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Symmetry of a Hydrogen Atom in a Weak Magnetic Field

Sadaaki Yanagawa
Department of Applied Physics, University of Tokyo, Tokyo, Japan
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The degeneracy problem of a hydrogen atom in a uniform weak magnetic field H is considered from the standpoint of the invariance group that the system obeys. Evidently the degeneracy space has a constant z component of the angular momentum. Under such a classification, the dynamical invariance of the problem is shown to be an isomorph to the Lie group of the linear transformation of the straight line.

I. INTRODUCTION AND THEORY

The degeneracy problem of a hydrogen atom in a uniform magnetic field seems to be interesting in the field of dynamical symmetry. When the field strength H tends toward negligibly small values and the Coulomb term becomes predominant, the invariance group for the system is just the one which the hydrogen atom obeys. This degeneracy has long been discussed since the Runge-Lenz vector[1,2] was discovered, and has been reviewed elsewhere in the textbooks.[3,4] This invariance group, as is well known, is $O(4)$. In the opposite limit, on the contrary, the Hamiltonian of a free electron moving in a uniform magnetic field has an invariance group $G(0,1)$, as pointed out by the authors previously.[5,6]

In this paper the first approach to the intermedi-

ate state is studied by taking into account the first-order term of H only—namely, Zeeman terms. The Hamiltonian for a hydrogen atom in a uniform weak magnetic field H directed to the z direction is

$$\mathcal{H} = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{r} + \frac{\hbar\omega_c}{2}L_z , \tag{1}$$

where L_z is the z component of the angular momentum L and

$$\omega_c = \frac{eH}{mc}.$$

Remembering the commutation relations of the Runge-Lenz vector A and L, we can easily verify that $\mathcal{H}$ commutes with the z component of the Runge-Lenz vector, A_z, as well as L_z. Introducing the linear combinations

$$M = \tfrac{1}{2}(L + A), \tag{2a}$$

$$N = \tfrac{1}{2}(L - A), \tag{2b}$$

as in the discussion for the hydrogen atom, one constructs the following operator:

$$M_+ N_- , \tag{3}$$

where

$$M_+ = M_x + iM_y , \quad N_- = N_x - iN_y .$$

Taking into account the relations

$$M \times M = iM , \quad N \times N = iN ,$$

it is easily verified that $M_+ N_-$ commutes with $\mathcal{H}$ and L_z; namely,

$$[M_+ N_-, \mathcal{H}] = 0 \tag{4a}$$

and

$$[M_+ N_-, L_z] = 0 . \tag{4b}$$

Thus the operators L_z, A_z, and $M_+ N_-$ commute with $\mathcal{H}$, and A_z, $M_+ N_-$ commute with L_z. Further, one finds the following relation:

$$[\tfrac{1}{2}A_z, M_+ N_-] = M_+ N_- . \tag{5}$$

From the above statement, one sees that the eigenvalue E of $\mathcal{H}$ is simultaneously characterized by the eigenvalues of L_z and $\frac{1}{2}A_z$. Let us denote them n and j, respectively, and label the corresponding eigenfunction as $\psi(n, j)$. When the $M_+ N_-$ is applied to the $\psi(n, j)$, the resulting function is to be written as $\psi(n, j+1)$ and has the same energy as $\psi(n, j)$.

II. INVARIANCE GROUP AND ITS REALIZATION

Let us consider the group of linear (real) transformations of the straight line

$$y = ax + b , \quad a > 0 .$$

The structure of this two-parameter Lie group is characterized by the following commutation rule:

$$[A, B] = B ,$$

where A and B are the infinitesimal operators of the group. If one denotes the group as L_1, one finds that the invariance group of our present problem is isomorphous to the direct product group of L_1 and L_z,

$$L_1 \times L_z . \tag{6}$$

Then the space of a degenerate energy is characterized by the eigenvalue n of L_z, and by the irreducible representation j of L_1. To get the irreducible basis of L_1 explicitly let us perform the coordinate transformation after Ravndal and Toyoda,[7]

$$x = \mu\nu\cos\phi ,$$

$$y = \mu\nu\sin\phi ,$$

$$z = \tfrac{1}{2}(\mu^2 - \nu^2) .$$

One gets for $\mathcal{H}$

$$\mathcal{H} = -\frac{\hbar^2}{2m}\left[\frac{1}{\mu^2+\nu^2}\left(\frac{\partial^2}{\partial\mu^2} + \frac{1}{\mu}\frac{\partial}{\partial\mu}\right) + \frac{1}{\mu^2+\nu^2}\left(\frac{\partial^2}{\partial\nu^2} + \frac{1}{\nu}\frac{\partial}{\partial\nu}\right) + \frac{1}{\mu^2\nu^2}\frac{\partial^2}{\partial\phi^2}\right] - \frac{2e^2}{\mu^2+\nu^2} + \frac{\hbar\omega_c}{2}\left(\frac{1}{i}\right)\frac{\partial}{\partial\phi}.$$

It is to be noted that in treating this equation one must always remember that $L_z \Rightarrow n$ as noted above. By setting

$$E = -\tfrac{1}{2}m\hbar^2\epsilon^2$$

and

$$m^2\epsilon^2 \pm \frac{m\omega_c}{\hbar}n = m^2\gamma^2(\pm n) \qquad (n > 0) ,$$

the eigenvalue problem is solved as

$$E(\pm n, j_\mu, j_\nu) = -\frac{me^4}{2\hbar^2}(n + j_\mu + j_\nu + 1) \pm \frac{\hbar\omega_c}{2}n ,$$

$$\psi(\pm n, j_\mu, j_\nu) = e^{\pm in\phi} e^{-[1/2m\gamma(\pm n)]\mu^2} e^{-[1/2m\gamma(\pm n)]\nu^2} \mu^n \nu^n L^n_{n+j_\mu}[m\gamma(\pm n)\mu^2] L^n_{n+j_\nu}[m\gamma(\pm n)\nu^2] .$$

The operators $A_z(\pm n)$, $M_+(\pm n)$, and $N_-(\pm n)$ are explicitly given as

$$A_z(\pm n) = -\frac{1}{4m\gamma(\pm n)}\left[\left(\frac{\partial^2}{\partial\mu^2}+\frac{1}{\mu}\frac{\partial}{\partial\mu}+\frac{1}{\mu^2}\frac{\partial^2}{\partial\phi_\mu^2}-m^2\gamma(\pm n)^2\mu^2\right)-\left(\frac{\partial^2}{\partial\nu^2}+\frac{1}{\nu}\frac{\partial}{\partial\nu}+\frac{1}{\nu^2}\frac{\partial^2}{\partial\phi_\nu^2}-m^2\gamma(\pm n)^2\nu^2\right)\right],$$

$$M_+(\pm n) = \frac{1}{2[m\gamma(\pm n)]^{1/2}}e^{-i\phi_\mu}\left(m\gamma(\pm n)\mu-\frac{\partial}{\partial\mu}+\frac{i}{\mu}\frac{\partial}{\partial\phi_\mu}\right)\frac{1}{2[m\gamma(\pm n)]^{1/2}}e^{-i\phi_\nu}\left(m\gamma(\pm n)\nu+\frac{\partial}{\partial\nu}-\frac{i}{\nu}\frac{\partial}{\partial\phi_\nu}\right),$$

and

$$N_-(\pm n) = -\frac{1}{2[m\gamma(\pm n)]^{1/2}}e^{i\phi_\mu}\left(m\gamma(\pm n)\mu-\frac{\partial}{\partial\mu}-\frac{i}{\mu}\frac{\partial}{\partial\phi_\mu}\right)\frac{1}{2[m\gamma(\pm n)]^{1/2}}e^{i\phi_\nu}\left(m\gamma(\pm n)\nu+\frac{\partial}{\partial\nu}+\frac{i}{\nu}\frac{\partial}{\partial\phi_\nu}\right).$$

When these operators are applied to $\psi(\pm n, j_\mu, j_\nu)$, the next formula is to be noted:

$$\phi = \phi_\mu + \phi_\nu .$$

Thus we see that the eigenvalue of $A_z(\pm n)$ is $j_\mu - j_\nu$, and $M_+(\pm n)N_-(\pm n)\psi(\pm n, j_\mu, j_\nu)$ will be just $\psi(\pm n, j_\mu+1, j_\nu-1)$. In these calculations, one refers to the following formulas:

$$e^{-i\theta}\left(\beta\rho-\frac{\partial}{\partial\rho}+\frac{i}{\rho}\frac{\partial}{\partial\theta}\right)e^{\pm im\theta}e^{-\beta\rho^2/2}\rho^m L_{m+j}^m(\beta\rho^2) = \begin{cases} 2(j+1)e^{i(m-1)\theta}e^{-\beta\rho^2/2}\rho^{m-1}L_{(m-1)+(j+1)}^{m-1}(\beta\rho^2) & (+) \\ -\dfrac{2\beta}{(m+j+1)}e^{-i(m+1)\theta}e^{-\beta\rho^2/2}\rho^{m+1}L_{m+1+j}^{m+1}(\beta\rho^2) & (-) \end{cases}$$

These arguments show that the value of $\frac{1}{2}A_z$ is changed from $\frac{1}{2}(j_\mu - j_\nu)$ to $\frac{1}{2}(j_\mu - j_\nu)+1$. The energy is determined by the values n and $J = j_\mu + j_\nu$, and the degenerate bases are characterized by n and values of $J+1$ pairs which run from $(0, J)$ to $(J, 0)$. Thus for $J = 0, 1, 2, \ldots$, the irreducible representations of L_1 can be realized.

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Fine Structure of the Ti $K\beta_1\beta'$ X-Ray Emission Spectrum*

M. Pessa, E.-K. Kortela, A. Suikkanen, and E. Suoninen†
Institute of Materials Research, University of Turku, 20500 Turku 50, Finland
(Received 20 February 1973)

A complex fine structure has been resolved in the $K\beta_1\beta'$ ($3p$-$1s$ transitions) x-ray emission spectrum of pure titanium metal. The measurement was performed with a double-crystal fluorescence spectrometer. The observed fine structure has been interpreted as originating from the interaction between the unpaired $3d$ electrons and the $3p$ hole in the final state of the $K\beta_1$ transition. The calculations are based on the relative energies and intensities for free-ion states of the $3p^5 3d^2 4s^2$ configuration in the Russell-Saunders coupling scheme with and without inclusion of configuration interaction. The Landé interval rule applied to these results has been found to be of minor influence on the appearance of the theoretical spectra.

In the iron transition metals with unpaired $3d$ electrons, the multiplet splitting of inner levels has been observed in x-ray photoelectron spectra[1–3] as well as in precision x-ray emission spectra.[4–8] The main advantage of x-ray emission spectroscopy (XS) over x-ray photoelectron spec-