

I. For Rectangle barrier

1. How is looks like Schrodinger equation for tunnel effect (topic 4.3) for regions I,II, and III ? Derive equations.
2. What does the Schrödinger equation and the continuity conditions looks like for the tunneling effect in the case $E > U_0$? Derive equations.
3. How looks like dependence of $R(E)$ and $T(E)$ on energy for rectangle barrier in **classical physics**? What does it mean the tunnel effect for rectangle barrier?
4. What does the Schrödinger equation and the continuity conditions looks like for the tunneling effect in the case $E < U_0$? Derive equations.
5. What does the **transparency window** mean (in case $E > U_0$) for a rectangular barrier and the conditions for its appearance?
6. Show that as U_0 tends to zero, the transfer coefficient $T(E)$ tend to 1 for both cases $E > U_0$ and $E < U_0$.
7. The electron falling on the barrier. The kinetic energy of particle is 8 eV and height of barrier 10 eV. How large the probability of transmission of electron through barrier. The width of barrier is 0.5 Å.

II. For infinite potential well:

8. Show that the probability current density (or wavefunction) inside of the walls (areas 1 and 3) should be zero? Why?
9. Prove that the eigenfunctions for infinite potential are orthonormal.
10. Calculate the average of the coordinate $\langle x \rangle$, the square of the coordinate $\langle x^2 \rangle$, and the square of the velocity $\langle v^2 \rangle$ for quantum numbers $n=1$ and $n=2$.
11. Why the solution for quantum number $n=0$ must be ignored? Give a physical justification.
12. What is the connection between the phenomenon of interference and the discreteness of the wave function and particle energy?
13. Calculate the probability current density “j” for quantum number $n=1$.

III. For finite potential well:

14. What does the Schrödinger equation and the continuity conditions looks like for **finite** potential well (for $E < U_0$)? Derive equations.
15. Can you show that equation for calculating energy of particle inside of **finite potential well**
$$\tan\left(\frac{a\sqrt{2mE}}{\hbar}\right) = \frac{2\sqrt{E(U_0-E)}}{2E-U_0}$$
 give the correct values for energy for **infinite potential well**
(topic 5.1) $E_n = \frac{(\pi \hbar)^2}{2Ma^2} \cdot n^2$, $n=1, 2, \dots$ in limit $U_0 \rightarrow \infty$?
16. Why zero energy solution ($E=0$) of equation $\tan\left(\frac{a\sqrt{2mE}}{\hbar}\right) = \frac{2\sqrt{E(U_0-E)}}{2E-U_0}$ should be ignored?
17. The wavefunction inside of **finite** potential well should be real or complex? Why?

18. Should the wave function inside the walls of a finite potential well be a complex number or a real number? What is your opinion, why?

IV. For Harmonic oscillator:

19. Why **asymptotical solution** of Schrodinger equation for harmonic oscillator is looks like so $\psi(\xi) = e^{-\frac{\xi^2}{2}}$? Why the option $\psi(\xi) = e^{\frac{\xi^2}{2}}$ should be ignored?

20. Show that for **classical harmonic oscillator** average value of kinetic and potential energies are equal $\langle E_{kin} \rangle = \langle E_{pot} \rangle$.

PS! The classical expression for calculate average value of classical physical quantity is

$$\langle A \rangle = \frac{1}{T} \int_0^T A(t) dt \quad \text{here } T - \text{ averaging time.}$$

21. Calculate the mean value of **x**-coordinate for harmonic oscillator $\int_{-\infty}^{+\infty} \psi_n^* \hat{x} \psi_n dx$. Tabular integral from lectures can be used. Results compare with the corresponding results for classical harmonic oscillator.

22. Calculate the mean value of momentum **p_x** for harmonic oscillator $\int_{-\infty}^{+\infty} \psi_n^* \hat{p}_x \psi_n dx$. Tabular integrals from lectures can be used. Results compare with the corresponding results for classical harmonic oscillator.

23. Calculate the mean value of square **x²**-coordinate for harmonic oscillator $\int_{-\infty}^{+\infty} \psi_n^* \hat{x}^2 \psi_n dx$. Tabular integrals from lectures can be used. Results compare with the corresponding results for classical harmonic oscillator.

24. Calculate the next matrix element for **x**-coordinate for harmonic oscillator $\int_{-\infty}^{+\infty} \psi_1^* \hat{x} \psi_3 dx$. Tabular integrals from lectures can be used.

25. Calculate matrix element for the dipole transition from the ground state to the first excited state for harmonic oscillator $\int_{-\infty}^{+\infty} \psi_0^* \hat{x} \psi_1 dx$. Tabular integrals from lectures can be used.

26. Why the power series $v(\xi) = \sum_{r=0} a_r \xi^r$ (here $a_{r+2} = \frac{2r+1-\lambda}{(r+2)(r+1)} a_r$) for the wave function of a harmonic oscillator should be limited? Why is it necessary to take into account only a limited number of terms of series?

27. Calculate the mean value of the square of the coordinate (the value of the square of the deviation from the equilibrium position) for **ground state** of harmonic oscillator.

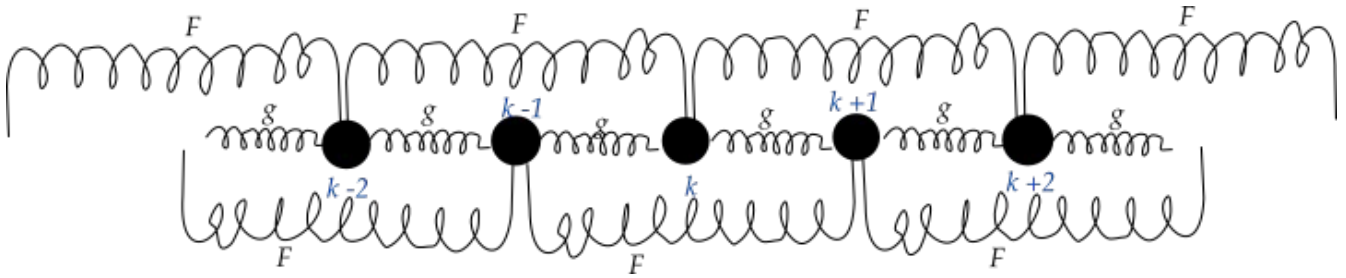
28. How can be calculate the energy of a harmonic oscillator at a non-zero temperature? (Don't forget that thermal motion is fully chaotic and can be described by a random force acting on a oscillating point mass).

NB! Can be used some ideas from calculation of heat capacity for 1d crystal lattice (next topic V).

V. For Heat capacity for 1d chain of atoms:

29. How looks like the expression for potential energy of the 1d chain of atoms if we assume that each atom interacted not only with the first neighbors but with with the second neighbors too. Here **g** and **F**

are force constant for different types of springs. It is enough to calculate the potential energy only for atom with number k



30. Can you proof that expression $u_k(t) = \frac{1}{\sqrt{N}} \cdot \sum_{q=-\pi/a}^{+\pi/a} A_q \cdot e^{i(\omega t + qak)}$ is a solution of the equation of motion

$$\ddot{u}_k = \frac{g}{m} [u_{k+1} - 2 \cdot u_k + u_{k-1}] \quad ?$$

31. Can you show that function $\omega(q) = \omega_0 \cdot \left| \sin\left(\frac{qa}{2}\right) \right|$ for $\omega(q)$ and $\omega\left(q + \frac{2\pi}{a}\right)$ describe the same harmonic wave $u_{k,q}(t) = A_q \cdot e^{i(\omega(q)t + qak)}$ (by other words show that $u_{k,q}(t) = u_{k, q + \frac{2\pi}{a}}(t)$) ?.

32. Potential energy of interacting nearby atoms in a 1d crystal is looks like so: $V = \frac{1}{2} g \sum_n (u_n - u_{n-1})^2$

Get the expression for force acting on atom with number $k+1$. Here u_n -displacement of atom with number n from its equilibrium position.

33. Give the physical meaning for density of vibration function (DOS) $g(\omega)$ (take the formula from the lecture). Calculate the value of next integral: $\int_0^{\omega_0} g(\omega) d\omega = ?$ Here $\omega_0 = \sqrt{\frac{4g}{m}}$. What is the physical meaning of the calculation result? <https://openstax.org/books/calculus-volume-1/pages/a-table-of-integrals> (integral 15 can help you).

34. Give a classical estimate of the heat capacity of a three-dimensional crystal (as was done for a one-dimensional lattice). Remember that atoms in a 3D crystal vibrate in all three dimensions it means that number of degrees of freedom must be increased (in compare with 1d lattice).

35. How the average value of the principal quantum number **for harmonic oscillator** depends on temperature. Please explain from a physical point of view the behavior of this function in the region of zero temperatures.

36. Why does the heat capacity tend to zero at low temperatures? Physical explanation.

37. Can you show that (for 1d crystal) **phase** and **group** velocities of harmonic waves are equal in limit of very long waves ($\lambda \rightarrow \infty$).

38. Calculate the quasi-classical amplitude of zero-point vibrations of a sodium atom in a NaCl crystal at a frequency of 2 THz.

39. How does classical harmonic motion emerge from the quantum mechanical description of a harmonic oscillator? (Outline the basic ideas.)