CHAPTER III

LENZ VECTOR IN THE COULOMB FIELD

In this chapter the Lenz Vector in the Coulomb field used by Pauli to solve the hydrogen atom problem is introduced. According to the matrix mechanics, all physical quantities taken from classical mechanics have to be replaced by analogously constructed matrix quantities which satisfy the equation of motion in classical mechanics. The vector matrix corresponds to the Lenz vector and its algebraic rules will be shown in section 3.2. By straightforward processes of noncommutative algebra, the system of matrix relations contributed by this vector matrix will be finally obtained

3.1 Historical Introduction

Consider a system of an electron, mass m_o, moving around the nucleus under the influence of a Coulomb field. If

$$\vec{L} = \vec{r} \times \vec{p} \tag{3.1}$$

denotes the time-independent angular momentum of the electron about the nucleus, and

$$\vec{p} = m_o\vec{v}$$

the linear momentum, then it can be shown directly from the equations of motion in classical mechanics that the vector

$$\vec{U} = \frac{1}{m_o e^2}(\vec{L} \times \vec{p}) + \frac{\vec{r}}{r} \tag{3.2}$$

is constant in time. To prove directly the property of this vector, we may start with Newton's law of motion for a particle in a Coulomb field,

$$\frac{d\vec{p}}{dt} = -\frac{e^2}{r^3}\vec{r}$$

Then

$$\vec{L} \times \frac{d\vec{p}}{dt} = -\frac{e^2}{r^3}(\vec{L} \times \vec{r}) = -\frac{e^2}{r^3} m_o(\vec{r} \times \frac{d\vec{r}}{dt}) \times \vec{r}$$

This works out to be

$$\frac{d}{dt}\left[\frac{1}{m_o e^2}(\vec{L} \times \vec{p}) + \frac{\vec{r}}{r} \right] = 0 \quad ,$$

showing that $\vec{U}$ is a constant of motion

Historically (6, 7) , when W. lenz made use of this vector to calculate the energy levels of perturbed Kepler motions on the basis of the old quantum theory, he referred to a text by C. Runge on vector analysis. Runge had briefly shown that in the Kepler problem, if the central force varies inversely as the square of the distance, another constant vector can be obtained from the equation of motion. This vector is then sometimes called "Runge-Lenz Vector".

Scalar multiplication with $\vec{r}$ in Eq. (3.2) then gives

$$\vec{U}.\vec{r} = -\frac{1}{m_o e^2} L^2 + r \qquad (3.3)$$

This is the equation of a conic section, and it can be seen that $\vec{U}$ lies along the major axis of the ellipse and that its magnitude is equal to the numerical eccentricity of the ellipse (see Appendix A) Squaring (3.2), one obtains

$$1 - U^2 = - \frac{2E}{m_o e^4} L^2 \qquad (3.4)$$

where E represents the energy

In the next section it will be shown that in the matrix mechanics, a time-independent vector matrix $\hat{\vec{U}}$ analogous to (3.2) can be introduced for which, together with the vector matrix of angualr momentum $\hat{\vec{L}}$ (also constant in time), relations analogous to (3.3) and (3.4) hold. Then, by the processes of noncommutative algebra, the system of matrix relations that comprise only the time-independent matrices $\hat{\vec{U}}$, $\hat{\vec{L}}$ and $\hat{E}$, will be obtained, the coordinates have been eliminated.

3.2 The Vector Matrix $\hat{\vec{U}}$ for Coulomb Forces. Elimination of the Coordinates

Let us first of all remark that we shall define, as in ordinary vector algebra, the scalar product of any two vector matrices $\hat{\vec{A}}$ and $\hat{\vec{B}}$ as the expression

$$\hat{\vec{A}} \cdot \hat{\vec{B}} = \hat{A}_x \hat{B}_x + \hat{A}_y \hat{B}_y + \hat{A}_z \hat{B}_z \qquad (3.5)$$

and the vector product $\hat{\vec{A}} \times \hat{\vec{B}}$, as a new vector matrix having components

$$(\vec{A} \times \vec{B})_x = \hat{A}_y \hat{B}_z - \hat{A}_z \hat{B}_y \, , \ldots \qquad (3.6)$$

In general, the order of the factors for $\hat{\vec{A}}$ and $\hat{\vec{B}}$ is important : the expressions $\hat{\vec{A}} \cdot \hat{\vec{B}} - \hat{\vec{B}} \cdot \hat{\vec{A}}$ and $(\hat{\vec{A}} \times \hat{\vec{B}}) + (\hat{\vec{B}} \times \hat{\vec{A}})$ do not in general vanish here, since the commutation law for multiplication does not apply. Also, the components of the vector product $\hat{\vec{A}} \times \hat{\vec{A}}$

of a matrix $\hat{\vec{A}}$ with itself are in general different from zero

$$(\hat{\vec{A}} \times \hat{\vec{A}})_x = \hat{A}_y\hat{A}_z - \hat{A}_z\hat{A}_y \ , \ldots \tag{3.7}$$

We now introduce a vector matrix

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} \tag{3.8}$$

which represents the angular momentum of the particle about the origin. This matrix satisfies the commutation rule (8) :

$$\left[\hat{L}_\alpha \ , \ \hat{x}_\beta\right] = - \frac{h}{2\pi i} \epsilon_{\alpha\beta\gamma} \hat{x}_\gamma \tag{3.9}$$

where $[\ ,\ ]$ denotes the commutator

and $\epsilon_{\alpha\beta\gamma}$ stands for the following anti-symmetrical tensor

$$\epsilon_{\alpha\beta\gamma} = \begin{cases} 0 & \text{if two indices are equal} \\ +1 & \text{if } \alpha, \beta, \gamma \text{ are obtained by even permutation of 1,2, 3} \\ -1 & \text{if } \alpha, \beta, \gamma \text{ are obtained by odd permutation of 1, 2, 3} \end{cases}$$

and also (8)

$$\left[\hat{L}_\alpha \ , \ \hat{p}_\beta\right] = - \frac{h}{2\pi i} \epsilon_{\alpha\beta\gamma} \hat{p}_\gamma \tag{3.10}$$

Further, we have the commutability of $\hat{r}$ with $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$,

$$\hat{r}\hat{\vec{L}} = \hat{\vec{L}}\hat{r} \quad \text{and} \quad \hat{r}\hat{L} = \hat{L}\,\hat{r}$$

Therefore every function $F(\hat{r})$ of $\hat{r}$ alone commutes with $\hat{\vec{L}}$. If we are dealing with central force, for which the potential energy depends only on $\hat{r}$,

$$\frac{1}{2} m_o \hat{\vec{v}}^2 + F(\hat{r}) = \hat{E} \quad \text{(diagonal matrix)} \tag{3.11}$$

it follows that

$$\hat{E}\hat{\vec{L}} = \hat{\vec{L}}\hat{E}$$

and hence the vector matrix $\hat{\vec{L}}$ remains constant with time

For the vector product of $\hat{\vec{L}}$ with itself (see (3.7)), it is easy to obtain a relation which will be of use later on,

$$\hat{\vec{L}} \times \hat{\vec{L}} = -\frac{h}{2\pi i} \hat{\vec{L}} \tag{3.12}$$

For example, from (3.9) and (3.10) we obtain for the z-component of $\hat{\vec{L}} \times \hat{\vec{L}}$

$$\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x = \hat{L}_x(\hat{z}\hat{p}_x - \hat{x}\hat{p}_z) - (\hat{z}\hat{p}_x - \hat{x}\hat{p}_z)\hat{L}_x$$

$$= (\hat{L}_x\hat{z} - \hat{z}\hat{L}_x)\hat{p}_x - \hat{x}(\hat{L}_x\hat{p}_z - \hat{p}_z\hat{L}_x)$$

$$= \frac{h}{2\pi i} (\hat{y}\hat{p}_x - \hat{x}\hat{p}_y) = -\frac{h}{2\pi i} \hat{L}_z$$

Let us now consider the hydrogen atom consisting of a proton having charge + e and exerting a Coulomb attraction on a single orbital electron of mass m_o and charge -e. For the Hamiltonian, we have to set

$$\frac{1}{2m_o} \hat{p}^2 - \frac{e^2}{\hat{r}} = \hat{E} \quad \text{(diagonal matrix)} \tag{3.13}$$

i.e., for this special case we set

$$F(\hat{r}) = -\frac{e^2}{\hat{r}}$$

in (3.13). And we now introduce a vector matrix $\hat{\vec{U}}$ analogously to classical mechanics (see (3.2)), defined by

$$\hat{\vec{U}} = \frac{1}{m_o e^2} \cdot \frac{1}{2} \left\{ \hat{\vec{L}} \times \hat{\vec{p}} - \hat{\vec{p}} \times \hat{\vec{L}} \right\} + \frac{\hat{\vec{r}}}{\hat{r}} \tag{3.14}$$

is constant with time in the special case of a Coulomb field of force (see Appendix B).

In spite of the differences between the classical and the quantum-theoretical varibles, we are convinced that the quantum-theoretical vector matrix, $\hat{\vec{U}}$, together with the angular momentum matrix, $\hat{\vec{L}}$, will provide the means for determining the energy eigenvalues of the hydrogen atom. We just go on to establish the following commutation relations, in which the coordinates $\hat{x}$, $\hat{y}$, $\hat{z}$, $\hat{r}$ have been entirely eliminated, leaving only the matrices $\hat{\vec{U}}$, $\hat{\vec{L}}$ and $\hat{E}$:

$$\hat{\vec{L}} \times \hat{\vec{L}} = -\frac{h}{2\pi i} \hat{\vec{L}} \tag{3.15a}$$

$$\left[\hat{L}_\alpha, \hat{U}_\beta\right] = -\frac{h}{2\pi i} \epsilon_{\alpha\beta\gamma} \hat{U}_\gamma \tag{3.15b}$$

$$\hat{\vec{U}} \times \hat{\vec{U}} = \frac{h}{2\pi i} \cdot \frac{2}{m_o e^4} \hat{E}\hat{\vec{L}} \tag{3.15c}$$

$$1 - \hat{\vec{U}}^2 = -\frac{2}{m_o e^4} \hat{E}\left(\hat{\vec{L}}^2 + \frac{h^2}{4\pi^2} \mathbb{1}\right) \tag{3.15d}$$

where $\hat{U}_\beta$ (β runs from 1, 2, 3) are x-, y- and z- component of $\hat{\vec{U}}$, respectively

Equation (3.15a) is identical with equation (3.12), (3.15b) is analogous with (3.9) in form, (3.15d) is analogous to the classical equation (3.4), the ocurrence of the additional term $\frac{h^2}{4\pi^2}\mathbf{1}$ is quantum correction. The proof of Eq. (3.15b), (3.15c), and (3.15d) will be shown in Appendix C, D, and E., respectively.

From the existence of the vector matrix $\hat{\vec{U}}$, constant in time, we can infer that the hydrogen atom constitutes a degenerate system. Namely, we can conclude from the relations derived above that in general $\hat{\vec{U}}\hat{\vec{L}}^2 - \hat{\vec{L}}^2\hat{\vec{U}}$ cannot vanish. Since, on the other hand $\hat{\vec{U}}\hat{E} - \hat{E}\hat{\vec{U}}$ vanishes, it is obvious that for every value of the energy $\hat{E}$ there is not just a single value of $\hat{\vec{L}}^2$, the system is thus in fact degenerate. In this case, the individual partial vibrations of a kinematic quantity which belong to the same frequency $\nu_m^n = (E_n - E_m)/h$ are not uniquely determined, nevertheless the energy values of these state are. Futhermore, matrices which are constant with time need not in general be diagonal, in as much as non-zero elements can occupy positions (n, m) which correspond to a vanishing frequency $\nu_m^n = 0$. In principle it should be possible to derive the energy spectrum from equations (3.15a) to (3.15d) without any further specifying assumptions as to the type of solution.

If the degeneracy is removed by an additional perturbing field whose Hamiltonian is H_1, then the time-average of the perturbation function $\bar{H}_1$, taken over the unperturbed motion, must be a diagonal matrix. In this case, this mean value depends not only on the energy E of the unperturbed motion but also on $\hat{\vec{L}}$ and $\hat{\vec{U}}$. If, in particular, the perturbing field is due to an additional non-Coulomb central force the above time average depends only on $\hat{\vec{L}}^2$ (apart from its E-dependence), since there exists no preferred direction in space here. Further, the perturbation energy of a magnetic field in the z-direction depends only on the momentum component $\hat{L}_z$, which is parallel to the field. The requirement that $\hat{\vec{L}}^2$ and $\hat{L}_z$ are to be diagonal matrices therefore leads to a special solution of

equations (3.15a) to (3.15d), i.e., the energy spectrum. The fact that the hydrogen atom can be perturbed in such a way that its degeneracy is removed and its energy eigenvalues are described by the eigenvalues of the matrices $\hat{L}^2$ and $\hat{L}_z$ play an important role in our calculation. We will treat this case in the next chapter.