IV
Electrodynamics

4.1 Introduction

This chapter is concerned with electric fields and charges encountered in different systems. Electricity is an ancient phenomenon already known by the Greeks. The experimental and theoretical basis of the current understanding of electrodynamical phenomena was established by two men: Michael Farady, the self-trained experimenter, and James Clerk Maxwell, the theoretician. The work of both were based on extensive material and knowledge by Coulomb. Farady, originally, a bookbinder, was most interested in electricity. His inquisitiveness in gaining knowledge on electrical phenomena made it possible to obtain an assistantship in Davy's lab. Farady (see Figure 4.1.1) was one of the greatest experimenters ever. In the course of his experiments, he discovered that a suspended magnet would revolve around a current bearing-wire. This observation led him to propose that magnetism is a circular force. He invented the dynamo in 1821, with which a large amount of our current electricity is generated. In 1831, he discovered electromagnetic induction. One of his most important contributions to physics in 1845 was his development of the concept of a field to describe magnetic and electric forces.

Michael Faraday: born September 22, 1791; died August 25, 1867.

Maxwell (see Figure 4.1.2) started out by writing a paper entitled "On Faraday's Lines of Force" (1856), in which he translated Faraday's theories into mathematical form. This description of Fara-

day's findings by means of mathematics presented the lines of force as imaginary tubes containing an incompressible fluid. In 1861, he published the paper "On Physical Lines of Force" in which he treated the lines of force as real entities. Finally, in 1865, he published a purely mathematical theory known as "On a Dynamical Theory of the Electromagnetic Field". The equations derived by Maxwell and published in "A Treaties on Electricity and Magnetism" (1873) are still valid and a source of basic laws for engineering as well as physics.

James Clerk Maxwell: born June 13, 1831; died November 5, 1879.

The aim of this chapter is to introduce basic phenomena and basic solution procedures for electric fields. The material discussed is a collection of examples. It is far from being complete by considering the huge diversity of electromagnetic phenomena. However, the examples discussed demonstrate how symbolic computations can be used to derive solutions for electromagnetic problems.

This chapter is organized as follows: Section 4.2 contains material on point charges. The exampl discuss the electric field of an assembly of discrete charges distributed in space. In Section 4.3, a standard boundary problem from electrostatics is examined to solve Poisson's equation for an angular segment. The dynamical interaction of electric fields and charged particles in a Penning trap is discussed in Section 4.4.

4.2 Potential and Electric Fields of Discrete Charge Distributions

In electrostatic problems, we often need to determine the potential and the electric fields for a certain charge distribution. The basic equation of electrostatics is Gauss' law. From this fundamental relation connecting the charge density with the electric field, the potential of the field can be derived. We can state Gauss' law in differential form by

$$\text{div}\,\vec{E} = 4\pi\rho(\vec{r}).$$

If we introduce the potential Φ by $\vec{E}$ = −grad Φ, we can rewrite Eq. (4.2.1) for a given charge distribution ρ in the form of a Poisson equation

$$\Delta\Phi = -4\pi\rho$$

where ρ denotes the charge distribution. To obtain solutions of Eq. (4.2..2), we can use the Green's function formalism to derive a particular solution. The Green's function $G(\vec{r}, \vec{r}')$ itself has to satisfy a Poisson equation where the continuous charge density is replaced by Dirac's delta function $\Delta_r G(\vec{r}, \vec{r}') = -4\pi\,\delta(\vec{r} - \vec{r}')$. The potential Φ is then given by

$$\Phi(\vec{r}) = \int_V G(\vec{r}, \vec{r}')\,\rho(\vec{r}')\,d^3r'.$$

In addition, we assume that the boundary condition $G \mid_V = 0$ is satisfied on the surface of volume V. If the space in which our charges are located is infinitely extended, the Green's function is given by

$$G(\vec{r}, \vec{r}') = \frac{1}{|\vec{r}-\vec{r}'|}$$

The solution of the Poisson equation (4.2.3) becomes

$$\Phi(\vec{r}) = \int \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}\,d^3r'.$$

Our aim is to examine the potential and the electric fields of a discrete charge distribution. The charges are characterized by a strength q_i and are located at certain positions $\vec{r}_i$. The charge density of such a distribution is given by

$$\rho(\vec{r}) = \sum_{i=1}^{N} q_i\,\delta(\vec{r}_i).$$

The potential of such a discrete distribution of charges is in accordance with Eq. (4.2.5):

$$\Phi(\vec{r}) = \sum_{i=1}^{N} \frac{q_i}{|\vec{r}-\vec{r}_i|},$$

where $\vec{r}_i$ denotes the location of the point charge. The corresponding electrical field is given by

$$\vec{E}(\vec{r}) = -\sum_{i=1}^{N} q_i\,\vec{r} - \frac{\vec{r}_i}{|\vec{r}-\vec{r}_i|^3}$$

and the energy density of the electric field of such a charge distribution is given by

$$w = \frac{1}{8\pi}\left|\vec{E}\right|^2.$$

Three fundamental properties of a discrete charge distribution are defined by Eqs. (4.2.7), (4.2.8), and (4.2.9). In the following, we write a *Mathematica* package which computes the potential, the electric field, and the energy density for a given charge distribution. With this package, we are able to create pictures of the potential, the electric field, and the energy density.

In order to design a graphical representation of the three quantities, we need to create contour plots of a three-dimensional space. To simplify the handling of the functions, we enter the cartesian coordinates of the locations and the strength of the charges as input variables in a list. Sublists of this list contain the information for specific charges. The structure of the input list is given by {{x_1, y_1, z_1, ρ_1}, {x_2, y_2, z_2, ρ_2}, …}. To make things simple in our examples, we choose the $y = 0$ section of the three-dimensional space. The package **PointCharge`**, located in the section on packages and programs, contains the equations discussed above. The package generates contour plots of the potential, the electric field, and the energy density.

In order to test the functions of this package, let us consider some ensembles of charges frequently discussed in literature. Our first example describes two particles carrying the opposite charge,

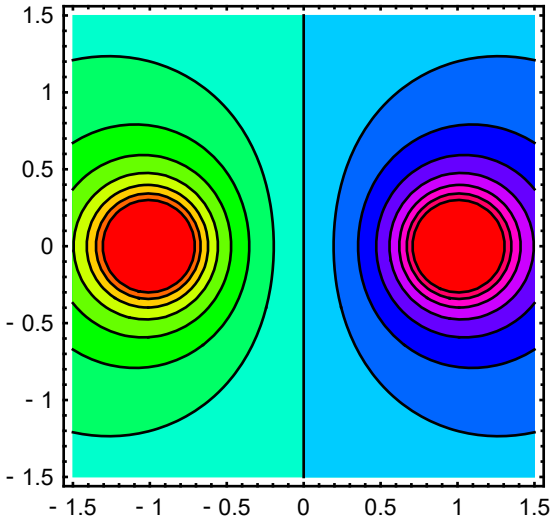
known as a dipole. Let us first define the charges and their coordinates by

```
charges = {{1,0,0,1},{-1,0,0,-1}}
```

```
{{1, 0, 0, 1}, {-1, 0, 0, -1}}
```

The charges are located in space at $x = 1$, $y = 0$, $z = 0$ and at $x = -1$, $y = 0$, $z = 0$. The fourth element in the sublists specifies the strength of the charges. The picture of the contour lines of the potential is created by calling

```
FieldPlot[charges,"Potential"];
```

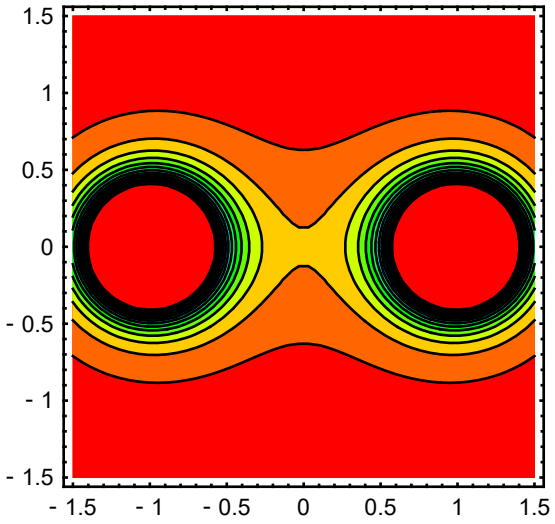


Contour plot of the potential for two charges in the (x, z)-plane. The particles carry opposite charges.

The second argument of **FieldPlot[]** is given as a string specifying the type of the contour plot. Possible values are *Potential*, *Field*, and *EnergyDensity*.

A graphical representation of the energy density follows by

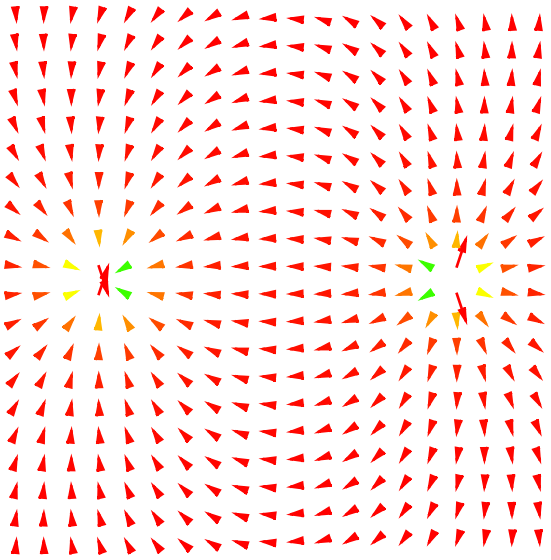
```
FieldPlot[charges,"EnergyDensity"];
```



Contour plot of the energy density of two charges in the (x, z)-plane.

The electrical field of the two charges are generated by

```
FieldPlot[charges, "Field"];
```



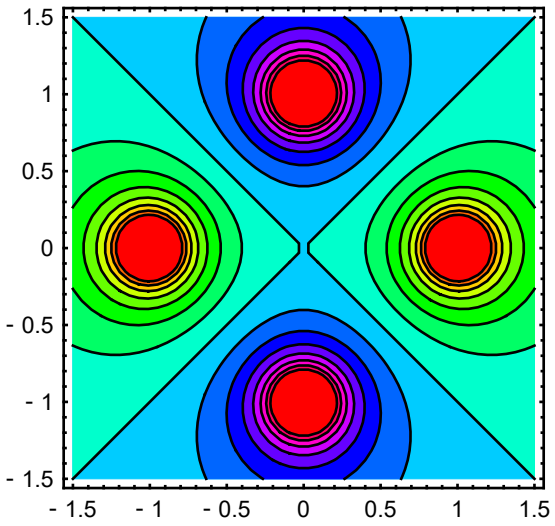
Since the generation of field plots is very flexible, we are able to examine any configuration of charges in space. A second example is given by a quadruple consisting of four charges arranged in a spatial configuration. The locations and strength of the charges are defined by

```
quadrupole = {{-1, 0, 0, -1}, {1, 0, 0, -1}, {0, 0, 1, 1}, {0, 0, -1, 1}}
```

```
{{-1, 0, 0, -1}, {1, 0, 0, -1}, {0, 0, 1, 1}, {0, 0, -1, 1}}
```

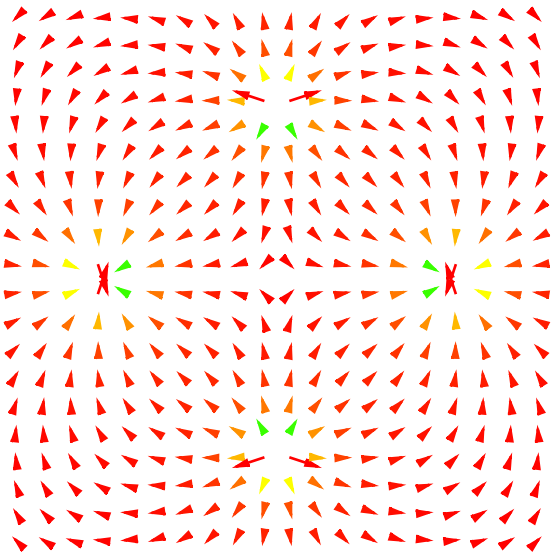
The potential is

```
FieldPlot[quadrupole, "Potential"];
```



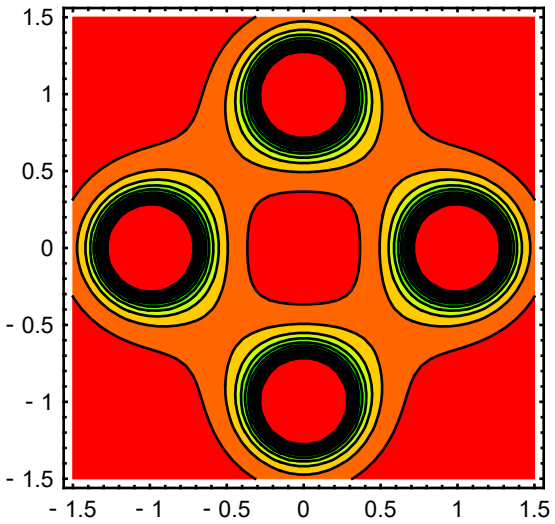
The field lines in the (x, z)-plane with $y = 0$ are

```
FieldPlot[quadrupole, "Field"];
```



The energy density looks like

```
FieldPlot[quadrupole, "EnergyDensity"];
```



4.3 Boundary Problem of Electrostatics

In the previous section, we discussed the arrangement of discrete charges. The problem was solved by means of the Poisson equation for the general case. We derived the solution for the potential using

$$\Delta\phi = 4\,\pi\rho.$$

Equation (4.3.10) is reduced to the Laplace equation if no charges are present in the space:

$$\Delta\phi = 0.$$

The Laplace equation is a general type of equation applicable to many different theories in physics, such as continuum theory, gravitation, hydrodynamics, thermodynamics, and statistical physics. In

this section, we use both the Poisson and the Laplace equations (4.3.10) and (4.3.11) to describe electrostatic phenomena. We show that Eqs. (4.3.10) and (4.3.11) are solvable by use of Green's function. If we know the Green's function of the equation, we are able to consider general boundary problems. A boundary problem is defined as follows: For a certain volume V, the surface of this volume, ∂V, possesses a specific electric potential. The problem is to determine the electric potential inside the volume given the value on the surface. This type of electrostatic boundary problem is called a Dirichlet boundary value problem. According to Eq. (4.3.10), there are charges inside volume V. The distribution or density of these charges is denoted by $\rho(\vec{x})$. The mathematical problem is to find solutions for Eq. (4.3.10) or (4.3.11) once we know the distribution of charges and the electric potential on the surface of the domain.

The Green's function allows us to simplify the solution of the problem. In our problem, we have to solve the Poisson equation (4.3.10) under certain restrictions. The Green's function related to the Poisson problem is defined by

$$\Delta G(\vec{x},\ \vec{x}') = -4\pi\delta(\vec{x} - \vec{x}')$$

under the specific boundary condition

$$G(\vec{x},\ \vec{x}')\Big|_{\partial V} = 0 \quad \text{with} \quad \vec{x}' \in \partial V$$

on the surface ∂V of volume V.

In the previous section, we discussed the Green's function for an infinitely extended space and found that the Green's function is represented by $G(\vec{x},\ \vec{x}') = 1/\left|\ \vec{x} - \vec{x}'\ \right|$. The present problem is more complicated than the one previously discussed. We need to satisfy boundary conditions for a finite domain in space.

For our discussion, we assume that the Green's function exists and that we can use it to solve the boundary problem. The proof of this assumption is given by Arfken [4.1]. The connection between the Green's function and the solution of the boundary problem is derived using Gauss's theorem. The first formula by Green

$$\int_V \operatorname{div} \vec{A}\, d^3x = \int_V \vec{A}\, d^2\vec{f},$$

along with an appropriate representation of the vector field $\vec{A} = \Phi\cdot\nabla G - \nabla\Phi\cdot G$ yields the second formula by Green:

$$\operatorname{div} \vec{A} = \Phi\cdot\Delta G - \Delta\Phi\cdot G.$$

Using the integral theorem of Gauss in the form of Eq. (4.3.14), we find

$$\int_V (\Phi\cdot\Delta G - \Delta\Phi\cdot G)\, d^3x = \int_{\partial V} \left(\Phi\frac{\partial G}{\partial n} - G\frac{\partial\Phi}{\partial n}\right) d^2 f,$$

where $\partial/\partial n = \vec{n}\cdot\nabla$ is the normal gradient. If we use relations (4.3.10), (4.3.12), and (4.3.13) in Eq. (4.3.16), we can derive the potential by the two integrals

$$\Phi(\vec{x}) = \int_V G(\vec{x},\ \vec{x}')\,\rho(\vec{x}')\, d^3x' -$$

$$\frac{1}{4\pi}\int_{\partial V} \Phi(\vec{x}')\,\frac{\partial G(\vec{x},\vec{x}')}{\partial n'}\ d^2 f'.$$

A comparison between Eqs. (4.3.17) and (4.2.3) reveals that the total potential in the Dirichlet problem depends on a volume part (consistent with Eq. (4.2.3) and on a surface part as well. The potential Φ at location $\vec{x}$ consists of a volume term containing the charges and of a surface term determined by the electric potential $\Phi(\vec{x})$. The potential $\Phi(\vec{x}')$ used in the surface term is known as a boundary condition. If there are no charges in the present volume, solution (4.3.17) reduces to

$$\Phi(\vec{x}) = -\frac{1}{4\pi}\int_{\partial V}\Phi(\vec{x}\,')\,\frac{\partial G(\vec{x},\vec{x}\,')}{\partial n'}\,d^2 f\,'.$$

For the charge-free case, the electric potential at a location $\vec{x}$ inside the volume V is completely determined by the potential on the surface $\Phi(\vec{x}\,')$. We are able to derive Eqs. (4.3.17) and (4.3.18) provided that the Green's function $G(\vec{x}, \vec{x}\,')$ vanishes on the surface of V. In other words, we assume the surface potential to be a boundary condition. This type of boundary condition is called a Dirichlet boundary condition. A second type is the so-called von Neumann boundary condition, which specifies the normal derivative of the electrostatic potential $\partial\Phi/\partial n$ on the surface. A third type used in potential theory is a mixture of Dirichlet and von Neumann boundary conditions. In the following, we will restrict ourselves to Dirichlet boundary conditions only.

If we take a closer look at solutions (4.3.17) and (4.3.18) of our boundary value problem, we observe that the Green's function as an unknown determines the solution of our problem. In other words, we solved the boundary problem in a form which contains an unknown function as defined by relation (4.3.12) and the boundary condition (4.3.13). The central problem is to find an explicit representation of the Green's function. One way to tackle this is by introducing an eigenfunction expansion [4.2]. This procedure always applies if the coordinates are separable. The eigenfunction expansion of the Green's function is based on the analogy between an eigenvalue problem and equations (4.3.10) and (4.3.11) for the potential.

The eigenvalue problem related to equation (4.3.10) is given by

$$\Delta\psi + (4\pi\rho + \lambda)\psi = 0.$$

For a detailed discussion of the connection, see [4.2]. We assume that solutions ψ of Eq. (4.3.19) satisfy the Dirichlet boundary conditions. In this case, the regular solutions of Eq. (4.3.12) only occur if parameter $\lambda = \lambda_n$ assumes certain discrete values. The λ_n's are the eigenvalues of Eq. (4.3.19). Their corresponding functions ψ_n are eigenfunctions. The eigenfunctions ψ_n are orthogonal and satisfy

$$\int_V \psi_m^*(\vec{x})\,\psi_n(\vec{x})\,d^3x = \delta_{mn}.$$

The eigenvalues of Eq. (4.3.19) can be discrete or continuous. In analogy to Eq. (4.3.12), the Green's function has to satisfy the equation

$$\Delta_x G(\vec{x}, \vec{x}\,') + (4\pi\rho + \lambda)\,G(\vec{x}, \vec{x}\,') = -4\pi\delta(\vec{x} - \vec{x}\,'),$$

where λ is different to the eigenvalues λ_n. An expansion of the Green's function with respect to the eigenfunctions of the related eigenvalue problem is possible if the Green's function satisfies the same boundary conditions. Substituting an expansion of the Green's function

$$G(\vec{x}, \vec{x}\,') = \sum_n a_n(\vec{x}\,')\,\psi_n(\vec{x})$$

into Eq. (4.3.21), we get

$$\sum_m a_m(\vec{x}\,')(\lambda - \lambda_m)\,\psi_m(\vec{x}) = -4\pi\delta(\vec{x} - \vec{x}\,').$$

Multiplying both sides of Eq. (4.3.23) by $\psi_n^*(\vec{x}\,)$ and integrating the result over the entire volume, we obtain the expansion coefficients $a_m(\vec{x}\,')$. Using the orthogonal relation (4.3.20) simplifies the sum. The expansion coefficients are defined by

$$a_n(\vec{x}\,') = 4\pi\,\frac{\psi_n^*(\vec{x}\,')}{\lambda_n - \lambda}.$$

With relation (4.3.24) we get the representation of the Green's function

$$G(\vec{x}, \vec{x}\,') = 4\pi\sum_n \frac{\psi_n^*(\vec{x}\,')\,\psi_n(\vec{x})}{\lambda_n - \lambda}.$$

So far, our considerations have assumed a discrete spectrum of eigenvalues. For a continuous distribution of eigenvalues λ_n, we need to replace the sum in Eq. (4.3.25) with an integral over the eigenvalues.

By using the representation of the Green's function (4.3.25), we can rewrite the solution of the potential (4.3.17) and (4.3.18) in the form

$$\Phi(\vec{x}) = \int_V 4\pi \sum_n \frac{\psi_n^*(\vec{x}')\psi_n(\vec{x})}{\lambda_n - \lambda} \rho(\vec{x}')\, d^3x' - \int_{\partial V} \Phi(\vec{x}') \sum_n \frac{\psi_n(\vec{x})}{\lambda_n - \lambda} \frac{\partial \psi_n^*(\vec{x}')}{\partial n'} d^2f'$$

$$= 4\pi \sum_n \frac{\psi_n(\vec{x})}{\lambda_n - \lambda} \int_V \psi_n^*(\vec{x}')\rho(\vec{x}')\, d^3x' - \sum_n \frac{\psi_n(\vec{x})}{\lambda_n - \lambda} \int_{\partial V} \Phi(\vec{x}') \frac{\partial \psi_n^*(\vec{x}')}{\partial n'} d^2f'.$$

If we know the eigenfunctions and eigenvalues of the problem, we can represent the potential by

$$\Phi(\vec{x}) = \sum_n (c_n - d_n)\psi_n(\vec{x}),$$

where the c_n's and the d_n's are expansion coefficients defined by

$$c_n = \frac{4\pi}{\lambda_n - \lambda} \int_V \psi_n^*(\vec{x}')\rho(\vec{x}')\, d^3x'$$

and

$$d_n = \frac{1}{\lambda_n - \lambda} \int_{\partial V} \Phi(\vec{x}') \frac{\partial \psi_n^*(\vec{x}')}{\partial n'} d^2f'.$$

For the charge-free case $\rho = 0$, we find

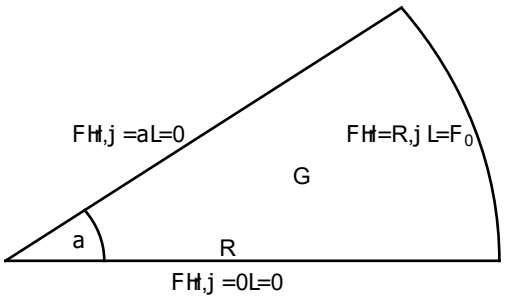
$$\Phi(\vec{x}) = -\sum_n \frac{\psi_n(\vec{x})}{\lambda_n - \lambda} \int_{\partial V} \Phi(\vec{x}') \frac{\partial \psi_n^*(\vec{x}')}{\partial n'} d^2f'.$$

which reduces to

$$\Phi(\vec{x}) = -\sum_n d_n \psi_n(\vec{x}).$$

The unknown quantities of this representation are the eigenfunctions ψ_n and the expansion coefficients c_n and d_n. By examining a specific planar problem, we show how these unknowns are calculated. To make things simple, we assume that no charges are distributed on the plane.

The problem under consideration examines in a section of a disk in which boundaries have fixed potential values $\Phi(r, \varphi = 0) = 0$, $\Phi(r, \varphi = \alpha) = 0$, and $\Phi(r = R, \varphi) = \Phi_0(\varphi)$. The specific form of the domain and the boundary values are given in Figure 4.3.5.



Boundary conditions on a disk segment. The domain G is free of charges.

The domain G is free of any charges and the potential $\Phi(r, \varphi)$ is regular and finite for $r \to 0$. To solve the problem efficiently, we choose coordinates which reflect the geometry of our problem. In this case, they are plane cylindrical coordinates. Since G is free of any charges, Laplace's equation in plane cylindrical coordinates takes the form

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \Phi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 \Phi}{\partial \varphi^2}=0.$$

When deriving the solution, we assume that the coordinates are separated. If we use the assumption of separating the coordinates, we are able to express the electric potential as $\Phi(r, \varphi) = g(r)\, h(\varphi)$. Substituting this expression into Eq. (4.3.32), we get

$$\frac{r}{g(r)}\frac{d}{dr}\left(r\frac{dg}{dr}\right)=-\frac{1}{h(\varphi)}\frac{d^2 h(\varphi)}{d\varphi^2}=\nu^2,$$

where v is a constant. Separating both equations, we get two ordinary differential equations determining g and h. g and h represent the eigenfunctions of the Green's function

$$\frac{r}{g(r)}\frac{d}{dr}\left(r\frac{dg}{dr}\right)=\nu^2,$$

$$\frac{1}{h(\varphi)}\frac{d^2 h(\varphi)}{d\varphi^2}=-\nu^2,$$

The eigenfunctions of the radial part of the potential are

$$g_\nu(r)=a_\nu r^\nu+b_\nu r^{-\nu}.$$

The angular part of the eigenfunctions defined in Eq. (4.3.35) is given by

$$h_\nu(\varphi)=A_\nu \sin(\nu\varphi)+B_\nu \cos(\nu\varphi).$$

The solutions (4.3.36) and (4.3.37) contain four constants a_v, b_v, A_v, and B_v for each eigenvalue v. These constants have to satisfy the boundary conditions and the condition of regularity at $r = 0$.

Let us first examine the radial part of the solution in the domain G. We find that for $\varphi = 0$, the relation

$$\Phi(r, \varphi=0)=g(r)\,h(\varphi=0)=0$$

needs to be satisfied. From condition (4.3.38), it follows that $h(\varphi = 0) = B_v = 0$. From the boundary condition at $\varphi=\alpha$ we get the condition

$$\Phi(r, \varphi=\alpha)=g(r)\,h(\varphi=\alpha)=0,$$

which results in $h(\alpha) = A_v \sin(v\alpha) = 0$. As a consequence, we get $v = n\pi/\alpha$ with $n = 0, 1, 2, 3, \ldots$. The angular part of the solution thus reduces to

$$h_n(\varphi)=A_n \sin\left(\frac{n\pi}{\alpha}\varphi\right).$$

From the condition of regularity $\Phi(r \to 0, \varphi) < \infty$, it follows from

$$\Phi(r, \varphi)=h_\nu(\varphi)\,(a_\nu r^\nu+b_\nu r^{-\nu})$$

that $b_v = 0$. The solution of the potential is thus represented by

$$\Phi(r, \varphi)=\sum_{n=0}^{\infty} d_n r^{n\pi/a}\sin\left(\frac{n\pi}{a}\varphi\right),$$

where $d_n = a_n A_n$. Expression (4.3.42) contains the unknown coefficients d_n, which we need to determine in order to find their explicit representations. Values for d_n are determined by applying the boundary condition on the circle $\Phi(r = R, \varphi) = \Phi_0(\varphi)$. If we take into account the orthogonality relation for the trigonometric functions

$$\frac{2}{\alpha}\int_0^\alpha \sin\left(\frac{n\pi}{\alpha}\varphi\right)\sin\left(\frac{m\pi}{\alpha}\varphi\right)d\varphi=\delta_{mn},$$

we are able to derive from the boundary condition of the circle a representation of d_n by

$$\begin{aligned}\int_0^\alpha \Phi_0(\varphi)\sin\left(\frac{n\pi}{\alpha}\varphi\right)d\varphi &= \sum_{m=0}^{\infty} d_m R^{m\pi/\alpha}\int_0^\alpha \sin\left(\frac{n\pi}{\alpha}\varphi\right)\sin\left(\frac{m\pi}{\alpha}\varphi\right)d\varphi\\ &= \sum_{m=0}^{\infty} d_m R^{m\pi/\alpha}\frac{\alpha}{2}\delta_{nm}\\ &= \frac{\alpha}{2}R^{n\pi/\alpha}d_n,\end{aligned}$$

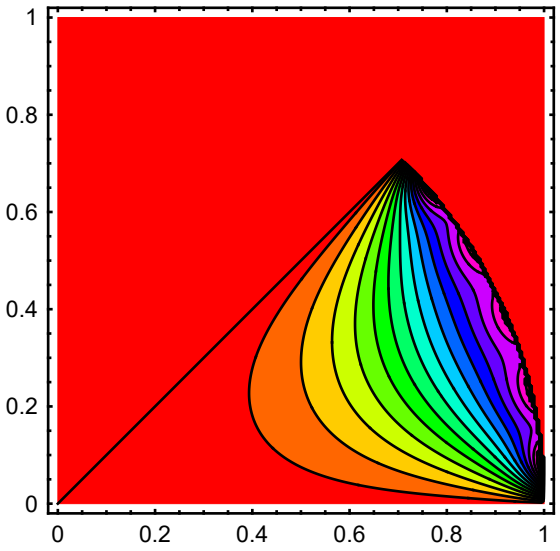
or in explicit form,

$$d_n = R^{-n\pi/\alpha}\,\frac{2}{\alpha}\int_0^{\alpha}\Phi_0(\varphi)\sin\left(\frac{n\pi}{\alpha}\varphi\right)d\varphi.$$

The representation of d_n by the integral (4.3.45) includes the boundary condition and only contains known parameters. Thus, we can determine d_n's numerical value if we know the boundary condition and if we specify the index m of the expansion in Eq. (4.3.42). The values of d_n are, however, only defined if the integral in Eq. (4.2.45) converges. The specific form of the Green's function is derivable if we compare the representation of the solution (4.3.42) with the definition of the Green's function.

With the above theoretical considerations, an explicit representation of the solution is now necessary. By specifying the geometrical parameters of the problem, the radius R of the segment, the angle α, the potential value along the rim of the disk and Eq. (4.3.42), we can calculate the potential in the domain G. The central quantities of the expansion (4.3.42) are the coefficients d_n. In order to make these factors available, we define the sum (4.3.42) and the integral (4.3.45) in the **Potential[]** function of the package **BoundaryProblem`** (see Section 4.6.2 for details). We define relations (4.3.42) and (4.3.45) to control the accuracy of the calculation using an upper summation index n (see also the definition of the function **Potential[]** in Section 4.6.2). An example of the potential for the parameters R=1, $\alpha = \pi/4$ and $\Phi_0(\varphi)$=1 is given in Figure 4.3.6. The calling sequence of **Potential[]** takes the form **Potential[*f*[*x*], *R*, *α*, *n*]**.

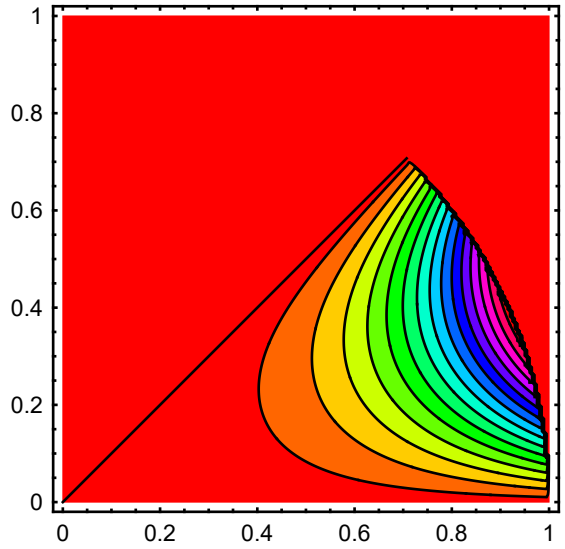
```
Potential[1, 1, π/4, 10];
```



Contour plot of the potential in the domain G. Boundary conditions and geometric parameters are $\Phi_0(\varphi)$= 1, R=1, $\alpha = \pi/4$ and n=10.

The result shows an approximation of the potential up to order 10. The contour lines show that the approximation shows some wiggles at the rim of the domain. The quality of the approximation can be checked by increasing the approximation order. The increase in quality is shown in the following sequence of plots (Figure 4.3.7):

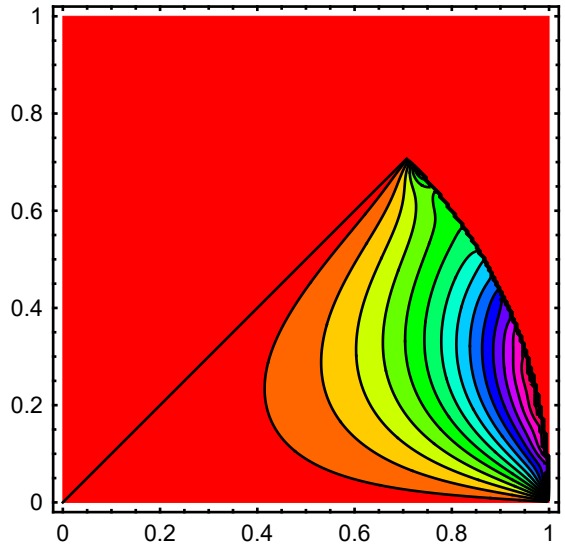
```
pl = Table[Potential[1, 1, π/4, i], {i, 1, 20, 2}];
```



Sequence of contour plot of the potential in the domain G. Boundary conditions and geometric parameters are $\Phi_0(\varphi)= 1$, R=1, $\alpha = \pi/4$ and $n\epsilon$[1,20,2].

At this place, a word of caution should be mentioned. The approximation of the potential shows that the procedure is sensitive in the approximation order. The kind of calculation is also sensitive on the boundary conditions, which is given as first argument in the function **Potential[]**. Although the calculated potential shows the expected behavior, it is not always possible to calculate the potential for a reasonable approximation order for arbitrary boundary conditions. This shortcoming is due to the calculation of integrals in the procedure. However, the reader should experiment with the function and test the limitations of the method to gain a feeling for the applicability. An example with a spatially varying boundary condition on the rim is presented in Figure 4.3.8.

```
Potential[2 + Sin[7 ϕ], 1, π/4, 20];
```



Contour plot of the potential in the domain G. Boundary conditions and geometric parameters are $\Phi_0(\varphi)= 2+\sin(7\varphi)$, R=1, $\alpha = \pi/4$ and n=10.

4.4 Two Ions in the Penning Trap

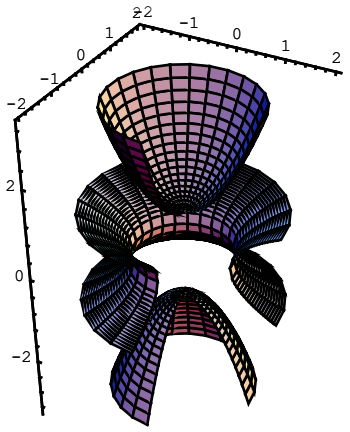
The study of spectroscopic properties of single ions requires that one or two ions are trapped in a cavity. Nowadays, ions can be successfully separated and stored by means of ion traps. Two techniques are used for trapping ions. The first method uses a dynamic electric field, while the second method uses static electric and magnetic fields. The dynamic trap was originally invented by Paul [4.3]. The static trap is based on the work of Penning [4.4]. Both traps use a combination of electric and magnetic fields to confine ions in a certain volume in space. Two paraboloids connected to a *dc*-source determine the kind of electric field in which the ions are trapped. The form of the paraboloids in turn determines the field of the trap's interior. Since the motion of the ions in Paul's trap is very complicated, we restrict our study to the Penning trap.

In our discussion of the Penning trap, the form of the quadrupole fields determined by the shapes of the paraboloids is assumed to be

$$\Phi = \frac{U_0}{r_0^2+2\,z_0^2}\left(x^2 + y^2 - 2\,z^2\right),$$

where U_0 is the strength of the source and $r_0$and $z_0$are the radial and axial extensions of the trap (see Figure 4.4.9). The shape of the potential is a consequence of the Laplace equation $\Delta\Phi=0$. The given functional shape of the potential is experimentally created by conducting walls which are connected to a dc-battery. The force acting on an ion carrying charge q in the trap is given by

$$\vec{F} = q\,\vec{E} = -q\,\nabla\Phi.$$



Cross-section of the Penning trap. The paraboloids are positioned on dc-potentials. A constant magnetic field is superimposed in the z vertical direction (not shown). The ions move in the center of the trap.

From the functional form of the electric field $\vec{E}$ of the trap

$$\vec{E} = -\nabla\,\Phi = -\frac{2\,U_0}{r_0^2+2\,z_0^2}\begin{pmatrix} x \\ y \\ -2\,z \end{pmatrix} = -\frac{2\,U_0}{r_0^2+2\,z_0^2}\,(\vec{x} - 3\,\vec{e}_z),$$

we detect a change of sign in the coordinates. This instability allows the ions to escape the trap. To prevent escape from the trap in the z-direction, Paul and co-workers used a high-frequency ac-field and Penning and co-workers used a permanent magnetic field $\vec{B} = B_0\vec{e}_z$.

In a static trap the forces acting on each of the two ions are determined by the electromagnetic force of the external fields and the repulsive force of the Coulomb interaction of the charges. The external

fields consist of the static magnetic field along the *z*-axis and the electric quadrupole field of the trap. The Coulomb interaction of the two particles is mainly governed by the charges which are carried by the particles. The total force on each particle is a combination of trap and Coulomb forces. Since we have a system containing only a few particles, we can use Newton's theory (see section 2.4) to write down the equations of motion in the form

$$m\,\vec{x}'' = (\vec{F})_i^T + (\vec{F})_i^{\text{Coul}} \qquad i=1,2.$$

In equation (4.4.49) the trap force $(\vec{F})_i^T$ denotes the Lorentz force of a particle in the electromagnetic field given by

$$(\vec{F})_i^T = q\,(\vec{E})_i + q\,(\vec{v}_i \times \vec{B}).$$

Since the magnetic field $\vec{B}$ is a constant field along the *z*-direction

$$\vec{B} = B_0 \vec{e}_z,$$

the total trap force on the *i*th ion is given by

$$(\vec{F})_i^T = -\frac{2\,U_0}{r_0^2+2\,z_0^2}\,(\vec{x} - 3\,z_i\,\vec{e}_z) + q\,(\vec{x}'_i \times \vec{B}).$$

The Coulomb forces between the first and the second ion are

$$(\vec{F})_{12}^{\text{Coul}} = \frac{q^2}{4\,\pi\varepsilon_0}\,\frac{\vec{x}_1-\vec{x}_2}{|\vec{x}_1-\vec{x}_2|^3},$$

$$(\vec{F})_{21}^{\text{Coul}} = \frac{q^2}{4\,\pi\varepsilon_0}\,\frac{\vec{x}_2-\vec{x}_1}{|\vec{x}_1-\vec{x}_2|^3}.$$

The explicit forms of the equations of motion are thus

$$m\,\vec{x}''_1 = -\frac{2\,U_0}{r_0^2+2\,z_0^2}\,(\vec{x}_1 - 3\,z_1\,\vec{e}_z) + q\,(\vec{x}'_1 \times \vec{B}) + \frac{q^2}{4\,\pi\varepsilon_0}\,\frac{\vec{x}_1-\vec{x}_2}{|\vec{x}_1-\vec{x}_2|^3},$$

$$m\,\vec{x}''_2 = -\frac{2\,U_0}{r_0^2+2\,z_0^2}\,(\vec{x}_2 - 3\,z_2\,\vec{e}_z) + q\,(\vec{x}'_2 \times \vec{B}) + \frac{q^2}{4\,\pi\varepsilon_0}\,\frac{\vec{x}_2-\vec{x}_1}{|\vec{x}_1-\vec{x}_2|^3}.$$

The two equations of motion (4.4.55) and (4.4.56) are coupled ordinary differential equations of the second order. They can be decoupled by introducing relative and center of mass coordinates:

$$\vec{r} = \vec{x}_1 - \vec{x}_2,$$
$$\vec{R} = \frac{1}{2}\,(\vec{x}_1 + \vec{x}_2).$$

Using Eqs. (4.4.57) in (4.4.55) and (4.4.56), we can describe the motion of the two ions in the center of mass and in relative coordinates. The two transformed equations read

$$\vec{R}'' = -\frac{2\,U_0}{m\left(r_0^2+2\,z_0^2\right)}\,(\vec{R} - 3\,Z\,\vec{e}_z) + \frac{q\,B_0}{m}\,(\vec{R}' \times \vec{e}_z),$$

$$\vec{r}'' = -\frac{2\,U_0}{m\left(r_0^2+2\,z_0^2\right)}\,(\vec{r} - 3\,z\,\vec{e}_z) + \frac{q\,B_0}{m}\,(\vec{r}' \times \vec{e}_z) + \frac{q^2}{2\,\pi\,m\,\varepsilon_0}\,\frac{\vec{r}}{|\vec{r}|^3}.$$

If we assume that the two ions carry a negative charge $q < 0$ and that the dc-potential U_0 on the paraboloids is positive ($U_0 > 0$), then we can introduce two characteristic frequencies and a scaled charge by

$$\omega_0^2 = \frac{2\,U_0}{m\left(r_0^2+2\,z_0^2\right)},$$

$$\omega_c = \frac{|q|\,B_0}{m},$$

$$Q^2 = \frac{q^2}{2\,\pi\,m\,\varepsilon_0}.$$

Constant ω_0 denotes the frequency of the oscillations along the *z*-direction. ω_c is the cyclotron frequency (i.e., the frequency with which the ions spin around the magnetic field). *Q* represents the scaled charge. Using these constants in the equations of motion (4.4.58) and (4.4.59), we get a simplified system of equations containing only three constants:

$$\vec{R}'' = \omega_0^2 \left(\vec{R} - 3\, Z\, \vec{e}_z\right) - \omega_c \left(\vec{R}' \times \vec{e}_z\right),$$

$$\vec{r}'' = \omega_0^2 \left(\vec{r} - 3\, z\, \vec{e}_z\right) - \omega_c \left(\vec{r}' \times \vec{e}_z\right) + Q^2 \frac{\vec{r}}{|\vec{r}|^3}.$$

In the following subsections, we discuss the two different types of motion resulting from these equations.

4.4.1 The Center of Mass Motion

The center of mass motion is determined by Eq. (4.4.63). Writing down the equations of motion in cartesian coordinates *X*, *Y*, and *Z*, we get a coupled system of equations:

$$X'' - \omega_0^2\, X + \omega_c\, Y' = 0,$$

$$Y'' - \omega_0^2\, Y - \omega_c\, X' = 0,$$

$$Z'' + 2\, \omega_0^2\, Z = 0.$$

The equations of motion for the *X*- and *Y*- components are coupled through the cross-product. The *Z*- component of the motion is completely decoupled from the *X* and *Y* coordinates. The last of these three equations is equivalent to a harmonic oscillator with frequency $\sqrt{2}\ \omega_0$. Thus, we immediately know the solution of the *Z*- coordinate given by

$$Z(t) = A \cos\left(\sqrt{2}\ \omega_0\, t + B\right).$$

The arbitrary constants *A* and *B* are related to the initial conditions of the motion by $Z(t = 0) = Z_0$ and $Z'(t = 0) = Z_0'$. Therefore, $A = Z_0^2 + Z'^2_0 / 2\, \omega_0^2$ and $\tan B = Z_0' \Big/ \sqrt{2}\ \omega_0 Z_0$.

A representation of the solution of the remaining two equations (4.4.65) and (4.4.66) follows if we combine the two coordinates *X* and *Y* by a complex transformation of the form $\mathcal{Y} = X + i\, Y$. Applying this transformation to the two equations delivers the simple representation

$$\ddot{\mathcal{Y}} - \omega_0^2\, \mathcal{Y} - i\, \omega_c\, \dot{\mathcal{Y}} = 0.$$

If we assume that the solutions of Eq. (4.4.69) are harmonic functions of the type $\mathcal{Y} = e^{i\, \omega\, t}$, we get the corresponding characteristic polynomial

$$\omega(\omega_c - \omega) - \omega_0^2 = 0.$$

The two solutions of this quadratic equation are given by the frequencies ω_1 and ω_2:

$$\omega_1 = \frac{\omega_c}{2} + \sqrt{\left(\frac{\omega_c}{2}\right)^2 - \omega_0^2}\ ,$$

$$\omega_2 = \frac{\omega_c}{2} - \sqrt{\left(\frac{\omega_c}{2}\right)^2 - \omega_0^2}\ .$$

The two frequencies are combinations of the cyclotron frequency ω_c and the axial frequency ω_0. The general solution of Eqs. (4.4.65) and (4.4.66) is thus given by

$$X(t) = B_r \cos(\omega_1\, t) + B_i \sin(\omega_1\, t) + A_r \cos(\omega_2\, t) + A_i \sin(\omega_2\, t),$$

$$Y(t) = A_r \sin(\omega_2 t) - A_i \cos(\omega_2 t) + B_r \sin(\omega_1 t) - B \cos(\omega_1 t).$$

The constants of integration A_r, A_i, B_r, and B_i are related to the initial conditions X_0, Y_0, X_0', and Y_0' by the relations

$$A_r = \frac{Y_0' - \omega_1 X_0}{\omega_2 - \omega_1},$$

$$A_i = \frac{X_0' + \omega_1 Y_0}{\omega_2 - \omega_1},$$

$$B_r = \frac{Y_0' - \omega_2 X_0}{\omega_1 - \omega_2},$$

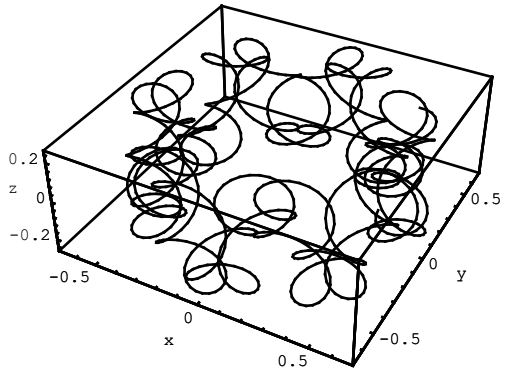
$$B_i = \frac{X_0' + \omega_2 Y_0}{\omega_1 - \omega_2}.$$

A special case of solutions (4.4.73) and (4.4.74) is obtained if we assume that the center of mass is initially located in the origin of the coordinate system $X_0 = Y_0 = 0$. We get from (4.4.75) $A_r = -B_r$, and $A_i = -B_i$. The solution then takes the form

$$X(t) = A_r \sin\left(\frac{\omega_c}{2} t\right) \sin\left(\sqrt{\left(\frac{\omega_c}{2}\right)^2 - \omega_0^2}\ t\right) - A_i \cos\left(\frac{\omega_c}{2} t\right) \sin\left(\sqrt{\left(\frac{\omega_c}{2}\right)^2 - \omega_0^2}\ t\right),$$

$$Y(t) = A_i \sin\left(\frac{\omega_c}{2} t\right) \sin\left(\sqrt{\left(\frac{\omega_c}{2}\right)^2 - \omega_0^2}\ t\right) - A_r \cos\left(\frac{\omega_c}{2} t\right) \sin\left(\sqrt{\left(\frac{\omega_c}{2}\right)^2 - \omega_0^2}\ t\right).$$

The above solutions show that the motion of the center of mass in the (X, Y)-plane is governed by two frequencies. The first frequency is one-half of the cyclotron frequency ω_c and the second frequency is a combination of the axial frequency and the cyclotron frequency given by $\sqrt{(\omega_c/2)^2 - \omega_0^2}$. A plot of the motion in center of mass coordinates is given in Figure 4.4.10. The three-dimensional motion of the center of mass is governed by three frequencies. The axial frequency $\sqrt{2}\ \omega_0$ determines the oscillation rate of the center of mass along the z-axis. The halved cyclotron frequency $\omega_c/2$ governs the spinning of the particles around the magnetic lines.



Motion of the center of mass in space for $t \in [0, 100]$. The initial conditions are $X_0 = 0.5 = Y_0$, $\dot{X}_0 = 0.1 = \dot{Y}_0$. The cyclotron frequency is fixed at ω_c=5.

4.4.2 Relative Motion of the Ions

The relative motion of the two ions is governed by Eq. (4.4.64)

$$\vec{r}'' = \omega_0^2 (\vec{r} - 3\, \overline{z}\vec{e}_z) - \omega_c (\vec{r}' \times \vec{e}_z) + Q^2 \frac{\vec{r}}{|\vec{r}|^3}.$$

Cylindrical coordinates are the appropriate coordinate system giving an efficient description of the relative motion of the particles. Location $\vec{r}$ of the relative particle is given in cylindrical coordinates by the representation

$$\vec{r} = \rho\ \vec{e}_\rho + \zeta\ \vec{e}_z,$$

where $\vec{e}_\rho$ and $\vec{e}_z$ represent the unit vectors in the radial and axial directions, respectively.

Using these coordinates in the equation of motion (4.4.81) gives the following representation:

$$\left(\rho'' - \rho\,\varphi'^2\right)\vec{e}_\rho + (2\,\rho'\,\varphi' + \rho\varphi'')\,\vec{e}_\varphi + \zeta''\,\vec{e}_z - \omega_0^2\left(\rho\,\vec{e}_\rho - 2\,\zeta\,\vec{e}_z\right) + \omega_c\left(-\rho'\,\vec{e}_\varphi + \rho\varphi'\,\vec{e}_\rho\right) = \frac{Q^2\left(\rho\,\vec{e}_\rho + \zeta\,\vec{e}_z\right)}{\left(\sqrt{\rho^2+\zeta^2}\right)^3}.$$

Separating each coordinate direction, we can split Eq. (4.4.83) into a system of equations for the coordinates ρ, φ, and ζ:

$$\rho'' - \rho\,\varphi'^2 - \omega_0^2\,\rho + \omega_c\,\rho\,\varphi' = \frac{Q^2\,\rho}{\left(\sqrt{\rho^2+\zeta^2}\right)^3},$$

$$2\,\rho'\,\varphi' + \rho\,\varphi' - \omega_c\,\rho = 0,$$

$$\zeta'' + 2\,\omega_0^2\,\zeta = \frac{Q^2\,\zeta}{\left(\sqrt{\rho^2+\zeta^2}\right)^3}.$$

By multiplying Eq. (4.4.85) by the radial coordinate ρ and integrating the result, we are able to derive an integral of motion. This integral of motion is given by an extended angular momentum containing the cyclotron frequency and is thus connected with the magnetic field. The conserved quantity is given by

$$\ell_B = \rho^2\,\varphi' - \frac{\omega_c}{2}\,\rho^2.$$

The integral of motion (4.4.87) eliminates the φ dependence in Eq. (4.4.84). The elimination of φ reduces the system of equations (4.4.84) and (4.4.86) to

$$\rho'' + \left(\left(\frac{\omega_c}{2}\right)^2 - \omega_0^2\right)\rho - \frac{\ell_B^2}{\rho^3} = \frac{Q^2\,\rho}{\left(\sqrt{\rho^2+\zeta^2}\right)^3},$$

$$\zeta'' + 2\,\omega_0^2\,\zeta = \frac{Q^2\,\zeta}{\left(\sqrt{\rho^2+\zeta^2}\right)^3}.$$

This system of equations contains a multitude of parameters. Our aim is to reduce these parameters by appropriately scaling the temporal and spatial coordinates. If we consider the expression $\beta = (\omega_c/2)^2 - \omega_0^2 > 0$ to be positive, time is scaled by $\tau = \beta\,t$. The radial and axial coordinates ρ and ζ are scaled by the factor $d = (Q/\beta)^{\frac{2}{3}}$. Introducing the abbreviations $v^2 = (l_B/\beta)^2$ and $\lambda^2 = \left(\sqrt{2}\ \omega_0^2/\beta\right)^2$ simplifies the system of equations (4.4.88) and (4.4.89) to

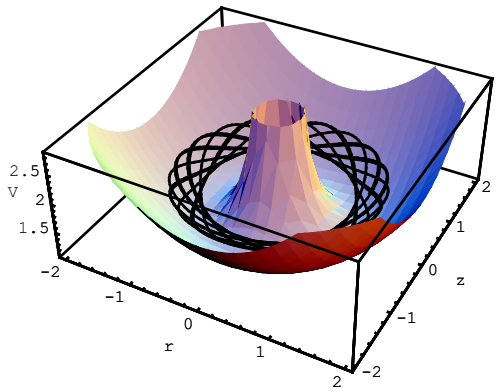
$$\rho'' + \rho - \frac{v^2}{\rho^3} = \frac{\rho}{\left(\sqrt{\rho^2+\zeta^2}\right)^3},$$

$$\zeta'' + \lambda^2\,\zeta = \frac{\zeta}{\left(\sqrt{\rho^2+\zeta^2}\right)^3},$$

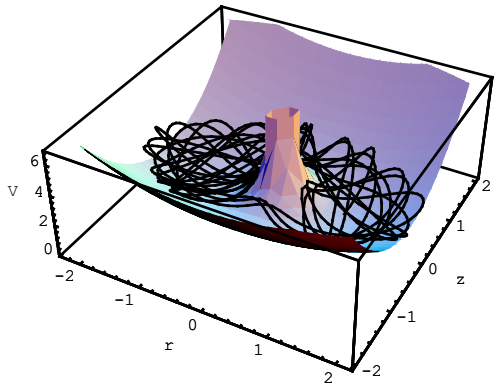
containing only two parameters v and λ. The handling of Eqs. (4.4.90) and (4.4.91) is easier than the four parameter representation in equations (4.4.88) and (4.4.89). Note that Eqs. (4.4.90) and (4.4.91) are equivalent to the secular equations of the Paul trap. Both systems of equations are derived from a Lagrangian given by

$$\mathcal{L} = \frac{1}{2}\left(\rho'^2 + \zeta'^2\right) - \left(\frac{1}{2}\left(\rho^2 + 2\,\lambda^2\,\zeta^2\right) + \frac{1}{\sqrt{\rho^2+\zeta^2}} + \frac{v^2}{2\,\rho^2}\right).$$

Equations (4.4.90) and (4.4.91) form a highly nonlinear coupled system of equations which can only be solved analytically given a special choice of parameters λ and ν [4.5]. If we wish to choose parameters, we need to integrate the equations numerically. *Mathematica* supports numerical integrations and we use this property to find numerical solutions for Eqs. (4.4.90) and (4.4.91). The package **Penning`,** a listing is given in Section 4.6.3, contains the necessary function **Penningl[]** to integrate Eqs. (4.4.90) and (4.4.91). Function **Penningl[]** also provides a graphical representations of the potential and the path of the relative particle. An example of a typical path in the potential is given in Figure 4.4.11. Parameters λ and ν of this figure have been chosen so that the motion of the relative particle is regular. Figure 4.4.12 shows a path for parameters λ and ν where chaotic motion is present.



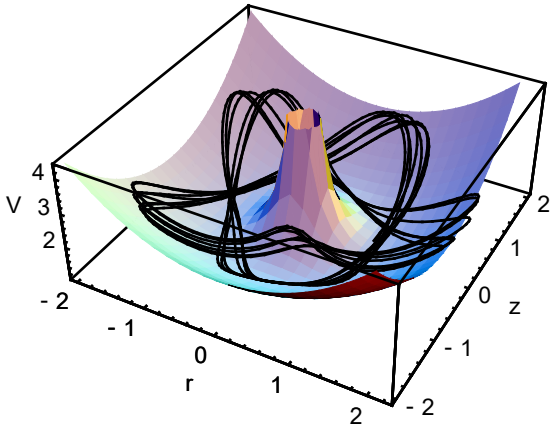
Relative motion in a Penning trap for $\lambda = 1$ and $\nu = 0$. The plot of the particle is superimposed on the effective potential. The numerical integration extends over $t \in [0,\ 100]$. The initial conditions are $\rho_0 = 1.1$, $\zeta_0 = 0.5$, $\dot{\rho}_0 = 0.0$, and $E = 2.0$.



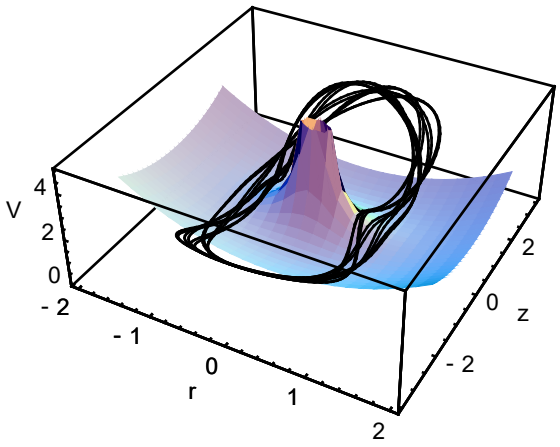
Relative motion in a Penning trap for $\lambda = 1.75$ and $\nu = 0$. The plot of the particle is superimposed on the effective potential. The numerical integration extends over $t \in [0,\ 100]$. Initial conditions are $\rho_0 = 1.0$, $\zeta_0 = 0.0$, $\dot{\rho}_0 = 0.0$, and $E = 3.0$.

Figures for different initial conditions and parameters can be generated for example by

```
PenningI[1.0, 0, 3, 0, 1.1, 100];
```

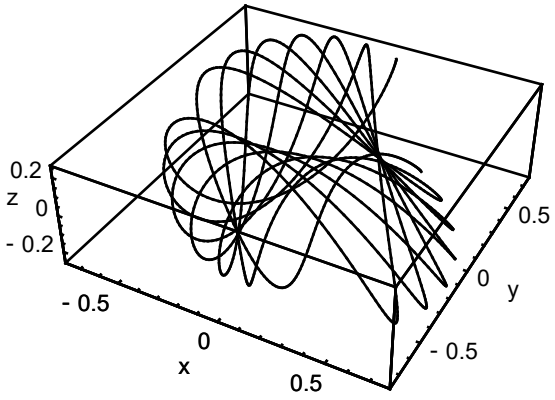



```
PenningI[1.0, 0.1, 3.6, 0, 1/Sqrt[2], 100];
```



The center of mass motion is accessible by the function **PenningCMPlot[]:**

```
PenningCMPlot[0.1, 0.2, 0.01, 0.01, 2.1];
```



4.5 Exercises

1. Create some pictures for a quadrupole arrangement of charges using the package **PointCharge'**. Choose the location of the charges in the representation plane of the potential section. What changes are required if your choice of coordinates for the charges is outside the representation plane? Perform some experiments with a larger number of charges.

2. Examine the electric potential of a disk segment under several boundary conditions using the package **BoundaryProblem'** (e.g., $\Phi_0 = \sin(\varphi)$ or $\Phi_0 = \varphi$). What changes occur in the potential if we change the angle α? Examine the influence of the upper summation index N on the accuracy of the solution.

3. Study the dynamic properties of two ions in a Penning trap for the following:

a) A vanishing angular momentum (ν=0) and different frequency ratios λ. Which λ values result in chaotic motion and in a regular motion of the particles?

b) Find solutions for $\nu \neq 0$, $\lambda = 1$ and $\lambda = 2$.

c) Examine the parameter combination $\nu = 0$ and $\lambda = \frac{1}{2}$.

4. Develop a *Mathematica* function to combine the relative and center of mass coordinates for a representation of motion in real space for the two-ion problem of a Penning trap.

5. Reexamine the Green's function formalism and discuss the problem of a rectangular boundary with one side carrying a constant charge distribution. The three other sides are fixed to the ground potential.

6. Examine a collection of three particles in a Penning trap.

7. Discuss the motion of two particles in a Penning trap for $\nu \neq 0$ and λ arbitrary.

4.6 Packages and Programs

4.6.1 Point Charges

Package for the generation of fields, potentials and energy densities.

```
BeginPackage["PointCharge`"];

(* --- load additional standard packages --- *)

Needs["Graphics`PlotField`"];

Clear[Potential,Field,EnergyDensity,FieldPlot];

(* --- export functions --- *)

Potential::usage = "Potential[coordinates_List] creates the potential of
an assembly of point charges. The cartesian coordinates of the locations of
the charges are given in the form of {{x,y,z,charge},{x,y,z,charge},...}.";

Field::usage = "Field[coordinates_List] calculates the electric field for
an ensemble of point charges. The cartesian coordinates are
lists in the form of {{x,y,z,charge},{...},...}.";

EnergyDensity::usage = "EnergyDensity[coordinates_List] calculates the
density of the energy for an ensemble of point charges. The cartesian
```

```
coordinates are lists in the form of {{x,y,z,charge},{...},...}.";

FieldPlot::usage = "FieldPlot[coordinates_List,typ_,options___] creates a
ContourPlot for an ensemble of point charges. The plot type (Potential,
Field, or Density) is specified as string in the second input variable. The
third argument allows a change of the Options of ContourPlot and
PlotGradientField.";

(* --- define the global variables x,y,z  --- *)

x::usage;
y::usage;
z::usage;

Begin["`Private`"];

(* --- determine the potential --- *)

Potential[coordinates_List]:=
      Block[{x,y,z},
      Fold[Plus,0,Map[(#[[4]]/Sqrt[(x-#[[1]])^2 +
                   (y-#[[2]])^2 +
                   (z-#[[3]])^2])&, coordinates]]];

(* --- calculate the field ---*)

Field[coordinates_List]:=
      Block[{field,x,y,z},
      field = - Fold[Plus,0,Map[(#[[4]]*({x,y,z}-Take[#,3])/
                  (Sqrt[(x-#[[1]])^2 +
                   (y-#[[2]])^2 +
                   (z-#[[3]])^2 ])^3)&,coordinates]];
      Simplify[field]
      ];

(* --- calculate the energy --- *)

EnergyDensity[coordinates_List]:=
      Block[{density,x,y,z,field},
      field = Field[coordinates];
      density = field.field/(8*Pi)
      ];

(* --- create plots  --- *)

FieldPlot[coordinates_List,typ_,options___]:=
    Block[
     {pot, ncharges, xmin, xmax, zmin, zmax, xcoord = {}, zcoord = {},
      pl1, pl2},
       ncharges = Length[coordinates];
(* --- determine limits for the plot --- *)
     Do[
     AppendTo[xcoord,coordinates[[i,1]]];
     AppendTo[zcoord,coordinates[[i,3]]],
     {i,1,ncharges}];
      xmax = Max[xcoord]*1.5;
      zmax = Max[zcoord]*1.5;
```

```
      xmax = Max[{xmax,zmax}];
      zmax = xmax;
      xmin = -xmax;
      zmin = xmin;
      Clear[xcoord,zcoord];

(* --- fix the type of the plot ---*)
      If[typ == "Potential",pot = Potential[coordinates] /. y -> 0,
      If[typ == "Field",pot = -Potential[coordinates] /. y -> 0,
      If[typ == "EnergyDensity",pot = EnergyDensity[coordinates] /. y -> 0,
      Print[" "];
      Print["  wrong key word! Choose "];
      Print["  Potential, Field or EnergyDensity  "];
      Print["  to create a plot "];
      Return[]
      ]]];

(* --- plot the pictures --- *)
       If[typ == "Field",
     pl1 = PlotGradientField[pot,{x,xmin,xmax},{z,zmin,zmax},
           options,
           PlotPoints->20,
           ColorFunction->Hue
        ],
     pl1= ContourPlot[pot,{x,xmin,xmax},{z,zmin,zmax},
          options,
          PlotPoints->50,
          ColorFunction->Hue,
          Contours->15]
      ]
       ];
End[];
EndPackage[];
```

4.6.2 Boundary Problem

The following package contains the main calculation steps for determining the expansion coefficients in the harmonic series representation of the potential.

```
BeginPackage["BoundaryProblem`", {"Calculus`Integration`"}];

Clear[Potential];

Potential::usage = "Potential[boundary_,R_,alpha_,n_] calculates the
potential in a circular segment. Input parameters are the potential on the
circle, the radius R of the circle and the angle of the segment of the circle.
The last argument n determines the number of expansion terms used to
represent the solution.";

Begin["`Private`"];

Potential[boundary_, R_, alpha_, n_] := Block[{listed = {}, int, boundaryh},
    (*---replace the independent variable in the input by Phi---*)
    boundaryh = boundary /. f_[x2_. * x1_] → f[x2 * phi];
    (*---calculate the coefficients of the expansion d_n---*)
    int = Integrate[boundaryh * Sin[m * Pi * phi / alpha], {phi, 0, alpha}] *
      R^(m * Pi / alpha) * 2 / alpha;
    Do[AppendTo[listed, If[m == 0, 0, int]], {m, 0, n}];
    (*---calculate the potential by using the sum---*)
    pot =
     Sum[listed[[n1 + 1]] * r^(n1 * Pi / alpha) * Sin[n1 * Pi * phi / alpha], {n1, 0, n}];
    (*---transform the potential to cartesian coordinates---*)
    pot1 = pot /. {r → Sqrt[x^2 + y^2], phi → ArcTan[x, y]};
    (*---graphical representation of the potential by ContourPlot---*)
    ContourPlot[ pot1 Boole[x^2 + y^2 ≤ R^2 && y > 0 && y ≤ Tan[alpha] x], {x, 0.0001, R},
     {y, 0, R} , PlotPoints -> 200, ColorFunction -> Hue, Contours → 15,
     PlotRange -> All, Epilog -> {Line[{{0, 0}, {R Cos[alpha], R Sin[alpha]}}]}]
  ];
End[];
EndPackage[];
```

4.6.3 Penning Trap

This package integrates the equations of motion for the Penning trap.

```
BeginPackage["Penning`"];

Clear[V,PenningI,PenningCMPlot];

PenningI::usage = "PenningI[r0_,z0_,e0_,n_,l_,te_] determines the numerical
solution of the equation of motion for the relative components. To integrate
the equations of motion, the initial conditions r0 = r(t=0), z0 = z(t=0) and
the total energy e0 are needed as input parameters. The momentum with respect
to the r direction is set to pr0=0. Parameters l and n determine the
shape of the potential. The last argument te specifies the end point of
the integration.";

PenningCMPlot::usage = "PenningCMPlot[x0_,y0_,x0d_,y0d_,w_] gives a graphical
representation of the center of mass motion for two ions in the Penning trap.
The plot is created for a fixed cyclotron frequency w in cartesian
```

```
coordinates (x,y,z). x0, y0, x0d, and y0d are the initial conditions for
integration.";

Begin["`Private`"];

(* --- potential --- *)
V[x_, y_, l_, n_] := (x^2 + l^2*y^2)/2 + n^2/(2*x^2) +
              1/(x^2 + y^2)^(1/2);

(*--- numerical integration of the relative motion ---*)

PenningI[r0_,z0_,e0_,n_,l_,te_]:=Block[{intk,pz0},
(* --- initial value of the momentum in z direction --- *)
    pz0 = Sqrt[2*(e0-V[r0,z0,l,n])];
(* --- numerical solution of the initial value problem --- *)
intk = NDSolve[{pr'[t] == n^2/r[t]^3 - r[t] +
              r[t]/(r[t]^2+z[t]^2)^(3/2),
        pz'[t] == -l^2*z[t] + z[t]/(r[t]^2+z[t]^2)^(3/2),
        r'[t]  == pr[t],
        z'[t]  == pz[t],
(* --- initial values --- *)
         r[0] == r0, z[0] == z0, pr[0] == 0, pz[0] == pz0},
     {r,z,pr,pz},{t,0,te}, MaxSteps->6000];
(* --- graphical representation --- *)

(* --- plot the potential --- *)
Show[
    Block[{$DisplayFunction=Identity},
      {Plot3D[V[x,y,l,n]-0.4,{x,-2,2},{y,-2,2},Mesh->False,
         PlotPoints->25],
(* --- plot the tracks by ParametricPlot3D --- *)
      ParametricPlot3D[Evaluate[{r[t],z[t],V[r[t],z[t],l,n]} /. intk],
             {t,0,te},PlotPoints->1000,
                  AxesLabel->{"r","z","V"}]}
      ],
                  AxesLabel->{"r","z","V"},
                  Prolog->Thickness[0.001],
                  ViewPoint->{1.3,-2.4,2}
    ]

                  ];


(* --- center of mass motion in the Penning trap --- *)

PenningCMPlot[x0_,y0_,x0d_,y0d_,w_]:= Block[{w0, a1, b1},
(* --- fix parameters Omega_0 = 1.0 --- *)
      w0 = 1.0;
      a1 = 0.25;
      b1 = 0.0;
      If[w <= 2*w0,Print[" "];
        Print[" cyclotron frequency too small"];
        Print[" choose w > 2"],
(* --- determine the amplitudes from the initial conditions --- *)
      gl1 = 2*ar + 2*br - x0 == 0;
      gl2 = -2*ai - 2*bi - y0 == 0;
      gl3 = 2*bi*w1 + 2*ai*w2 - x0d == 0;
```

```
      gl4 = 2*br*w1 + 2*ar*w2 - y0d == 0;
      result = Flatten[N[Solve[{gl1,gl2,gl3,gl4},{ar,ai,br,bi}]]];
(* --- solutions for the center of mass motion --- *)
x = 2*br*Cos[w1*t] + 2*bi*Sin[w1*t] + 2*ar*Cos[w2*t] + 2*ai*Sin[w2*t];
y = 2*ar*Sin[w2*t] - 2*ai*Cos[w2*t] + 2*br*Sin[w1*t] + 2*bi*Cos[w1*t];
z = a1*Cos[Sqrt[2 w0]*t + b1];
(* --- define frequencies --- *)
w1 = wc/2 + Sqrt[(wc/2)^2 - w0];
w2 = wc/2 - Sqrt[(wc/2)^2 - w0];
(* --- substitute the results result into the variables x, y, and z --- *)
x = Simplify[x /. result];
y = Simplify[y /. result];
x1 = x /. wc -> w;
x2 = y /. wc -> w;
x3 = z /. wc -> w;
(* --- plot the solution --- *)
ParametricPlot3D[{x1,x2,x3},{t,0,60},AxesLabel->{"x","y","z"},
         PlotPoints->1000,
         Prolog->Thickness[0.001]]
      ]];
End[];
EndPackage[];
```

Next Notebook