Particles and Waves (10 points)

Part A. Quantum particle in a box (1.4 points)

A.1 (0.4 points)

The width of the potential well (L) should be equal to the half of the wavelength of the de Broglie standing wave $\lambda_{\mathrm{dB}} = h/p$, here h is the Planck's constant and p is the momentum of the particle. Thus $p = h/\lambda_{\mathrm{dB}} = h/(2L)$, and the minimal possible energy of the particle is

$$E_{\min} = \frac{p^2}{2m} = \frac{h^2}{8mL^2}.$$

A.1 (0.4 pt)

$$E_{\min} = \frac{h^2}{8mL^2}.$$

A.2 (0.6 points)

The potential well should fit an integer number of the de Broglie half-wavelengths: $L = \frac{1}{2}\lambda_{\mathrm{dB}}^{(n)} \cdot n$, $n = 1, 2, \ldots$. Therefore, particle's momentum, corresponding to the de Broglie wavelength $\lambda_{\mathrm{dB}}^{(n)}$ is

$$p_n = \frac{h}{\lambda_{\mathrm{dB}}^{(n)}} = \frac{hn}{2L},$$

and the corresponding energy is

$$E_n = \frac{p_n^2}{2m} = \frac{h^2 n^2}{8mL^2}, \qquad n = 1, 2, 3, \ldots. \tag{1}$$

A.2 (0.6 pt)

$$E_n = \frac{h^2 n^2}{8mL^2} = E_{\min} n^2.$$

A.3 (0.4 points)

The energy of the emitted photon, $E = hc/\lambda$ (here c is the speed of light and λ is the photon's wavelength) should be equal to the energy difference $\Delta E = E_2 - E_1$, therefore

$$\lambda_{21} = \frac{hc}{E_2 - E_1} = \frac{8mcL^2}{3h}.$$

A.3 (0.4 pt)

$\lambda_{21} = \frac{8mcL^2}{3h}$.

Part B. Optical properties of molecules (2.1 points)

B.1 (0.8 points)

Taking into account the Pauli exclusion principle, each energy level E_n is occupied by two electrons with spins oriented in the opposite directions. As a results, 10 electrons fill the lowest 5 states, and the absorption of the photon of the longest wavelength corresponds to the transition of one electron from the occupied E_5 to the unoccupied E_6 energy state:

$$\frac{hc}{\lambda} = E_6 - E_5,$$

where E_6 and E_5 can be found from Eq. 1, where m is replaced with the electron mass m_e. Hence we obtain:

$$\lambda = \frac{c \cdot 8m_e L^2}{h\,(6^2 - 5^2)} = \frac{10.5^2 \cdot 8}{11}\frac{m_e c l^2}{h} = \frac{882}{11}\frac{m_e c l^2}{h} \approx 647\,\text{nm}.$$

This result correspond precisely to the experimental value the peak position of the Cy5 absorption spectrum.

B.1 (0.8 pt)

Expression: $\lambda = \frac{882}{11}\frac{m_e c l^2}{h}$. Numerical value: $\lambda = 647\,\text{nm}$.

B.2 (0.4 points)

In the similar model for the Cy3 molecule, there are 8 electrons in the box of length $L = 8.5l$, thus photon's absorption corresponds to the $E_4 \longrightarrow E_5$ transition. Taking into account the result of question B1, we obtain

$$\lambda_{\text{Cy3}} = \frac{8.5^2 \cdot 8}{(5^2 - 4^2)}\frac{m_e c l^2}{h} \approx 518\,\text{nm},$$

i. e. the absorption spectrum of the Cy3 molecule is shifted by $\Delta\lambda \approx 129\,\text{nm}$ to the blue comparing to that of the Cy5 molecule. The experimental value is $\lambda_{\text{Cy3}}^{(\text{exp})} = 548\,\text{nm}$, so that our model catches general properties of these dye molecules rather well.

B.2 (0.4 pt)

Absorption spectrum of Cy3 is shifted to the (check): ☒ **bluer** ☐ redder

spectral region by $\Delta\lambda \approx 129\,\text{nm}$.

B.3 (0.7 points)

Let us assume

$$K = k\varepsilon_0^{\alpha} h^{\beta} \lambda^{\gamma} d^{\delta}. \tag{2}$$

The SI units of the relevant quantities are:

$$[\varepsilon_0] = \frac{\text{A}^2 \cdot \text{s}^4}{\text{kg} \cdot \text{m}^3}, \qquad [h] = \frac{\text{kg} \cdot \text{m}^2}{\text{s}}, \qquad [\lambda] = \text{m}, \qquad [d] = \text{A} \cdot \text{s} \cdot \text{m}, \qquad [K] = \text{s}^{-1}.$$

By plugging these expressions into Eq. 2 we obtain a simple system of linear equations for the unknown powers α, β, γ, and δ:

$$2\alpha + \delta = 0, \qquad -\alpha + \beta = 0, \qquad 4\alpha - \beta + \delta = -1, \qquad -3\alpha + 2\beta + \gamma + \delta = 0.$$

By solving this system we get:

$$\alpha = \beta = -1, \qquad \gamma = -3, \qquad \delta = 2,$$

so that the rate of spontaneous emission is

$$K = \frac{16\pi^3}{3} \frac{d^2}{\varepsilon_0 h \lambda^3}. \tag{3}$$

B.3 (0.7 pt)

$$K = \frac{16\pi^3}{3} \frac{d^2}{\varepsilon_0 h \lambda^3}.$$

B.4 (0.2 points)

By using the result of question B.2 and expressing transition dipole moment as $d = 2.4\,el$, we obtain from Eq. 3:

$$\tau_{\text{Cy5}} = \frac{3}{16\pi^3} \frac{\varepsilon_0 h}{2.4^2 l^2 e^2} \lambda^3 \approx 3.3\,\text{ns}.$$

B.4 (0.2 pt)

Numerical value: $\tau_{\text{Cy5}} \approx 3.3\,\text{ns}$.

Part C. Bose-Einstein condensation (1.5 points)

C.1 (0.4 points)

At temperature T, the average kinetic energy of translational motion is $\frac{3}{2}k_B T$. Equating this result to $p^2/(2m)$, we obtain typical momentum $p = \sqrt{3mk_B T}$ and the de Broglie wavelength

$$\lambda_{dB} = \frac{h}{p} = \frac{h}{\sqrt{3mk_B T}}.$$

C.1 (0.4 pt)

$p = \sqrt{3mk_B T}$. $\lambda_{dB} = \frac{h}{\sqrt{3mk_B T}}$.

C.2 (0.5 points)

The volume per particle V/N is a good estimate for ℓ^3. We obtain $\ell = n^{-1/3}$, with $n = N/V$ and equate $\ell = \lambda_{dB}$ to express $T_c = h^2 n^{2/3}/(3mk_B)$.

C.2 (0.5 pt)

$\ell = n^{-1/3}$. $T_c = \frac{h^2 n^{2/3}}{3mk_B}$.

C.3 (0.6 points)

Using the answer to the previous question, we express $n_c = (3mk_B T_c)^{3/2}/h^3$. Equation of state for the ideal gas gives $n_0 = p/(k_B T)$. Numerical estimations yield $n_c \approx 1.59 \cdot 10^{18}\ \mathrm{m}^{-3}$ and $n_0/n_c \approx 1.5 \cdot 10^7$.

C.3 (0.6 pt)

Expression: $n_c = \frac{(3 \cdot 87\, m_{amu} k_B T_c)^{3/2}}{h^3}$. Numerical value: $n_c \approx 1.59 \cdot 10^{18}\ \mathrm{m}^{-3}$.

Expression: $n_0 = p/(k_B T)$. Numerical value: $n_0/n_c \approx 1.5 \cdot 10^7$.

Part D. Three-beam optical lattices (5.0 points)

D.1 (1.4 points)

We sum the three electric fields (z components)

$$E(\vec{r},t) = E_0 \sum_{i=1}^{3} \cos\left(\vec{k}_i\cdot\vec{r} - \omega t\right), \tag{4}$$

and square the result

$$\begin{aligned} E^2(\vec{r},t) &= E_0^2 \sum_{i=1}^{3}\sum_{j=1}^{3} \cos\left(\vec{k}_i\cdot\vec{r} - \omega t\right)\cos\left(\vec{k}_j\cdot\vec{r} - \omega t\right) \\ &= \frac{E_0^2}{2}\sum_{i=1}^{3}\sum_{j=1}^{3}\left\{\cos\left[\left(\vec{k}_i - \vec{k}_j\right)\cdot\vec{r}\right] + \cos\left[\left(\vec{k}_i + \vec{k}_j\right)\cdot\vec{r} - 2\omega t\right]\right\}. \end{aligned} \tag{5}$$

Time averaging gives

$$\langle E^2(\vec{r},t)\rangle = \frac{E_0^2}{2}\sum_{i=1}^{3}\sum_{j=1}^{3}\cos\left[\left(\vec{k}_i - \vec{k}_j\right)\cdot\vec{r}\right], \tag{6}$$

we analyse the 9 terms and simplify to

$$\langle E^2(\vec{r},t)\rangle = E_0^2\left(\frac{3}{2} + \sum_{j=1}^{3}\cos\vec{b}_j\cdot\vec{r}\right). \tag{7}$$

Here $\vec{b}_{1,2,3} = (\vec{k}_2 - \vec{k}_3), (\vec{k}_3 - \vec{k}_1), (\vec{k}_1 - \vec{k}_2)$ or in terms of the Levi-Civita symbol, $\vec{b}_k = \varepsilon_{ijk}(\vec{k}_i - \vec{k}_j)$. Incidentally, they are known as the reciprocal lattice vectors.

D.1 (1.4 pt)

$$V(\vec{r}) = -\alpha E_0^2\left(\frac{3}{2} + \sum_{j=1}^{3}\cos\vec{b}_j\cdot\vec{r}\right).$$

$\vec{b}_1 = \vec{k}_2 - \vec{k}_3,\qquad \vec{b}_2 = \vec{k}_3 - \vec{k}_1,\qquad \vec{b}_3 = \vec{k}_1 - \vec{k}_2.$

D.2 (0.5 points)

D.2 (0.5 pt)

Argument: Observe that rotation by 60° maps the three vectors $\vec{b}_{1,2,3}$ into the relabelled triplet of $-\vec{b}$'s.

D.3 (1.2 points)

We find

$$V(x,y) = -\alpha E_0^2 \left\{ \frac{3}{2} + \cos\left(ky\sqrt{3}\right) + \cos\left(\frac{3kx}{2} + \frac{ky\sqrt{3}}{2}\right) + \cos\left(\frac{3kx}{2} - \frac{ky\sqrt{3}}{2}\right) \right\}, \tag{8}$$

and deduce

$$V_X(x) = -\alpha E_0^2 \left\{ \frac{5}{2} + 2\cos\frac{3kx}{2} \right\}. \tag{9}$$

The potential has a simple cosine form, and the origin in an obvious minimum. Its replica appear at multiples of $\Delta x = 4\pi/(3k)$. In the midpoint between any two minima, e.g. at $x = \Delta x/2 = 2\pi/(3k)$, the function $V_X(x)$ has its maxima.

Concerning the behaviour along the y axis, we have

$$V_Y(y) = -\alpha E_0^2 \left\{ \frac{3}{2} + \cos 2\varphi + 2\cos\varphi \right\}, \qquad \varphi = \sqrt{3}ky/2. \tag{10}$$

Looking for the extrema, we find the equation

$$\sin 2\varphi + \sin\varphi = 0. \tag{11}$$

- $\varphi = 0$ is the 'deep' minimum – the lattice site;
- $\varphi = \pi$ is the 'shallow' minimum (later shown to be a saddle point of $V(x,y)$);
- $\varphi = 2\pi/3$ and $\varphi = 4\pi/3$ are maxima.

D.3 (1.2 pt)

$V_X(x) = -\alpha E_0^2 \left\{ \frac{3}{2} + 2\cos\frac{3kx}{2} \right\}.$

$V_Y(y) = -\alpha E_0^2 \left\{ \frac{3}{2} + \cos 2\varphi + 2\cos\varphi \right\},$ here $\varphi = \sqrt{3}ky/2.$

Minimum (-a) of $V_X(x)$: $x = 0$.
Maximum (-a) of $V_X(x)$: $x = \frac{2\pi}{3k}$.

Minimum (-a) of $V_Y(y)$: $y = 0$ ('deep') and $y = \frac{2\pi}{\sqrt{3}k}$ ('shallow').
Maximum (-a) of $V_Y(y)$: $y = \frac{4\pi}{3\sqrt{3}k}$ and $y = \frac{8\pi}{3\sqrt{3}k}$.

D.4 (0.8 points)

We review the minima found in the previous question and eliminate the saddle point at $(0, 2\pi/3\sqrt{3}k)$. The actual minima of the 2D potential landscape $V(x, y)$ are:

- $(0, 0)$ – at the origin;
- $(4\pi/(3k), 0)$ – nearest to the origin in the positive direction along the x axis. On the grounds of symmetry we argue that there are six equivalent nearest minima in the directions $0°$, $\pm 60°$, $\pm 120°$, and $180°$ with respect to the x axis.

Distance between nearest minima (the lattice constant) $a = 4\pi/(3k)$. Given that the laser wavelength is $\lambda_{\text{las}} = 2\pi/k$, we have $a = \Delta x = 2\lambda_{\text{las}}/3$.

D.4 (0.8 pt)

Ratio of the lattice constant to the laser wavelength: $a/\lambda_{\text{las}} = \frac{2}{3}$

Positions of all equivalent minima nearest to the origin: **in the directions 0°, ±60°, ±120°, and 180° with respect to the *x* axis**.

D.5 (1.1 points)

The atom's core electrons (all but the one promoted to to a state with a high principal quantum number n) shield the electric field of the nucleus so that the effective potential for the outer electron resembles that of a hydrogen atom. The attractive force acting on that electron, $F = e^2/(4\pi\varepsilon_0 r^2)$, gives rise to its centripetal acceleration $a = v^2/r$. Equating $F = m_e a$ and using the expression for the angular momentum $m_e v r = n\hbar$ to eliminate the velocity, we find the quantum number n corresponding to the orbit with the radius $r = \lambda_{\text{las}}$:

$$n = \frac{e}{\hbar}\sqrt{\frac{m_e \lambda}{4\pi\varepsilon_0}} \approx 85. \tag{12}$$

D.5 (1.1 pt)

Expression: $n = \frac{e}{\hbar}\sqrt{\frac{m_e \lambda}{4\pi\varepsilon_0}}$. Numerical value: $n \approx 85$.