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T.Paszkiewicz

CONSTRUCTION OF THE TIME-REVERSED WAVE FUNCTION FOR A CHARGED PARTICLE MOVING IN A HOMOGENEOUS DC MAGNETIC FIELD

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The property of invariance under the time reversal is an important source of selection rules for matrix elements, statistical mean values, correlation functions, kinetic coefficients, etc. The derivation of such rules is essentially based on the (formal) use of "time-reversed" state vectors, or "time-reversed" wave functions (cf. Martin [1]). For kinetic coefficients, such as the tensor of electric conductivity σ, this microscopic approach yields the famous Onsager relations. These relations connect the elements of such tensors. For example, in the case of electric conductivity in the DC homogeneous magnetic field $\vec{h}$ these relations read

$$\sigma_{\alpha\beta}(\vec{h}) = \sigma_{\beta\alpha}(-\vec{h}).$$

The reason why one should change the orientation of the magnetic field $\vec{h}$ is clear. One can use the classical arguments. Since the time-reversed state means the state of reversed motion, to get such a motion in the magnetic field, one should reverse the valocities of charged particles and also reverse the orientation of the magnetic field (cf. Gottfried [2]).

The macroscopic derivation of the Onsager relation is based on the principle of positive production of the entropy in the nonequilibrium state (cf. de Groot, Mazur [3]). The microscopic quantum mechanical theory gives the explicit expressions for kinetic coefficients but it needs the use of time-reversed (the motion-reversed) states. In the framework of quantum mechanics and in the case of absence of the magnetic field such a discussion is presented in many textbooks (cf. Chapter 26 of Wigner's Group Theory [4] , Sec.39 of Gottfried's Quantum Mechanics [2], or Sec.1.46 of Roman's Advanced Quantum Theory [5]). It seems, however, that there is lack of such a discussion in the case of motion in the magnetic field. It is the purpose of this paper to present such a discussion.

For reasons of simplicity we like to consider the simplest exactly solvable example. We choose a free charged particle in the DC homogeneous magnetic field. This problem was firstly solved by Landau in 1930, his discussion can be found, for example, in Quantum Physics by Gasiorowicz [6]. Landau has shown that the motion in the plane perpendicular to the vector of the magnetic field $\vec{h}$ (transversal motion) separates from the motion along an axis parallel to $\vec{h}$. After Landau we assume that the magnetic field $\vec{h}$ is chosen to define the z-direction. He has also shown that the transversal motion is bounded and the orbits are circular. Thus the motion is quantized and is characterized by the Larmore frequency $\Omega = eh/(\mu c)$ and by the so-called classical radius of the ground (Landau) level $\ell = \sqrt{\hbar/\mu\Omega}$. Here e is the charge, μ is the mass of a particle, c is the velocity of light. Landau has shown that the discussed problem is equivalent to the problem of linear harmonic oscillator. Johnson and Lippmann /7/ and later Feldman and Kahn /8/ proposed an elegant algebraic formulation of it. In section 1 we consider a minor generalization of the results obtained by Feldman and Kahn /8/. They discuss the motion of a charged particle in the field oriented parallel to the z axis. We shall introduce the matrix notation for both orientations, parallel and antiparallel, simultaneously. In Sec.2 the properties of state vectors and wave functions are discussed. The matrix notation allows us to introduce the operator of the time-reversal in a rather natural way. An example of the derivation of the selection rule is given in Sec.4.

1. THE ALGEBRA OF VARIABLES

Since the magnetic field $\vec{h}$ is directed along the z axis, parallel or antiparallel, the vector potential is

$$\vec{A} = \pm\left(-\frac{\mu c\Omega}{2} y,\ \frac{\mu c\Omega}{2} x,\ 0 \right).$$

To take into account both allowed orientations of the magnetic field, we shall introduce the direct product representation for variables related to the transverse motion. The general discussion of this representation is given, for example, by Byron and Fuller /9/. The transverse components of the kinematic momentum Π_x, Π_y in this representation are

$$\Pi_x = I_2 \otimes p_x - \frac{1}{2}\mu\Omega\sigma_z \otimes y, \quad \Pi_y = I_2 \otimes p_y + \frac{1}{2}\mu\Omega\sigma_z \otimes y, \qquad (1a,b)$$

I_2 being the unit matrix in the two-dimensional linear space C_2, σ_z is the 2x2 matrix $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$. The operators p_x, p_y, x, y are acting in space L_2 as respective components of the momentum and position operators satisfying the canonical commutation relations. The operators Π_x, Π_y act in the Hilbert space $\mathcal{H} = C_2 \otimes L_2$. As vectors of the basis in C_2 we choose the eigenvectors of the operator σ_z, which we denote by u_σ

$$\sigma_z u_\sigma = \sigma u_\sigma \qquad (\sigma = \pm 1).$$

The Hamiltonian of transverse motion is

$$H_t = \frac{1}{2\mu}(\Pi_x^2 + \Pi_y^2). \qquad (2)$$

This Hamiltonian commutes with the operator of the z components of the angular momentum $I_2 \otimes L_z$ /8/

Let us introduce raising and lowering operators, which we shall denote by a, a^+ respectively

$$a^+ = (2\mu\hbar\Omega)^{-1/2}\,\Pi_+, \qquad (3a)$$

$$a = (2\mu\hbar\Omega)^{-1/2}\,\Pi_-, \qquad (3b)$$

where Π_+, Π_- are linear combinations of Π_x, Π_y

$$\Pi_\pm = \Pi_x \pm i\sigma_z \Pi_y. \qquad (4a,b)$$

The operators a, a^+ are easily seen to obey the commutation rule

$$[a, a^+] = I_2 \otimes I_t,$$

where I_t is the unit operator acting in L_2.

The transverse motion Hamiltonian can be expressed in terms of a^+, a as

$$H_t = \hbar\Omega\left(a^+ a + \frac{1}{2} I_2 \otimes I_t\right). \qquad (5)$$

It is well known that spectrum of H_t is bounded from below. The spectrum of the operator of number of quanta $N = a^+ a$ is $0, 1, 2, \ldots$. The raising and lowering operators do not commute with $I_2 \otimes L_z$

$$[I_2 \otimes L_z, a^+] = \hbar a^+ \sigma_z, \quad [I_2 \otimes L_z, a] = -\hbar a \sigma_z. \qquad (6a,b)$$

However, the operator $I_2 \otimes L_z$ commutes with N, hence, also with H_t

$$[H_t, I_2 \otimes L_z] = 0.$$

We shall introduce the operator of orientation of the magnetic field

$$S = \sigma_z \otimes I_t.$$

This operator commutes with the all introduced operators. This means that the Hilbert space $\mathcal{H}$ can be decomposed into mutually orthogonal subspaces $\mathcal{H}_+$, $\mathcal{H}_-$. Since the state vectors are labelled by the eigenvalues of the operators N, $I_2 \otimes L_z$, σ_z, these subspaces are spanned by the vectors $|n,m,+\rangle = \begin{pmatrix} |n,m\rangle_+ \\ 0 \end{pmatrix}$, $|n,m,-\rangle = \begin{pmatrix} 0 \\ |n,m\rangle_- \end{pmatrix}$, respectively. We denote these vectors by $|n,m,\sigma\rangle$. The state vectors $|n,m\rangle_+$ were introduced by Johnson and Lippmann /7/ (cf. also Feldman and Kahn /8/). The component $|n,m\rangle_-$ corresponds to a state in the magnetic field oriented antiparallel with n excited quanta and the azimuthal quantum number m. We have

$$N|n,m\sigma\rangle = n|n,m,\sigma\rangle, \quad I_2 \otimes L_z|n,m,\sigma\rangle = \hbar m|n,m,\sigma\rangle, \quad S|n,m,\sigma\rangle = \sigma|n,m,\sigma\rangle.$$

Thus, the state $|n,m,\sigma\rangle$ with $n \neq 0$ corresponds to the excited state since the energy in this state is greater than in the ground state with $n=0$.

The matrix element of any physical observable taken between two different subspaces $\mathcal{H}_+$ and $\mathcal{H}_-$ vanishes. Similarly, one can show that a vector of $\mathcal{H}$ which has components in different subspaces cannot represent a physical state of the system. (This is a special case of the superselection rule. The simple presentation of this problem is given by Roman /5/). The wave function of the state (n,m,σ) is

$$\Psi_{nm\sigma}(x,y) = \langle x,y|n,m\rangle_\sigma$$

hence, the independent two-component wave functions are

$$u_\sigma \otimes \Psi_{nm\sigma}(x,y), \quad (\sigma = \pm 1).$$

We complete the algebraic structure of the problem by introducing additionally two operators which raise or lower only the azimuthal quantum number m. These operators, which we denote by X_+, X_- are related to coordinates of the center of orbit (Kubo et al. /10/)

$$X_+ = \frac{1}{2} I_2 \otimes (x+iy) + \frac{i}{(\mu\Omega)} \sigma_z \otimes (p_x + ip_y), \tag{7a}$$

$$X_- = \frac{1}{2} I_2 \otimes (x-iy) + \frac{i}{(\mu\Omega)} \sigma_z \otimes (p_x - ip_y). \tag{7b}$$

They satisfy the commutation rules

$$[X_+, X_-] = 2\ell^2 \sigma_z \otimes I_t, \tag{8}$$

$$[I_2 \otimes L_z, X_+] = \hbar X_+, \quad [I_2 \otimes L_z, X_-] = -\hbar X_-. \tag{9a,b}$$

Using the relations

$$X_+ X_- = \frac{2}{\mu\Omega}(\hbar N - \sigma_z \otimes L_z) + \frac{\hbar}{\mu\Omega}(I_2 + \sigma_z) \otimes I_t, \tag{10a}$$

$$X_- X_+ = \frac{2}{\mu\Omega}(\hbar N - \sigma_z \otimes L_z) + \frac{\hbar}{\mu\Omega}(I_2 - \sigma_z) \otimes I_t, \tag{10b}$$

and Eqs. (9a,b), we can easily check that the operators commute with H_t

$$[H_t, X_+] = 0, \quad [H_t, X_-] = 0. \tag{11}$$

2. CONSTRUCTION OF STATE VECTORS AND WAVE FUNCTIONS

Now, we consider the state vectors. Suppose that there exist two degenerated ground states $|0,0,\sigma\rangle$

$$N|0,0,\sigma\rangle = 0, \quad I_2 \otimes L_z|0,0,\sigma\rangle = 0, \quad S|0,0,\sigma\rangle = \sigma|0,0,\sigma\rangle. \tag{12}$$

These relations are consistent with

$$a|0,0,\sigma\rangle = 0, \tag{13}$$

and in virtue of (10a,b) with

$$X_\sigma|0,0,\sigma\rangle. \tag{14}$$

We can construct the vectors of an excited state $|n,m,\sigma\rangle$ with the help of operators a^+ and $X_{-\sigma}$. Let us construct such a state vector. First of all, we shall find restrictions on the allowed values of m. With the use of the commutation rules (9a,b) and formulas (10a,b) a little algebra shows that

$$X_+|n,m,+\rangle = \sqrt{2\ell^2(n-m)}\,|n,m+1,+\rangle, \quad X_-|n,m,+\rangle = \sqrt{2\ell^2(n-m+1)}\,|n,m-1,+\rangle$$

$$X_+|n,m,-\rangle = \sqrt{2\ell^2(n+m)}\,|n,m-1,-\rangle, \quad X_-|n,m,+\rangle = \sqrt{2\ell^2(n+m+1)}\,|n,m+1,-\rangle$$

So, the states $X_+|n,n,+\rangle$, $X_+|n,-n,-\rangle$ vanish. Hence, for the state $|n,m,+\rangle$

$$-\infty \le m \le n$$

and for $|n,m,-\rangle$

$$-n \le m \le \infty.$$

The general state $|n,m,\sigma\rangle$ is obtained with the help of the operators $a^+, X_{-\sigma}$

$$|n,m\sigma\rangle = \frac{(X_{-\sigma})^{(n-\sigma m)}(a^+)^n}{\sqrt{(2\ell^2)^{(n-m\sigma)}(n-\sigma m)!n!}}|0,0,\sigma\rangle . \tag{15}$$

Similarly as in the case of an ordinary linear harmonic oscillator the conditions (13), (14) for matrix elements of the operators a , $X_{+\sigma}$ between the states $u_\sigma \otimes |x,y\rangle$ and $|0,0,\sigma\rangle$ yield the differential equations for the wave functions of ground states. The wave function of an excited state can be obtained in the way familiar to the theory of linear harmonic oscillator (cf. Baym/11/).

3. TIME-REVERSAL OPERATION

Now we shall construct the operator of the time-reversal T. We demand that operators Π_a transform in the familiar way

$$T\Pi_a T^{-1} = -\Pi_a \quad (a = x,y). \tag{16}$$

From the commutation rule for Π_x, Π_y

$$[\Pi_x, \Pi_y] = -i\mu\hbar\Omega\sigma_z \otimes I_t$$

we see that this relation is preserved if

$$T = \sigma_x \otimes \theta , \tag{17}$$

where θ is an antilinear operator. The definitions of the operators Π_x, Π_y show that θ is the familiar operator which changes the sign of momentum

$$\theta p_a \theta^{-1} = -p_a \quad (a = x,y,z).$$

In the coordinate basis θ is simply the operator of complex conjugation K (Wigner /4/, cf. also Gottfried /2/, Chern and Tubis /12/)

$$\langle\vec r|\theta|\vec r'\rangle = K\,\delta(\vec r - \vec r'),$$

where for any complex number a

$$Ka = a^* K, \quad (K = K^{-1} = K^+).$$

We should show that the Hamiltonian is invariant under the time-reversal operation. For this purpose we shall study the transformation properties of the operators a , a^+ under time reversal. By (17) and (3a,b) we have

$$TaT^{-1} = -a, \qquad Ta^+T^{-1} = -a^+ . \tag{18a,b}$$

Thus, the Hamiltonian H_t is invariant under the time reversal

$$TH_t T^{-1} = H_t .$$

This relation follows also from Eqs. (16) and (3a,b). The operator $I_2 \otimes L_z$ is odd

$$TI_2 \otimes L_z T^{-1} = -I_2 \otimes L_z . \tag{19}$$

The operators X_+, X_- transform quite differently

$$TX_+T^{-1} = X_- , \quad TX_-T^{-1} = X_+ . \tag{20}$$

The obtained rules of transformation allow us to verify that all commutation rules remain unchanged. We conclude that the introduced time-reversal operation does not change the algebraic structure of the theory.

Let us now study the transformation properties of state vectors and wave functions. It is easy to check that the vector $T|n,m,\sigma\rangle$ is proportional to $|n,-m,-\sigma\rangle$. Indeed, $T|n,m,\sigma\rangle$ corresponds to the reversed direction of the magnetic field and to the azimuthal quantum number $(-m)$

$$ST|n,m,\sigma\rangle = T\,T^{-1}ST|n,m,\sigma\rangle = -\sigma\,T|n,m,\sigma\rangle , \tag{21a}$$

$$I_2 \otimes L_z T|n,m,\sigma\rangle = TT^{-1}I_2 \otimes L_z T|n,m,\sigma\rangle = -\hbar m T|n,m,\sigma\rangle . \tag{21b}$$

The same consequences follow from relations (15), (18a,b), and (20). Since

$$(\langle n,m,\sigma|T)(T|n,m,\sigma\rangle) = \langle n,m\sigma|n,m,\sigma\rangle = 1$$

the vectors $|n,-m,-\sigma\rangle$, $T|n,m\sigma\rangle$ differ only by a phase factor.

$$T|n,m,\sigma\rangle = e^{i\delta}|n,-m,-\sigma\rangle . \tag{22}$$

Since we know the operator of the time-reversal in the coordinate basis, we can find the time-reversed wave function. We have

$$(\sigma_x \otimes K)u_\sigma \otimes \psi_{nm\sigma}(x,y) = u_{-\sigma} \otimes \psi^*_{nm\sigma}(x,y) = u_{-\sigma} \otimes \psi_{n,-m,\sigma}(x,y).$$

Thus, we conclude that we get the time-reversed wave function if we interchange the components of the two-component wave function and change the sign of the azimuthal quantum number.

4. THE SELECTION RULE FOR THE TENSOR OF ELECTRIC CONDUCTIVITY

For illustrative purposes we shall derive the selection rule for the tensor of electric conductivity $\sigma_{\mu\nu}$. For simplicity we shall consider only components of this tensor connected with the transverse motion. This means that $\mu,\nu = x,y$. To introduce the electric conduct tensor, we should define the current density operator $\vec{j}$. The electric current is both due to the motion of center and due to the orbital motion of charged particles. So, we shall introduce the relative coordinates of the cyclotron motion (Kubo et al. /10/)

$$\xi = (\Omega\mu)^{-1}\,\Pi_y\,, \qquad \eta = -(\Omega\mu)^{-1}\,\Pi_x\,,$$

and its center coordinates

$$X = (I_2 \otimes x - \xi), \qquad Y = (I_2 \otimes y - \eta).$$

Components of the current carried by a particle in the plane can be written as

$$j_x = e(\dot{X} + \dot{\xi})\,, \qquad j_y = e(\dot{Y} + \dot{\eta})\,, \tag{23}$$

where $\dot{X}$, $\dot{\xi}$, etc., mean the commutator with H_t , e.g.,

$$\dot{X} = \frac{i}{h}[H_t\,, X]\,.$$

All kinetic coefficients, i.e., the components of the tensor of electric conductivity, are connected with the statistical mean values. Such mean values are traces with the density operator ρ. However, we should remember that here we should exclude the averaging over two possible directions of the magnetic field. This means that for any variable A the mean value for a system in the magnetic field $\sigma|\vec{h}|\,\hat{z}$ is

$$\langle A\rangle_\sigma = \frac{\mathrm{Tr}(P_\sigma A P_\sigma \rho)}{\mathrm{Tr}(P_\sigma \rho)} = \frac{1}{2}\langle P_\sigma A P_\sigma\rangle\,,$$

where P_σ is the projection operator onto the subspace $\mathcal{H}_\sigma$. In the basis of vectors $|n,m,\sigma\rangle$ we have

$$\langle A\rangle_\sigma = \frac{\sum\limits_{n,m} \langle n,m,\sigma|A|n,m,\sigma\rangle\, e^{-\beta E_n}}{\sum\limits_{n,m} e^{-\beta E_n}}\,.$$

The time-reversal operation couples the mean values $\langle A\rangle_\sigma$, $\langle A\rangle_{-\sigma}$.

The Fourier transform of the electric conductivity tensor $\sigma_{\mu\nu}(\omega,\sigma)$ is given by the Kubo formula (Kubo et al. /10/)

$$\sigma_{\mu\nu}(\omega,\sigma) = \frac{1}{2V}\int_0^\infty dt\, e^{-i\omega t}\int_0^\beta d\lambda\, \langle P_\sigma\, j_\nu(-i\hbar\lambda)\, j_\mu(t) P_\sigma\rangle\,.$$

7. Johnson M.H., Lippmann B.A. Phys.Rev., 1949, 76, p.828.
8. Feldman A., Kahn A.H. Phys.Rev., 1970, 81, p.4584.
9. Byron F.W., Fuller W. Mathematics of Classical and Quantum Physics. Addison-Wesley, Reading MA, 1973, sect. 3.11.
10. Kubo R., Miyake S.J., Hashitsume N. Solid State Physics, 1965, 17, p.269.
11. Baym G. Lectures on Quantum Mechanics. Benjamin, Reading MA, 1974, p.123.
12. Chern B., Tubis A. Am.J.Phys., 1967, 35, p.254.

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