V(x) e^{k_4 - k_1} dx$	$\int V(x) e^{k_4 - k_2} dx$	$\int V(x) e^{k_4 - k_3} dx$	$\frac{\hbar^2 k_4^2}{2m}$

=

E_1			
	E_2		
		E_3	
			E_4

具体例:

平面波設計:

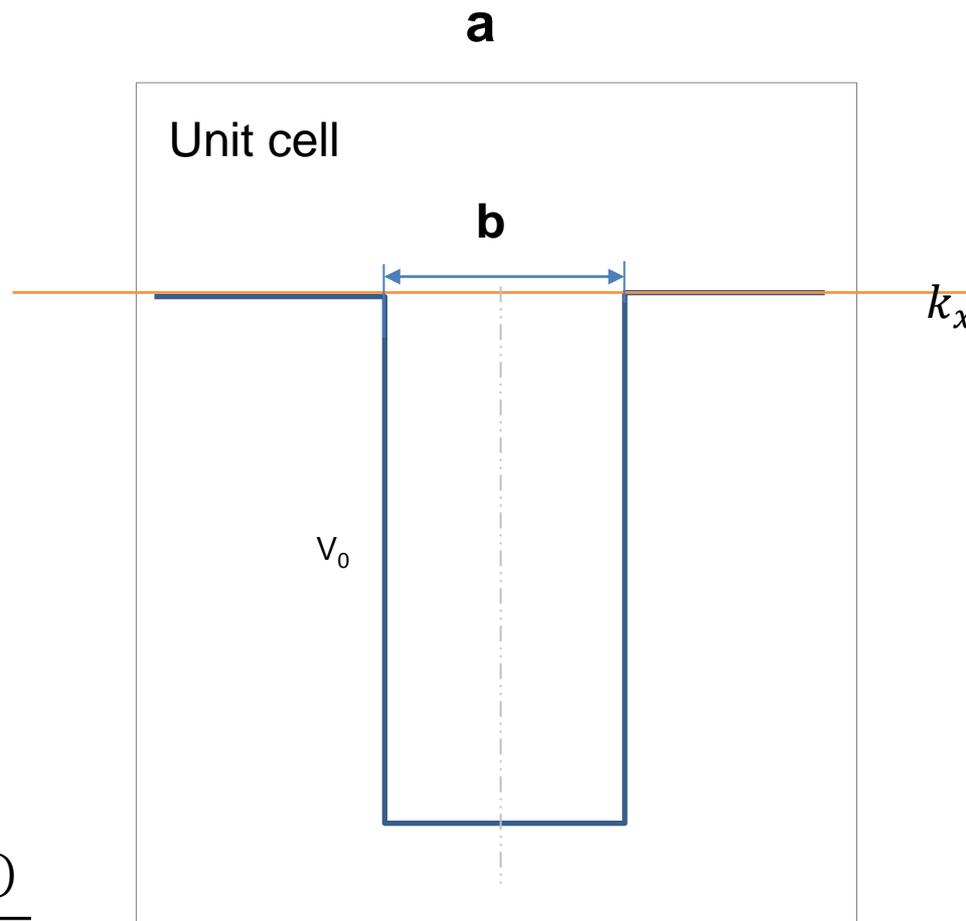
$$\Phi(x) = \sum_i c_i \frac{1}{\sqrt{a}} e^{ik_i x}$$

$$k_i = \frac{2\pi}{a} i$$

$$i = 0, \pm 1, \pm 2, \pm 3, \dots, \pm N$$

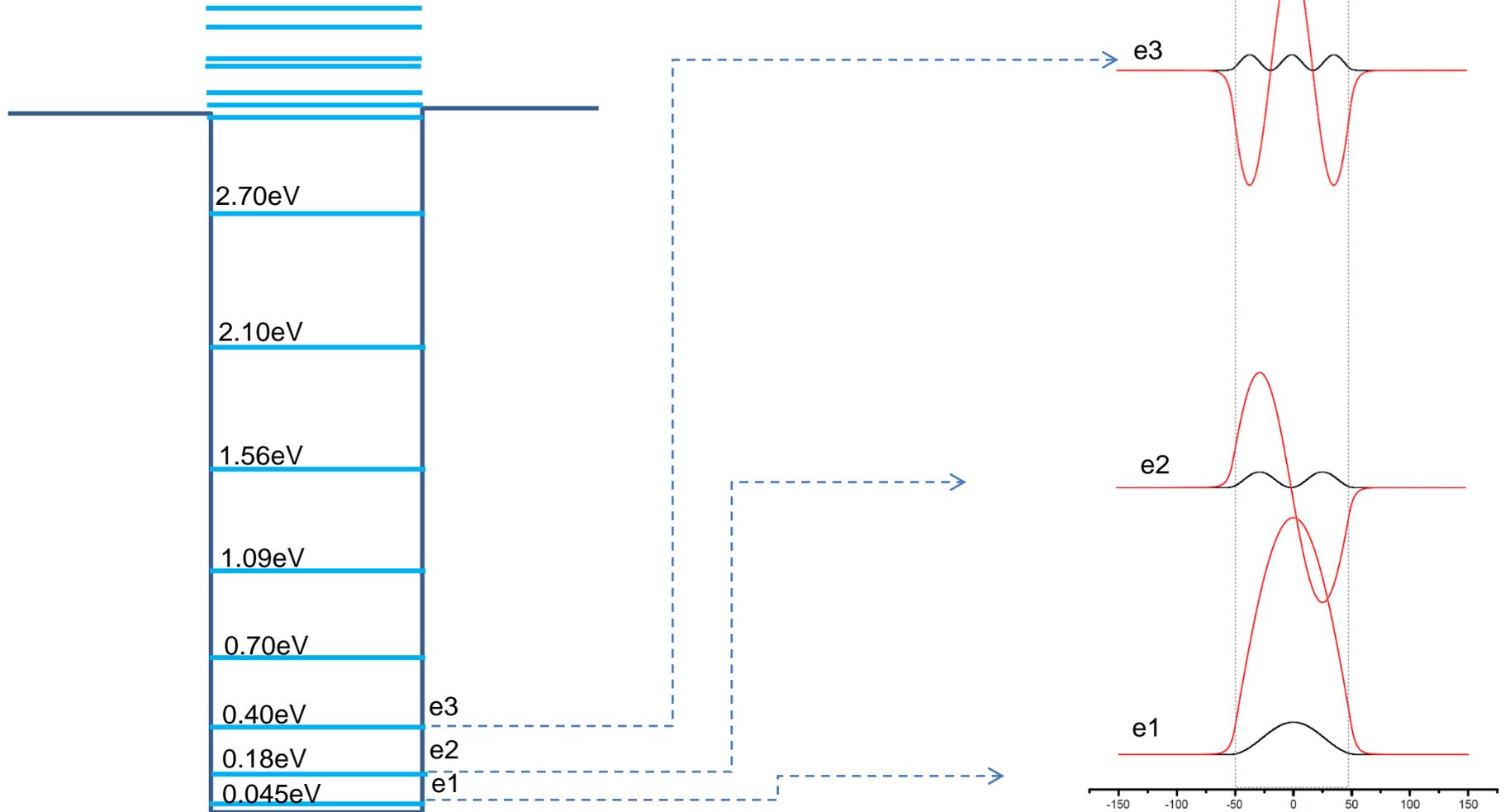
$$V(x)$$

$$\int V(x) e^{k_i - k_j} dx = \frac{V_0}{a} * \frac{\text{Sin}(b * (\frac{k_i - k_j}{2}))}{(\frac{k_i - k_j}{2})}$$



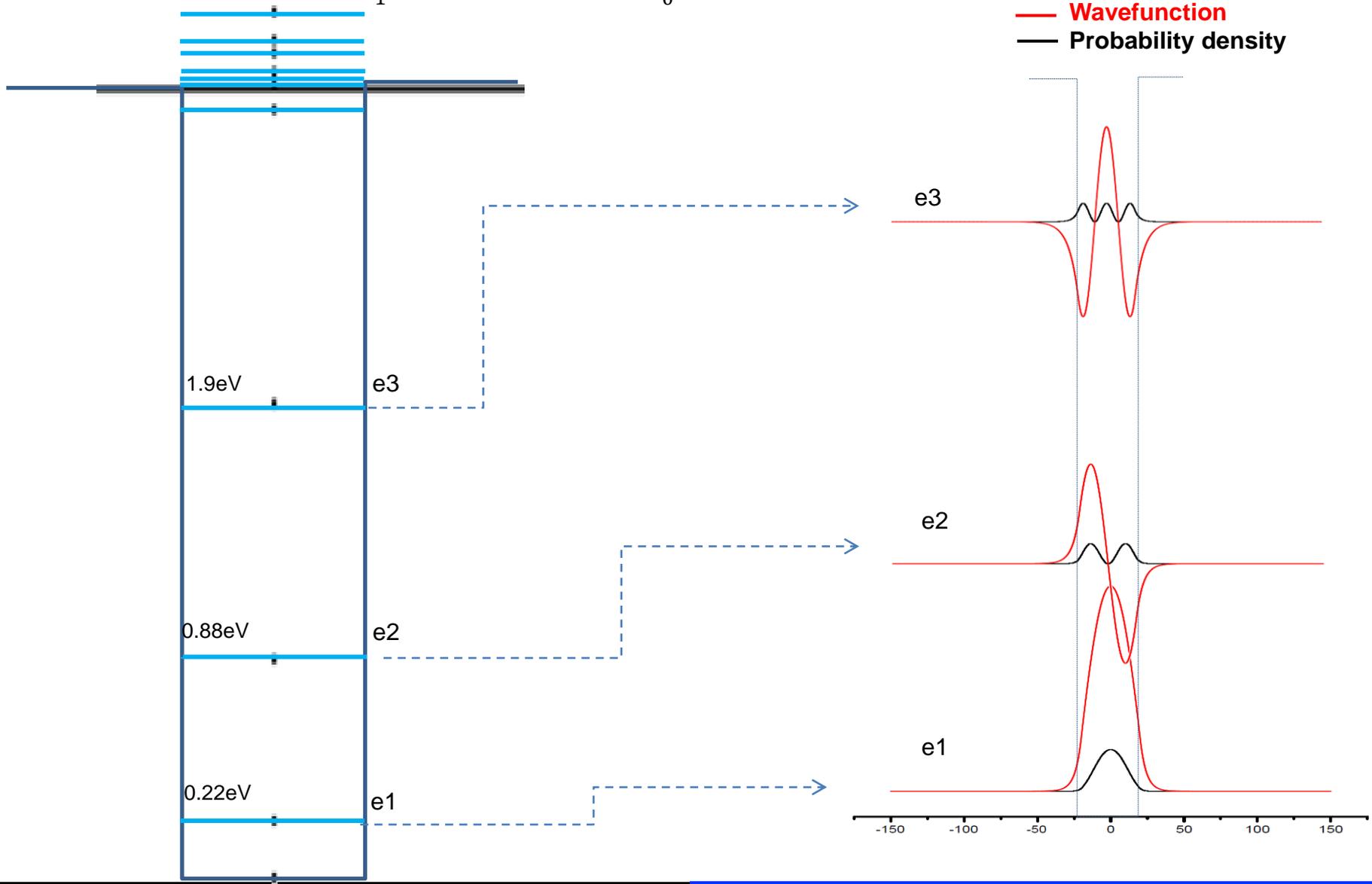
計算結果： $a=30\text{nm}$ $b=10\text{nm}$

N : Mesh size 1000 Number of plane wave = $2*N+1=2001$
 a : unite cell size 30nm $\Delta E_1 = 3.2\text{eV}$ $m^* = 0.26m_0$



計算結果: $a=30\text{nm}$ $b=4\text{nm}$

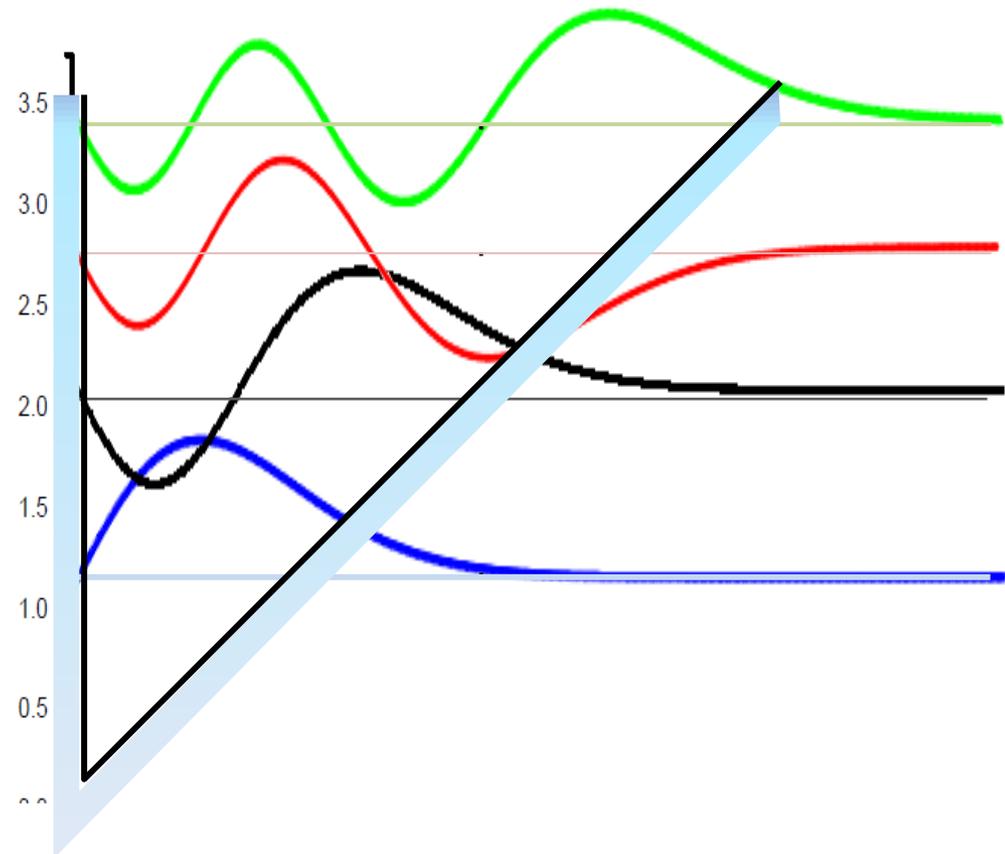
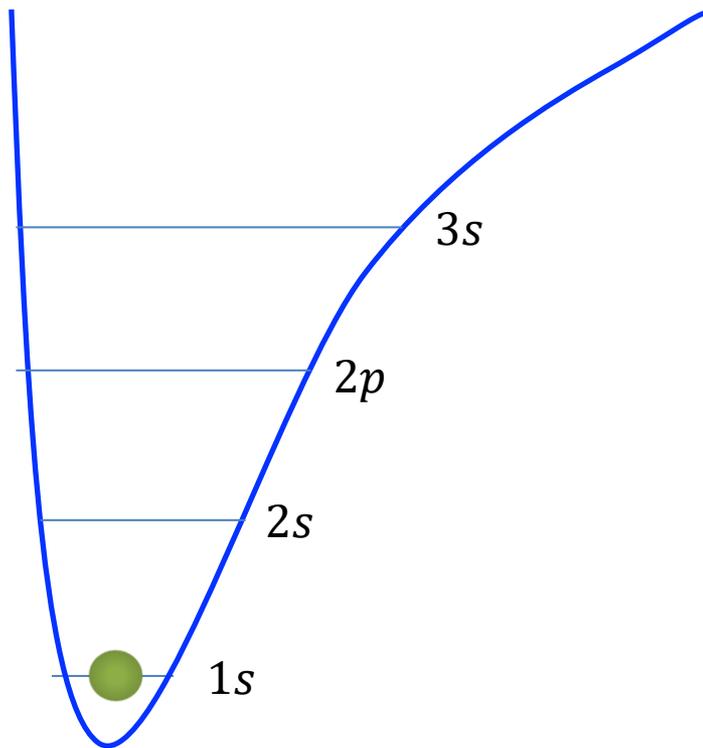
N : Mesh size 1000 Number of plane wave = $2*N+1=2001$
 a : unite cell size 30nm $\Delta E_1 = 3.2\text{eV}$ $m^* = 0.26m_0$

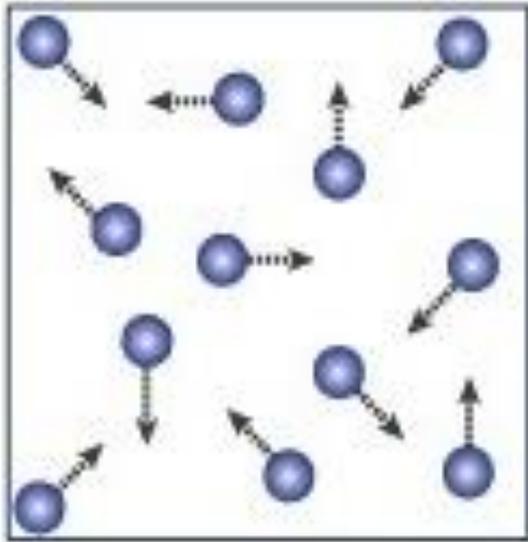


水素原子

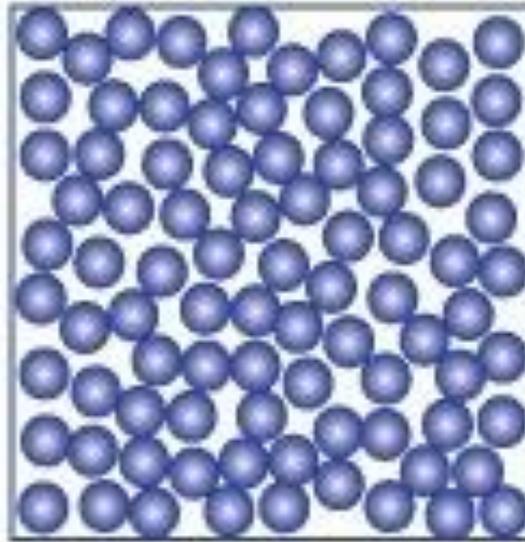
簡易型ポテンシャル

$$V(x) = x$$

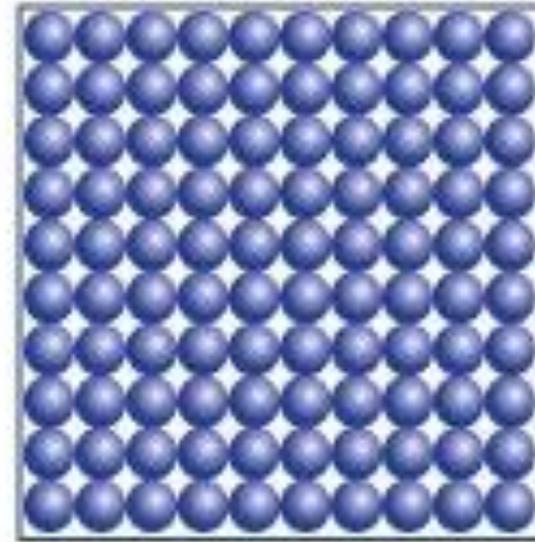




気
体
(原子、分子)



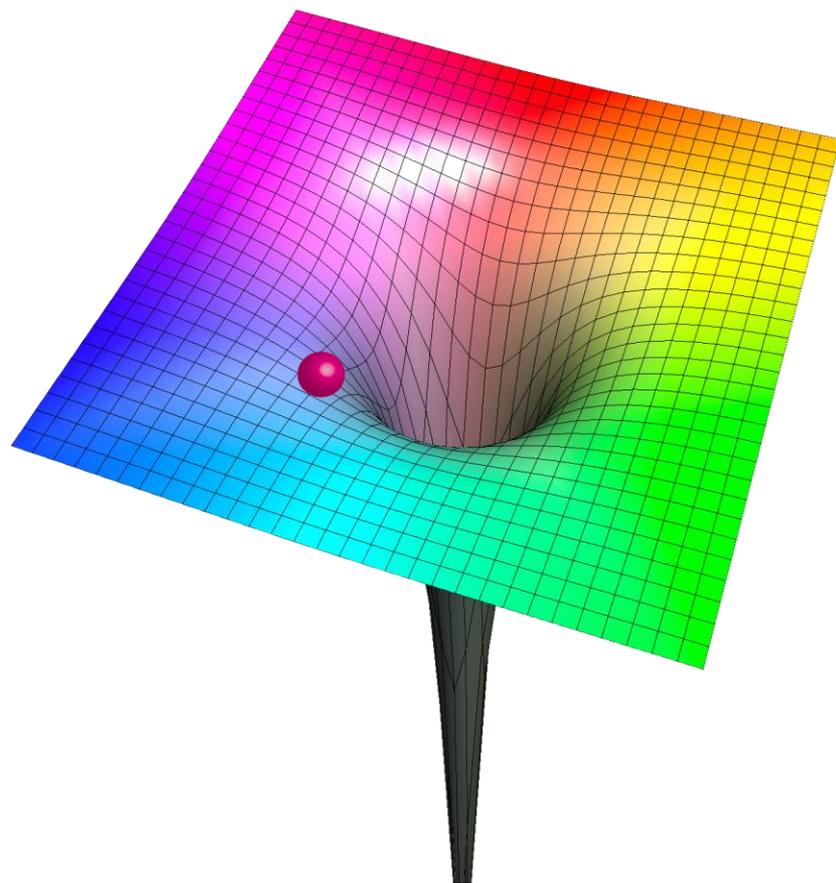
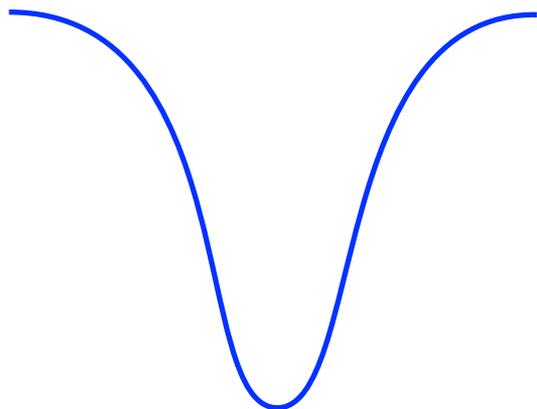
液
体



固
体

水素原子:

$$V = -\frac{1}{r}$$



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

球座標変換

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \psi + V(r)\psi = E\psi$$

計算結果:



s

Angular Part $Y(\theta, \phi)$

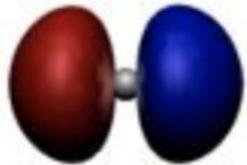
$$\ell = 0 \left\{ Y_s = \left(\frac{1}{4\pi} \right)^{1/2} \right.$$

Radial Part $R_{n\ell}(r)$

$$R_{1s} = 2 \left(\frac{Z}{a_0} \right)^{3/2} \exp(-\sigma)$$

$$R_{2s} = \frac{1}{2\sqrt{2}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \sigma) \exp(-\sigma/2)$$

$$R_{3s} = \frac{2}{81\sqrt{3}} \left(\frac{Z}{a_0} \right)^{3/2} (27 - 18\sigma + 2\sigma^2) \exp(-\sigma/3)$$

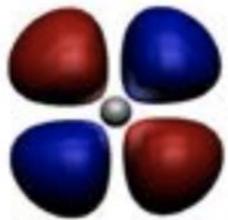


p

$$\ell = 1 \left\{ \begin{array}{l} Y_{p_x} = \left(\frac{3}{4\pi} \right)^{1/2} \sin \theta \cos \phi \\ Y_{p_y} = \left(\frac{3}{4\pi} \right)^{1/2} \sin \theta \sin \phi \\ Y_{p_z} = \left(\frac{3}{4\pi} \right)^{1/2} \cos \theta \end{array} \right.$$

$$R_{2p} = \frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma \exp(-\sigma/2)$$

$$R_{3p} = \frac{4}{81\sqrt{6}} \left(\frac{Z}{a_0} \right)^{3/2} (6\sigma - \sigma^2) \exp(-\sigma/3)$$

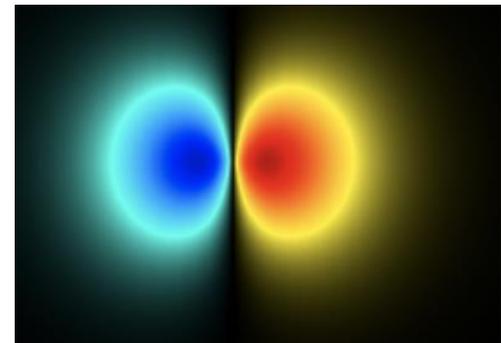
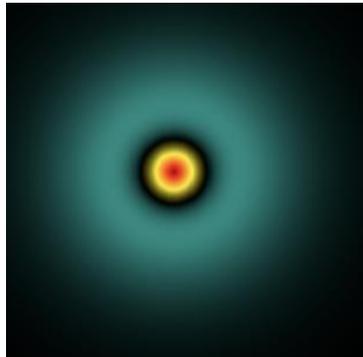
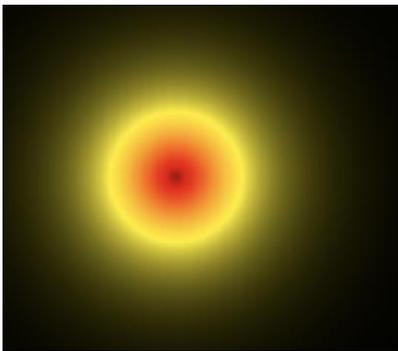
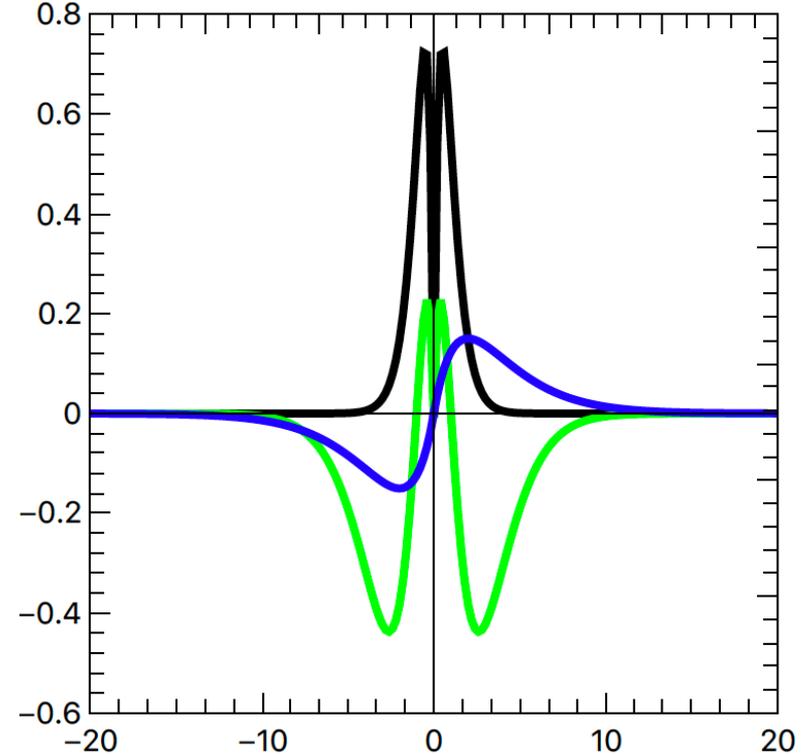
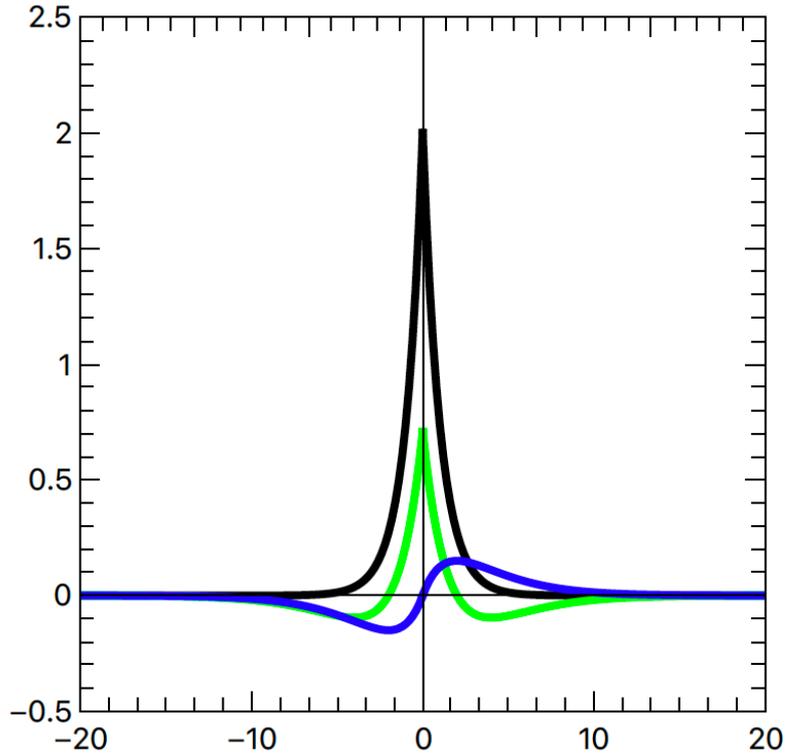


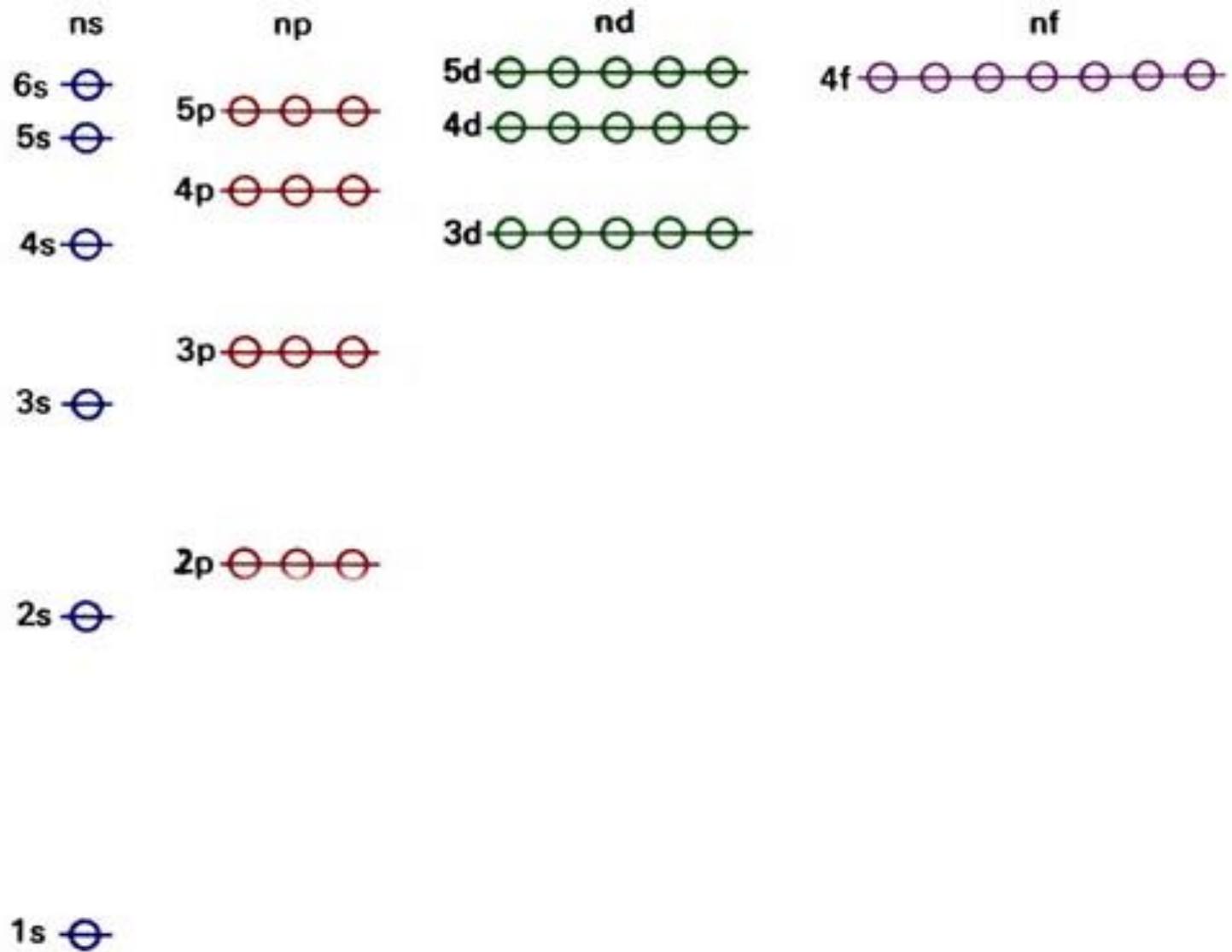
d

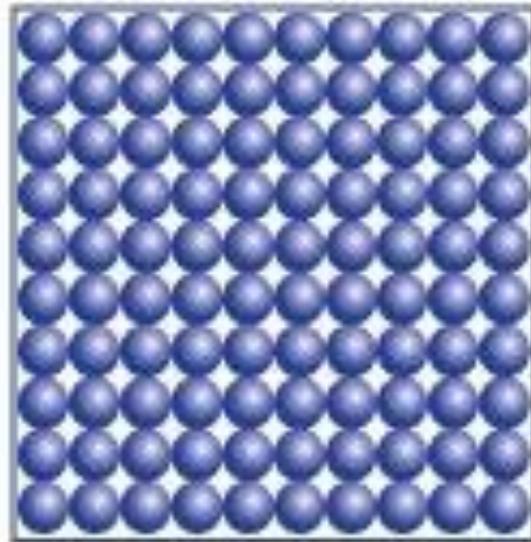
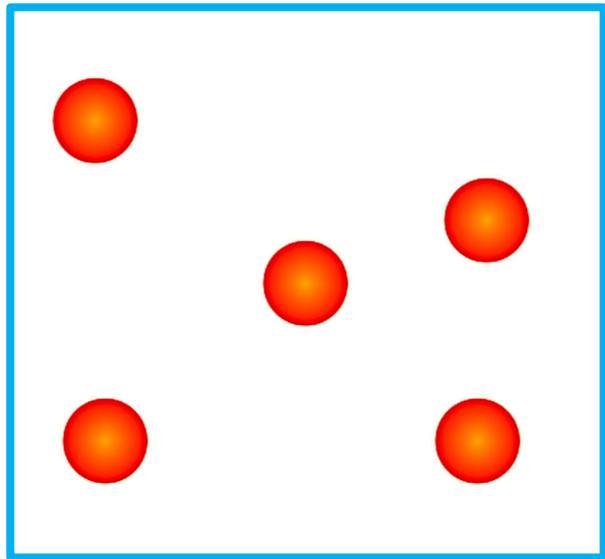
$$\ell = 2 \left\{ \begin{array}{l} Y_{d_{z^2}} = \left(\frac{5}{16\pi} \right)^{1/2} (3 \cos^2 \theta - 1) \\ Y_{d_{xz}} = \left(\frac{15}{4\pi} \right)^{1/2} \sin \theta \cos \theta \cos \phi \\ Y_{d_{yz}} = \left(\frac{15}{4\pi} \right)^{1/2} \sin \theta \cos \theta \sin \phi \\ Y_{d_{xy}} = \left(\frac{15}{16\pi} \right)^{1/2} \sin^2 \theta \sin 2\phi \\ Y_{d_{x^2-y^2}} = \left(\frac{15}{16\pi} \right)^{1/2} \sin^2 \theta \cos 2\phi \end{array} \right.$$

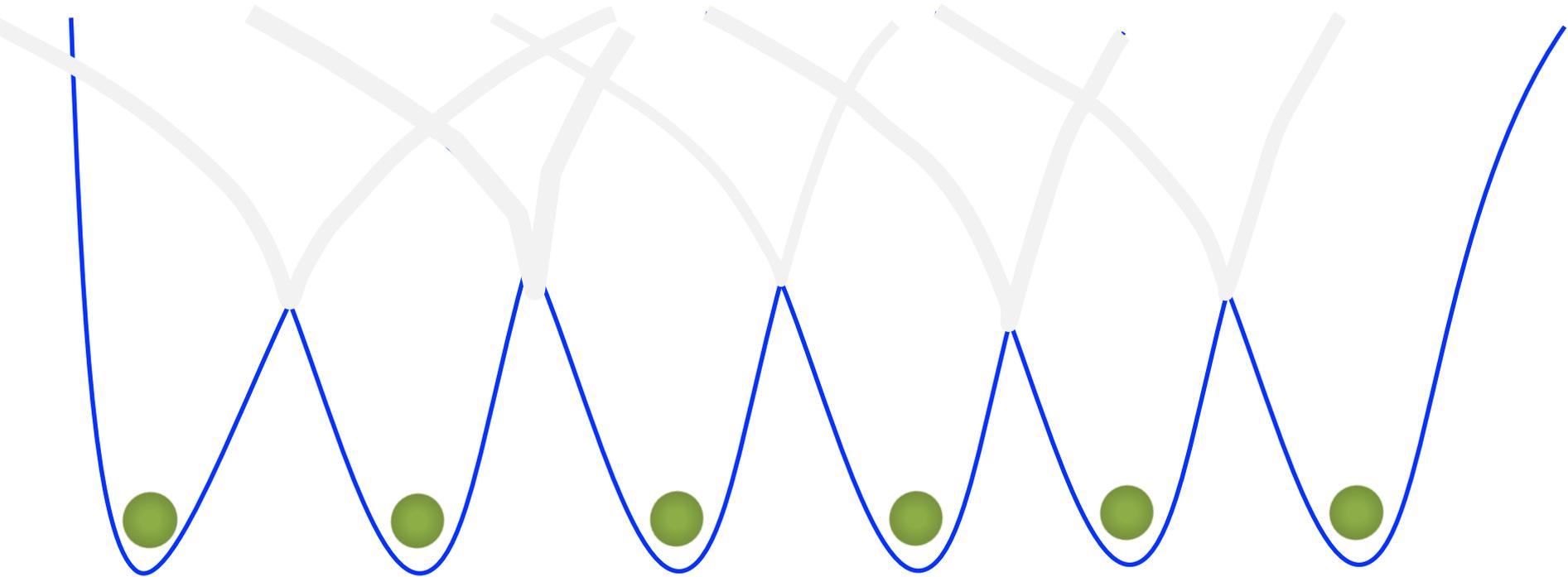
$$R_{3d} = \frac{4}{81\sqrt{30}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma^2 \exp(-\sigma/3)$$

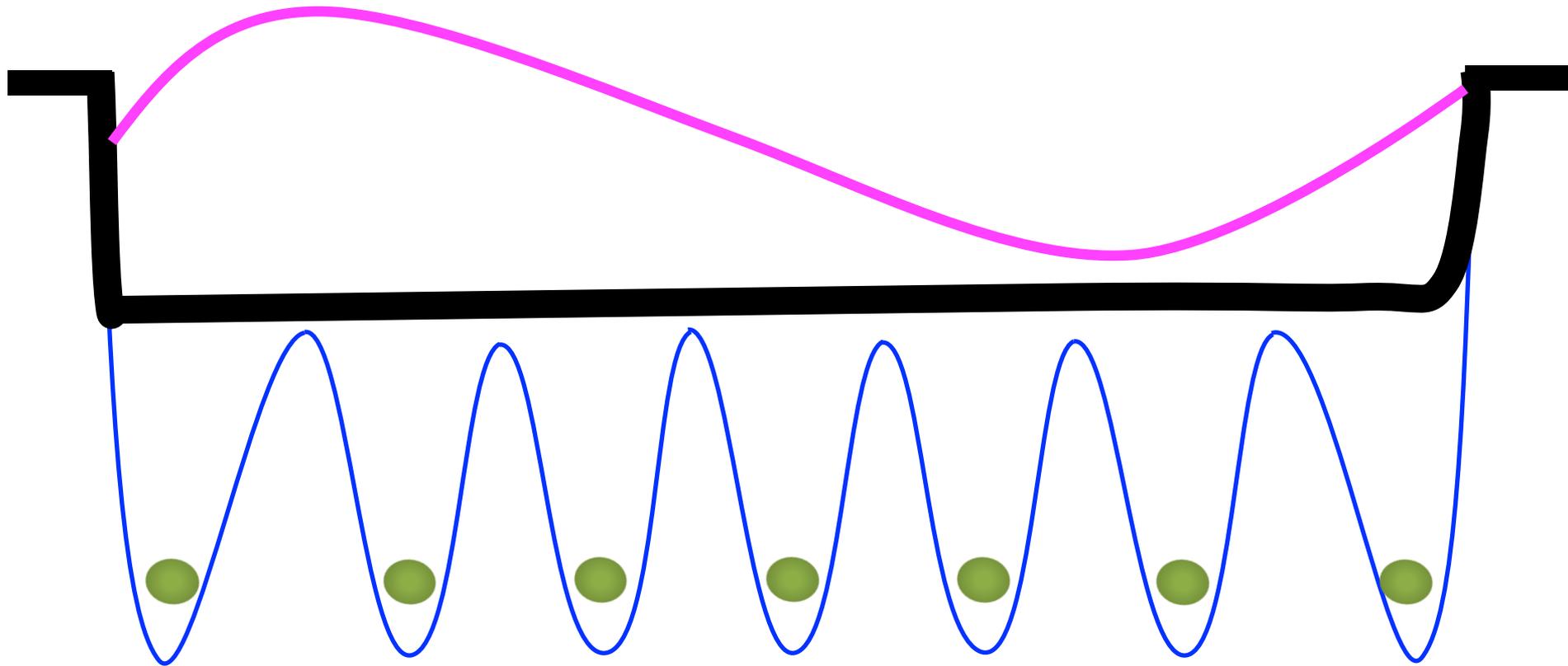
水素原子：波動関数

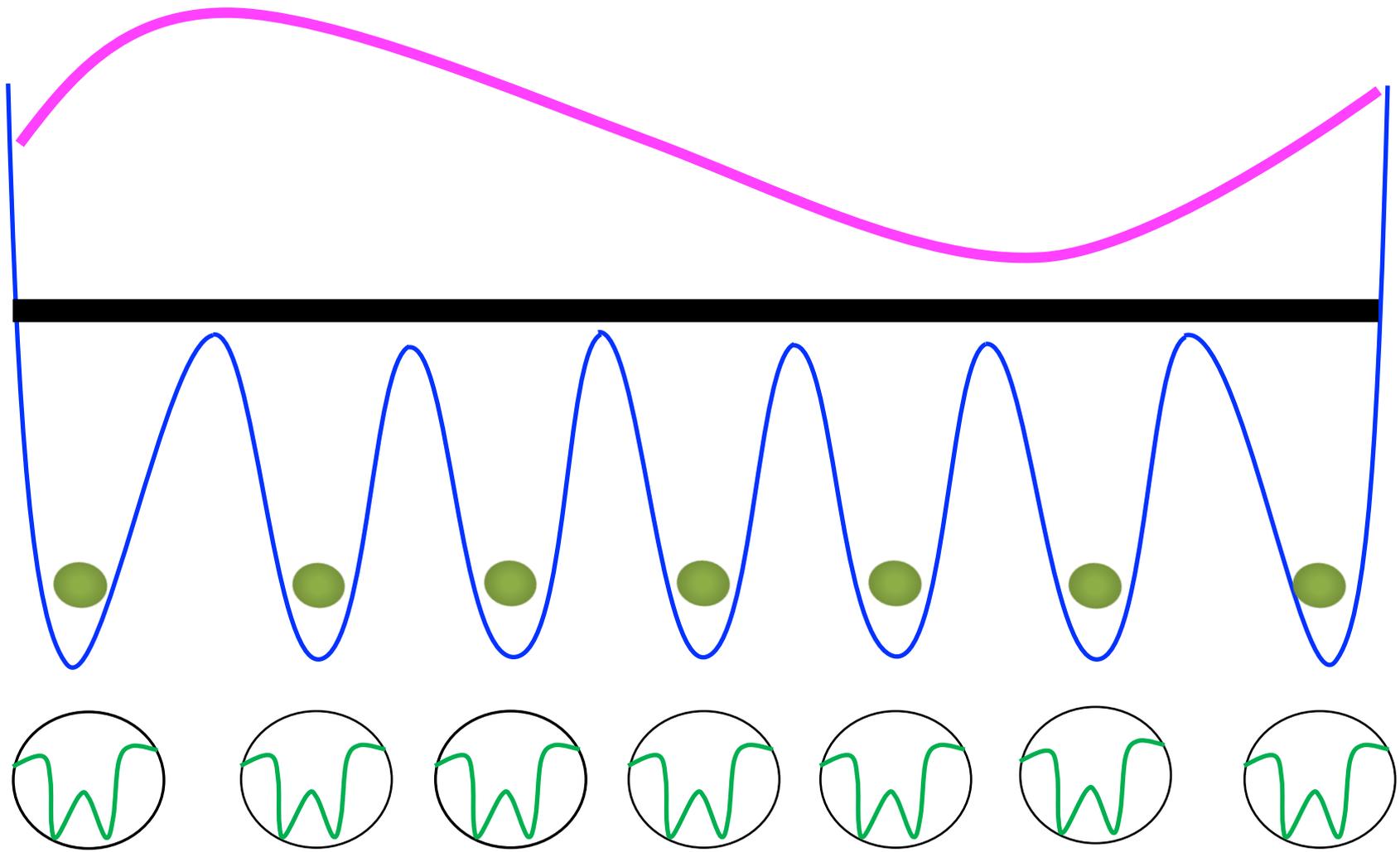


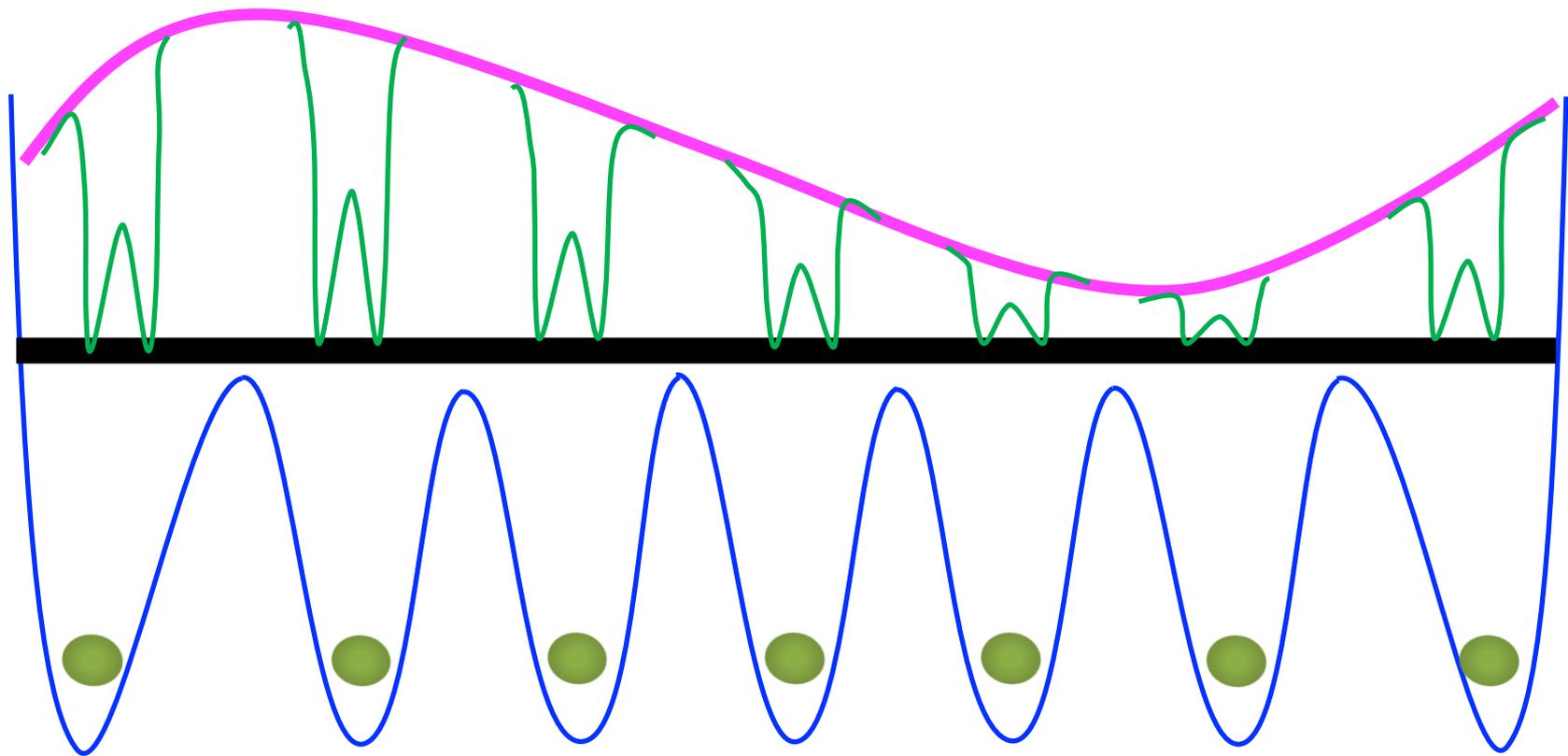


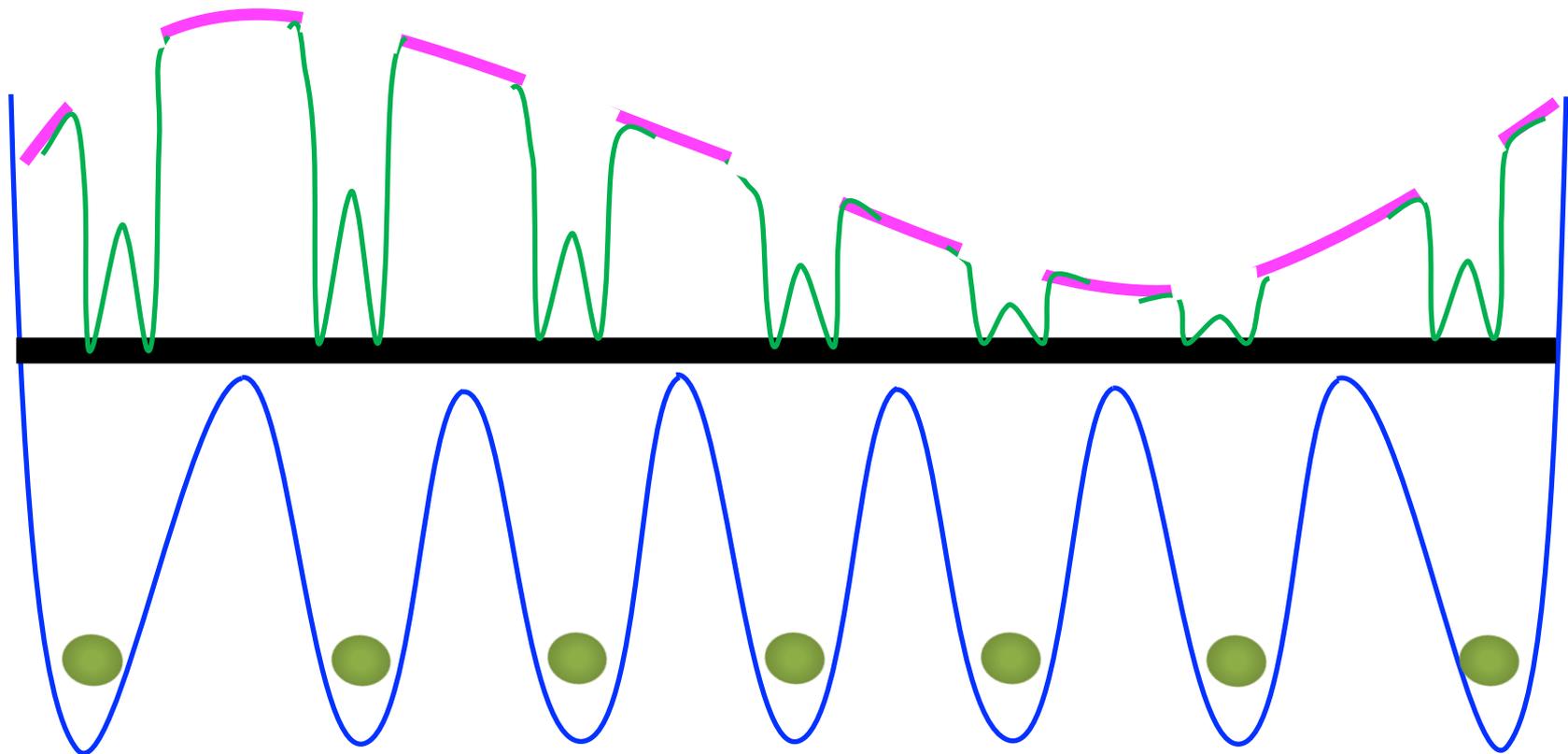




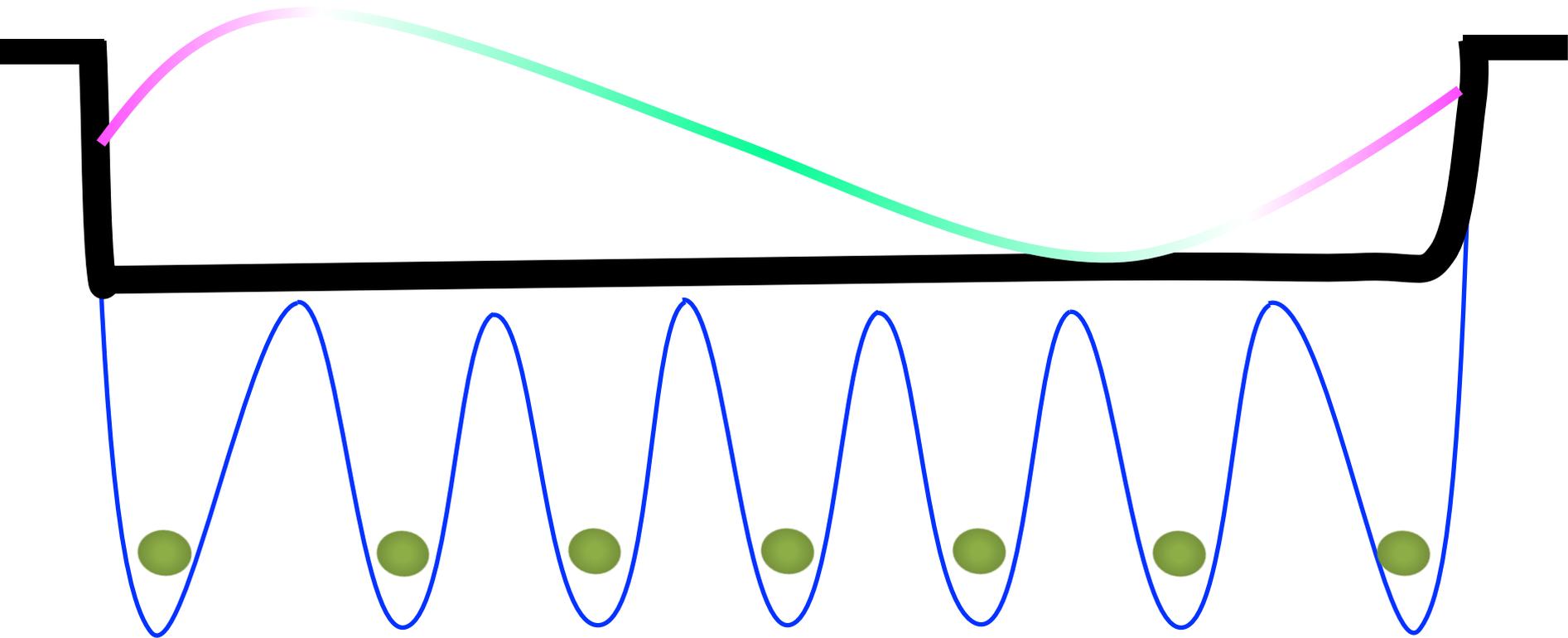






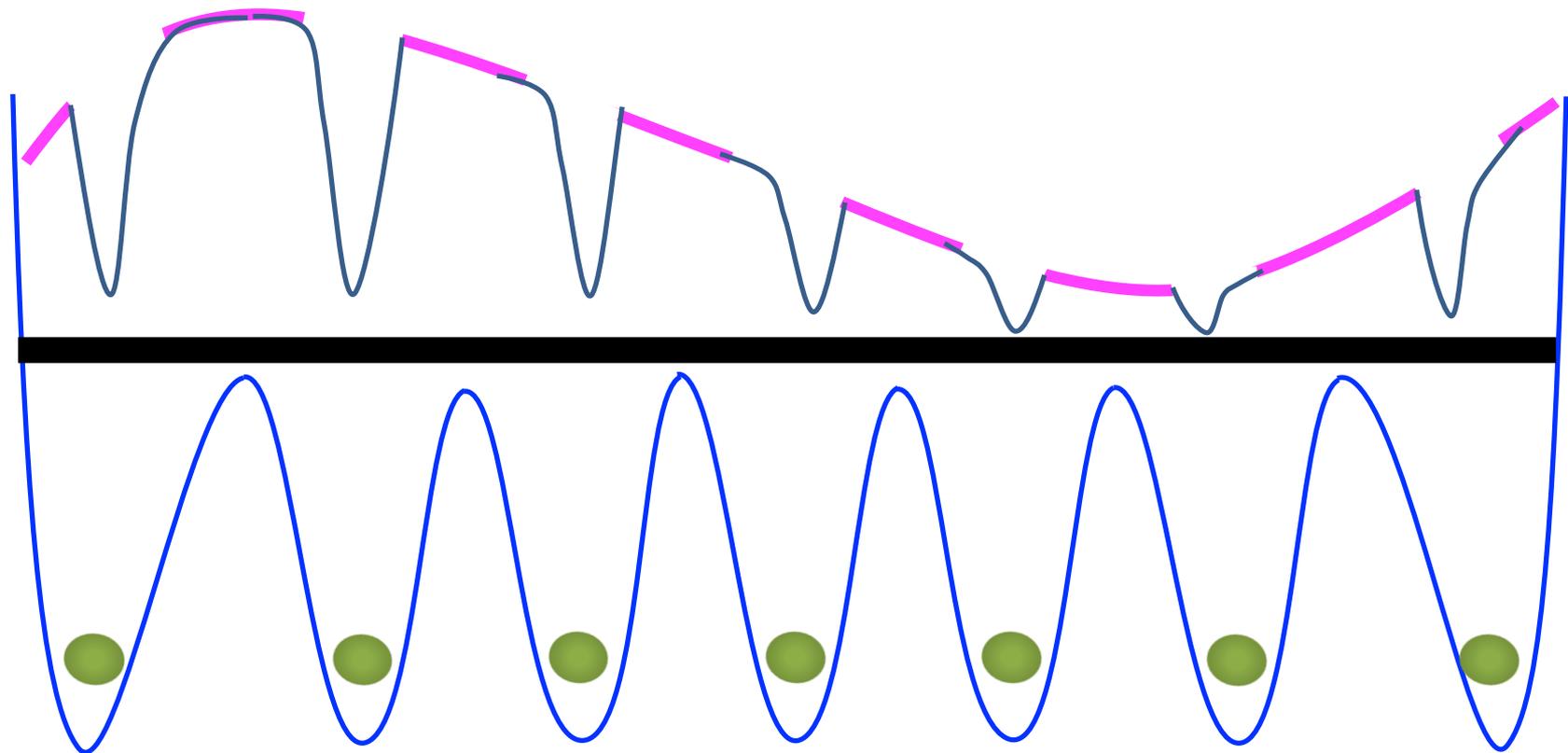


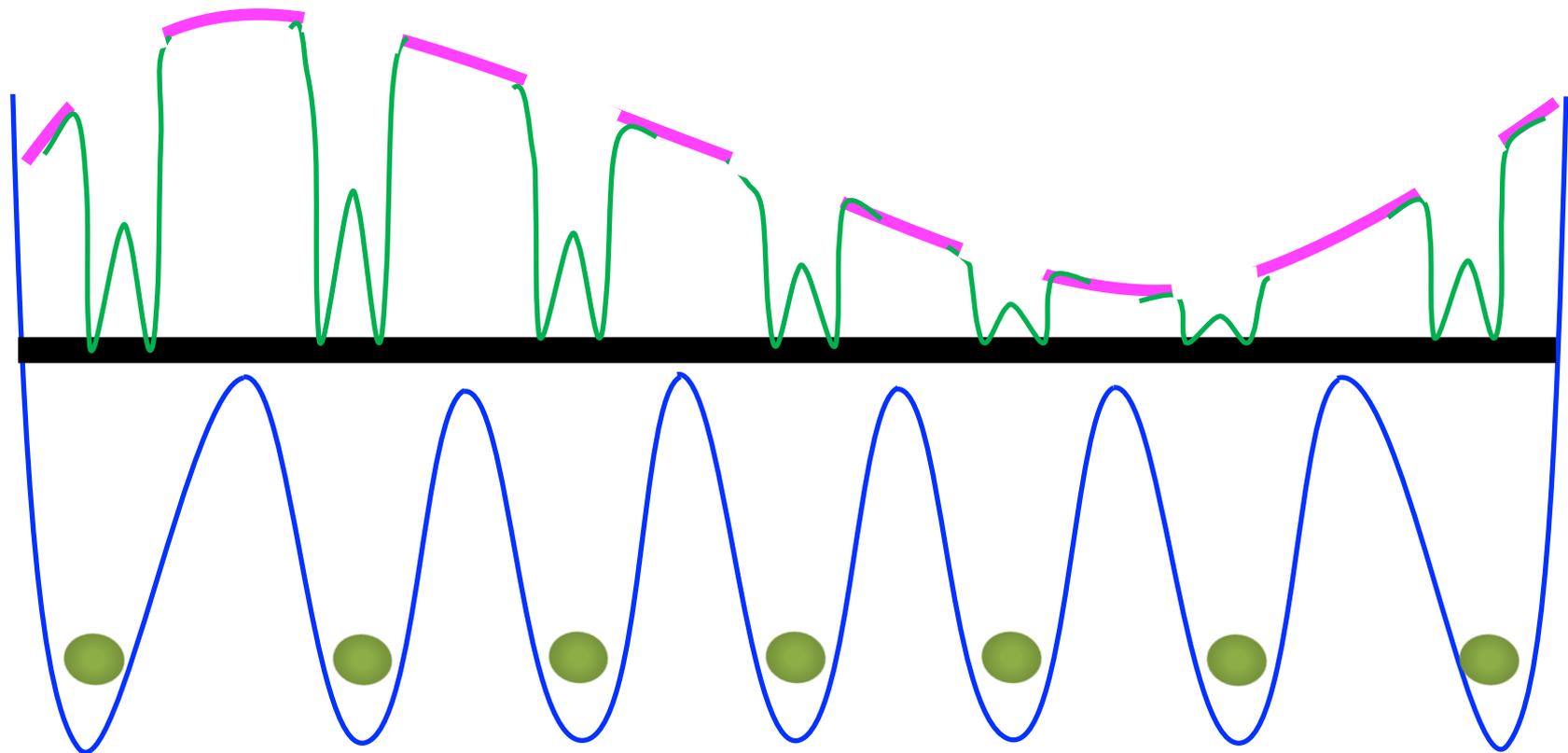
有効質量法： m^* の導入



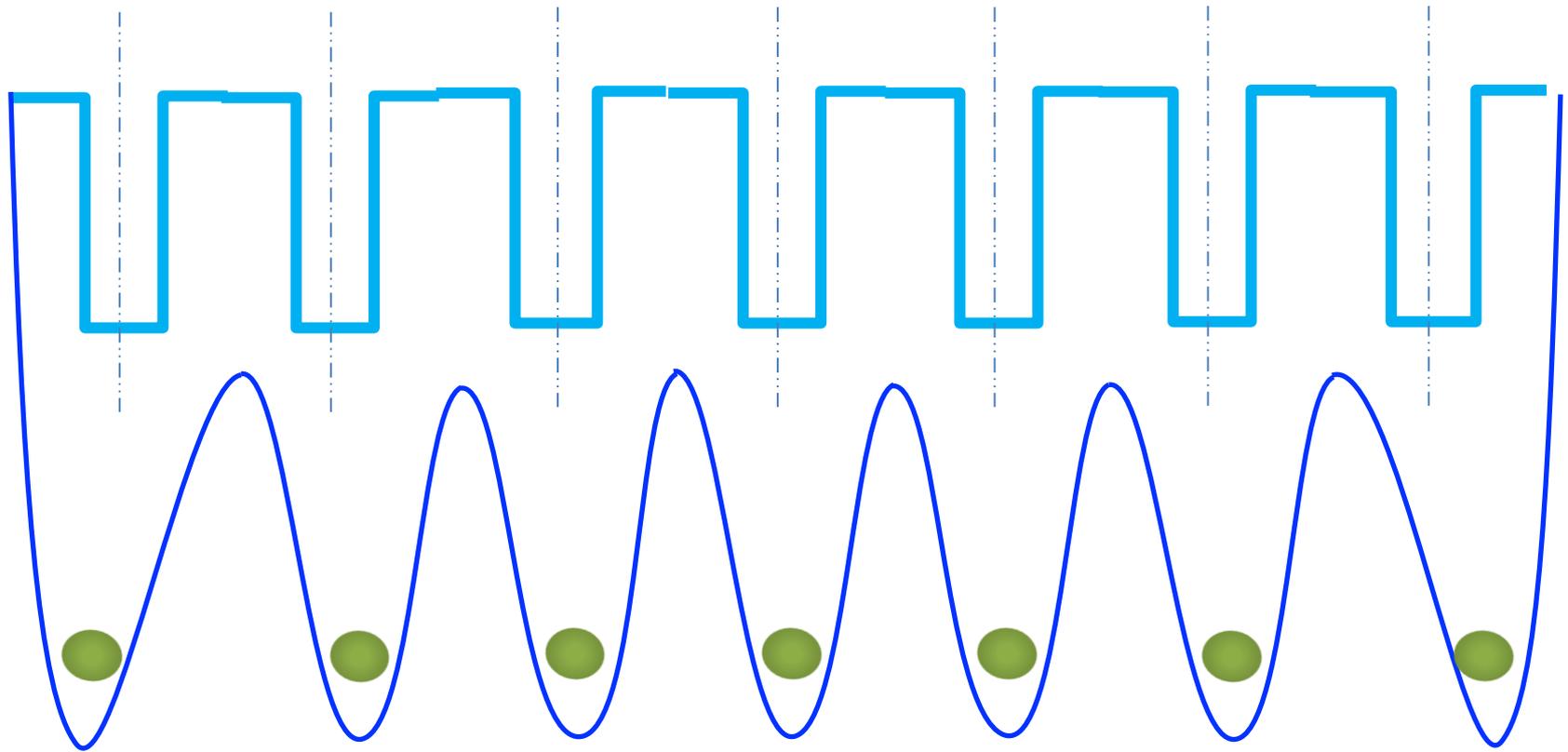
$$-\frac{\hbar^2}{2m^*} \frac{\partial^2 \Psi(x)}{\partial x^2} + V\Psi(x) = E\Psi(x)$$

擬ポテンシャル法:

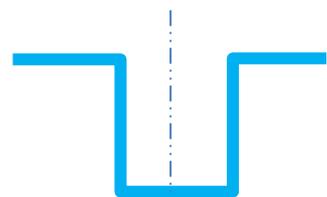




有効質量法： m^* の計算



周期構造:



$$H = \frac{p^2}{2m^*} + V(x)$$

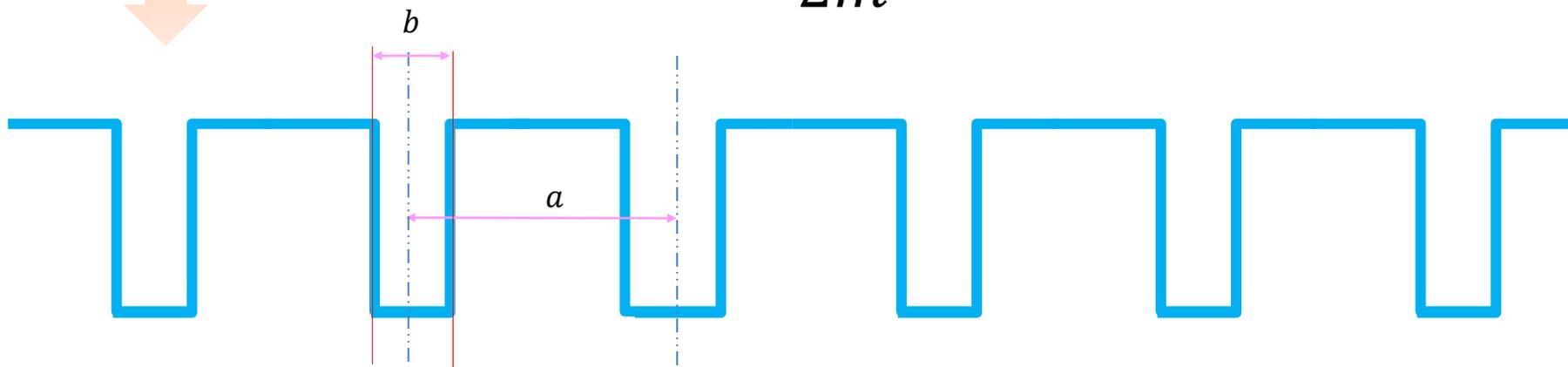
with $G = \frac{2\pi}{a}$

$$V(x) = \sum_n v(x - na) = \sum_G V_G e^{iG \cdot x}$$

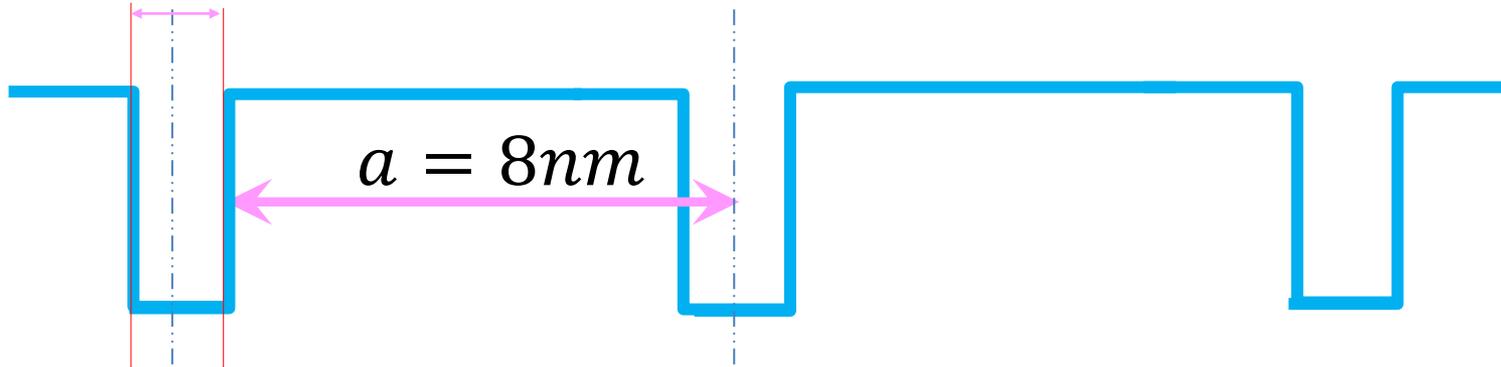
$$\Psi(x) = \sum_{G'} c_{G'} \frac{1}{\sqrt{a}} e^{i(k_i + G'(n))x}$$

with $G' = \frac{2\pi}{a}n$

$$H_{G'G''} = \frac{\hbar^2 (k_i + G'')^2}{2m^*} \delta_{G'G''} + V_{G''-G'}$$



$$b = 2\text{nm}$$



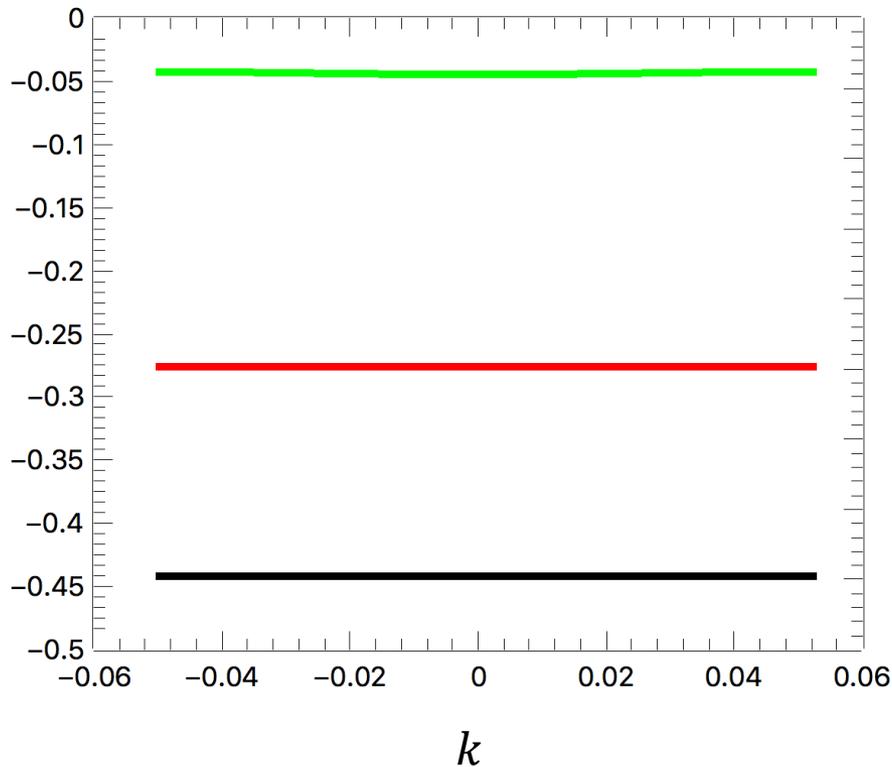
$$a = 8\text{nm}$$

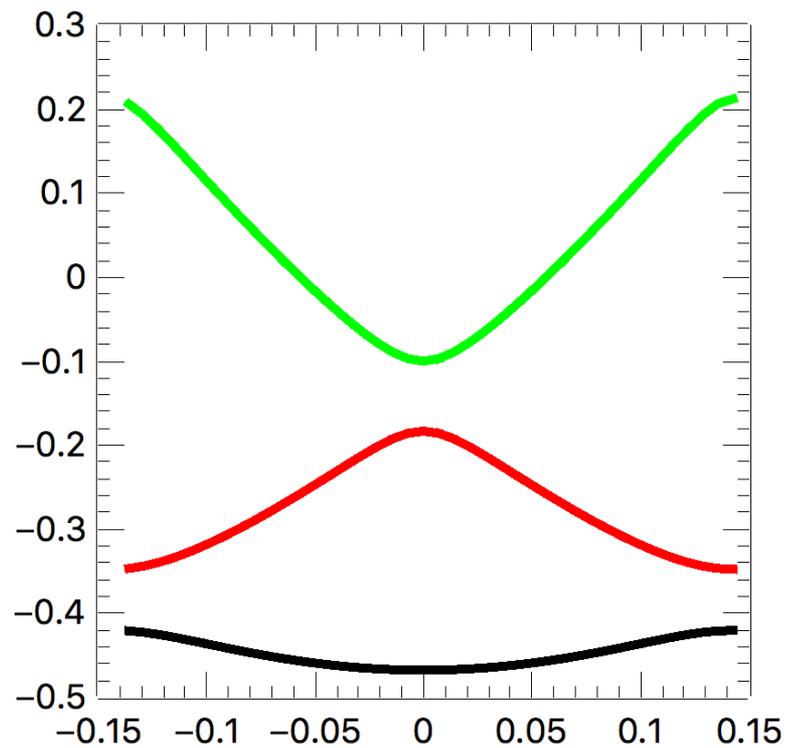
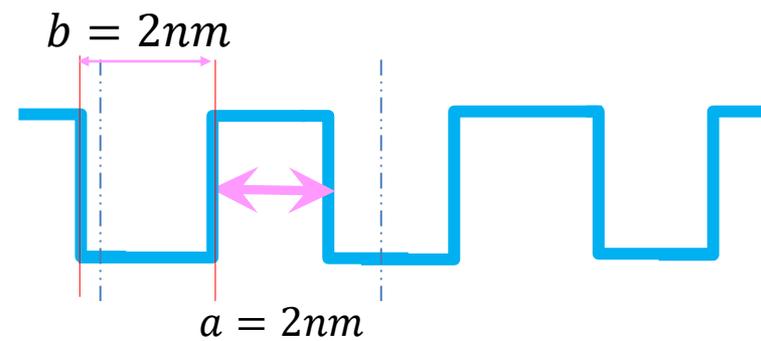
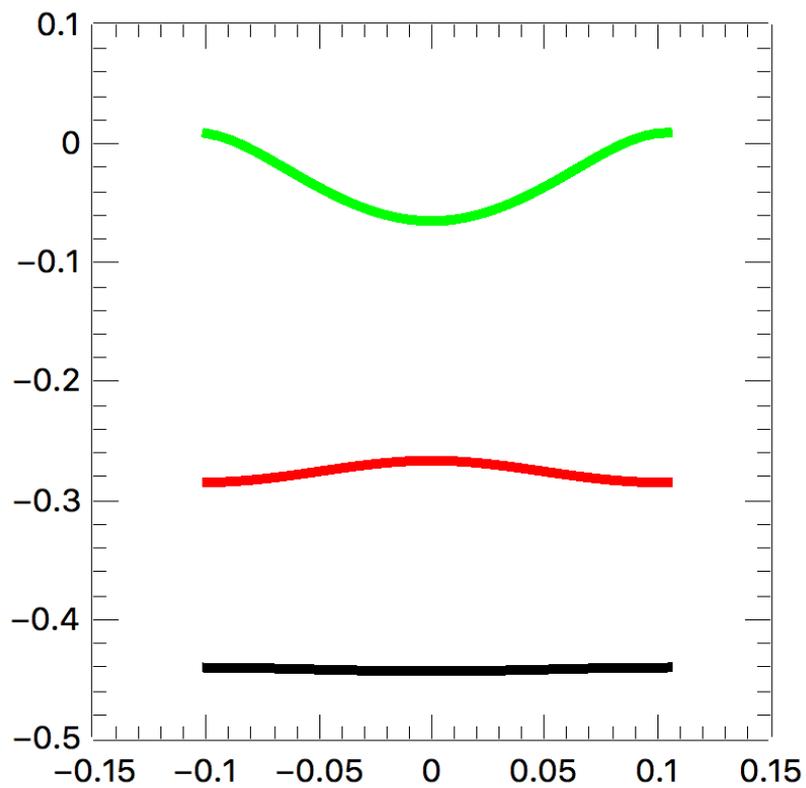
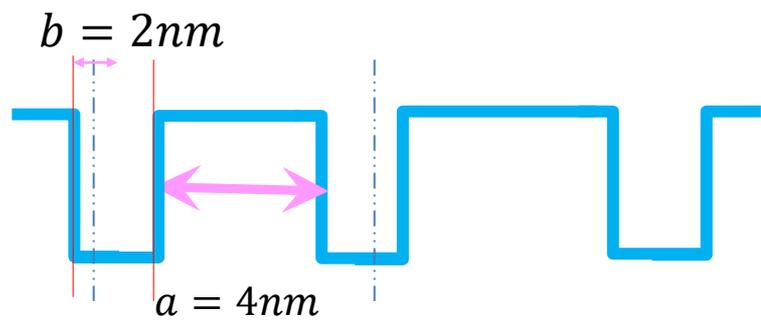
$$k_i = \frac{\pi}{Na} i \quad (i = -N : N)$$

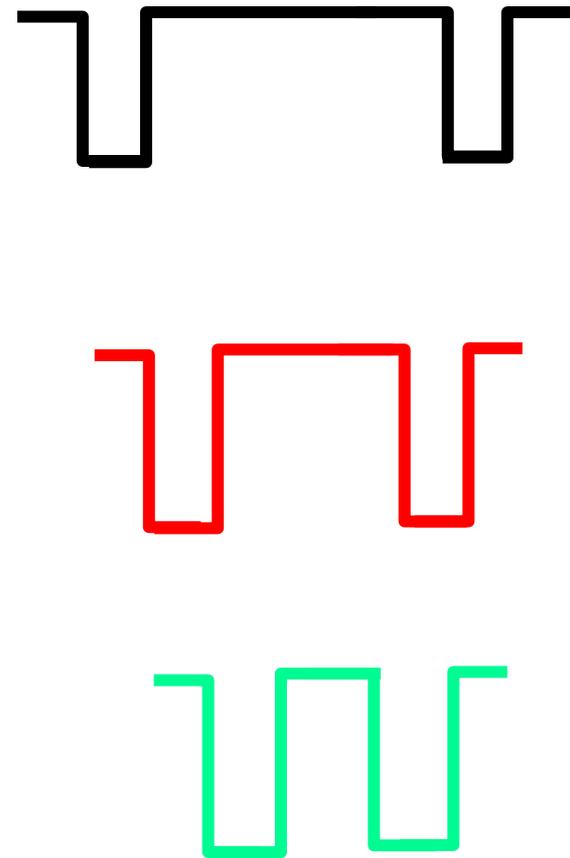
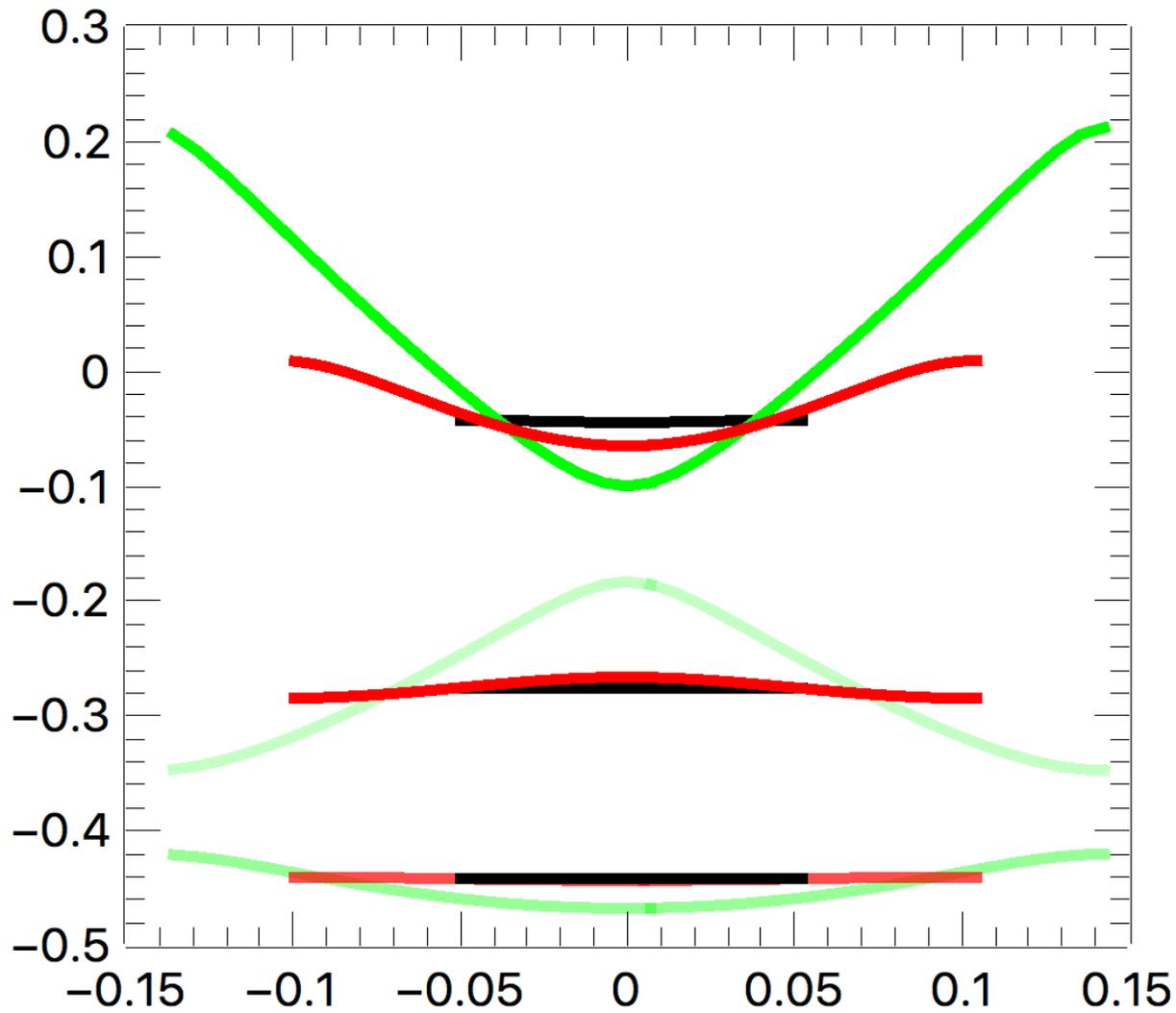
$$k_i = \frac{\pi}{10a} i \quad k_0 = 0$$

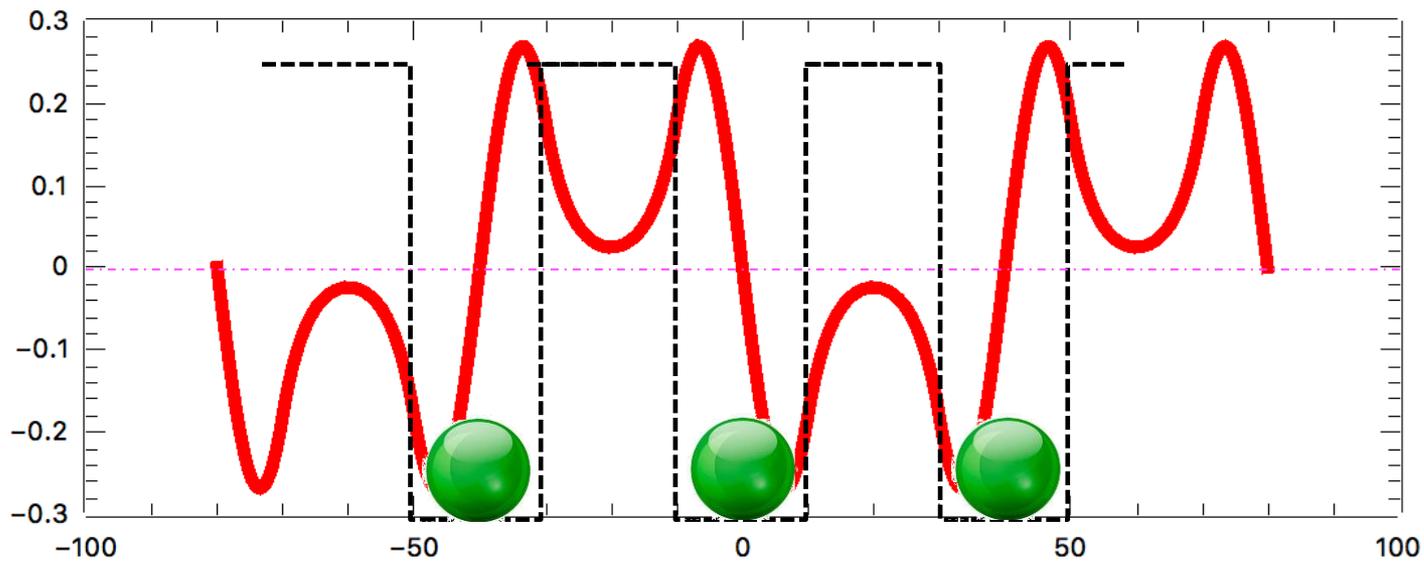
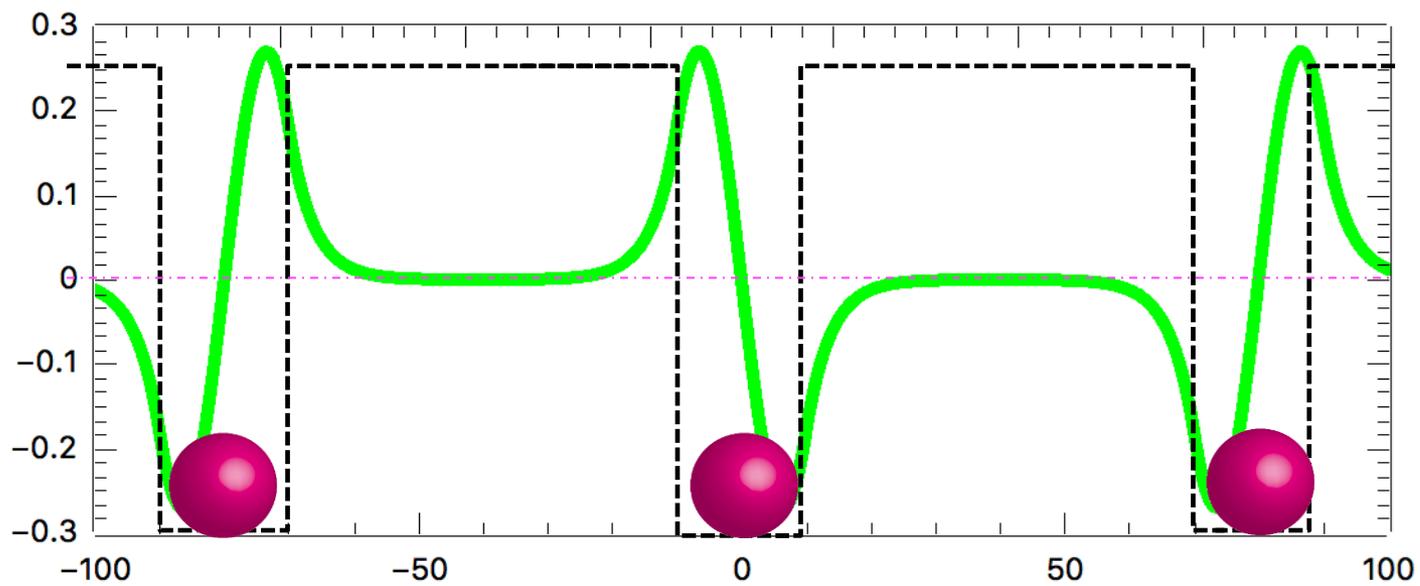
$$k_{1,-1} = \pm \frac{1}{10} \frac{\pi}{a} \quad k_{10,-10} = \pm \frac{\pi}{a}$$

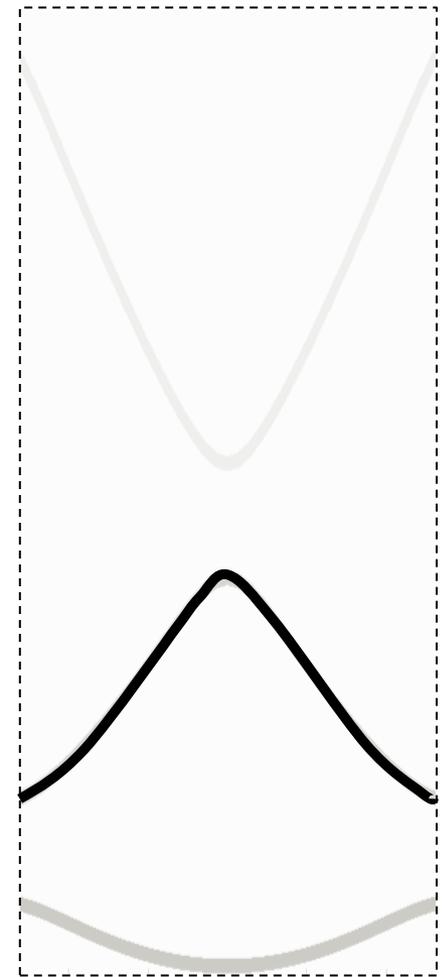
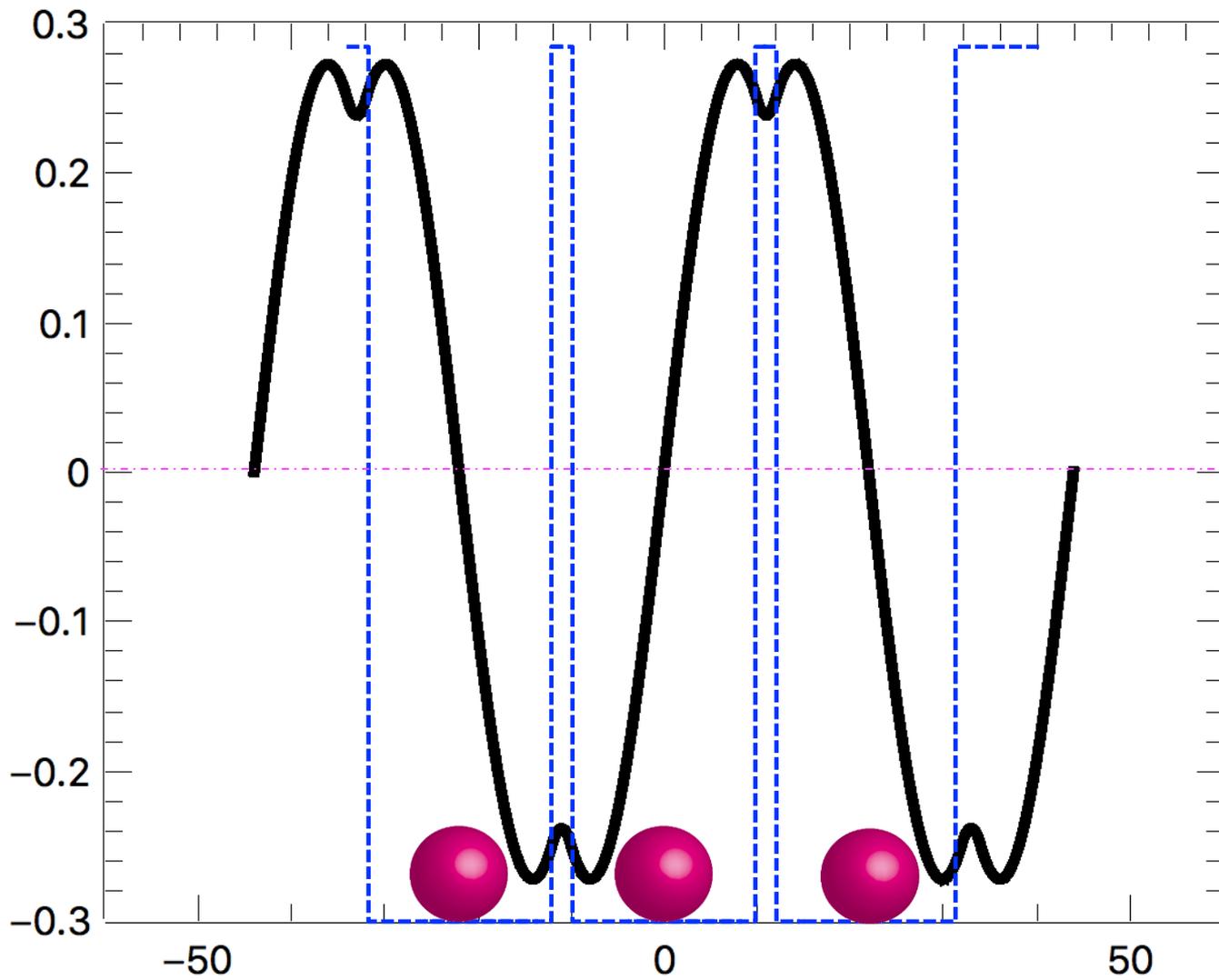
$$E = \frac{p^2}{2m} = \frac{\hbar^2}{2m} k^2$$



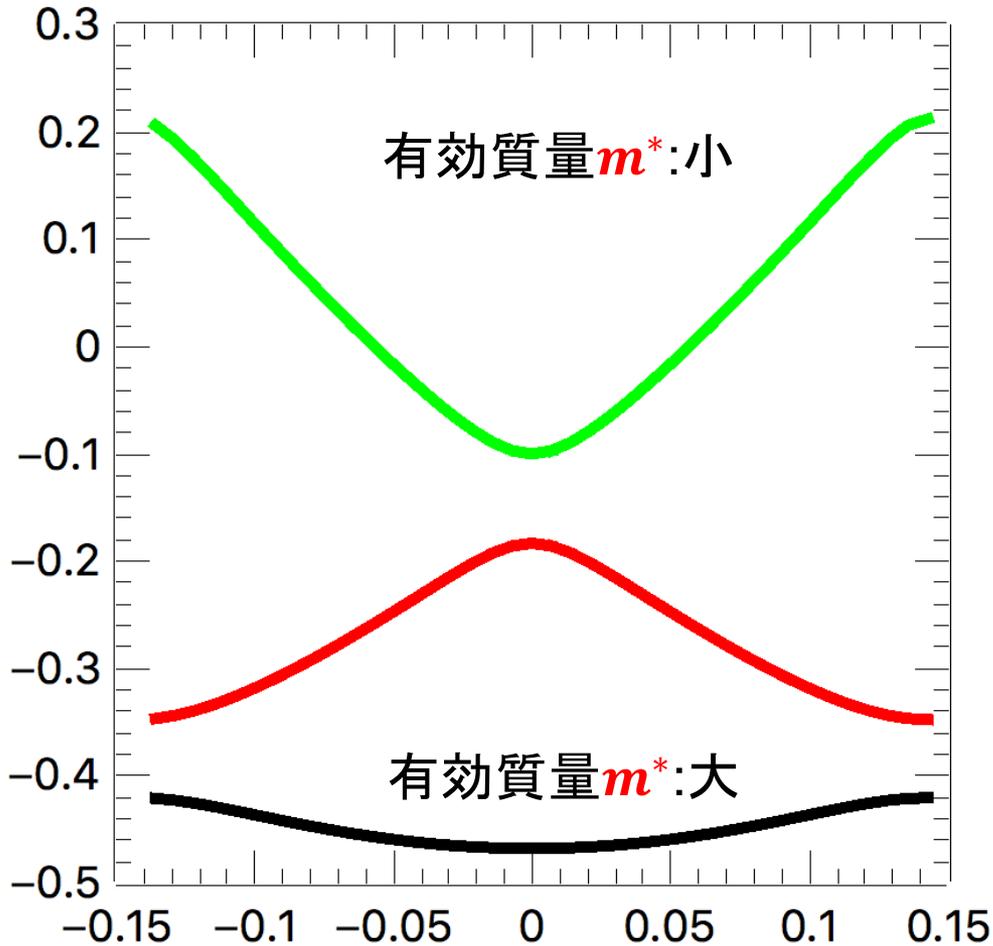








有効質量 m^* が小さくなればなるほど、自由電子に似ていく



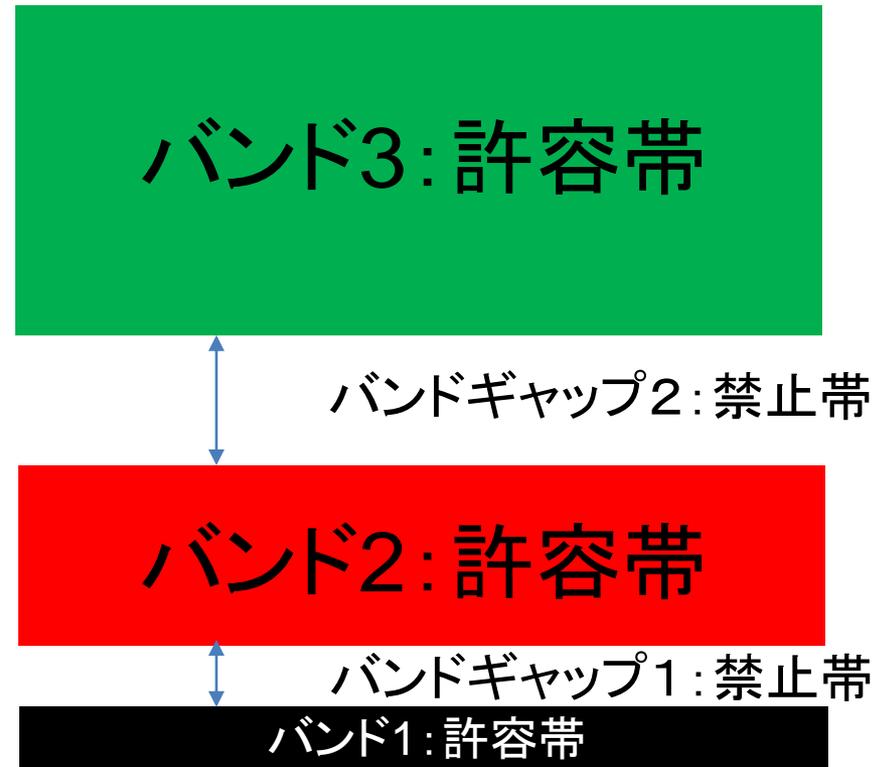
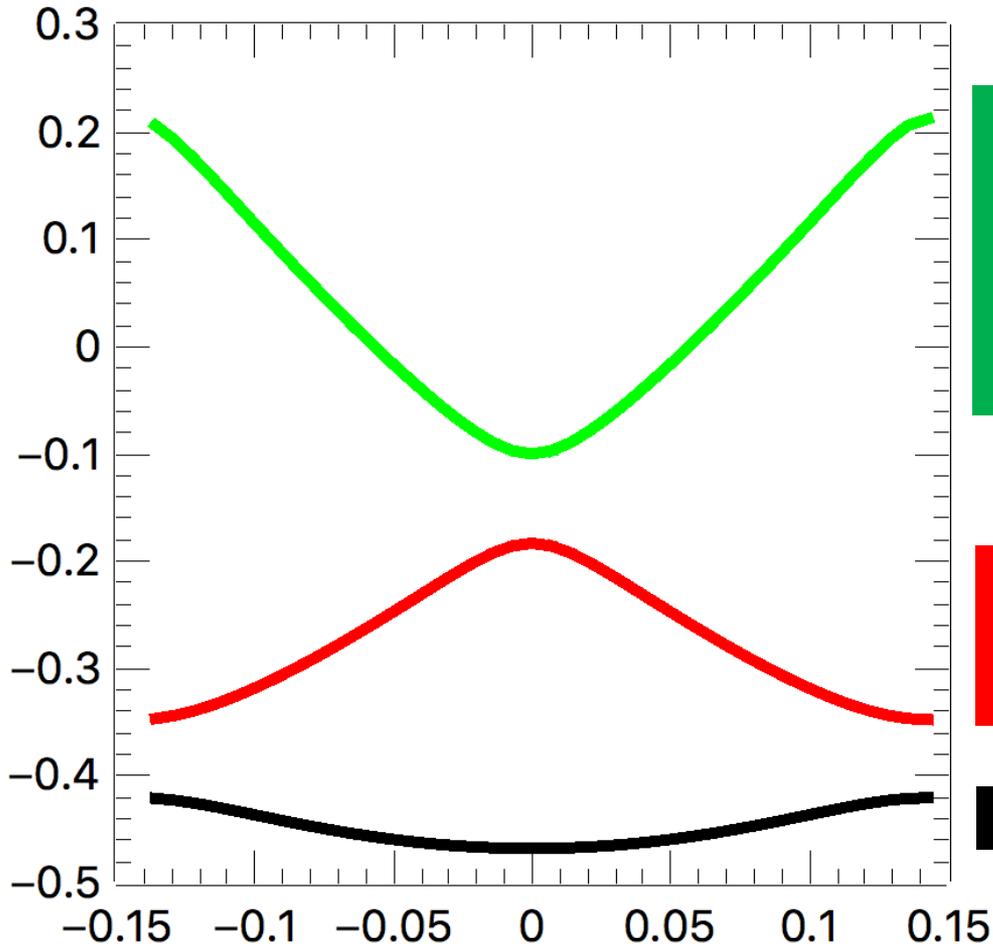
$$E = \frac{\hbar^2}{2m^*} k^2$$

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

$$m^* = \hbar^2 \left(\frac{\partial^2 E}{\partial k^2} \right)^{-1}$$

バンドとバンドギャップ

有効質量 m^* が大きいとバンド幅は大きくなる



有効質量 m^* が大きいとバンド幅が小さくなり、バンドは平らになる