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About the Solutions of Dirac's Equations in the Presence of New Magnetic Fields

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Dirac's equations are completely solved for four entirely new configurations of the external magnetic field. The use of the quaternionic formalism simplifies the problem of separation of variables. For three of those new magnetic fields the radial equations just obtained are not classical. Section II studies them and gives their solutions in term of usual transcendental functions. When energy is quantized, energy levels are given.

The problem of finding all electrical or magnetical fields which allow a complete integration of Dirac's equations has always interested physicists. Lam[1] and Stanciu[2] have established a quasicomplete bibliography about that problem. However they omitted an important contribution of Harish-Chandra.[3] We bring our contribution by solving Dirac's equation for four entirely new configurations of the external magnetic field. The mathematical problem involved is rather complicated, and may easily be solved only if we use the following two-step procedure:

(I) separation of variables by a quaternionic method we have previously indicated,[4]

(II) resolution of the separated differential equations which, as we shall see, are not classical.

I. SEPARATION OF VARIABLES

(A) Let us first consider Dirac's equations in cylindrical coordinates:

$$ie^{-k\varphi}\frac{\partial u}{\partial r}+\frac{1}{r}\,je^{-k\varphi}\frac{\partial u}{\partial \varphi}+k\frac{\partial u}{\partial z}=-u\left(\frac{m_0c}{\hbar}\,j+\frac{\sqrt{-1}E}{c\hbar}i\right)-\frac{\epsilon\sqrt{-1}}{\hbar}\,(\mathrm{vect}P)u, \quad (1)$$

where i, j, k are the symbols of quaternions, $\sqrt{-1}$ the symbol of complex number, $\mathrm{vect}P = i\,A_x + jA_y + kA_z$ the magnetic potential, ϵ the charge of the electron.

The solution of (1) may be found under the separated form ($m = \cdots, -2, -1, 0, 1, 2, \cdots$)

$$u = e^{k\varphi/2}\; e^{(\sqrt{-1}/\hbar)p_z z}\; e^{\sqrt{-1}(m+1/2)\varphi}\times(R_1 + iR_2 + jR_3 + kR_4) \quad (2)$$

if and only if

$$\mathrm{vect}P = e^{k\varphi/2}\,(jS_3 + kS_4)e^{-k\varphi/2},$$

where S_3 and S_4 are arbitrary functions of r.

The corresponding magnetic field may be deduced; in vectorial familiar notation it is written ($r^2 = x^2 + y^2$).

$$\mathbf{B} = \mathrm{curl}\mathbf{A} = \left(\frac{y}{r}\frac{dS_4}{dr}, -\frac{x}{r}\frac{dS_4}{dr}, \frac{dS_3}{dr}+\frac{S_3}{r}\right). \quad (3)$$

Introducing (2) into (1), we deduce the radial equation for the quaternion $R = R_1 + iR_2 + jR_3 + kR_4$:

$$ir\frac{dR}{dr}+\tfrac{1}{2}\,iR+j\sqrt{-1}\,(m+\tfrac{1}{2})R+\frac{\sqrt{-1}}{\hbar}\,p_z rkR+rR\left(\frac{m_0c}{\hbar}\,j+\frac{\sqrt{-1}E}{c\hbar}\,i\right)+\frac{\epsilon\sqrt{-1}}{\hbar}\,r\,(jS_3+kS_4)R=0. \quad (4)$$

This quaternionic equation is equivalent to a system of four coupled differential equations. The extreme complexity of that system can be avoided by using the quaternionic notation. Multiplying (4) at both sides by the constant quaternion $Q = (m_0c/\hbar)\,j + (\sqrt{-1}E/c\hbar)\,i$, we see that the equation remains unchanged if we consider the new unknown function RQ. Therefore, we have

$$RQ = \lambda R, \quad \lambda = \text{scalar}.$$

That equation is equivalent to an algebraic homogeneous system of four equations; it is compatible only if

$$\lambda^2 = a^2 - b^2 \quad \text{where} \quad a = E/c\hbar \quad \text{and} \quad b = m_0c/\hbar.$$

Equation (4) is then equivalent to a coupled system of two differential equations plus two algebraic relations which give R_1 and R_4, for example, when R_2 and R_3 are known. Eliminating R_1 and R_4 and putting

$$T_2 = R_2 + R_3\sqrt{-1}, \quad T_3 = R_3 + R_2\sqrt{-1},$$

there only remains the following differential system:

$$\begin{cases} r\dfrac{dT_2}{dr}+(m+1)\,T_2+(a+b)\dfrac{p_z+\lambda\hbar+\epsilon S_4}{\lambda\hbar}\,rT_3+\dfrac{\epsilon}{\hbar}\,S_3rT_2=0, \\ r\dfrac{dT_3}{dr}-mT_3+(a-b)\dfrac{p_z-\lambda\hbar+\epsilon S_4}{\lambda\hbar}\,rT_2-\dfrac{\epsilon}{\hbar}\,S_3rT_3=0. \end{cases} \quad (5)$$

That system is exactly soluble in four cases. Let us study them. We first point out that $S_4 = $ const and $S_3 = \alpha/r$ are to be rejected because they lead to $\mathbf{B} = 0$.

1. $S_3 = (B/2)r, \quad S_4 = 0.$

Thus $\mathbf{B} = (0, 0, B) = $ constant magnetic field. This problem is classical.[5] The following are new.

2. $S_3 = \alpha \quad (= \text{const}), \quad S_4 = 0.$

Thus $\mathbf{B} = (\alpha/\sqrt{x^2+y^2})(0,0,1)$.

Decoupling system (5), we obtain second-order differential equations for T_2 and T_3 which are confluent hypergeometric equations (we deal with the case $m \geq 0$; analogous calculations hold when $m < 0$):

$$\begin{cases} T_2 = \mathrm{const}\,r^{m+1}e^{-\sqrt{N}r}F(1-n; 2m+3; 2\sqrt{N}r), \\ T_3 = \mathrm{const}\,r^{m}\,e^{-\sqrt{N}r}F(-n; 2m+1; 2\sqrt{N}r), \end{cases}$$

where

$$N = AD + \left(\frac{\epsilon\alpha}{\hbar}\right)^2 \quad \text{and} \quad A = (a+b)\frac{p_z+\lambda\hbar}{\lambda\hbar},$$

$$D = (a-b)\frac{p_z-\lambda\hbar}{\lambda\hbar},$$

$n = 0, 1, 2, 3, \cdots$, when $n = 0$, $F(1; 2m + 3; 2\sqrt{N}r)$ is not a polynomial, but in this case $T_2 = 0$ because the constant it contains is zero on account of (5).

The energy levels are given by the polynomial condition:

$$E^2 = m_0^2 c^4 + c^2 p_z^2 + (\epsilon \alpha c)^2 \frac{4n(n + 2m + 1)}{(2n + 2m + 1)^2}$$

3. $S_3 = 0, \quad S_4 = \gamma/r.$

Thus $\mathbf{B} = [\gamma/(x^2 + y^2)^{3/2}](-y, x, 0)$.

Decoupling system (5), we obtain nonclassical second-order differential equations for T_2 and T_3:

$$\begin{aligned} & r^2[d(a + b) - Ar] \frac{d^2 T_2}{dr^2} \\ & + \{Ar^2 + 2[d(a + b) - Ar]r\} \frac{dT_2}{dr} \\ & + \{(m + 1)Ar - m(m + 1)[d(a + b) - Ar] \\ & - [d(a - b) - Dr][d(a + b) - Ar]^2\} \, T_2 = 0 \end{aligned} \qquad (6)$$

(with $d = -\epsilon\gamma/\lambda\hbar$) (idem for T_3).

Problem 4 leads to the same conclusion.

4. $S_3 = \alpha, \quad S_4 = \gamma/r.$

$$\mathbf{B} = \frac{1}{\sqrt{x^2 + y^2}} \left(\frac{-\gamma y}{x^2 + y^2}, \frac{\gamma x}{x^2 + y^2}, \alpha \right)$$

is in fact the superposition of the two former fields. The theorems contained in Sec. II are necessary to solve completely problems 3 and 4.

(B) Before enunciating these theorems, we shall solve the same problem in spherical coordinates. We start with Dirac's equations in the quaternionic formalism:

$$k e^{k\varphi/2} e^{-j\theta} e^{-k\varphi/2} \frac{\partial u}{\partial r} + i e^{-k\varphi/2} e^{-j\theta} e^{-k\varphi/2} \frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{j e^{-k\varphi}}{r \sin\theta} \frac{\partial u}{\partial \varphi} = -uQ - \frac{\epsilon\sqrt{-1}}{\hbar} (\text{vect}\, P) u \qquad (7)$$

The solution of (7) may be found under the separated form ($m = \cdots, -2, -1, 0, 1, 2, \cdots$)

$$u = e^{k\varphi/2} e^{j\theta/2} e^{\sqrt{-1}(m+1/2)\varphi} \textcircled{u}(\theta) R(r),$$

where $\textcircled{u} = \textcircled{u}_1 + k\textcircled{u}_4$ and $R = (R_1 + iR_2)(1 - j)$ if $\text{vect}\, P = (1/r) e^{k\varphi/2} e^{j\theta/2} j g(\theta) e^{-j\theta/2} e^{-k\varphi/2}$.

The corresponding magnetic field is

$$\mathbf{B} = (g \cot\theta + g')\mathbf{r}/r^3.$$

g is an arbitrary scalar function of θ (except $1/\sin\theta$ because $\mathbf{B} = 0$ in that case). Both $\textcircled{u}$ and R satisfy a quaternionic equation. The R equation is analogous to the radial equation when there is no magnetic field. The $\textcircled{u}$ equation is identical to the corresponding $\textcircled{u}$ equation in the relativistic hydrogen problem apart from a factor depending upon g:

$$j \frac{d\textcircled{u}}{d\theta} - \frac{\sqrt{-1}(m + \frac{1}{2})}{\sin\theta} i\textcircled{u} + \tfrac{1}{2} j \cot\theta\, \textcircled{u} - \frac{\epsilon\sqrt{-1}}{\hbar} g i \textcircled{u} = a\textcircled{u} i.$$

That equation which becomes real if we put

$$\begin{cases} 2\textcircled{u}_1 = T_1 + \sqrt{-1}T_4 \\ -2\textcircled{u}_4 = T_4 + \sqrt{-1}T_1 \end{cases}$$

is generally insoluble except in the two following cases.

1. $g = \mu \cot\theta.$

We deduce $\mathbf{B} = \mu\mathbf{r}/r^3.$

Harish-Chandra[3] has solved that problem when there is no electrical field. Yet equations are also soluble when Coulomb field is simultaneously considered: It might be shown that the $\textcircled{u}$ equations remains unchanged while the radial equation is analogous to the hydrogen radial equation except that $(j + \frac{1}{2})^2$ must be replaced by $(j + \frac{1}{2})^2 - (\epsilon\mu/\hbar)^2$. The energy levels are therefore given by

$$E^2 = m_0^2 c^4 \left(1 + \frac{Z^2\alpha^2}{[n + \sqrt{(j + \frac{1}{2})^2 - (\epsilon\mu/\hbar)^2 - Z^2\alpha^2}]^2}\right)^{-1}$$

2. $g = \nu \tan\theta$

We deduce $\mathbf{B} = \nu(1 + r^2/z^2)\mathbf{r}/r^3.$

If $m \geqslant 0$, the $\textcircled{u}$ equation when decoupled leads to $[u = \cos^2(\theta/2);\ T_1 = u^{m/2}(1 - u)^{(m+1)/2}(1 - 2u)^{\epsilon\nu/h} V_1]$

$$\begin{aligned} & u(1 - u)(1 - 2u)V_1'' + [(1 - 2u)(m + 1 - 2mu - 3u) \\ & - (4\epsilon\nu/\hbar)u(1 - u)]V_1' + (A + Bu)V_1 = 0, \end{aligned} \qquad (8)$$

where A and B are constants. The theorems of Sec. II (idem for V_4) are absolutely necessary to solve completely that problem.

II. THREE NEW DIFFERENTIAL EQUATIONS

We have studied the three following second-order differential equations:

$$DP'' + (az^2 + bz + c)P' + (d + ez + fz^2)P = 0,$$

where $D \equiv z, z(z - 1)$ or $z(1 - z)(\alpha - z)$.

They give rise to the following theorems.

Theorem 1: $zP_n'' + (az^2 + bz + c)P_n' + (d + ez + fz^2)P_n = 0$ admits polynomial solutions if

$$\begin{cases} \left.\begin{aligned} e &= -an \\ f &= 0 \end{aligned}\right\} \text{necessary conditions} \quad (n = 0, 1, 2, \cdots) \\ c = -j \quad (= 0, -1, -2, \cdots \text{ fixed}) \\ \begin{vmatrix} S_0 & T_0 & & \\ R_1 & S_1 & T_1 & \\ \cdot & \cdot & \cdot & \\ & \cdot & \cdot & \cdot \\ & \cdot & \cdot & \cdot \\ & R_{j-1} & S_{j-1} & T_{j-1} \\ & & R_j & S_j \end{vmatrix} = 0, \end{cases}$$

where $\begin{cases} R_k = a(k - 1 - n), \\ S_k = d + bk, \\ T_k = (k + 1)(k + c). \end{cases}$

The polynomials are written as a linear combination of $j+1$ Hermite polynomials:

$$\boxed{P_n = \sum_{k=0}^{j} A_k H_{n-k}\,\frac{(az+b)}{\sqrt{-2a}}}\,, \qquad H_0 = 1,\ H_1 = 2x, \text{ etc.}$$

The A_k are solutions of the recurrent system

$$\mathcal{R}_k A_{k-1} + \mathcal{S}_k A_k + \mathcal{T}_k A_{k+1} = 0$$

$$\text{with}\ \begin{cases} \mathcal{R}_k = -\sqrt{-2a}(n-k+1)(k-j-1), \\ \mathcal{S}_k = (d+bk), \\ \mathcal{T}_k = -\frac{1}{2}\sqrt{-2a}\,(k+1). \end{cases}$$

Theorem 2: $z(z-1)P_n'' + (az^2+bz+c)P_n' + (d+ez+fz^2)P_n = 0$ admits polynomial solutions if

$$\begin{cases} \left.\begin{array}{l} e = -an \\ f = 0 \end{array}\right\} \text{necessary conditions} \quad (n = 0, 1, 2, \cdots) \\ c = j \quad (= 0, 1, 2, \ldots \text{ fixed}) \\ \begin{vmatrix} S_0 & T_0 & & & \\ R_1 & S_1 & T_1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & \cdot & \cdot & \cdot \\ & & R_{j-1} & S_{j-1} & T_{j-1} \\ & & & R_j & S_j \end{vmatrix} = 0, \end{cases}$$

$$\text{where}\ \begin{cases} R_k = a(k-1-n), \\ S_k = d + k(b+k-1), \\ T_k = (k+1)(c-k). \end{cases}$$

The polynomials are written as a linear combination of $j+1$ Laguerre polynomials:

$$\boxed{P_n = \sum_{k=0}^{j} A_k F[k-n, a+b+c; a(1-z)]}$$

$$F(a, b, y) = 1 + \frac{a}{b}\frac{y}{1!} + \cdots .$$

The A_k are solutions of the recurrent system

$$\mathcal{R}_k A_{k-1} + \mathcal{S}_k A_k + \mathcal{T}_k A_{k+1} = 0$$

$$\text{with}\ \begin{cases} \mathcal{R}_k = (k-1-c)(k-1-n), \\ \mathcal{S}_k = d - cn + k(b+2c-2k+2n), \\ \mathcal{T}_k = (k+1)(k+1-n-a-b-c). \end{cases}$$

Remark 1: Another solution deduces from the former if we simultaneously replace

z by $1-z$, $\quad c$ by $-(a+b+c)$,
a by $-a$, $\quad d$ by $d-an$,
b by $2a+b$, $\quad n$ by n.

Theorem 3: $z(1-z)(\alpha-z)P_n'' + (az^2+bz+c)P_n' + (d+ez+fz^2)P_n = 0$ admits polynomial solutions if

$$\begin{cases} \left.\begin{array}{l} e = -n(n+a-1) \\ f = 0 \end{array}\right\} \begin{array}{l}\text{necessary conditions} \\ (n = 0, 1, 2, \cdots)\end{array} \\ c = -\alpha j \quad (= 0, -\alpha, -2\alpha, \cdots \text{ fixed}) \\ \begin{vmatrix} S_0 & T_0 & & & \\ R_1 & S_1 & T_1 & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & \cdot & \cdot & \cdot \\ & & R_{j-1} & S_{j-1} & T_{j-1} \\ & & & R_j & S_j \end{vmatrix} = 0, \end{cases}$$

$$\text{where}\ \begin{cases} R_k = (k-1)(a+k-2) - n(n+a-1) \\ S_k = d + bk - (\alpha+1)k(k-1), \\ T_k = (k+1)(c+\alpha k). \end{cases}$$

The polynomials are written as a linear combination of $j+1$ Jacobi polynomials:

$$\boxed{P_n = \sum_{k=0}^{j} A_k F\left(k-n, n-k+a+j-1; \frac{a+b+c}{1-\alpha}; \frac{1-z}{1-\alpha}\right)}\,.$$

The A_k are solutions of the recurrent system

$$\mathcal{R}_k A_{k-1} + \mathcal{S}_k A_k + \mathcal{T}_k A_{k+1} = 0$$

with

$$\begin{cases} \mathcal{R}_k = \dfrac{(\alpha-1)(k-1-n)[(a+b+c)/(1-\alpha) - n + k - a - j](2n-k+a+j)(k-j-1)}{(2n-2k+a+j+1)(2n-2k+a+j)}, \\ \mathcal{S}_k = d - \alpha Bk - \alpha n(k-j) - \dfrac{1-\alpha}{(B-A-1)(B-A+1)} \\ \qquad \times \{jAB(2C-B-A-1) - [Bk + n(k-j)](1-B^2-A^2-C+CB+CA)\}, \\ \mathcal{T}_k = \dfrac{(\alpha-1)(n-k+a+j-2)[(a+b+c)/(1-\alpha) - k - 1 + n](k+1)(2n+a-k-2)}{(2n-2k+a+j-3)(2n-2k+a+j-2)}, \end{cases}$$

with $A = k - n$, $B = n - k + a + j - 1$, and $C = (a + b + c)/(1 - \alpha)$.

Remark 2: As in Theorem 2, other solutions occur when we replace in the starting equation

(a) z by $1 - z$, (c) z by $(\alpha - 1)z + 1$,
(b) z by $\alpha(1 - z)$, (d) z by $(1 - \alpha)z + \alpha$,
(e) z by αz.

The demonstrations are similiar for the three theorems. Here we prove only Theorem 3. We start from the equation

$$z(1 - z)(\alpha - z)P_n'' + (az^2 + bz + c)P_n' + (d + ez + fz^2)P_n = 0. \quad (9)$$

Let us introduce into (9) the polynomial form $P_n = \sum_{k=0}^{n} \lambda_k z^k$; it follows that $f = 0$ and $e = -n(n + a - 1)$ are necessary and that

$$\begin{aligned}&[(k - 1)(a + k - 2) - n(n + a - 1)]\lambda_{k-1} \\ &\quad + [d + bk - (\alpha + 1)k(k - 1)]\lambda_k \\ &\quad + (k + 1)(c + \alpha k)\lambda_{k+1} \\ &\quad = R_k\lambda_{k-1} + S_k\lambda_k + T_k\lambda_{k+1} = 0.\end{aligned}$$

That condition is satisfied if

$$\begin{vmatrix} S_0 & T_0 & & & \\ R_1 & S_1 & T_1 & & \\ \cdot & \cdot & \cdot & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & R_{n-1} & S_{n-1} & T_{n-1} \\ & & & R_n & S_n \end{vmatrix} = 0. \quad (10)$$

It seems very difficult to deduce the general polynomial solution because the order of the determinant increases with the order n of the polynomial. However, if we suppose $c = -\alpha j$ (j *fixed* integer) $T_j = 0$ and condition (10) may be replaced by

$$\begin{vmatrix} S_0 & T_0 & & & \\ R_1 & S_1 & T_1 & & \\ \cdot & \cdot & \cdot & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & R_{j-1} & S_{j-1} & T_{j-1} \\ & & & R_j & S_j \end{vmatrix} = 0$$ whose order does not depend upon n.

Now let us introduce $P_n = \sum_{k=0}^{j} A_k F(k - n, n - k + a + j - 1; (a + b + c)/(1 - \alpha); (1 - z)/(1 - \alpha))$ into equation (9) taking into account the differential equation satisfied by the F functions, the following remains to be proved:

$$\sum_{k=0}^{j} A_k \left\{ j(1 - z)(\alpha - z)\frac{dF(k - n)}{dz} + \left[(2kn - k^2 + ak - k + jk - nj)z - d\right] \times F(k - n) \right\} = 0.$$

Remembering the recurrence relations existing between $(1 - z)(\alpha - z)dF(k - n)/dz$ and $zF(k - n)$ on one side, $F(k - 1 - n)$ and $F(k + 1 - n)$ and $F(k - n)$ on another side, it follows that

$$\sum_{k=0}^{j} F(k - n)\left\{\mathcal{R}_k A_{k-1} + \mathcal{S}_k A_k + \mathcal{T}_k A_{k+1}\right\} = 0,$$

where $\mathcal{R}_k$, $\mathcal{S}_k$, and $\mathcal{T}_k$ are given above. Therefore, our theorem is proved and the A_k are solutions of $\mathcal{R}_k A_{k-1} + \mathcal{S}_k A_k + \mathcal{T}_k A_{k+1} = 0$. Moreover, for our three theorems the reader will verify the curious equality correct for all j-values:

$$\begin{vmatrix} S_0 & T_0 & & \\ R_1 & S_1 & T_1 & \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \\ R_{j-1} & S_{j-1} & T_{j-1} & \\ & R_j & S_j & \end{vmatrix} = \begin{vmatrix} \mathcal{S}_0 & \mathcal{T}_0 & & \\ \mathcal{R}_1 & \mathcal{S}_1 & \mathcal{T}_1 & \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \\ \mathcal{R}_{j-1} & \mathcal{S}_{j-1} & \mathcal{T}_{j-1} & \\ & \mathcal{R}_j & \mathcal{S}_j & \end{vmatrix}$$

Remarks:

(a) Those theorems remain entirely valid when n is not an integer. In that case of course the solutions are not polynomial.
(b) In the third theorem we deduce from Remark 2 that condition $c = -\alpha j$ can be replaced by $a + b + c = -j(1 - \alpha)$ or by

$$a\alpha^2 + b\alpha + c = -j\alpha(\alpha - 1) \quad (11)$$

following the case.

III. APPLICATION TO THE PROBLEMS OF SEC. I

A. Dirac's Equations in the Magnetic Field,

$$\mathbf{B} = \frac{1}{\sqrt{x^2 + y^2}}\left(\frac{-\gamma y}{x^2 + y^2}, \frac{\gamma x}{x^2 + y^2}, \alpha\right)$$

The radial equations for T_2 and T_3 may be solved by using Theorem 2 of Sec. II. It is easily seen that $j = 1$. T_2 and T_3 appear as linear combinations of two confluent hypergeometric functions while energy levels are given by the polynomial condition

$$E^2 = m_0^2c^4 + c^2p_z^2 + (\epsilon\alpha c)^2 - \left(\frac{\epsilon\alpha c(2m + 1) + 2cp_z\epsilon\gamma/\hbar}{2n + \sqrt{(2m + 1)^2 + 4(\epsilon\gamma/\hbar)^2}}\right)^2.$$

We pass over the explicit writing of T_2 and T_3 for the sake of brevity.

B. Dirac's Equations in the Magnetic Field,

$$\mathbf{B} = \nu(1 + r^2/z^2)\,\mathbf{r}/r^3$$

The θ functions T_1 and T_4 may be found by Theorem 3 of Sec. II only if one among the three relations (11) may be satisfied. Only the third may be, provided that

$$\nu = -j\hbar/2\epsilon \quad \text{(remember } j \text{ is an integer).} \qquad (12)$$

Remembering that ν has the dimensions of a magnetic pole, we see that relation (12) is absolutely identical with Dirac's rule of quantization concerning magnetic poles,[6] rule he has established in a very different way. Therefore, we may conclude with this very curious remark: Dirac's equation are exactly soluble only when the parameter ν is quantized following the rules of quantum mechanics.

We omit again the explicit writing of the functions T_1 and T_4. They appear as linear combinations of $j+1$ hypergeometric functions. Energy would be quantized if we added Coulomb electrical field.

1 L. Lam, Phys. Letters **31A**, 406 (1970).
2 G. N. Stanciu, Phys. Letters **23A**, 232 (1966).
3 Harish-Chandra, Phys. Rev. **74**, 883 (1948).
4 André Hautot, Physica **48**, 609 (1970).
5 I. I. Rabi, Z. Phys. **49**, 507 (1928).
6 P. A. M. Dirac, Phys. Rev. **74**, 817 (1948).

Two-Time Spin-Pair Correlation Function of the Heisenberg Magnet at Infinite Temperature. II

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The two-time spin-pair correlation function $\sigma(R,t)$ is expressed as a product of a Gaussian distribution function and a power series with respect to time. The width of the Gaussian distribution function is determined by the second derivative with respect to time of the autocorrelation function $\sigma(0,t)$. The coefficients of the power series are determined up to terms of order t^8 for the square and s.c. isotropic Heisenberg and XY magnets of spin $\frac{1}{2}$ at infinite temperature, and up to terms of t^{10} for the linear magnets. The expressions obtained by truncating the power series to the exactly known terms give a very good fit at short times to the exact expression for the linear XY model, and to the results of the computer simulation due to Windsor for the s.c. Heisenberg ferromagnet. The Fourier-time transforms of the expressions thus obtained are shown to be the Gram–Charlier expansions. Thus we conclude that the Gram–Charlier expansion of the Fourier-time transform of $\sigma(R,t)$, $\tilde{\sigma}(R,\omega)$, and that of its Fourier-space transform $I(k,t)$, $S(k,\omega)$, is especially useful in the cases when the short-time behavior of $\sigma(R,t)$ or $I(k,t)$ is considered important; generally speaking, this is the case at large k or at ω which is not very small. When the width of the Gaussian distribution function is determined by the second derivative of $I(k,t)$, a convergent result is not obtained for small values of k. For larger k, the convergence is as good as for the case when the width is determined by the autocorrelation function.

1. INTRODUCTION

The two-time spin-pair correlation function is the quantity of primary importance in the theory of neutron scattering from magnetic materials.[1,2] In a number of papers,[3–8] calculations are focused on the function at infinite temperature, for simplicity of the treatment. For example, Windsor[4] performed a computer simulation calculation for the Heisenberg magnet of classical spins at infinite temperature. Carboni and Richards[5] gave an exact calculation, for a finite chain, of the Heisenberg magnet of spin $\frac{1}{2}$ at infinite temperature.

In the preceding paper,[9] the author gave the numerical values of the coefficients of the expansion in powers of time of the two-time spin-pair correlation function $\langle s_i^z(t)s_f^z(0)\rangle$ of spin $\frac{1}{2}$ at infinite temperature. In the present paper, we express $\langle s_i^z(t)s_f^z(0)\rangle$ and its Fourier-space transform $\langle S_k^z(t)S_{-k}^z(0)\rangle$ as a product of a Gaussian distribution function and a power series.

It is noted that the Fourier-time transform of this expression gives the Gram–Charlier expansion, which was proposed by Collins and Marshall[7] for the analysis of the Fourier-time transform of $\langle S_k^z(t)S_{-k}^z(0)\rangle$. The convergence of those expansions is discussed for the Heisenberg magnet and the XY magnet. For the one-dimensional XY magnet, the results are compared with the exact solution.

In the remaining part of this introduction, definitions adopted in this paper are given. The Hamiltonian of the system is

$$H = -\sum_f \sum_g [J_\perp(f,g)s_f^- s_g^+ + J_\parallel(f,g)s_f^z s_g^z], \qquad (1.1)$$

where $J_\perp(f,g)$ and $J_\parallel(f,g)$ are equal to $J_\perp$ and $J_\parallel$, respectively, when f and g are nearest neighbors of each other and zero otherwise. For the Heisenberg magnet, $J_\perp = J_\parallel \equiv J$. If $J_\parallel = 0$ and the system is one-dimensional, the system is the XY model. We shall call the case of $J_\parallel = 0$ the XY magnet in general. The two-time spin-pair correlation function $\sigma(R_{if},t)$ is defined by

$$\sigma(R_{if},t) = \langle s_i^z(t)s_f^z(0)\rangle - \langle s_i^z\rangle\langle s_f^z\rangle, \qquad (1.2)$$

where

$$s_i^z(t) = e^{iHt}s_i^z e^{-iHt}.$$

We shall introduce the Fourier-space transform of $s_i^z(t)$ by

$$S_k^z(t) = \sum_f s_f^z(t)e^{ik\cdot R_f}. \qquad (1.3)$$

The Fourier-space transform of $\sigma(R_{if},t)$ is the so-called "intermediate scattering function." It will be denoted by $I(k,t)$:

$$I(k,t) = \sum_f \sigma(R_{if},t)e^{ik\cdot R_{if}}. \qquad (1.4)$$

It is the correlation function of $S_k^z(t)$:

$$I(k,t) = N^{-1}\langle S_k^z(t)S_{-k}^z(0)\rangle, \qquad k \neq 0, \qquad (1.5)$$

where N is the total number of spins in the system. We shall focus our attention mainly on $\sigma(R_{if},t)$ in Secs. 2 and 3, and on $I(k,t)$ in Sec. 4.