Solid State Physics
Lecture 61
Quenching of Orbital Angular Momentum

Lecture - 61

Hello. Earlier we discussed about crystal field and its consequence on the magnetic properties of a material. Mostly 3-D and other d-elements or f-elements transition metals in their magnetic properties. Now, we shall discuss about the influence of orbital angular momentum rather the quenching of orbital angular momentum. Orbital angular momentum is a fundamental property of an electron and therefore, it must have implications on the magnetic properties, but in case of 3-D transition metal elements, the orbital angular momentum usually gets quenched. We will try to understand why. (Refer Slide Time: 01:10)

In an electric field directed towards the fixed nucleus, the plane of classical orbital is fixed in a space. So, all the orbital angular momentum components that is $L_x,\ L_y,\ L_z$; they would be constants. But in quantum theory, one angular momentum component we usually take it as L_z and the square of the total angular momentum that is L^2; these are constants in central field; that means, L_z and L^2, these two quantities are constant in quantum theory. These two operators have simultaneous eigen states and $L_x,\ L_y,\ L_z$; they would be constants only in classical theory. If we consider a non central field, the plane of the orbit will move around the angular momentum components and it is no longer constant and may average out to 0; if we consider a non central field applying on it. In a crystal, L_z will no longer be a constraint of motion. Although to a good approximation, L^2 can be a constant of motion. When $\langle L_z \rangle$ = 0, the angular momentum is said to be quenched. So, $\langle L_z \rangle$ = 0 means, orbital angular momentum quenched. The magnetic moment of a state is given by the average values of the magnetic moment operator; that is expressed as $\mu_B(\overrightarrow{L} + 2\overrightarrow{S}$. In a magnetic field along the z-direction, the orbital contribution to the magnetic moment is proportional to the quantum expectation value of L_z. The orbital magnetic moment is quenched, if the mechanical moment L_z is quenched. As an example, we consider a single electron with orbital quantum number L = 1; just we take an example of this single electron. It is moving about a nucleus and the hole being placed in an inhomogeneous crystalline electric field. And we do not consider the electron spin in this case, because that is not useful. So, we have an inhomogeneous crystalline crisp electric field. Now, in a crystal of orthorhombic symmetry, the charge of neighboring ions will produce an electrostatic potential about the nucleus. We can write that electrostatic potential multiplied by the charge of an electron the charge of a proton $e\phi = Ax^2 + By^2 - (A+B)z^2$,phi is the electrostatic potential Here, A and B are constants. This expression is the lowest degree polynomial in x, y and z which is a solution of the Laplace equation. The Laplace equation would be $\Delta^2\phi = 0$ that a potential electrostatic potential must satisfy. And this would be the lowest order polynomial solution that is allowed for this Laplace equation. And this is compatible with the symmetry of the crystal. In free space, the ground state is three-fold degenerate with magnetic quantum numbers m_L = 1, 0 and -1. This is valid in free space. In a magnetic field, these levels are split by energies proportional to the magnetic field B. In a crystal, the picture may be different. (Refer Slide Time: 07:43)

We take as the three wave functions associated with the unperturbed ground state of the ion. We take three potentials U_x. We take three wave functions; $U_x = xf(r)$, $U_y = yf(r)$ and $U_z = zf(r)$. These wave functions are orthogonal and we assume that they are normalized. Each of the U's can be shown to have the property that L^2U_i any of these U's. I can take values from x, y and z. $L^2U_i = L(L+1)U_i$; that means, that is the same as $2U_i$, where L^2 is the operator for the square of the orbital angular momentum and we have written it in the units of $\hbar$. The results confirm that the selected wave functions are in fact, p functions, p orbitals having L = 1. We observe now, that the U's are diagonal with respect to the perturbation as by symmetry, the non-diagonal elements vanish. The non-diagonal elements would be like $\langle U_x|e\phi|U_y\rangle = \langle U_x|e\phi|U_z\rangle = \langle U_y|e\phi|U_z\rangle = 0$. Let us consider an example. $\langle U_x|e\phi|U_y\rangle = \int xy|f(r)|^2[Ax^4+By^2x^2-(A+B)z^2x^2]dxdydz$. This quantity is $A(I_1-I_2)$. We can write it in this form, if we define $I_1 = \int |f(r)|^2x^4dxdydz$. And $I_2 = \int |f(r)|^2x^2y^2dxdydz$. Clearly, they would be equal and this difference goes to 0. And additionally, we can write $\langle U_y|e\phi|U_y\rangle = B(I_1-I_2)$ doing similar algebra. And $\langle U_z|e\phi|U_z\rangle = -(A+B)(I_1-I_2)$ this is what we obtained. The three eigen states in the crystal field are p functions, as we said earlier with their angular lobes directed along x, y and z directions. (Refer Slide Time: 13:07)

The orbital moment of each of the levels are 0, because we can we know that $\langle U_x|L_z|U_x\rangle = \langle U_y|L_z|U_y\rangle = \langle U_z|L_z|U_z\rangle = 0$. The level still has a definite total angular momentum, since L^2 is diagonal and gives L = 1, but the projection goes to 0, but the spiral component of the angular momentum are not constants of the motion and their time average is 0 in the first approximation. Therefore, the components of the orbital angular momentum also vanish in the same approximation. The role of the crystal field in quenching process is to split the originally degenerate levels into magnetic levels separated by an energy. The energy is $\gg \mu H$, because that comes from crystal fields; so that, the magnetic field is a small perturbation in comparison with the crystal field. Magnetic field. When the magnetic field is a small perturbation compared to the crystal field, then the orbital angular momentum quenches and that happens most of the times in a crystal. At a lattice site of cubic symmetry, there is no term in the potential of the form of $e\phi$ that we mentioned here. If we have cubic symmetry, there is no term in the potential of this form; that means, quadratic in electron coordinates that kind of term does not exist for cubic symmetry. Now, the ground state of an ion with p-electron or with 1 hole in the p shell whatever; that has similar kind of wave function will be triply degenerate; however, the energy of the ion will be lowered, if the ion displaces itself with respect to the surroundings that; that means, it creates a non cubic potential effect which was shown earlier. Such a spontaneous displacement of an ion is known as the Jahn-Teller effect. Jahn-Teller effect is a spontaneous displacement of an ion that has a consequence on the quenching of the orbital momentum and many other things in the electronic structure of a crystal of a system. And this is often large and important particularly with $Mn^{+3} ions$ and Cu^{+2} ions and with holes in alkali and silver halides.