EM field, tracking and scattering simulations for the KATRIN experiment

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Abstract. The aim of the KATRIN experiment is to determine the absolute neutrino mass scale in a model independent way, by measuring the electron energy spectrum shape near the endpoint of tritium beta decay. For this purpose, the KATRIN experiment uses two spectrometers with high voltage, and many superconducting and air coils, to create the necessary electric and magnetic fields. In order to design the spectrometer electrodes and the coils, and to investigate and understand the various background processes and systematic effects, one needs various accurate electric and magnetic field, charged particle tracking and scattering computations, for which we use mainly our self-written C and C++ codes.

1. The KATRIN experiment
Neutrino oscillation studies during the past 15 years have proved that the neutrinos have non-zero masses. However, they yield no information on the absolute neutrino mass scale. Neutrinoless double beta decay experiments and cosmological observations are sensitive to the absolute neutrino mass scale, but they are rather model dependent. The KATRIN (Karlsruhe Tritium Neutrino) experiment [1] plans to determine the absolute neutrino mass scale in a direct and model independent way with a sensitivity of 200 meV, by measuring the integral electron energy spectrum shape close to the tritium beta decay endpoint (18.6 keV).

Fig. 1 shows the experimental setup of the KATRIN experiment. The electrons are created in the windowless gaseous tritium source by beta decay of T$_2$ molecules and are guided by high magnetic field (a few T) of many superconducting coils in the transport system towards the spectrometers. The pumping section reduces the tritium flow towards the spectrometers by many orders of magnitude. The main spectrometer (length: 23 m, diameter: 10 m, magnetic field at center: 0.3 mT) collimates the electrons by the inverse magnetic mirror effect and analyzes their energy by its high negative potential (around -18.6 kV). Inside the main spectrometer a complicated wire electrode system has been installed; this consists of 0.2 and 0.3 mm diameter wires with 40 km total length, and its main task is to reduce the background.

The KATRIN experiment requires various detailed electromagnetic field, charged particle tracking and scattering computations. For this purpose, we use mainly our self-written C and C++ codes developed in the past 10 years. The C++ package KASSIOPEIA [2] is now the standard simulation framework of the KATRIN experiment.
2. Electromagnetic field computations

2.1. Magnetic field

The KATRIN system contains about 70 superconducting and air coils. In addition, these magnets are surrounded by a lot of magnetic materials. The precise and reliable computation of the magnetic field from these sources is an important task of the KATRIN experiment.

For the calculation of the axisymmetric coils we use the zonal harmonic expansion. This is a special version of the spherical harmonic method, applied for axisymmetric systems. It can be 100–1000 times faster than the more widely known elliptic integral method, and it is more general than the similar radial series expansion. It has not only high speed but also high accuracy, which makes the method especially appropriate for trajectory calculations of charged particles. Due to these properties, no interpolation is necessary when the magnetic field during particle trajectories is computed with the aid of the zonal harmonic method.

The zonal harmonic field series formulas are convergent at field points within the central and remote regions, which have spherical boundaries, and their center, the source point, can be arbitrarily chosen on the symmetry axis. The rate of convergence of the field series depends on the distance of the field and the source point; smaller distance for central field points and larger distance for remote field points correspond to higher convergence rate. The zonal harmonic method is applicable also for special three-dimensional magnetic systems, whose components (coils or magnetic materials) are axially symmetric in their own local coordinate systems. See Ref. [3] for more details.

Some of the KATRIN coils (earth field compensation coils, dipole coils) are not axisymmetric; they are computed by integrated Biot-Savart formulae. In order to accelerate the speed of these calculations we use three-dimensional Hermite interpolation. The field of the magnetic materials in the KATRIN buildings is computed by equivalent (fictitious) magnetic charges.

2.2. Electric field

Some parts of the KATRIN electrode system are approximately axisymmetric. In order to compute the electric field of axisymmetric electrodes, one can use again the zonal harmonic expansion method, like in the case of magnetic field [4]. The sources of the electric field — the charges on the electrode surfaces — are usually not known in the beginning of the field calculation. The most natural way to compute the charge densities is by the boundary element method (BEM). With BEM, one has to discretize only the two-dimensional surface of the electrodes, not the whole three-dimensional space of the electrode system, as it is the case using the finite difference and finite element methods. The electrode system is then approximated by \( N \) subelements (e.g. axisymmetric conical elements): in our method, the charge density of each element is assumed to be constant over the element surface. The Coulomb matrix elements \( C_{ij} \), defined as the potential at the centre of element \( i \) due to the element \( j \) with unit charge...
density, can be computed by some routines in our codes. The potential $U_i$ of the element $i$ is connected with the charge densities $\sigma_j$ by the linear equation system: $U_i = \sum_{j=1}^{N} C_{ij} \sigma_j$. The $N$ charge densities can be computed by some direct method (like Gauss-Jordan elimination). The source constants that are needed for the zonal harmonic expansions can be calculated using these charge density values.

The BEM is also useful for general 3-dimensional electric field computations. It is especially advantageous for electrodes having small scale structures within large volumes, like the wire electrode system of KATRIN. In order to get a sufficient discretization of the KATRIN wire electrode system of KATRIN. In order to get a sufficient discretization of the KATRIN wire electrodes, more than 1 million subelements are necessary. On the other hand, using the above scheme, the number of different charge densities $N$ cannot be more than several 10000, otherwise the Coulomb matrix does not fit into the computer main memory (and the charge density computation time becomes also extremely large). One method to solve this problem is by using the approximate rotational symmetry of the wire electrodes. For example, in the cylindrical part of the KATRIN main spectrometer there are 1200 wires in the azimuthal direction, and all of them have approximately the same charge density. Using this symmetry, the number of geometrical subelements can be much larger than the number of different charge densities.

Another possibility to overcome the charge density number limit is by using an iterative method to solve the above linear algebraic equation system. The Robin Hood method [5], which is similar to the well-known Gauss-Seidel iterative algorithm, has several advantages relative to the direct method: i, the memory requirement grows only linearly with $N$, instead of quadratically; ii, it can be easily parallelized; iii, the computation time grows quadratically with $N$, instead of the third power.

3. Relativistic charged particle tracking with explicit Runge-Kutta method
The first-order differential equation system $\dot{y}(t) = f(y, t)$, $y(t_0) = y_0$ (the $y$, $y_0$ and $f$ vectors having generally $n$ components) can be solved by the explicit $s$-stage Runge-Kutta method defined by

$$y(t_0 + h) = y_0 + h \sum_{j=1}^{s} b_j k_j, \quad (1)$$

$$k_j = f(y_0 + h \sum_{l=1}^{j-1} a_{jl} k_l, t_0 + h c_j) \quad (j > 1), \quad k_1 = f(y_0, t_0). \quad (2)$$

The coefficients $b_j$, $c_j$, $a_{jl}$ ($j = 1, \ldots, s; l = 1, \ldots, j-1$) can be found in various Runge-Kutta tables (see e.g.: [6, 7, 8, 9]). The number of function evaluations during a Runge-Kutta step is proportional to the stage $s$. The local and the global errors are proportional to $h^{p+1}$ and $h^{p}$, respectively, where $p$ is the order of the Runge-Kutta method. The classical Runge-Kutta method has $p = 4$ and $s = 4$. The Runge-Kutta methods of [6, 7, 8] have $p = 8$ (eighth-order) and require $s = 13$ stages. According to our experience, these eighth-order Runge-Kutta methods are much more efficient (have much better precision for a given computation time) than the fourth-order classical Runge-Kutta method.

The relativistic charged particle motion can be expressed by the first order differential equations $\dot{x} = v$, $\dot{v} = F_L$, where $x$, $v$ and $p$ are the space coordinate, velocity and relativistic momentum 3-vectors, and $F_L = Q (E + v \times B)$ denotes the Lorentz force ($Q$ is the charge of the particle, $E$ and $B$ are the electric and magnetic field vectors). In this case the vectors $y$ and $f$ both have 6 components: the first 3 components are defined by $y_i = x_i$ and $f_i = v_i$ ($i = 1, \ldots, 3$); the second 3 components are then $y_i = p_{i-3}$ and $f_i = F_{Li-3}$ ($i = 4, \ldots, 6$).

The time step $h$ should be automatically controlled by the computer code. For this control we use several different methods. For example, $h = P_c/m$, where $P_c$ denotes the cyclotron motion period, and the $m$ integer is around 20 to 50 (higher $m$ value corresponds to higher accuracy
level, but more computation time). Another simple possibility is \( h = s/v \), where \( s \) is some user-defined distance and \( v \) the particle velocity. The widely used time step control is by local error estimation and embedded Runge-Kutta formulae [10].

In the case of time-independent fields, the accuracy of our trackings can be tested by energy conservation. Due to the high accuracy of our fields and to the high order of our Runge-Kutta method, the relative change of the energy of our tracked charged particles was in many cases order of \( 10^{-10} \) or smaller, even for very large tracking time values. In addition, in order to estimate the global error of a charged particle trajectory, one can perform the tracking with two different time step series (e.g. the second tracking can have twice smaller steps than the first one), and then one compares the coordinate and velocity values of the two tracks corresponding to the same tracking time. Often, these coordinate and velocity values agree quite well, even for large tracking time, certifying again the high accuracy of our field and tracking computations. On the other hand, in the case of higher energy stored electrons in the KATRIN main spectrometer, it occurs often that after some time value the two trajectories start to deviate (diverge) strongly from each other. It turned out that these divergences of the trajectories with different time steps are due to chaotic motion of non-adiabatic electrons; in this case, it is not possible to improve significantly the long-time accuracy of the numerical tracking method.

In addition to exact tracking described above, we use also adiabatic tracking. In this case we compute first the motion of the guiding center in the adiabatic approximation, assuming that for the motion along the magnetic field line the first adiabatic invariant is constant [11], and using also the magnetron drift perpendicularly to the magnetic field line. The gyration of the charged particle along the guiding centre is also taken into account. The adiabatic tracking can be used only if the charged particle motion is approximately adiabatic. But in this case the adiabatic tracking can be 100 times faster than the exact tracking.

4. Electron–hydrogen molecule scattering

The KATRIN source contains molecular tritium with a few times \( 10^{-3} \) mbar pressure, and the beta decay electrons can have collisions with \( T_2 \) molecules. In addition, \( H_2 \) molecules are expected to provide the main part of the residual gas in the KATRIN vacuum system, and stored electrons can collide with these \( H_2 \) molecules even if the vacuum pressure is as low as \( 10^{-11} \) mbar. Therefore, to investigate and understand various background processes and systematic effects, one has to perform electron-\( H_2(T_2) \) scattering simulations. In our codes, we use total and angular differential cross sections for elastic, electronic excitation, ionization, vibrational and rotational excitation scatterings [12, 13, 14], for electron kinetic energy range from a few meV up to a few times 100 keV.

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