Theory of Electron Diffraction by Crystals

I. Green's Function and Integral Equation

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A general theory of electron diffraction by crystals is developed. The crystals are assumed to be infinitely extended in two dimensions and finite in the third dimension. For the scattering problem by this structure two-dimensionally expanded forms of Green's function and integral equation are at first derived, and combined in single three-dimensional forms. Ewald's method is applied to sum up the series for Green's function.

The fundamental theory of electron diffraction by crystals is Bethe's dynamical theory [1]. In this theory the wave field inside the crystal is represented by a superposition of Bloch waves and continued into the vacuum by a superposition of plane waves. The main problem is to solve the eigenvalue problem for the wave vector (propagation vector) of Bloch waves. In one dimension this is represented by Hill's determinantal equation (Whittaker–Watson [2], p. 415). In three dimensions, however, the solubility of the corresponding determinantal equation is somewhat problematic. In contrast to the one-dimensional case, we cannot secure the absolute convergence of the infinite determinant. In fact, Bethe argues that the problem is not exactly soluble (l. c. [1], p. 73, § 4) and confines himself to approximate solutions.

Apart from this difficulty in fundamental principle, Bethe's assumption of geometrically plane surfaces will not be valid especially in practical application to low-energy electron diffraction.

In the present paper we propose an alternative formulation of the problem which appears to be more fundamental and more widely applicable than Bethe's. We consider, as Bethe, non-relativistic elastic scattering and an infinitely extended crystal slab, but assume that the potential is periodic only in two dimensions parallel to the surface. The variation of the potential in the third dimension is at first almost arbitrary. This assumption allows us to apply the theory to monatomic layers and to crystals with regularly distributed adsorbed atoms or steps on their surface. These cases are important for low-energy electron diffraction.

We formulate the problem at first as a boundary-value problem for the Schrödinger equation, but go over at once to the equivalent integral equation. The integral equation is convenient for mathematical analysis and renders the *exact* solution of the problem. The integral equation is also a convenient tool for investigating various existing theories of electron diffraction (including Bethe's theory) and provides an unifying view over these theories.

§ 1. General Survey of Green's Functions

Before going into our problem let us consider at first some related problems and corresponding Green's functions to clarify our point of view.

The most general form of the integral equation for potential scattering may be

$$\psi(\boldsymbol{r}) = \psi^{(0)}(\boldsymbol{r}) + \int G(\boldsymbol{r} \mid \boldsymbol{r}')\, V(\boldsymbol{r}')\, \psi(\boldsymbol{r}')\, \mathrm{d}\tau', \qquad (1)$$

where $\psi(\boldsymbol{r})$ is a solution of Schrödinger's equation

$$\nabla^2\psi + (\varkappa^2 - V(\boldsymbol{r}))\,\psi = 0\,, \qquad (2)$$

$\psi^{(0)}(\boldsymbol{r})$ is the incident wave, and Green's function

$$G(\boldsymbol{r} \mid \boldsymbol{r}') = -\frac{\exp\{i\varkappa|\boldsymbol{r}-\boldsymbol{r}'|\}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} \qquad (3)$$

is constructed to satisfy

$$\nabla_r^2 G + \varkappa^2 G = +\delta(\boldsymbol{r}-\boldsymbol{r}') \qquad (4)$$

and the condition of outgoing waves. This Green's function is valid only for scattering objects which are *finite* in three dimensions. Therefore, it is questionable to use this Green's function in our problem of infinitely extended slabs.

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[1] H. Bethe, Ann. Phys. (4) **87**, 55 [1928].

[2] E. T. Whittaker and G. N. Watson, A Course of Modern Analysis, Cambridge University Press 1927 (2nd ed.).

Another extreme case of crystals *infinite* in three dimensions appears in the theory of BLOCH functions (for example, KOHN and ROSTOKER [3]). GREEN's function for the integral equation of BLOCH function is

$$G(\boldsymbol{r}\,|\,\boldsymbol{r}') = \frac{1}{\tau}\sum_{g}\frac{\exp\{i(\boldsymbol{k}+\boldsymbol{B}_g)\cdot(\boldsymbol{r}-\boldsymbol{r}')\}}{\varkappa^2-(\boldsymbol{k}+\boldsymbol{B}_g)^2}, \qquad (5)$$

where τ is the volume of the unit cell, $\boldsymbol{k}$ is the propagation vector, and $\boldsymbol{B}_g$ are the reciprocal lattice vectors. This GREEN's function is constructed to satisfy (4) and to have the periodic property of BLOCH functions. Owing to this periodicity the range of integration in the integral equation [which has the form (1) with $\psi^{(0)}=0$] is confined to one unit cell or to one WIGNER–SEITZ cell.

In the present problem with two-dimensionally infinite crystals the geometry requires that the solution should have a periodic property like a BLOCH function in two directions parallel to the surfaces (cf. § 2). In the third direction perpendicular to the surfaces the solution should have the property of outgoing waves as required for (3). Thus, it is clear that the GREEN's function should have a mixed type between the above two forms (3) and (5).

FUJIWARA [4] who investigated the same problem as ours, used the spectral representation for GREEN's function

$$G(\boldsymbol{r}\,|\,\boldsymbol{r}') = \frac{1}{(2\pi)^3}\int\frac{\exp\{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')\}}{\varkappa^2-|\boldsymbol{k}|^2}\mathrm{d}\boldsymbol{k}, \qquad (6)$$

and put it in the iterative solution of the integral equation (1). This GREEN's function appears to be effectively that what we want. However, the form (6) is not very convenient to be used in further mathematical investigations, because it contains a somewhat indefinite contour integral. Although FUJIWARA's treatment appears to be satisfactory so far as the iterative solution is concerned, he could not prove its convergence. His solution appears hence to be a formal one. In any case his result is identical with the iterative solution of TOURNARIE's system of integral equations [5], which is discussed in § 2, and consequently should be identical also with our exact solution if the iteration is convergent.

[3] W. KOHN and N. ROSTOKER, Phys. Rev. **94**, 1111 [1954].
[4] K. FUJIWARA, J. Phys. Soc. Japan **14**, 1513 [1959].
[5] N. TOURNARIE, J. Phys. Soc. Japan **17**, Suppl. B-II, 98 [1962].
[6] M. VON LAUE, Phys. Rev. **37**, 53 [1931].

§ 2. Expansion in Two Dimensions

The two-dimensional periodicity of the potential allows us to expand the solution in a kind of FOURIER series. This process has been applied already in several cases (von LAUE [6], ATTREE and PLASKETT [7], TOURNARIE [5], HIRABAYASHI and TAKEISHI [8]). Although we would prefer to work with the three-dimensional form (1), it seems to be convenient to start with the two-dimensional expansion because we can write down relatively easily an explicit form of the boundary conditions and corresponding GREEN's function.

In the SCHRÖDINGER equation (2) the "potential" $V(\boldsymbol{r})$ is now periodic in two dimensions

$$V(\boldsymbol{r}+n_1\boldsymbol{a}_1+n_2\boldsymbol{a}_2)=V(\boldsymbol{r}), \qquad (7)$$

where $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are the two-dimensional basis vectors, and n_1 and n_2 are arbitrary integers. In the third dimension, for which we take the z-axis perpendicular to $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$, the non-zero region of $V(\boldsymbol{r})$ is assumed to be confined to a finite range $z_\mathrm{i}<z<z_\mathrm{e}$. Thus

$$V(\boldsymbol{r})=0 \quad \text{if} \quad z\leqq z_\mathrm{i} \quad \text{or} \quad z\geqq z_\mathrm{e}. \qquad (8)$$

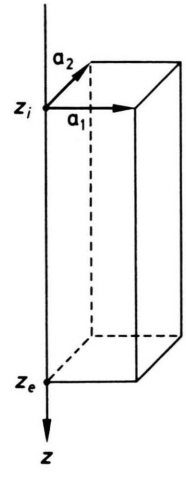

Fig. 1. The column of reference.

This restriction is introduced only to simplify the mathematics, and can be removed afterwards by the process of shifting z_i and z_e to $-\infty$ and $+\infty$ respectively.

[7] R. W. ATTREE and J. S. PLASKETT, Phil. Mag. (8) **1**, 885 [1956].
[8] K. HIRABAYASHI and Y. TAKEISHI, Surface Sci. **4**, 150 [1966].

We call the planes $z=z_i$ and $z=z_e$ the surfaces, the space $z_i<z<z_e$ the crystal, the spaces $z<z_i$ and $z>z_e$ the vacuum.

The potential $V(\boldsymbol{r})$ needs not necessarily be periodic as a function of z in the crystal. If $V(\boldsymbol{r})$ should represent a perfect crystal, however, the above assumption requires nothing but that the surfaces are parallel to one of the netplanes of the crystal. The vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ can be properly chosen in this netplane and may not be identical to the conventional basis vectors of the crystal itself.

We assume that a plane-parallel electron wave falls on the crystal from the "upper" vacuum $z<z_i$ with the wave vector $\boldsymbol{K}_0$. We call it the primary wave and write

$$\psi^{(0)}(\boldsymbol{r}) = \exp\{i\,\boldsymbol{K}_0\cdot\boldsymbol{r}\}\,, \tag{9}$$

where $\boldsymbol{K}_0$ has a positive z-component. The surfaces $z=z_i$ and $z=z_e$ are called then the surface of incidence and exit respectively.

It is shown in Appendix 1 that the solution ψ has the periodicity like a BLOCH function in two dimensions

$$\psi(\boldsymbol{r}+n_1\,\boldsymbol{a}_1+n_2\,\boldsymbol{a}_2) = \exp\{i\,\boldsymbol{K}_0\cdot(n_1\,\boldsymbol{a}_1+n_2\,\boldsymbol{a}_2)\}\,\psi(\boldsymbol{r})\,. \tag{10}$$

We can put therefore

$$\psi(\boldsymbol{r}) = \exp\{i\,\boldsymbol{K}_{0t}\cdot\boldsymbol{r}_t\}\sum_m \psi_m(z)\,\exp\{i\,\boldsymbol{B}_{mt}\cdot\boldsymbol{r}_t\}\,, \tag{11}$$

where $\boldsymbol{K}_{0t}$ and $\boldsymbol{r}_t$ are the components of $\boldsymbol{K}_0$ and $\boldsymbol{r}$ tangential to the surfaces. $\boldsymbol{B}_{mt}$ are given by

$$\boldsymbol{B}_{mt} = m_1\,\boldsymbol{B}_{1t}+m_2\,\boldsymbol{B}_{2t}\,, \tag{12}$$

where the index m stands for the pair of integers m_1 and m_2. $\boldsymbol{B}_{1t}$ and $\boldsymbol{B}_{2t}$ are the *two*-dimensional reciprocal basis vectors which are determined from $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ to satisfy

$$\boldsymbol{a}_i\cdot\boldsymbol{B}_{jt} = 2\,\pi\,\delta_{ij} \quad (i,j=1,2)\,. \tag{13}$$

$\boldsymbol{B}_{1t}$ and $\boldsymbol{B}_{2t}$ may not be identical with the conventional basis vectors of the three-dimensional reciprocal lattice.

Putting (11) into the SCHRÖDINGER equation (2) we obtain

$$\frac{d^2}{dz^2}\psi_m(z)+\Gamma_m{}^2\,\psi_m(z)-\sum_n V_{m-n}(z)\,\psi_n(z)=0\,, \tag{14}$$

where $\Gamma_m{}^2$ is given by

$$\Gamma_m{}^2 = \varkappa^2-|\boldsymbol{K}_{mt}|^2, \tag{15}$$

where

$$\boldsymbol{K}_{mt} = \boldsymbol{K}_{0t}+\boldsymbol{B}_{mt}\,. \tag{16}$$

For the later purposes Γ_m is made unique by the convention

$$\Gamma_m = +\sqrt{\varkappa^2-|\boldsymbol{K}_{mt}|^2} \quad \text{if } \varkappa^2>|\boldsymbol{K}_{mt}|^2, \tag{17a}$$

and

$$\Gamma_m = +i\sqrt{|\boldsymbol{K}_{mt}|^2-\varkappa^2} \quad \text{if } \varkappa^2<|\boldsymbol{K}_{mt}|^2 \tag{17b}$$

We assume at first

$$\varkappa \neq |\boldsymbol{K}_{mt}| \quad \text{for all} \quad m\,. \tag{18}$$

$V_m(z)$ in (14) is the two-dimensional expansion coefficient of the potential $V(\boldsymbol{r})$ according to the periodicity (7). Thus

$$V(\boldsymbol{r}) = \sum_m V_m(z)\,\exp\{i\,\boldsymbol{B}_{mt}\cdot\boldsymbol{r}_t\}\,. \tag{19}$$

In the vacuum $z<z_i$ and $z>z_e$ we have

$$\nabla^2\psi+\varkappa^2\,\psi=0\,. \tag{20}$$

Therefore we can write for $z<z_i$

$$\psi_m(z) = \Psi_m\exp\{i\,\Gamma_m\,z\}+R_m\exp\{-i\,\Gamma_m\,z\}, \tag{21a}$$

and for $z>z_e$

$$\psi_m(z) = T_m\exp\{i\,\Gamma_m\,z\}+\Phi_m\exp\{-i\,\Gamma_m\,z\}. \tag{21b}$$

Ψ_m, R_m, T_m, and Φ_m are constants and can be interpreted, if Γ_m is real, as the amplitudes of plane waves going upwards or downwards, and, if Γ_m is imaginary, as the amplitudes of "evanescent waves" [9] which increase or decrease exponentially. The condition of outgoing waves can be adapted to the present problem in the form

$$\Psi_m = \delta_{0m_1}\,\delta_{0m_2}, \tag{22a}$$

and

$$\Phi_m = 0 \quad \text{for all} \quad m\,. \tag{22b}$$

From the continuity of ψ and $\partial\psi/\partial z$ on the surfaces it is found at once that the solution ψ inside the crystal must satisfy the boundary conditions

$$\left(\psi_m+\frac{1}{i\,\Gamma_m}\frac{d\psi_m}{dz}\right)_{z=z_i} = 2\,\delta_{0m_1}\,\delta_{0m_2}\exp\{i\,\Gamma_0\,z_i\} \tag{23a}$$

and

$$\left(\psi_m-\frac{1}{i\,\Gamma_m}\frac{d\psi_m}{dz}\right)_{z=z_e}=0 \quad \text{for all } m\,. \tag{23b}$$

This is an explicit form of the condition of outgoing waves (SOMMERFELD [10], p. 179).

[9] Cf. for example M. BORN and K. WOLF, Principles of Optics, Pergamon Press, London 1959, p. 560. — J. A. RATCLIFFE, Rep. Progr. Phys. **19**, 188 [1956].

[10] A. SOMMERFELD, Vorlesungen über theoretische Physik, Bd. 6, Partielle Differentialgleichungen der Physik, Akadem. Verlagsges. Leipzig 1958 (4. Aufl.).

Thus we have a boundary value problem for an *infinite* system of ordinary differential equations (14) in the finite region $z_i \leqq z \leqq z_e$ with the boundary conditions (23 a, b). Our aim is to find from the solution of this problem the amplitudes of the waves going out from the crystal, i. e. R_m and T_m of Eqs. (21 a, b).

In analogy to the one-dimensional problem (SOMMERFELD [10], p. 180, MORSE–FESHBACH [11], p. 1071) it is easy to find the system of GREEN's functions ("GREEN matrix" of TOURNARIE [5])

$$G_m(z\,|\,z') = \frac{1}{2\,i\,\Gamma_m} \exp\{i\,\Gamma_m\,|\,z-z'\,|\}\,. \qquad (24)$$

These GREEN's functions satisfy the equations [the main part [12] of (14)]

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}\,G_m(z\,|\,z') + \Gamma_m{}^2\,G_m(z\,|\,z') = +\delta(z-z') \qquad (25)$$

and the homogeneous boundary conditions corresponding to (23a, b), that is, if $z_i < z' < z_e$,

$$G_m(z_i\,|\,z') + \frac{1}{i\,\Gamma_m}\left[\frac{\mathrm{d}}{\mathrm{d}z}\,G_m(z\,|\,z')\right]_{z=z_i} = 0\,, \qquad (26\,\mathrm{a})$$

and

$$G_m(z_e\,|\,z') - \frac{1}{i\,\Gamma_m}\left[\frac{\mathrm{d}}{\mathrm{d}z}\,G_m(z\,|\,z')\right]_{z=z_e} = 0\,. \qquad (26\,\mathrm{b})$$

The system of integral equations is

$$\psi_m(z) = \delta_{0m_1}\,\delta_{0m_2}\exp\{i\,\Gamma_0\,z\} + \int_{z_i}^{z_e} G_m(z\,|\,z')\sum_n V_{m-n}(z')\;\psi_n(z')\;\mathrm{d}z', \qquad (27)$$

or with (24)

$$\psi_m(z) = \delta_{0m_1}\,\delta_{0m_2}\exp\{i\,\Gamma_0\,z\} + \frac{1}{2\,i\,\Gamma_m}\exp\{i\,\Gamma_m\,z\}\int_{z_i}^{z}\exp\{-i\,\Gamma_m\,z'\}\sum_n V_{m-n}(z')\;\psi_n(z')\;\mathrm{d}z'$$
$$+\frac{1}{2\,i\,\Gamma_m}\exp\{-i\,\Gamma_m\,z\}\int_{z}^{z_e}\exp\{i\,\Gamma_m\,z'\}\sum_n V_{m-n}(z')\;\psi_n(z')\;\mathrm{d}z'. \qquad (28)$$

If we have obtained the solution of this system we can calculate the amplitudes of the outgoing waves by

$$R_m = \frac{1}{2\,i\,\Gamma_m}\int_{z_i}^{z_e}\exp\{i\,\Gamma_m\,z'\}\sum_n V_{m-n}(z')\;\psi_n(z')\;\mathrm{d}z', \qquad (29\,\mathrm{a})$$

$$T_m = \delta_{0m_1}\,\delta_{0m_2} + \frac{1}{2\,i\,\Gamma_m}\int_{z_i}^{z_e}\exp\{-i\,\Gamma_m\,z'\}\sum_n V_{m-n}(z')\;\psi_n(z')\;\mathrm{d}z'. \qquad (29\,\mathrm{b})$$

§ 3. Recombination in Three Dimensions

The infinite system derived in § 2 have a satisfactorily explicit and simple form to be used for further mathematical analysis or for practical calculations. For example, VON LAUE's theory [6] of electron diffraction by monatomic layers is nothing but the first iterated solution of (28). In many cases, however, it is more convenient to have one integral equation in three dimensions in the form (1). This is particularly true for low-energy electron diffraction as well be shown in a separate paper [12a]. In fact, the forms of the systems in § 2 suggest that these can be obtained by expansion of single three-dimensional equations.

For the beginning, it is obvious that the system of differential equations (14) is an expanded form of (2). The periodicity (10) shows that the *three*-dimensional boundary-value problem may be confined to a column parallel to the z-axis ("column of reference") (Fig. 1). Its cross-section is a unit cell of the two-dimensional lattice, that is, a parallelo-

[11] P. M. MORSE and H. FESHBACH, Methods of Theoretical Physics, 2 Vols., McGraw-Hill, New York 1953.

[12] It should be noted that the choice of the main part is somewhat arbitrary. Thus, we can write

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}\,G_m(z\,|\,z') + (\Gamma_m{}^2 - \beta_m)\;G_m(z\,|\,z') = \delta(z-z'),$$

where the constant β_m can be chosen arbitrarily. We arrive in this way at various forms of existing theories. This will be shown in a later paper.

[12a] K. KAMBE, Z. Naturforschg. **22 a**, 322 [1967].

gramm of the basis vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$. The top and bottom of the column are parts of the surfaces of incidence and exit respectively.

On the side planes of the column of reference the boundary conditions are given, in accordance with (10), by

$$\psi(\boldsymbol{r}_{s1}+\boldsymbol{a}_1)=\exp\{i\,\boldsymbol{K}_{0t}\cdot\boldsymbol{a}_1\}\,\psi(\boldsymbol{r}_{s1}), \quad (30\,a)$$

and

$$\psi(\boldsymbol{r}_{s2}+\boldsymbol{a}_2)=\exp\{i\,\boldsymbol{K}_{0t}\cdot\boldsymbol{a}_2\}\,\psi(\boldsymbol{r}_{s2}), \quad (30\,b)$$

where $\boldsymbol{r}_{s1}$ and $\boldsymbol{r}_{s2}$ are points on one of the pairs of side planes. The points $\boldsymbol{r}_{s1}+\boldsymbol{a}_1$ and $\boldsymbol{r}_{s2}+\boldsymbol{a}_2$ are then situated on the opposite side planes.

The boundary conditions on the top and bottom are derived from (23 a, b). We get, by multiplying with $\exp\{i\,\boldsymbol{K}_{mt}\cdot\boldsymbol{r}_t\}$, summing over m, writing $\psi(\boldsymbol{r})=\psi(\boldsymbol{r}_t,z)$ and applying *at first formally* PARSEVAL's theorem, on the top surface $z=z_i$

$$\psi(\boldsymbol{r}_t,z_i)+\int A(\boldsymbol{r}_t-\boldsymbol{r}_t')\;\psi_z(\boldsymbol{r}_t',z_i)\,ds' = 2\,\psi^{(0)}(\boldsymbol{r}_t,z_i), \quad (31\,a)$$

and on the bottom surface $z=z_e$

$$\psi(\boldsymbol{r}_t,z_e)-\int A(\boldsymbol{r}_t-\boldsymbol{r}_t')\;\psi_z(\boldsymbol{r}_t',z_e)\,ds'=0, \quad (31\,b)$$

where

$$\psi_z(\boldsymbol{r}_t,z)=\frac{\partial}{\partial z}\psi(\boldsymbol{r}_t,z), \quad (32)$$

and

$$A(\boldsymbol{r}_t-\boldsymbol{r}_t')=\frac{1}{A}\sum_m\frac{1}{i\,\Gamma_m}\exp\{i\,\boldsymbol{K}_{mt}\cdot(\boldsymbol{r}_t-\boldsymbol{r}_t')\}, \quad (33)$$

where A is the area of the cross-section of the column, that is, the two-dimensional unit cell. The surface integral $\int ds'$ of (31 a, b) is taken for $\boldsymbol{r}_t'$ over the top and bottom surfaces respectively.

(31 a, b) are the explicit forms of the conditions of outgoing waves which has been stated by FUJIWARA [4] somewhat vaguely in words. They are, however, at first purely formal, since we do not know whether the double series (33) converges.

We obtain GREEN's function by recombining the system (24) in a similar manner as

$$G(\boldsymbol{r}\,|\,\boldsymbol{r}')=\frac{1}{A}\sum_m\frac{1}{2\,i\,\Gamma_m}\exp\{i\,\Gamma_m\,|\,z-z'\,|+i\,\boldsymbol{K}_{mt}\cdot(\boldsymbol{r}_t-\boldsymbol{r}_t')\} \quad (34)$$

to satisfy the Eq. (4) and the boundary conditions on the side planes, that is, if the point $\boldsymbol{r}'$ lies inside the column

$$G(\boldsymbol{r}_{s1}+\boldsymbol{a}_1\,|\,\boldsymbol{r}')=\exp\{i\,\boldsymbol{K}_{0t}\cdot\boldsymbol{a}_1\}\,G(\boldsymbol{r}_{s1}\,|\,\boldsymbol{r}'), \quad (35\,a)$$

and

$$G(\boldsymbol{r}_{s2}+\boldsymbol{a}_2\,|\,\boldsymbol{r}')=\exp\{i\,\boldsymbol{K}_{0t}\cdot\boldsymbol{a}_2\}\,G(\boldsymbol{r}_{s2}\,|\,\boldsymbol{r}'). \quad (35\,b)$$

Further, if the point $\boldsymbol{r}_1=(\boldsymbol{r}_{t1},z_1)$ lies inside the column, the boundary conditions on the top and bottom surfaces are

$$G(\boldsymbol{r}_t,z_i\,|\,\boldsymbol{r}_{t1},z_1)+\int A(\boldsymbol{r}_t-\boldsymbol{r}_t')\,G_z(\boldsymbol{r}_t',z_i\,|\,\boldsymbol{r}_{t1},z_1)\,ds'=0, \quad (36\,a)$$

$$G(\boldsymbol{r}_t,z_e\,|\,\boldsymbol{r}_{t1},z_1)-\int A(\boldsymbol{r}_t-\boldsymbol{r}_t')\,G_z(\boldsymbol{r}_t',z_e\,|\,\boldsymbol{r}_{t1},z_1)\,ds'=0, \quad (36\,b)$$

where

$$G_z=\partial G(\boldsymbol{r}_t',z\,|\,\boldsymbol{r}_{t1},z_1)/\partial z\,.$$

The form (34) shows that it is really a mixed type between (3) and (5) as was expected in § 1. Thus (34) is hermitic just as (5) for the interchange of variables $\boldsymbol{r}_t$ and $\boldsymbol{r}_t'$, and complex symmetric just as (3) for the interchange of variables z and z'.

Obviously the double series (34) is absolutely and uniformly convergent if $z\neq z'$, but for $z=z'$ we do not know whether it converges. We note that we have the relation

$$A(\boldsymbol{r}_t-\boldsymbol{r}_t')=2[G(\boldsymbol{r}\,|\,\boldsymbol{r}')]_{z=z'}, \quad (37)$$

where z' may be arbitrarily chosen as zero.

The integral equation having the GREEN's function (34) is obtained from the system (28) in the recombined form (1), where $\psi^{(0)}(\boldsymbol{r})$ is given by (9) and the range of integration is extended over the "column of reference".

If we have found the solution of the integral equation the amplitudes of the outgoing waves can be calculated as

$$R_m = \frac{1}{A} \exp\{i\,\Gamma_m z_i\} \int\int \exp\{-i\,\mathbf{K}_{mt}\cdot\mathbf{r}_t\}\, G(\mathbf{r}_t, z_i \mid \mathbf{r}')\, V(\mathbf{r}')\, \psi(\mathbf{r}')\, \mathrm{d}\tau'\, \mathrm{d}s\,, \tag{38 a}$$

$$T_m = \delta_{0m_1}\delta_{0m_2} + \frac{1}{A} \exp\{-i\,\Gamma_m z_e\} \int\int \exp\{-i\,\mathbf{K}_{mt}\cdot\mathbf{r}_t\}\, G(\mathbf{r}_t, z_e \mid \mathbf{r}')\, V(\mathbf{r}')\, \psi(\mathbf{r}')\, \mathrm{d}\tau'\, \mathrm{d}s\,, \tag{38 b}$$

where the surface integral $\int \mathrm{d}s$ is taken for $\mathbf{r}_t$ over the cross-section of the column.

It remains to investigate the convergence of the series (34) for $z = z'$.

§ 4. Green's Function in an Explicit Form

To evaluate the sum of (34), in particular for the case $z = z'$, we apply EWALD's method [13] for summing the series (5). The method is essentially a generalization of RIEMANN's method (WHITTAKER–WATSON [2], p. 273) for evaluating zeta functions. Its main feature is to derive the unknown sum of a series by analytic continuation of another series whose sum is known to be an analytic function of a parameter. The proposed series for (34) is (see Appendix 2) its generalized form

$$G_s(\mathbf{R}) = \frac{1}{2\,i\,A}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \sum_m \left(\frac{|Z|}{\Gamma_m}\right)^{\frac{1}{2}s} H^{(1)}_{-s/2}(\Gamma_m \mid Z|)\, \exp\{i\,\mathbf{K}_{mt}\cdot\mathbf{R}_t\}\,, \tag{39}$$

where $\mathbf{R} = \mathbf{r} - \mathbf{r}'$, $\mathbf{R}_t = \mathbf{r}_t - \mathbf{r}_t'$, $Z = z - z'$, s is a complex parameter, and $H^{(1)}_{-s/2}(\Gamma_m \mid Z|)$ is a HANKEL function. This *double* series is absolutely and uniformly convergent (with respect to s, $\mathbf{R}_t$, and Z) if $\Re\mathrm{e}(s) > 2$, so that it is an analytic function of s in that domain. By means of an integral representation of HANKEL functions we obtain, on applying RIEMANN's method, the analytic continuation of it into the domain $\Re\mathrm{e}(s) \leqq 2$, and particularly $G(\mathbf{R})$ for $s = 1$. In an explicit form it can be written

$$\begin{aligned} G(\mathbf{R}) = &-\frac{1}{2\,\pi\,A}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \sum_m \exp\{i\,\mathbf{K}_{mt}\cdot\mathbf{R}_t\} \int_{\omega}^{\infty \exp\{i\varphi_m\}} \zeta^{-\frac{1}{2}} \exp\left\{\frac{1}{2}\left(\Gamma_m{}^2\,\zeta - \frac{Z^2}{\zeta}\right)\right\} \mathrm{d}\zeta \\ &-\frac{1}{4\,\pi^2}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \sum_n \exp\{-i\,\mathbf{K}_{0t}\cdot\mathbf{a}_{nt}\} \int_{1/\omega}^{\infty} \zeta^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}\left(|\,\mathbf{R} + \mathbf{a}_{nt}\,|^2\,\zeta - \frac{\varkappa^2}{\zeta}\right)\right\} \mathrm{d}\zeta\,, \end{aligned} \tag{40}$$

where $\varphi_m = \pi - 2\arg\Gamma_m$, $\mathbf{a}_{nt} = n_1\,\mathbf{a}_1 + n_2\,\mathbf{a}_2$ (n stands for a pair of integers n_1 and n_2), and ω is a complex number which can be chosen arbitrarily in the domain $\Re\mathrm{e}(\omega) > 0$, $|\omega| < \infty$. These integrals can be expressed after EWALD [13] by error functions.

(4) can be modified to (cf. Appendix 2)

$$\begin{aligned} G(\mathbf{R}) = &\frac{1}{A} \sum_m \exp\{i\,\mathbf{K}_{mt}\cdot\mathbf{R}_t\} \left[\frac{\exp\{i\,\Gamma_m|Z|\}}{2\,i\,\Gamma_m} + \frac{1}{2\sqrt{2}\,\pi} \int_{1/\omega}^{\infty} t^{-3/2} \exp\left\{\frac{1}{2}\left(Z^2\,t - \frac{\Gamma_m{}^2}{t}\right)\right\} \mathrm{d}t\right] \\ &-\frac{1}{4\,\pi^2}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \sum_n \exp\{-i\,\mathbf{K}_{0t}\cdot\mathbf{a}_{nt}\} \int_{1/\omega}^{\infty} t^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}\left(|\,\mathbf{R} + \mathbf{a}_{nt}\,|^2\,t - \frac{\varkappa^2}{t}\right)\right\} \mathrm{d}t\,, \end{aligned} \tag{41}$$

where $\omega > 0$ and the integrals are taken on the real axis. A comparison with (34) shows that to each term of (34) the second term in the square bracket is added to make the series convergent. These terms are compensated by the second series.

It can be proved directly (Appendix 3) that $G(\mathbf{R})$ given by (40) or (41) satisfies the equation (4) and the boundary conditions (35 a) – (36 b). Therefore it *is* the required GREEN's function.

$A(\mathbf{R}_t)$ given by (33) can be obtained from (40) according to the relation (37). We find easily that the integrals of (31 a, b) exist if ψ_z is a continuous function of $\mathbf{r}_t'$.

[13] P. P. EWALD, Ann. Phys. (4) **64**, 253 [1921]. – O. EMERSLEBEN, Phys. Z. **24**, 73 [1923]. – The author is greatly indebted to Prof. Dr. K. MOLIÈRE for calling his attention to these papers.

In this way it is proved that the three-dimensional form of § 3 is consistent quite independent of its derivation from the form of § 2 [14].

The formal expressions (33) and (34) are the limit of (40) for $|\omega| \to 0$ (Appendix 2). Another formal expression can be obtained (Appendix 2) in the limit $|\omega| \to \infty$. Thus

$$G(\boldsymbol{R}) = -\sum_n \frac{1}{4\pi(\boldsymbol{R}+\boldsymbol{a}_{nt})} \times \exp\{i\varkappa|\boldsymbol{R}+\boldsymbol{a}_{nt}| - i\boldsymbol{K}_{0t}\cdot\boldsymbol{a}_{nt}\}. \quad (42)$$

This is apparently a two-dimensional lattice of unit sources of spherical waves. One source lies within the column of reference at the point $\boldsymbol{r}'$, that is, $|\boldsymbol{R}| = 0$. The other sources lie outside the column at the points $\boldsymbol{r}' - \boldsymbol{a}_{nt}$ which are generated from $\boldsymbol{r}'$ by repeated lattice translations $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$.

Finally it is to be noted that the case $\Gamma_m^2 = 0$, which is excluded in the present treatment, can be taken into account by means of a modified GREEN's function (MORSE–FESHBACH [11], p. 822).

§ 5. Discusssion

The form of GREEN's function (40) is only an alternative of the expanded form (24) of TOURNARIE [5] and the spectral representation (6) of FUJIWARA [4]. Our form has, however, the advantage of being explicit and relatively rapidly convergent (particularly in the case of low-energy electrons). The main disadvantage is that it contains somewhat cumbersome integrals. For analytical calculations it is often more convenient to use the function $G_s(\boldsymbol{R})$ given by (39) at first, and to put $s = 1$ in the result if analytic continuation is allowed (cf. [14]).

The explicit form of our GREEN's function allows us, in virtue of the *finite* integration range (that is, the column of reference), to derive the *exact* solution of our problem, namely, the FREDHOLM's series. This will be shown in a succeeding paper. Although the FREDHOLM's series is more complicated than the iterated (NEUMANN's) series, the convergence of the series is guaranteed for a wide range of potential functions $V(\boldsymbol{r})$. The exact solution is no doubt a valuable help to prove various approximation methods.

The rapid convergence of our representation (40) is significant particularly for low-energy electron diffraction, for which we can apply the cellular method of the band theory of metals (e. g. KOHN–ROSTOKER [3]), in virtue of the fact that the partial wave expansion of the single-atom scattering is rapidly convergent for slow electrons [12a].

The author wishes to thank Prof. Dr. K. MOLIÈRE for his encouragement to this work.

Appendix 1. Periodicity of Solution

If $\boldsymbol{K}_0$ is perpendicular to the surface we see at once that the solution should be two-dimensionally periodic in the whole space with the same periods as those of the two-dimensional lattice. For, if we observe two points $\boldsymbol{r}$ and $\boldsymbol{r}' = \boldsymbol{r} + n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2$ with arbitrarily chosen integers n_1 and n_2, then the geometry of the problem is completely identical for $\boldsymbol{r}$ and $\boldsymbol{r}'$. Thus the solution has the form (11) with $|\boldsymbol{K}_{0t}| = 0$.

If $\boldsymbol{K}_0$ is not perpendicular to the surface, then the geometry is not quite the same for $\boldsymbol{r}$ and $\boldsymbol{r}'$. The only difference is, however, that the primary wave has different phases at $\boldsymbol{r}$ and $\boldsymbol{r}'$, the phase difference being equal to $\exp\{i\boldsymbol{K}_0\cdot(n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2)\}$. If we shift the phase of the primary wave by this amount, then the geometrical condition for $\boldsymbol{r}$ is again identical to the geometrical condition for $\boldsymbol{r}'$ *before* the phase shift. As we have a time-stationary problem, the phase shift of the primary wave should only change the phase of the solution by the same amount. Thus (10) follows.

[14] The question which arises now is whether the form of § 2 can be derived from the form of § 3. The difficulty lies in the fact that PARSEVAL's theorem cannot be applied directly in the expansion in two-dimensions, because the functions $G(\boldsymbol{R})$ for $Z=0$ and $A(\boldsymbol{R}_t)$ are not quadratically integrable for the surface integral $\int ds$ (HOBSON [15], Vol. 2, p. 718). We can, however, circumvent this difficulty by expanding at first the function $G_s(\boldsymbol{R})$, which is quadratically integrable for $\Re e(s) > 2$, applying PARSEVAL's theorem, and then deriving from the expanded expression the form for $s=1$ by analytic continuation. In this way the form in § 2 proves to be really equivalent to the form in § 3.

[15] E. W. HOBSON, Functions of a Real Variable, 2 Vols., Cambridge University Press 1926–1927.

Appendix 2. Derivation of Green's Function

The expression (34) can be modified to the series of HANKEL functions

$$G(\boldsymbol{R}) = \frac{1}{2\,i\,A}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \sum_m \left(\frac{|Z|}{\Gamma_m}\right)^{\frac{1}{2}} H^{(1)}_{-\frac{1}{2}}(\Gamma_m|Z|)\exp\{i\,\boldsymbol{K}_{mt}\cdot\boldsymbol{R}_t\}\,. \tag{A 1}$$

We consider the generalized series (39). The power $(|Z|/\Gamma_m)^{\frac{1}{2}s}$ is made definite by the convention that (WHITTAKER–WATSON [2], p. 589)

$$\left(\frac{|Z|}{\Gamma_m}\right)^{\frac{1}{2}s} = \exp\left\{\frac{s}{2}\left(\mathrm{Log}\left|\frac{Z}{\Gamma_m}\right| - i\arg\Gamma_m\right)\right\} \tag{A 2}$$

and the argument of Γ_m takes the value 0 or $\pi/2$ according to (17 a, b). The series (39) can be easily seen to be an analytic function of s for all values of $\boldsymbol{R}=(\boldsymbol{R}_t, Z)$ if $\mathfrak{Re}(s)>2$, because then the double series $\sum_m |\Gamma_m|^{-s}$ is convergent (WHITTAKER–WATSON [2], p. 51). We want to find the analytic continuation of (39) for a domain containing $s=1$ to obtain the sum of (A 1), that is, of (34).

From an integral representation of HANKEL functions (WATSON [16], p. 178) we obtain the expression

$$\left(\frac{|Z|}{\Gamma_m}\right)^{\frac{1}{2}s} H^{(1)}_{-\frac{1}{2}s}(\Gamma_m|Z|) = \frac{1}{i\,\pi}\int_{0+}^{\infty\exp\{i\varphi_m\}} \zeta^{\frac{1}{2}s-1}\exp\left\{\frac{1}{2}\left(\Gamma_m{}^2\zeta - \frac{Z^2}{\zeta}\right)\right\}\mathrm{d}\zeta\,, \tag{A 3}$$

where

$$\varphi_m = \pi - 2\arg\Gamma_m\,. \tag{A 4}$$

The lower limit $0+$ indicates that the contour integral starts from 0 in the direction of the positive real axis. On putting (A 3) into (39) we have

$$\begin{aligned} G_s(\boldsymbol{R}) = &-\frac{1}{2\,\pi\,A}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \sum_m^{\Gamma_m{}^2>0} \exp\{i\,\boldsymbol{K}_{mt}\cdot\boldsymbol{R}_t\}\int_{0+}^{-\infty}\zeta^{\frac{1}{2}s-1}\exp\left\{\frac{1}{2}\left(\Gamma_m{}^2\zeta - \frac{Z^2}{\zeta}\right)\right\}\mathrm{d}\zeta \\ &-\frac{1}{2\,\pi\,A}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \sum_m^{\Gamma_m{}^2<0} \exp\{i\,\boldsymbol{K}_{mt}\cdot\boldsymbol{R}_t\}\int_{0+}^{+\infty}\zeta^{\frac{1}{2}s-1}\exp\left\{\frac{1}{2}\left(\Gamma_m{}^2\zeta - \frac{Z^2}{\zeta}\right)\right\}\mathrm{d}\zeta\,. \end{aligned} \tag{A 5}$$

We note that the first sum has only a limited number of terms so that the order of integration and summation can be inverted.

We apply now the theta-transformation formula in two dimensions (KRAZER and PRYM [17], p. 88; KRAZER [18], p. 108; EPSTEIN [19], p. 624) which is valid for $\mathfrak{Re}(\zeta)>0$

$$\sum_m \exp\left\{-\frac{\zeta}{2}|\boldsymbol{K}_{0t}+\boldsymbol{B}_{mt}|^2 + i(\boldsymbol{K}_{0t}+\boldsymbol{B}_{mt})\cdot\boldsymbol{R}_t\right\} = \frac{A}{2\,\pi\,\zeta}\sum_n \exp\left\{-\frac{1}{2\,\zeta}|\boldsymbol{R}_t+\boldsymbol{a}_{nt}|^2 - i\,\boldsymbol{K}_{0t}\cdot\boldsymbol{a}_{nt}\right\}, \tag{A 6}$$

where $\boldsymbol{a}_{nt}=n_1\boldsymbol{a}_1+n_2\boldsymbol{a}_2$ (n stands for the pair of indices n_1 and n_2). From this formula we find (in a similar manner as described in WHITTAKER–WATSON [2], p. 273) that the order of integration and summation of the second sum of (A 5) can be inverted if $\mathfrak{Re}(s)>4$ and if always $\mathfrak{Re}(\zeta)>0$ on the contour. After the inversion we split the integrals in two parts by taking a point ω somewhere in the domain $\mathfrak{Re}(\omega)>0$, $|\omega|<\infty$ (WHITTAKER–WATSON [2]: $\omega=1$). On applying (A 6) for the parts of the integrals from 0 to ω, and putting into this part $1/\zeta$ instead of ζ, we obtain

$$\begin{aligned} G_s(\boldsymbol{R}) = &-\frac{1}{2\,\pi\,A}\left(\frac{\pi}{2}\right)^{\frac{1}{2}}\left[\int_{\omega}^{-\infty}\zeta^{\frac{1}{2}s-1}\sum_m^{\Gamma_m{}^2>0}\exp\left\{\frac{1}{2}\left(\Gamma_m{}^2\zeta - \frac{Z^2}{\zeta}\right) + i\,\boldsymbol{K}_{mt}\cdot\boldsymbol{R}_t\right\}\mathrm{d}\zeta\right. \\ &\left.+\int_{\substack{\omega\\ \mathfrak{Re}(\zeta)>0}}^{+\infty}\zeta^{\frac{1}{2}s-1}\sum_m^{\Gamma_m{}^2<0}\exp\left\{\frac{1}{2}\left(\Gamma_m{}^2\zeta - \frac{Z^2}{\zeta} + i\,\boldsymbol{K}_{mt}\cdot\boldsymbol{R}_t\right\}\mathrm{d}\zeta\right] \\ &-\frac{1}{4\,\pi^2}\left(\frac{\pi}{2}\right)^{\frac{1}{2}}\int_{\substack{1/\omega\\ \mathfrak{Re}(\zeta)>0}}^{+\infty}\zeta^{-\frac{1}{2}s}\sum_n\exp\left\{-\frac{1}{2}\left(|\boldsymbol{R}+\boldsymbol{a}_{nt}|^2\zeta - \frac{\varkappa^2}{\zeta}\right) - i\,\boldsymbol{K}_{0t}\cdot\boldsymbol{a}_{nt}\right\}\mathrm{d}\zeta\,. \end{aligned} \tag{A 7}$$

[16] G. N. WATSON, Theory of BESSEL Functions, Cambridge University Press 1944 (2nd ed.).

[17] A. KRAZER and F. PRYM, Neue Grundlagen einer Theorie der allgemeinen Thetafunktionen, Teubner, Leipzig 1892 (referred to by EPSTEIN [19]).

[18] A. KRAZER, Lehrbuch der Thetafunktionen, Teubner, Leipzig 1903 (referred to by EWALD [13]).

[19] P. EPSTEIN, Math. Ann. **56**, 615 [1903].

This expression can be proved (again in a similar manner as WHITTAKER–WATSON [2], p. 273) to be an analytic function of s for *all values* of s if $|\boldsymbol{R}| \neq 0$. It represents the analytic continuation of (39) for $\Re\mathrm{e}(s) \leqq 2$. On putting $s=1$ and inverting again the order of summation and integration (since it can be proved to be allowed) we obtain (40). The restriction $\Re\mathrm{e}(\zeta) > 0$ can then be removed.

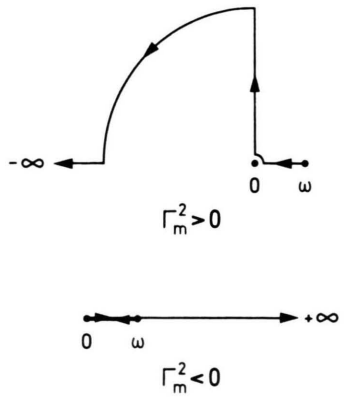

Fig. 2. The paths of integrals for Eq. (41).

We take ω on the real axis ($\omega > 0$) and the contours shown in Fig. 2 for the integrals of (40). We consider at first the case ${\Gamma_m}^2 > 0$. On applying JORDAN's lemma (WHITTAKER–WATSON [2], p. 115) to the infinitely large and infinitely small quadrants of circles we find that the integrals on these vanish (WATSON [16], p. 180). We obtain from the part 0 to $i\,\infty$ on the imaginary axis

$$-\sqrt{2\pi}\,\frac{\exp\{i\,\Gamma_m |Z|\}}{i\,\Gamma_m}, \tag{A 8}$$

and from the part ω to 0 on the real axis

$$-\int_{1/\omega}^{\infty} t^{-3/2} \exp\left\{-\frac{1}{2}\left(|Z|^2 t - \frac{{\Gamma_m}^2}{t}\right)\right\} \mathrm{d}t. \tag{A 9}$$

In the case ${\Gamma_m}^2 < 0$ we obtain (A 8) from the part 0 to $+\infty$ and (A 9) from the part ω to 0. It follows then (41).

To derive the form (42) we assume, just as EWALD [13] did, that $\varkappa$ has a small positive imaginary part. We put then in the expression (40)

$$\omega \to \infty \exp\{i\varphi\},$$

where

$$\tfrac{1}{2}\pi - 2\arg\varkappa < \varphi < \tfrac{1}{2}\pi. \tag{A 10}$$

Then the contours of the first integrals can be represented by segments of an infinitely large circle from $\infty \exp\{i\varphi\}$ to $\infty \exp\{i\varphi_m\}$. By applying JORDAN's lemma one can prove that these integrals vanish. The second integrals of (40) can be transformed to the form (EWALD [13])

$$\sqrt{2\pi}\,\frac{\exp\{i\varkappa|\boldsymbol{R}+\boldsymbol{a}_{nt}|\}}{|\boldsymbol{R}+\boldsymbol{a}_{nt}|}, \tag{A 11}$$

so that (42) follows.

Appendix 3.

Proof of the Properties of Green's Function

If $Z = z - z' \neq 0$ the termwise differentiation of (34) is allowed, and it follows at once that $G(\boldsymbol{R})$ satisfies

$$\nabla^2_{\boldsymbol{R}}\, G(\boldsymbol{R}) + \varkappa^2 G(\boldsymbol{R}) = 0. \tag{A 12}$$

If $Z = 0$ and $\Re\mathrm{e}(s) > 2$ we find that the termwise differentiation of (39) is allowed. On applying the properties of BESSEL functions (WATSON [16], p. 74) we obtain, if $|\boldsymbol{R}| \neq 0$,

$$\nabla^2_{\boldsymbol{R}}\, G_s(\boldsymbol{R}) = -\varkappa^2 G_s(\boldsymbol{R}) - (s-1) G_{s-2}(\boldsymbol{R}). \tag{A 13}$$

The right-hand side is an analytic function of s, so that (A 12) follows for $s=1$ if $|\boldsymbol{R}| \neq 0$.

The expression (A 7) shows that $G_s(\boldsymbol{R})$ is a smooth function of $\boldsymbol{R}$ if $|\boldsymbol{R}| \neq 0$. In the neighbourhood of $|\boldsymbol{R}| = 0$ the term with $|\boldsymbol{a}_{nt}| = 0$ in the last series of (A 7) becomes predominant if $s = 1$.

Thus

$$\begin{aligned} G(\boldsymbol{R}) \underset{|\boldsymbol{R}|\to 0}{\to} & -\frac{1}{4\pi^2}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \int_{1/\omega}^{\infty} t^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}\left(|\boldsymbol{R}|^2 t - \frac{\varkappa^2}{t}\right)\right\} \mathrm{d}t \\ = & -\frac{1}{4\pi^2}\left(\frac{\pi}{2}\right)^{\frac{1}{2}} \sum_n \frac{1}{n!}\left(\frac{\varkappa^2}{2}\right)^n \left(\frac{|\boldsymbol{R}|^2}{2}\right)^{n-\frac{1}{2}} \int_{|\boldsymbol{R}|^2/2\omega}^{\infty} x^{-\frac{1}{2}-n} \exp\{-x\}\,\mathrm{d}x \qquad \text{(A 14)} \\ \to & -\frac{1}{4\pi|\boldsymbol{R}|}. \end{aligned}$$

This equation shows, combined with (A 12), valid for $|\boldsymbol{R}| \neq 0$, that $G(\boldsymbol{R})$ satisfies (4) (MORSE–FESHBACH [11], p. 809).

The function $G(\boldsymbol{R})$ satisfies the boundary conditions on the side planes (35 a, b) as it can be seen directly from (40).

The boundary conditions (36 a, b) are also satisfied. This can be proved as follows. For example, for (36 a) we consider at first the integral

$$I_s = 2 \int G_s(\boldsymbol{r}_t, 0 \,|\, \boldsymbol{r}_t', 0)\; G_{sz}(\boldsymbol{r}_t', z_i \,|\, \boldsymbol{r}_{t1}, z_1)\; \mathrm{d}s', \tag{A 15}$$

where $G_{sz} = \partial G_s / \partial z$. If $\Re\mathrm{e}(s) > 2$ we obtain from the expression (39), using the known properties of HANKEL functions,

$$I_s = -\frac{1}{i\,A}\, 2^{\frac{1}{2}s-2} \exp\left\{ i\,\frac{s\,\pi}{2} \right\} \Gamma\left(\frac{s}{2}\right) \sum_m \frac{|z_i - z_1|^{\frac{1}{2}s}}{\Gamma_m^{\frac{3}{2}s-1}}\, H^{(1)}_{-\frac{1}{2}s+1}\,(\Gamma_m\,|\,z_i - z_1\,|)\; \exp\{i\,\boldsymbol{K}_{mt}\cdot(\boldsymbol{r}_t - \boldsymbol{r}_{t1})\}\,. \tag{A 16}$$

Since it is assumed that $z_i \neq z_1$ this expression is an analytic function of s except at the poles of $\Gamma(\frac{1}{2}\,s)$. Hence putting $s = 1$ we have

$$I_1 = 2 \int G(\boldsymbol{r}_t, 0 \,|\, \boldsymbol{r}_t', 0)\; G_z(\boldsymbol{r}_t', z_i \,|\, \boldsymbol{r}_{t1}, z_1)\; \mathrm{d}s' = -G(\boldsymbol{r}_t, z_i \,|\, \boldsymbol{r}_{t1}, z_1)\,. \tag{A 17}$$

This proves (36 a). (36 b) can be proved in the same way.

Gravitationsinstabilitäten eines Plasmas bei differentieller Rotation

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Herrn Prof. Dr. L. BIERMANN *zum 60. Geburtstag gewidmet*

In this paper an instability calculation is given for an axially symmetric gas distribution which has a differential rotation and in which a magnetic field is present. It is a generalization of similar calculations given by CHANDRASEKHAR and BEL and SCHATZMAN. The generalization becomes necessary for the study of problems of the formation of planetary systems and star formation.

The instability conditions and the critical wave lengths are calculated for plane-wave-like disturbances. For disturbances running perpendicularly to the axis of rotation instability can occur only if the gas density exceeds a critical value which depends on the differential rotation at the considered distance only as long as pressure gradients and gradients of the magnetic field strength are negligible. If the gas density exceeds this critical value the shortest unstable wave length is proportional to the square root of $v_T^2 + v_B^2$, where v_T means the velocity of sound and v_B the ALFVÉN-velocity.

For disturbances running parallel to the axis of rotation in addition to the JEANS instability a new type of instability occurs due to the simultaneous action of the magnetic field and the differential rotation; for rigid rotation this instability vanishes.

In vielen astrophysikalischen Untersuchungen spielt die Frage nach den Gravitationsinstabilitäten eines unter seiner Eigengravitation stehenden Gases eine wichtige Rolle. JEANS [1] führte als erster Instabilitätsrechnungen dieser Art aus. Erweiterungen auf kompliziertere Gaskonfigurationen ohne und mit Magnetfeld sind in unserer Zeit u. a. von CHANDRASEKHAR und FERMI [2], FRICKE [3], CHANDRASEKHAR [4], BEL und SCHATZMAN [5], SAFRONOV [6] und GLIDDON [7] ausgeführt worden. Die hier durchgeführte ist eine Verallgemeinerung der von CHANDRASEKHAR [4] und BEL und SCHATZMAN [5]. Sie geht aus neueren Untersuchungen zur Entstehung von Sternen und Planetensystemen hervor [8].

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