Particle in a box (infinite well)

Note

-2011

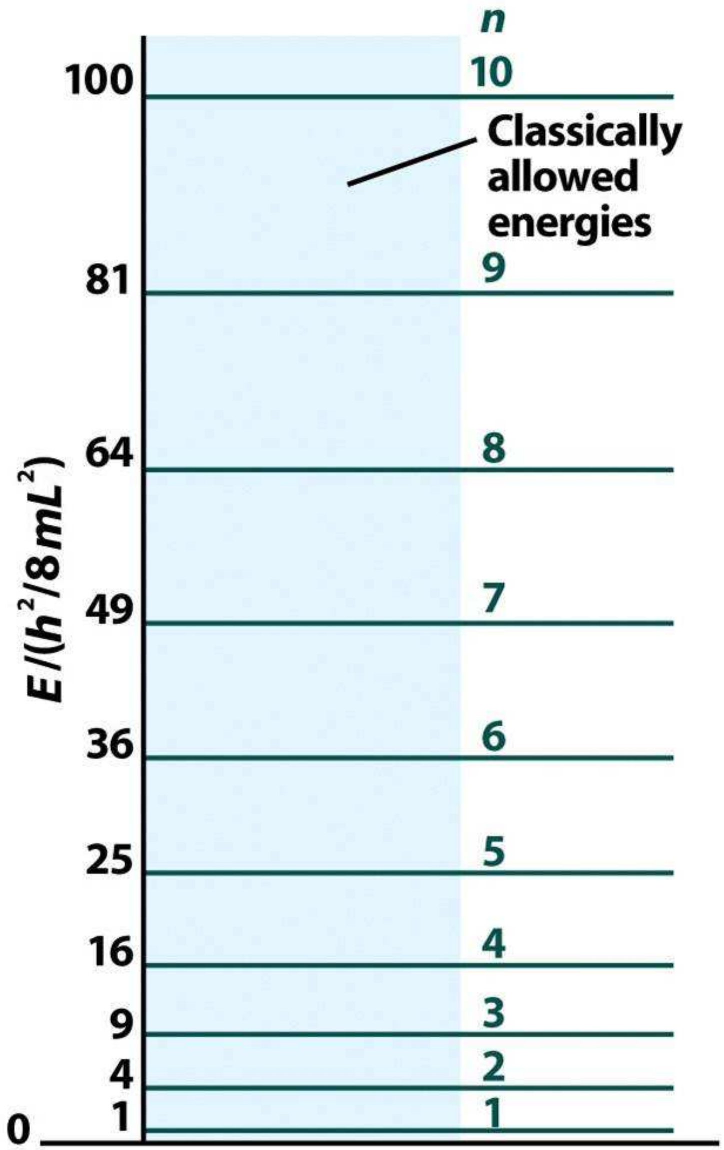

Figure 9-2
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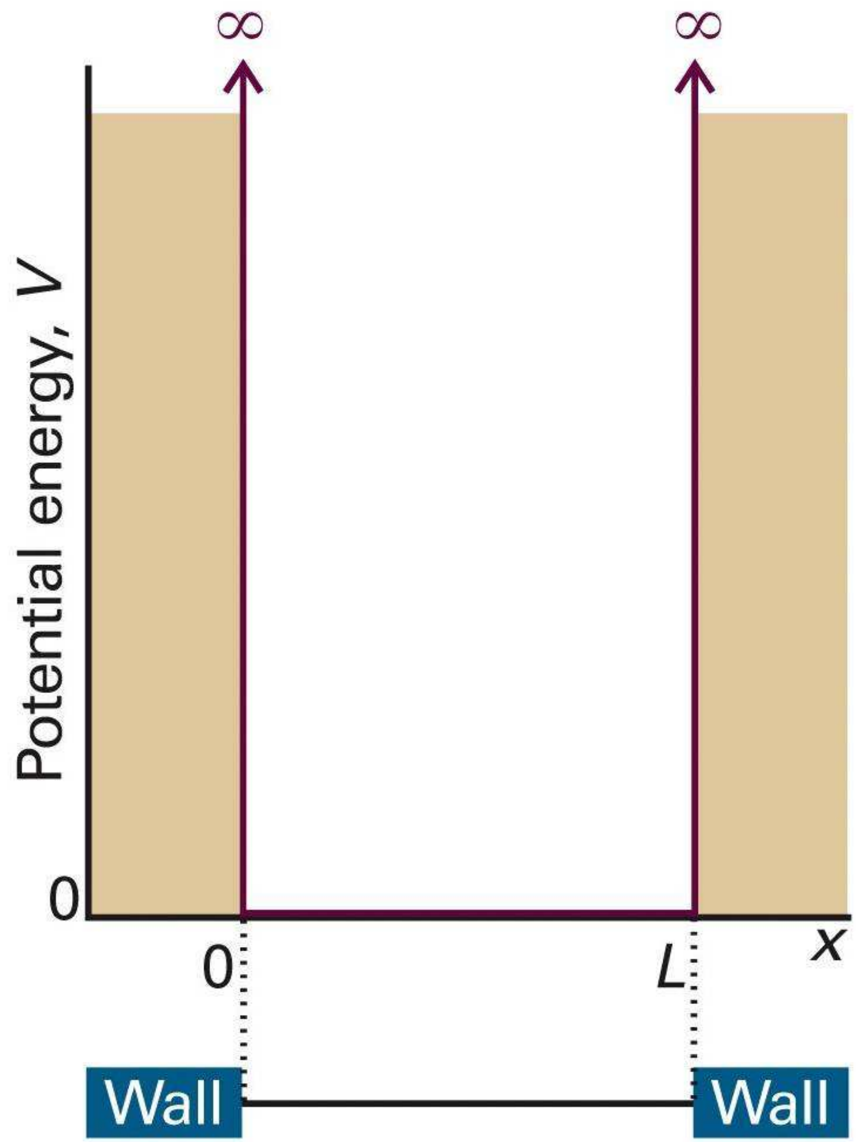


Figure 9-1
Atkins Physical Chemistry, Eighth Edition

Given $u_n(x) = A \sin(k x) + B \cos(k x)$, the boundary condition, $u(0) = 0$, implies what?

A) $A = 0$

B) $B = 0$

C) $k = 0$

D) $k = n\pi$, $n = 1, 2, 3 \ldots$

E) None of these

Given $u_n(x) = A \sin(k x)$
the boundary condition, $u(a) = 0$,
implies what?

A) $A = 0$

B) $B = 0$

C) $k = 0$

D) $k = n \pi$, $n = 1, 2, 3 \ldots$

E) None of these

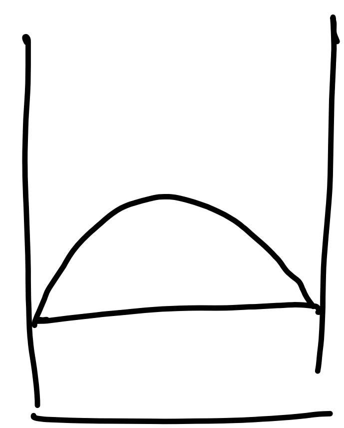
$$\int f^* \hat{O}_p \, g \, d\tau = \int \underline{(\hat{O}_p f)}^* g \, d\tau$$

$$\int \psi^* \hat{O}_p \, \psi \, d\tau \qquad \qquad \int f^* g \, d\tau = 0$$

$$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad n = 1, 2, 3, \ldots$$

$$\langle x \rangle = \int_0 \psi_1^* \, x \, \psi_1 \, dx = a/2$$

$$\text{Prob} = |\psi|^2 = \psi^2$$



$$\Delta x \, \Delta p_x \geq \hbar/2$$

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2}$$

$$\langle x^2 \rangle = ?$$

$$\langle x \rangle = \frac{a}{2}$$

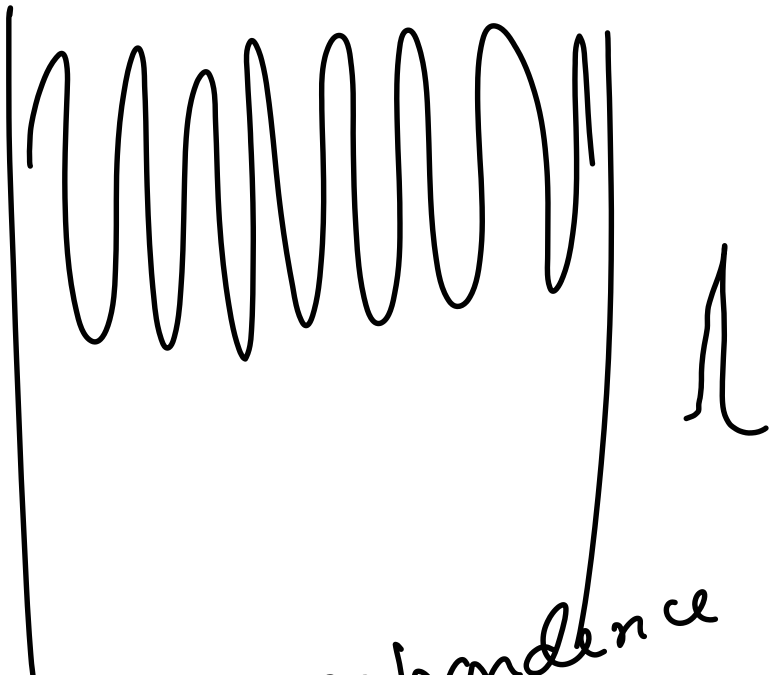
$$\langle p_x \rangle = \int \psi_1^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi_1 \, dx$$

$$= 0$$

$$\langle p_x^2 \rangle = \langle 2mE \rangle$$

$$= 2m \boxed{\langle E \rangle}$$

n large



Bohr correspondence principle

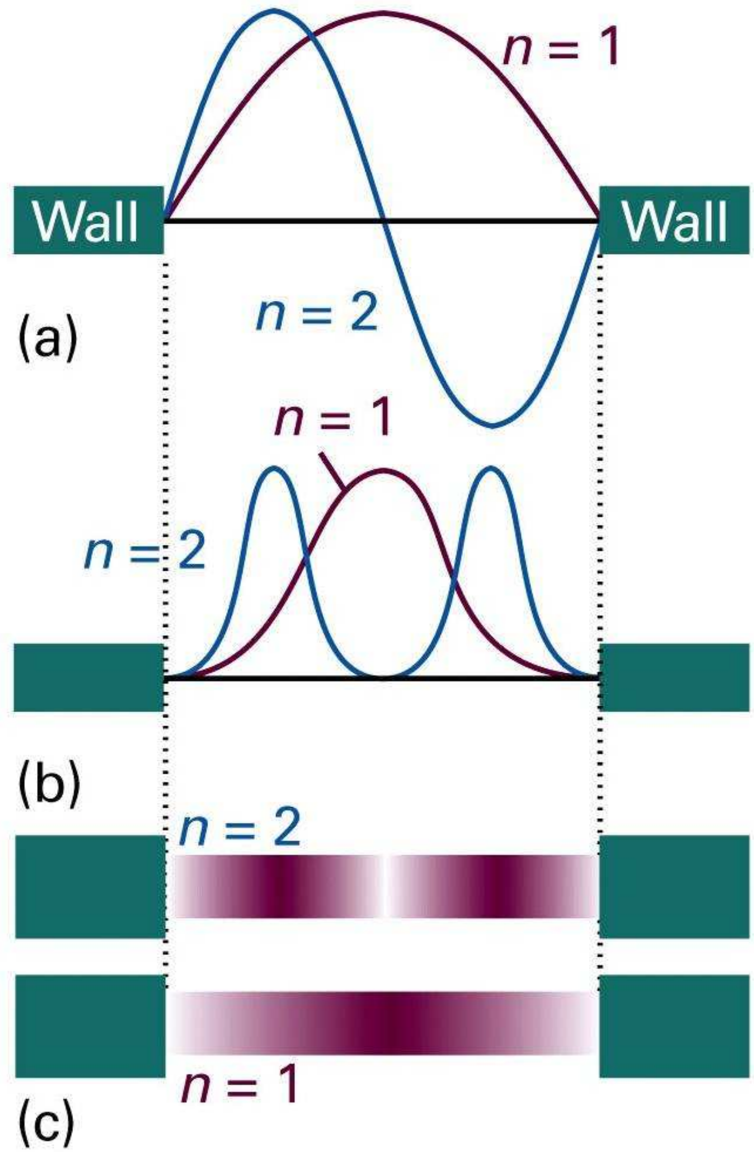


Figure 9-4
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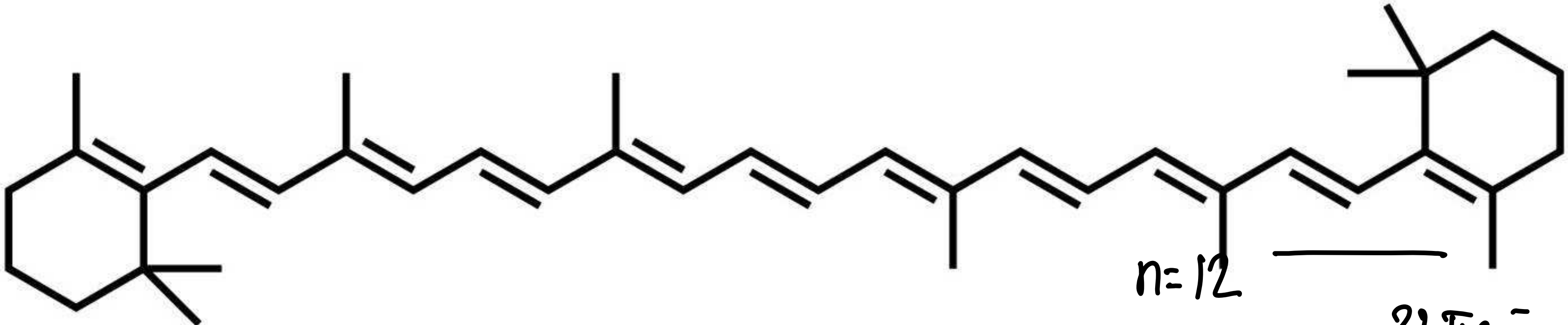
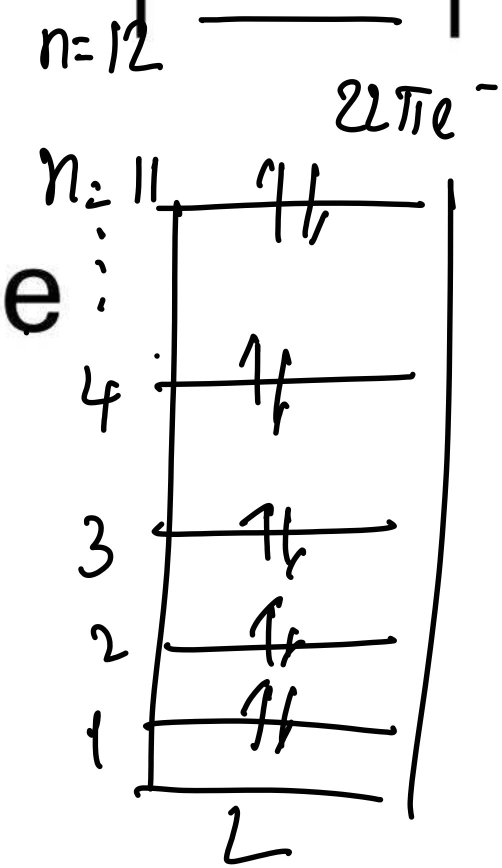
Optical behavior of carotene



1 β-carstene



Marginal 9-1
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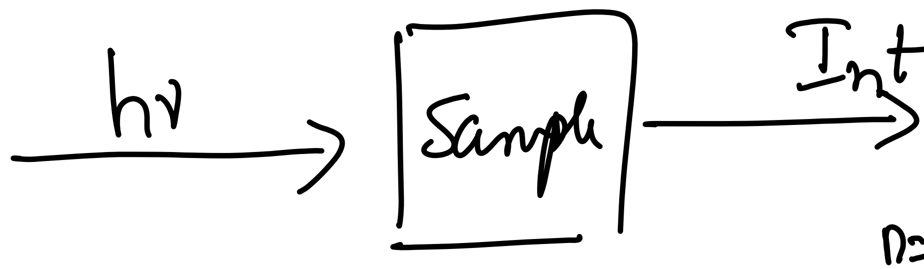
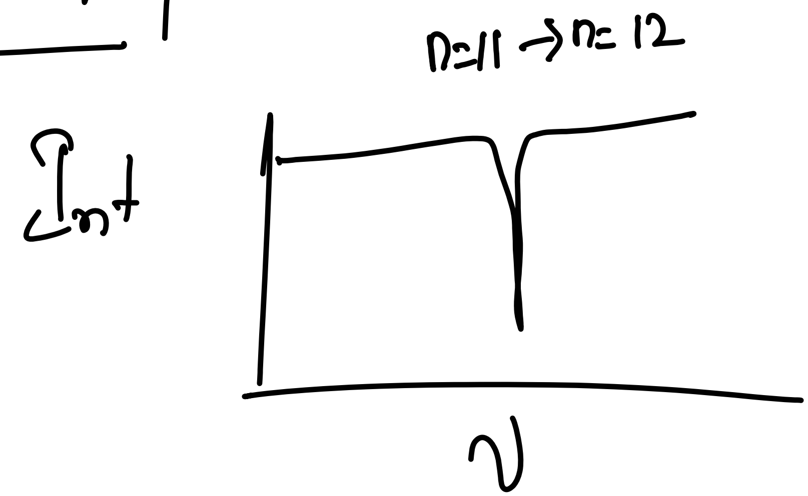
$$-\frac{\hbar^2}{2m_e}\frac{d^2\psi}{dx^2} = E\psi$$


hν
Sample
Int


n=11 → n=12
Int
ν

"Porphyrins"

Hemoglobin

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

$$\boxed{\psi(x,y) = f(x)\,g(y)}$$

One differential equation in x, & another in y

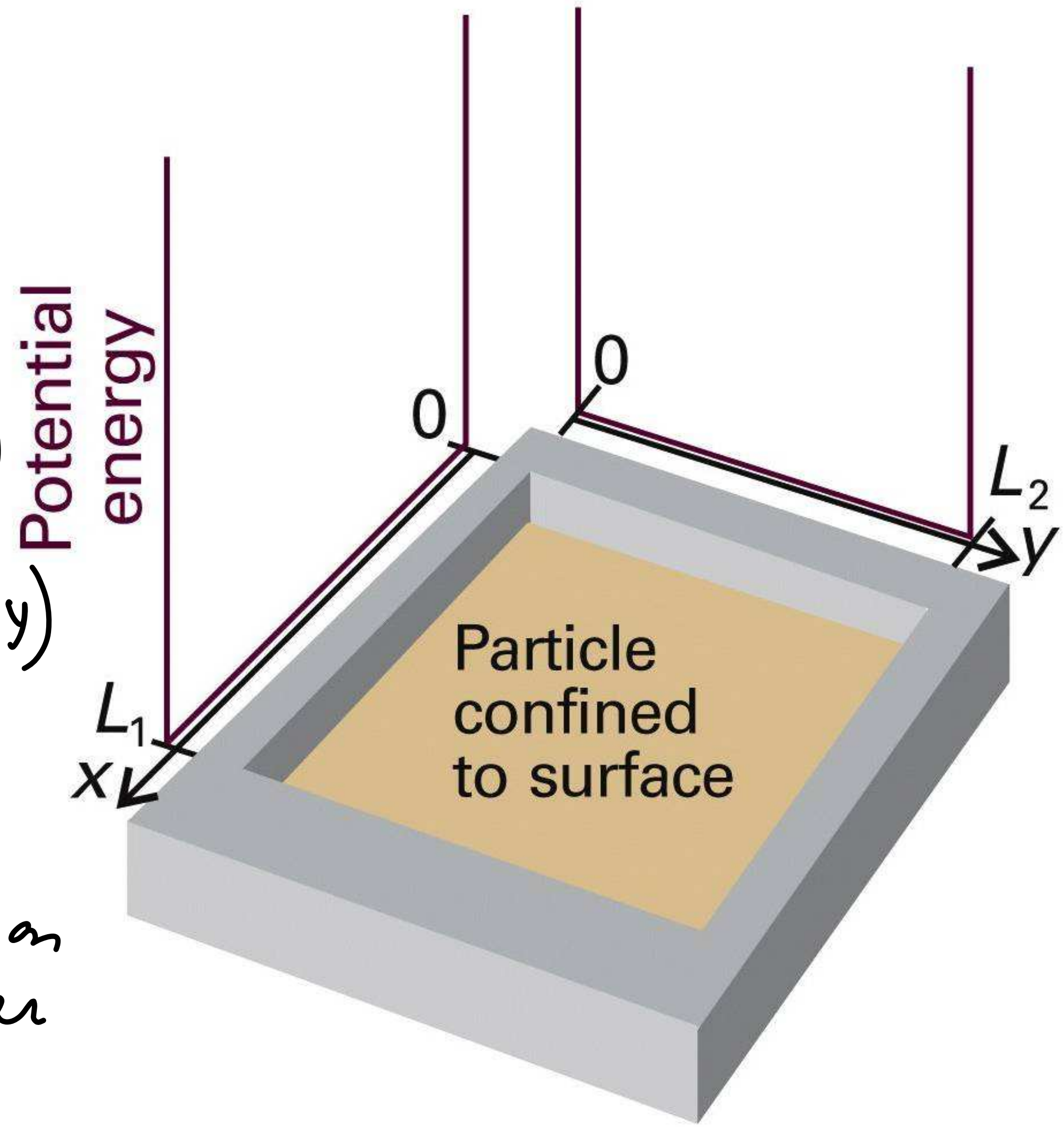


Figure 9-6
Atkins Physical Chemistry, Eighth Edition

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2}\right) f(x)\, g(y) = E f(x)\, g(x)$$

$$\frac{1}{g(y)f(x)} \times \left[\underbrace{-\frac{\hbar^2}{2m}\, g(y)\, \frac{d^2 f}{dx^2}}_{x \text{ dependent}} - \underbrace{\frac{\hbar^2}{2m}\, f(x)\, \frac{d^2 g}{dy^2}}_{y\text{-dependent}} \right] = E f(x)\, g(y)$$

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2 + \hat{\mathcal{H}}_3 + \dots$$

$$\hat{H}_1 \psi_1 = E_1 \psi_1$$

$$\hat{H}_2 \psi_2 = E_2 \psi_2$$

$$\vdots$$

$$\psi = \psi_1 \psi_2 \cdots \psi_n$$

$$E = E_1 + E_2 + \cdots E_n$$

$$E = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2\right)$$

$n_x = 1, 2, 3, \ldots$

$n_y = 1, 2, 3, \ldots$

degeneracy

$n_x = 1$, $n_y = 2$

$n_x = 2$, $n_y = 1$ $\rightarrow$ $A \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right)$

$A \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right)$

—— $1, 1$

n_x n_y