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T1. Stability in Paul trap

An ion trap is a device that uses a spatially inhomogeneous electric field to store, separate, and study the quantum properties of charged particles.

Part A. Theoretical background

Here is the simplest equation for the electric potential in which a particle might be held

$$\Phi = \frac{U}{2r_0^2}\left(\alpha x^2 + \beta y^2 + \gamma z^2\right),$$

where U is the voltage in the setup, r_0 is a typical size of the field inhomogeneity, α, β, γ are dimensionless constants.

This potential is created in a vacuum by external electrodes, therefore, it should satisfy the Poisson equation $\Delta\Phi = 0$ (we can substitute $\vec{E} = -\operatorname{grad}\Phi$ in Maxwell's equation $\operatorname{div}\vec{E} = \rho/\varepsilon_0$ for vacuum, i.e. for $\rho = 0$), where Δ is the Laplacian. The Laplacian of Φ is defined by:

$$\Delta\Phi = \frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} + \frac{\partial^2\Phi}{\partial z^2}.$$

A1	From the Poisson equation, obtain an expression which establishes a relationship between the coefficients α, β and γ.

The above expression shows that it's impossible to create such a static potential where the particle is stable in all three directions. This problem is solved by adding an oscillating with radio frequency electric field to the static field:

$$\Phi = \frac{U}{2r_0^2}\left(\alpha x^2 + \beta y^2 + \gamma z^2\right) + \frac{V}{2r_0^2}\cos(\omega_{\text{rf}} t)\left(\tilde{\alpha} x^2 + \tilde{\beta} y^2 + \tilde{\gamma} z^2\right),$$

where V is the amplitude of the AC voltage in the setup, $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$ are dimensionless constants.

It is important, that ω_{fr} the frequency of the radio band, since this frequency range corresponds to wavelengths much larger than the characteristic size of the ion trap ($r_0 \approx 1$ mm) and therefore, wave effects can be neglected (in particular, this generally allows us to introduce a potential for an electric field).

A2	Calculate the maximum frequency $\omega_{\text{fr,max}}$ for which the wavelength λ is $n = 100$ times greater than r_0.

So, if $\omega_{\text{fr}} < \omega_{\text{fr,max}}$ then the coefficients $\tilde{\alpha}$, $\tilde{\beta}$ and $\tilde{\gamma}$ satisfy the same equation, as the coefficients α, β and γ. The motion along each axis is independent and can be described by the Mathieu equation:

$$\frac{d^2x}{d\xi^2} + (a_x - 2q_x\cos 2\xi)x = 0, \tag{1}$$

where ξ is a dimensionless variable which depends on the time, a_x and q_x are dimensionless constants.

A3	Using the equation $\vec{E} = -\operatorname{grad}\Phi$, find the x-component of the electric field $\vec{E}$, in which the motion of the ion occurs.

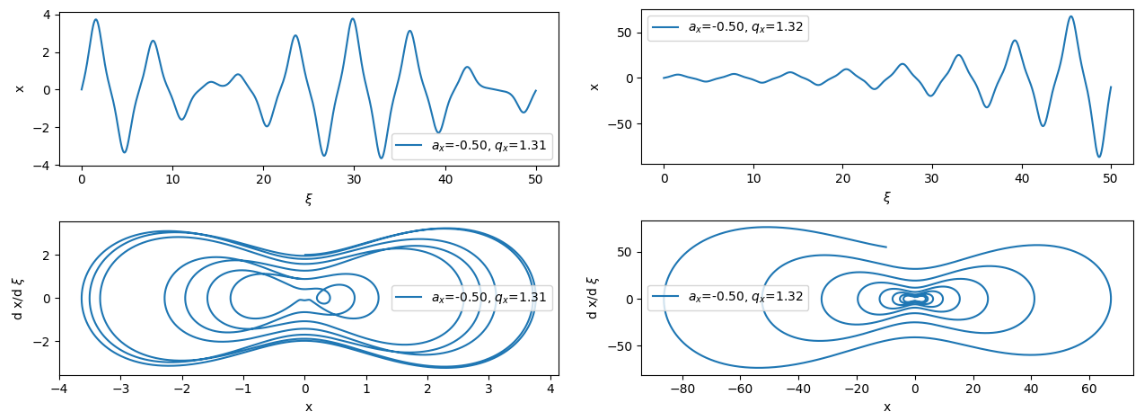
Consider that the only force acting on the ion is the force of interaction with an electric field $\vec{E}$.

A4	Write an expression for ξ, a_x and q_x using time t and parameters of the system: voltage U, radio frequency ω_{rf}, the amplitude V of the AC voltage, mass m of the ion, it's charge Ze, typical size of the setup r_0 and coefficients α and $\tilde{\alpha}$.

Solutions of the Mathieu equation for different constants a_x and q_x can be stable and unstable. You can study this issue yourself with the program Mathieu.py by setting a_x and q_x in the code (lines 7 and 8). This program implements the simplest numerical integration (Euler's method). During the program cycle, the variable ξ runs through the value from 0 to ξ_{max} in increments of $\Delta\xi$. According to the known values of x, ξ the value of $d^2x/d\xi^2$ is calculated with respect to the equation (1) at each iteration of the loop. Next, the approximation formulas

$$\Delta\left(\frac{dx}{d\xi}\right) = \frac{d^2x}{d\xi^2}\Delta\xi, \quad \Delta x = \frac{dx}{d\xi}\Delta\xi,$$

are used to calculate the values x and $dx/d\xi$ for the next step of the program.



An example of a stable (left) and unstable (right) solution of the Mathieu equation for different parameters a_x, q_x. The plot on the left: $a_x = 0.5, q_x = 1.31$, the plot on the right $a_x = 0.5, q_x = 1.32$. As can be seen, the nature of the dependence $x(\xi)$ changes qualitatively even with a small transition beyond the region of stability.

To study the stability for a large number of pairs of parameters a_x and q_x, we will develop the following criterion for the automatic analysis. We will consider the solution stable if the maximum value of $x_{\text{max},1/2}$ reached in half of the simulation time differs less than 10% from the maximum value of x_{max} during the entire simulation time.

This algorithm is implemented in the program Mathieu-stab.py. In 31-37 lines you can define the ranges for a_x and q_x to study the stability. If you don't have programming skills in Python it is highly recommended to run this program ones with high resolution for both axes (it may possibly take several minutes) and manually write down some coordinates of the the stability region boundaries. Our criteria of stability are not perfect, so the graph may have some artifacts. You can manually precisely examine any region of parameters with the Matheiu.py.

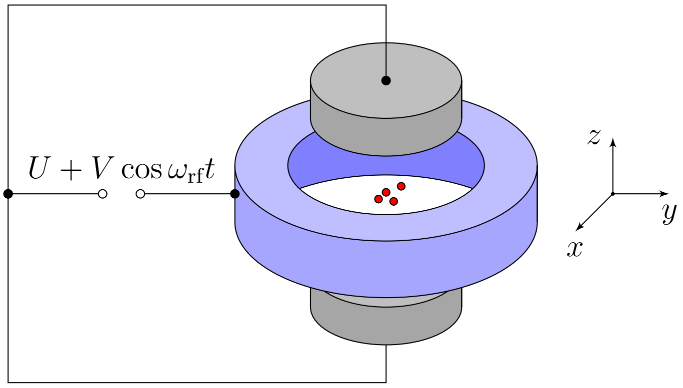
Note that replacing $q_x \to -q_x$ does not affect the stability of the solution. This can be shown as follows: since $-q_x\cos(2\xi) = q_x\cos(-\pi + 2\xi)$, the simultaneous replacement of $q_x \to -q_x$, $\xi \to \xi - \pi/2$ does not change the form of the equation. It only changes the initial conditions, so it does not affect the stability of the solution.

A5	Qualitatively plot the subset of a_x and q_x parameter values that result in the stable motion along the x-axis. Consider the range $a_x \in [-3;\ 7]$ and $q_x \in [0;\ 5]$.

Part B. Common implementations

The first common implementation of an ion trap is a cylindrical symmetric 3D RF trap. This trap has the geometry shown in the figure and the following selection of constants corresponds to this geometry.

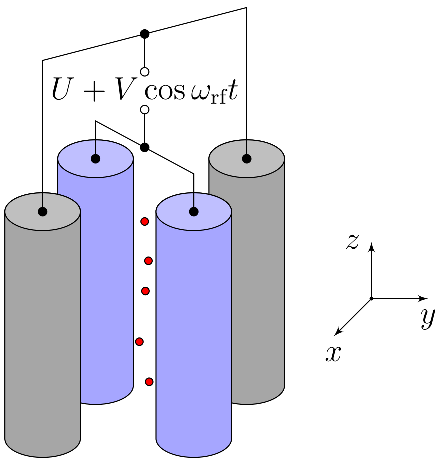
$\alpha = 1$	$\beta = 1$	$\gamma = -2$
$\tilde{\alpha} = 1$	$\tilde{\beta} = 1$	$\tilde{\gamma} = -2$



B1	Qualitatively plot the subset of U and V parameter values that result in stable ion motion in the 3D RF trap. Calculate the values of the characteristic points of the stability region for $\omega_{\rm rf} = 3 \cdot 10^7\ \text{s}^{-1}$, $r_0 = 1$ mm and the ions of rubidium $^{87}\text{Rb}^+$. Consider that the generator in the lab allows you to get this range of voltage values $\lvert U\rvert \in [0;\ 200]$ V and $\lvert V\rvert \in [0;\ 400]$ V.

The second common implementation of an ion trap is the linear RF trap, which is used for mass spectrometry. This trap has the geometry shown in the figure and the following set of constants corresponding to it:

$\alpha = 1$	$\beta = -1$	$\gamma = 0$
$\tilde{\alpha} = 1$	$\tilde{\beta} = -1$	$\tilde{\gamma} = 0$



B2	Qualitatively plot the subset of U and V parameter values that result in different stability for $^{87}\text{Rb}^+$ and $^{86}\text{Rb}^+$ ions. Consider the case where the $^{87}\text{Rb}^+$ ions fly through the trap and the $^{86}\text{Rb}^+$ ions are ejected from the trap. Calculate the values of the characteristic points of the stability region for $\omega_{\rm rf} = 3 \cdot 10^7\ \text{s}^{-1}$ and $r_0 = 1$ mm.

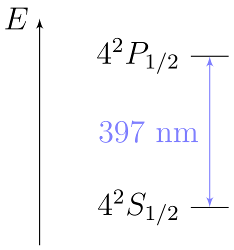
T2. "Photo" of ion

Ions inside ion traps interact with the light shining on them, allowing us to obtain their "photographs". This can be achieved using fluorescence: a process of spontaneous transition between two states of a system, followed by the emission of light.

Considering any system from the perspective of quantum mechanics leads to the fact that this system has discrete energy levels and their corresponding states. In other words, the stationary state of a quantum system (as opposed to a classical one) cannot be any state whatever you want. There is a certain discrete set of stationary states for each quantum system.

To describe a huge number of properties of quantum objects, it is sufficient to use a two-level system (TLS), i.e. to consider transitions of the system only between two of its levels.

In particular, let's consider two levels in the $^{41}Ca^+$ ion. To distinguish them, we will call them $4^2S_{1/2}$ and $4^2P_{1/2}$. The energy difference between them corresponds to the energy of a photon with a wavelength of $\lambda = 397$ nm. The energy of a photon is given by the equation $\hbar\omega$, where $\hbar = 1.05 \cdot 10^{-34}$ J $\cdot$ s is the Planck constant, and $\omega = 2\pi c/\lambda$ is the photon frequency. The speed of light is $c = 2.98 \cdot 10^8$ m/s, and the elementary charge is $e = 1.602 \cdot 10^{-19}$ C.



A1	Find the energy difference $\Delta E = E_{4^2P_{1/2}} - E_{4^2S_{1/2}}$ between the states $4^2S_{1/2}$ and $4^2P_{1/2}$ in electron volts.

Every two-level system (TLS) doesn't exist in a pure vacuum but in a "bath" of electromagnetic radiation, with which it can exchange energy. This leads to the fact that if a TLS is not in the lowest energy state, it can **spontaneously** emit a photon with a certain probability. In our case, if the ion $^{41}Ca^+$ is in the state $4^2P_{1/2}$, then with a probability per unit time $\Gamma = dP/dt$, it will spontaneously relax to the state $4^2S_{1/2}$ while emitting a photon with a wavelength $\lambda = 397$ nm. This phenomenon is called fluorescence.

Similarly, an ion in the state $4^2S_{1/2}$ can be excited by shining light of wavelength of $\lambda = 397$ nm. With some probability, it will absorb a photon and change its state to the $4^2P_{1/2}$.

Let's consider an ion in the 3D RF Paul's ion trap. Its motion along each axis is described by the Mathieu equation:

$$\begin{cases} \dfrac{d^2x}{d\xi^2} + (a - 2q\cos 2\xi)x = 0 \\ \dfrac{d^2y}{d\xi^2} + (a - 2q\cos 2\xi)y = 0 \\ \dfrac{d^2z}{d\xi^2} - 2(a - 2q\cos 2\xi)z = 0 \end{cases},$$

where $\xi = \omega_0 t/2$ is a dimensionless variable proportional to time, ω_0 is the characteristic frequency of the electric field oscillations in the ion trap, a and q are dimensionless constants.

Perform further studies for the following constant values: $a_x = -0.1$, $q_x = 0.8$.

A2	Using the program Mathieu.py, find the ratio $A = x_{\max}/(dx/d\xi)_{\max}$ of the maximum value of x to the maximum value of $dx/d\xi$ during the oscillations. Show that this quantity does not depend on the initial conditions $x(0)$ and $dx/d\xi(0)$ which are defined in the 12th and 13th lines of the program.

The Heisenberg's indeterminacy principle states that for any quantum object, there is an inherently unavoidable uncertainty σ_p in the value of the momentum p and an uncertainty σ_x in the value of the coordinate x, which are related by the expression

$$\sigma_p \cdot \sigma_x \geq \frac{\hbar}{2}.$$

A3	Estimate the minimum possible uncertainty σ_x in the position of the $^{41}Ca^+$ ion in the trap, assuming that $\sigma_x/\sigma_{dx/d\xi} = A$. Express the answer in terms of the ion's mass m, ω and A. Calculate the value of σ_x for $\omega_0 = 9.4 \cdot 10^9$ s^{-1}. Compare σ_x with the wavelength λ.

The absorption of light by ions and fluorescence is used to reduce their kinetic energy, i.e., for cooling. This method is called Doppler cooling. The idea is that a moving ion absorbs light not at a wavelength λ but of a wavelength $\lambda + \delta\lambda$ due to the Doppler effect.

In the laboratory frame, the four-momentum of a photon moving along the x-axis is given by $p^\mu = (E/c, p_x, p_y, p_z) = (\hbar\omega/c, \hbar\omega/c, 0, 0)$. In a frame moving with velocity V along the x-axis, the four-momentum of the photon changes according to the Lorentz transformations:

$$p'^\mu = \begin{pmatrix} \hbar\omega'/c \\ \hbar\omega'/c \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma V/c & 0 & 0 \\ -\gamma V/c & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \hbar\omega/c \\ \hbar\omega/c \\ 0 \\ 0 \end{pmatrix} = \Lambda^\mu{}_\nu p^\nu,$$

where $\gamma = (1 - V^2/c^2)^{-1/2}$ is the Lorentz factor, and $\Lambda^\mu{}_\nu$ is the Lorentz transformation matrix.

A4	Let the ion move with velocity $v \ll c$ along the x-axis. A photon with frequency $\omega + \delta\omega$ travels along the same axis. At what value of $\delta\omega = \delta\omega_0$ does the energy of the photon in the rest frame of the ion coincide with the energy difference $\hbar\omega$ between the levels of the ion?

A5	What is the photon flux $\Phi = dN/dt$ per unit area in a laser beam of intensity I and photon frequency ω?

When an ion absorbs a photon, it gains a momentum of $\hbar\omega/c$. Conversely, during fluorescence, the ion gives the emitted photon a momentum of $\hbar\omega/c$. However, the momentums of the absorbed photons are directed in one direction, while the momentums of the emitted photons are directed randomly. Therefore, by illuminating the ion with light of frequency $\omega + \delta\omega$, we act on it with a non-zero force on average.

A6	Find the average change in the ion's momentum δp after absorbing and emitting a photon of frequency $\omega + \delta\omega$ that has traveled in the direction of the x-axis. Assume that $\delta\omega \ll \omega$ and the velocity of the ion is $v \ll c$.

To find the change in the ion's momentum, an energy analysis is also possible, but it requires a more detailed study of the phenomenon: most of the energy $\hbar\omega$ goes into changing the energy of a specific electron, and a small part of $\hbar\omega$ goes into changing the kinetic energy of the entire ion. The relationship between these quantities can be estimated using the conservation of momentum law.

What's more important for us is that in reality, the absorption spectrum of an ion has a certain width. This means that the ion absorbs photons not only with a frequency (in the ion's rest frame) exactly equal to the transition frequency ω. The nature of the absorption spectrum is directly related to the probability per unit time Γ of spontaneous transition. If the photon frequency (in the ion's rest frame) is equal to $\omega + \Delta\omega$, then the absorption probability is given by:

$$P = \frac{\Gamma^2}{\Delta\omega^2 + \Gamma^2}.$$

Note that P is not the probability per unit time, but simply the probability of absorption when a photon passes through the effective cross-sectional area σ of the ion.

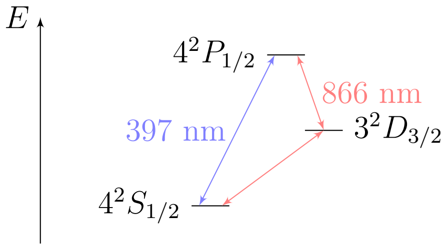
A7	Estimate the average lifetime of the ion's excited state, denoted as τ_1', measured in its own rest frame. Express the answer in terms of Γ.

A8	Find the average force F acting on the ion moving at velocity v in a laser beam of intensity I and frequency $\omega + \delta\omega$ (this frequency is given in the laboratory frame). In the resulting expression, the constant component is of no interest. So extract the variable component F_{var}, which depends on the velocity v. Assuming that the time the ion spends in the excited state is much shorter than in the unexcited state, and also assuming that $\Gamma \gg \delta\omega v/c$ and $v/c \ll 1$, write the expression for F_{var} in terms of v, ω, $\delta\omega$, Γ, I, and σ, c.

A9	What sign of $\delta\omega$ should be chosen to cool the ion, i.e. to reduce its kinetic energy over time?

After cooling the ion, we can proceed to study its interaction with various physical objects. In the process, we can obtain a "photo" of the ion. As discussed earlier, the ion interacts with light. However, it is inconvenient to use the light from the cooling laser to take an image of the ion, and an alternative method is usually used.

Let's add a 3rd level $3^2D_{3/2}$ to our model. This way the ion in the excited state will not only spontaneously relax during the transitions $4^2P_{1/2} \to 4^2S_{1/2}$ with emitting a photon with a wavelength $\lambda = 397$ nm but also spontaneously relax through $4^2P_{1/2} \to 3^2D_{3/2}$ with emitting a photon with a wavelength $\lambda_1 = 866$ nm and $3^2D_{3/2} \to 4^2S_{1/2}$ with emitting a photon with a wavelength λ_2.



A10	What is the value of λ_2?

The fluorescent light with a wavelength of λ_1 could be used to obtain an image of the ion. To do this, we place an optical filter that is nontransparent to λ and λ_2, followed by a flat lens with a diameter D and a focal length f, and then a photosensitive matrix. The distance from the plane of the lens to the ion is a.

A11	At what distance b from the plane of the lens to the photosensitive matrix does the clearest image of the ion form on it? Estimate the size of the clearest image of the ion for a lens with $f = 0.6$ nm, $D = 0.2$ nm.