quantum multipole expansion

(automated transcription)

In this session we will combine the concept of a multipole expansion with the concept of perturbation theory. Multipole expansion that we discussed a few sessions ago, and we applied it to a classical system of two gravitationally interacting mass distributions. We also discussed perturbation theory, and now we will combine these two concepts. We will apply the multipole expansion to a quantum system, and we will realize how important perturbation theory is in order to turn that into manageable expressions. Let us first look at the ingredients which will appear in our problem. What is our problem? We have a nucleus interacting with an electron cloud. So let's first formally describe a nucleus, a free nucleus, there are no electrons around yet. The Hamiltonian that describes this free nucleus is a Hamiltonian that gives you the kinetic energy of the different nucleons, protons and neutrons inside the nucleus, and the strong interaction between the nucleons. If we would know that Hamiltonian, and nuclear physics is not yet to that level that it completely knows it, but if we would know that Hamiltonian we could apply it to the nuclear states and find the eigenvalues and eigenstates of a nucleus. These are these levels that are separated by a few kiloelectronvolts to megaelectronvolts that we saw in the first very important picture about this course. Then we turn our attention to the electrons, we forget about the nucleus and we look formally at a system of interacting electrons, there is no nucleus with which they interact. Then we have completely analogously to the nucleus problem the kinetic energy of the electrons and a term describing the electron-electron interaction. Then we can apply this Hamiltonian to a set of electrons and if there is no nucleus around we will find unbound solutions and these electrons just repel each other and try to go away from each other as far as they can. In the next step we describe these two separate problems, the free nucleus and the free electrons, in one. So there is still no interaction yet between nucleus and electrons, but we describe the two systems formally as one system. So our eigenvalues will be the sum of the eigenvalues of the nuclei and the eigenvalues of the electron system, the eigenstates will be direct products between the nuclear states and the electron states and the total Hamiltonian of the system is a Hamiltonian that works only on the nucleus subspace and a Hamiltonian that works only on the electron subspace. Why do we write that problem in such an admittedly rather artificial way? Well, because now it becomes very easy to switch on the nucleus-electron interaction and that switching on is represented by an extra term to the Hamiltonian that operates as well on the nuclear space as on the electron space. And by giving them the symbols Q-hat and V-hat you already get a hint to which kind of quantity this will be. This nucleus-electron interaction can be potentially very complicated, especially if the nucleus has a complicated shape, that is what we studied in the gravitational example, and therefore it will not be surprising that we can manage that complication by making a multipole expansion of that particular term. And in this way we can recognize in this problem again the familiar energy scales, we had already the nuclear energy scales, keV to MeV, if we take the first order term, the monopole term of this interaction Hamiltonian, then we have the atomic energy levels, energy of electron volts, and if you deal with the relativistic version of the problem, then you can have this MeV fine structure splitting, and if you now consider the higher order multipole terms, the more fine details of the electron-nucleus interaction, then you will find this micro eV splitting that corresponds to the hyperfine structure. So that is a formal translation of our gravitational problem into a nucleus interacting with electrons. Now we have to merge this with the concept of perturbation theory. Look at the Hamiltonian this way, we have the nuclear Hamiltonian which we know, and knowing doesn't mean that we can completely solve the nuclear problem from scratch, but we know the nuclear properties from experiments, and we can represent the relevant Hamiltonian of the nucleus by something that contains that experimental information. For instance, the spin operator of the nucleus, if that is for a spin 5.5 nucleus, that will be a spin 5.5 operator. So the nuclear part of the Hamiltonian is known, the interaction between the nucleus and the electron cloud up to the monopole term, that is something you studied in quantum physics, you solve the hydrogen atom in that way, and that's your usual way to think about atoms. So up to this point the Hamiltonian is known, and now you add the extra interactions due to the complicated shape of the nucleus, and that will be your perturbing Hamiltonian. So this is where you need perturbation theory. You will make use of the knowledge of the system which you already solved, your quantum physics up to now, in order to find the eigenvalues and eigenstates of the more complicated system that you don't know yet. That is repeated in this picture here, the first half of the slide, that is something you already knew, the eigenvalues and eigenstates of an atom up to the monopole term, and now you use these eigenstates together with the Hamiltonian that describes the first order corrections due to the shape of the nucleus, and by perturbation theory you find the energy corrections that are due to this complicated shape of the nucleus. Let us more exactly make the transition from the gravitational problem to the problem of an atom. This first line here gives a chain of reasoning that starts at the very left with a dot product between two identical nuclear states, which you can represent by the symbol psi n, or by the symbol i, referring to the spin of the nucleus, and because these are eigenstates of a quantum system, these states are normalized so that dot product should give 1. You could also write that dot product in an integral expression, integral over the entire space occupied by the nucleus of the complex conjugate of the nuclear wave function times the nuclear wave function itself, and in this expression you recognize something that is related to the charge density of the nucleus, or the probability density of the nucleus, so if we take that symbol rho index n as meaning the charge density of the nucleus, well if we integrate over that charge density we get the total charge of the nucleus, so if we divide by the total charge we get 1 again, as our normalization requested. A set of identities that helps to recognize the symbols that we used at the very right in the gravitational problem to something at the very left that is more familiar to the quantum context. You can do the same for the electrons. And if we now look at our fundamental expression for the gravitational potential energy in the system of interacting mass distributions, that was this expression here, well by this identification of symbols we can transform it into a quantum expression. The full energy of an atom, energy due to the interaction between the charge distribution of the nucleus and the charge distribution of the electrons can be described in this way, and what is the complicated feature here, this is this 1 over r electron minus r nucleus for which we have to use a multipole expansion. If we do that multipole expansion with the Laplace expression, and if we assume for a while that all nuclear coordinates are smaller in length than all electron coordinates, then we can write this expression here for the Hamiltonian. And this we can fill out in our formal description that we developed in the previous slides, so this complete electrostatic energy depends on a nuclear part that is known, that corresponds to this kilo electron volt to mega electron volt separation, a part that is related to the nucleus electron interaction, and that corresponds to this right hand side of the picture where up to the fine structure term you take only the monopole term of this nucleus electron interaction into account, and if you go to the hyperfine structure you take the higher order multipoles into account. How do these higher order multipoles look like, well we have them separated here in the second line of this slide, so the monopole term enters here in the first line, all higher order multipoles are in the second line, and in a quantum language you could write them in this way, so for instance the nuclear quadrupole moment tensor of a nucleus would be one where n equals two, and which has five components Q, and that is found from properties of the nuclear state I, so you make, you squeeze a particular operator R to the power n times this spherical harmonic in between the nuclear state I, and you find the corresponding component of the nuclear quadrupole moment tensor. But this can be generally done for all higher order multipoles. If we focus on the charge-charge interaction, the interaction between the nuclear charge distribution and the charge distribution of the electron cloud, then the leading term in this set of higher order multipoles will be the quadrupole term, because the dipole term turns out to vanish, that is something we have shown before. The next term would be the octupole term, which vanishes as well, so the next next term that is non-vanishing would be the hexadecapole term, which is really small. So what we will have to focus on is finding matrix elements of this operator, which is indicated here as perturbing operator H1, into the states of the unperturbed system. That was for the charge-charge interaction. How would that look like for the current-current interaction? Let's just in one slide summarize the mathematical reasoning. So we have a current distribution due to the electron cloud, a current distribution which is indicated here by a current vector J at the position R', and that current distribution gives rise to a vector potential, A of R. Now we wonder what is the energy represented by the nuclear current distribution, Jn, in the presence of this vector potential due to the electron current distribution, and that's this expression here. Now you fill out the electron vector potential that was on the first line, and you get this general expression for the current-current interaction energy based on the two current distributions Jn and Je. And again that's a complicated expression to solve, especially if these current distributions are non-trivial, so you make a multipole expansion, which is mathematically somewhat more involved now because you are dealing with these vector properties, J, but it can be done. Mathematicians have developed that formalism. So you make a multipole expansion, and the leading non-zero term is the dipole term, where you have the obnuclear property, the magnetic dipole moment of the nucleus, interacting with an electron property, the magnetic field due to that electron current distribution at the position of the nucleus. That is our leading perturbing Hamiltonian for the current-current case. So our complete perturbing Hamiltonian, where we take the charge-charge interaction as well as the current-current interaction into account, will look like this one. The quadrupole term from the charge-charge multipole expansion, the dipole term from the current-current multipole expansion. That is summarized in this overview table here. So what do we see? The first two lines deal with the charge-charge interaction. The third and fourth line deal with the current-current interaction. And in the vertical direction we have monopole, dipole, quadrupole, octupole contributions. Let's concentrate for the time being on the situations without overlap, which means that the property Rn is smaller than any Re is always fulfilled. So that will be this first line here for the charge-charge interaction, and the third line for the current-current interaction. Current-current interaction will come in later chapters. For the next few sessions we will deal with the charge-charge interaction. So what is the situation you have studied so far? That is the one that is labeled by A, and that letter A will return in the table on the next slide. So that is one where you only looked at the monopole contribution of the charge-charge interaction. We have seen in the gravitational case that there is a correction which is called the quadrupole interaction, and which is due to the shape of the charge distribution of the nucleus. If we allow overlap, if we allow Rn being larger than some of the Re's, and we will see in the next session an example of that, so if we would allow for that more general situation we will get a correction term here, actually a series of correction terms. And the same can be told about the quadrupole interaction, but there this correction will be extremely small. So only for the charge-charge interaction this same information is summarized in a slightly different table, and in order to identify the different contributions you have the same letters A, B, C, D, E here as on the previous slide. So we have in the first column all contributions that appear in the situation without overlap, so the monopole, quadrupole, hexadecapole contributions. And now for each of these multipole contributions there is an infinite series of corrections that become smaller and smaller if you would go in the horizontal direction in this table, an infinite series of corrections that takes into account this overlap. So there will be a first order overlap correction to the monopole term, a second order overlap correction to the monopole term, and so on, and then a first order overlap correction to the quadrupole term, a second order overlap correction to the quadrupole term, and so on. Whatever is indicated here in this table in red is very very small and will not be discussed in this course, whatever is indicated in black will be discussed at some point. So now we have understood why we need perturbation theory if we want to use the multipole expansion in a quantum situation, and we have an overview of the kind of terms this will lead to, interactions that we will focus on in the next sessions.