The potential model treatment of the scattering of electrons by atoms and the existence of negative ions

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The low energy scattering of electrons by different neutral atoms has been treated by assuming that the atomic wave functions remain unchanged even at the presence of the scattered particle and by neglecting the exchange between the scattered electron and the bound electrons. The potential term in the differential equation of the scattered particle is exactly the atomic potential of the neutral atom and is approximated by analytical expressions, yielding the potential scattering equation. The variational treatments of Hulthén, Kohn and a related one suggested by Malik, are applied to solve this equation for a Hartree atom with $l=0$. The scattering by He, C and N is treated explicitly and the results of He indicate that in this way one may get some good result without going into the great complexity of the many body problem. It is further pointed out that the study of scattering by neutral atoms near zero energy under this model may serve as a possible mean to investigate the existence of different negative ions and their number of bound states. It seems from this point of view that He^-, C^- and N^- for this model may exist and have one bound s-state.

The elastic scattering of electrons by neutral atoms as well as the formation of the negative ions are of great interest in connection with upper atmosphere physics as well as astrophysics. Apart from that the partial scattering cross sections are needed in order to calculate the diffusion cross sections. Since the energy where only the elastic scattering takes place, is of the order of 0 to 50 eV, the usual treatment by the Born approximation loses its validity. On the other hand the accurate treatment of the scattering by atoms is a very complicated problem. Accurate accounts are available only for scattering by Hydrogen and to a certain extent by Helium[1], Argon[2], Krypton[3], and Sodium[4]. We shall try here to formulate a semi-phenomenological method which may be termed as potential scattering model. Although it may not have the same accuracy as when one would treat each case separately it is simple and may give appreciably better results than the Born approximation. Furthermore it seems that this method may serve as a mean to establish the existence of different negative ions as well as the number of bound states available. The scattering by the Thomas–Fermi atom for elements $Z=57$ to $Z=90$ has been investigated by Robinson[5] who integrated the wave equation for the scattered electron numerically. Tietz[6] has used the Born approximation with the same type of potential used here. A perturbational approach of the type of Brueckner and Watson[7] to this problem has been studied by Lippman, Mittleman and Watson[8, 9] who try to get a scattering potential by rearranging different perturbation series. But it seems that their approach may have similar limitations as other methods and is quite complicated. It is in fact difficult to see the amount of labour that will be involved and the accuracy that may be obtained unless some concrete problem is worked out by their approach.

I. Derivation of the scattering equation

In deriving the scattering equation, we shall usually neglect the Pauli principle and the so-called polarisation effect but we shall all along sketch the type of modification that will come in due to Pauli's principle and at the end indicate a possible approach to consider polarisation. In general we shall refer to the scattering of electrons by atoms but it is obvious that the method works also for the scattering of any particle.

Assuming the nucleus to be at rest having infinite mass and charge Z, the non-relativistic Hamiltonian

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[1] B. L. Moiseiwitsch, Proc. Roy. Soc., Lond. A **219**, 102 [1953].

[2] J. Holtsmark, Z. Phys. **55**, 437 [1929].

[3] J. Holtsmark, Z. Phys. **66**, 49 [1930].

[4] P. A. Salmona et P. Frenkiel, J. Phys. Radium **20**, 492 [1959].

[5] L. B. Robinson, Phys. Rev. **117**, 1281 [1960].

[6] T. Tietz, Ann. Phys. (7) **3**, 105 [1959].

[7] see ref. [8, 9].

[8] M. H. Mittleman and K. M. Watson, Phys. Rev. **113**, 198 [1959].

[9] B. A. Lippman, M. H. Mittleman and K. M. Watson, Phys. Rev. **116**, 920 [1960].

of the system with the nucleus and $(N+1)$ charged particles having only COULOMB interaction between them may be written as

$$H=\sum_{i=1}^{N+1}\left(-\frac{1}{2}\Delta_i-\frac{Z}{r_i}\right)+\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N+1}\frac{1}{|\mathfrak{r}_i-\mathfrak{r}_j|}\qquad(1)$$

where we have used the atomic units of HARTREE i. e. $\hbar=m=e=1$.

$\mathfrak{r}_i$ is the position vector of the i-th electron from the nucleus, $r_i=|\mathfrak{r}_i|$, and Δ_i is LAPLACE's operator acting on the i-th coordinate.

(1) can obviously be written as

$$H=H_{\mathrm{A}}+H_{N+1},$$

$$H_{\mathrm{A}}=\sum_{i=1}^{N}\left(-\frac{1}{2}\Delta_i-\frac{Z}{r_i}\right)+\frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{|\mathfrak{r}_i-\mathfrak{r}_j|},\qquad(2)$$

$$H_{N+1}=-\frac{1}{2}\Delta_{N+1}-\frac{Z}{r_{N+1}}+\sum_{i=1}^{N}\frac{1}{|\mathfrak{r}_{N+1}-\mathfrak{r}_i|}.\qquad(3)$$

If $\psi(\mathfrak{q}_1,\mathfrak{q}_2\dots\mathfrak{q}_{N+1})$ be the wave function of the system, the SCHRÖDINGER equation is

$$H\,\psi(\mathfrak{q}_1\dots\mathfrak{q}_{N+1})=E\,\psi(\mathfrak{q}_1\dots\mathfrak{q}_{N+1})\qquad(4)$$

where E is the total energy of the system and $\mathfrak{q}_1$, $\mathfrak{q}_2\dots\mathfrak{q}_{N+1}$ are the configuration and spin coordinates.

Let Φ_{A} be the total wave function of the atom, given by

$$H_{\mathrm{A}}\,\Phi_{\mathrm{A}}(\mathfrak{q}_1\dots\mathfrak{q}_N)=E_{\mathrm{A}}\,\Phi_{\mathrm{A}}(\mathfrak{q}_1\dots\mathfrak{q}_N).\qquad(5)$$

We write

$$\psi(\mathfrak{q}_1\dots\mathfrak{q}_{N+1})=\Phi_{\mathrm{A}}(\mathfrak{q}_1\dots\mathfrak{q}_N)\,F(\mathfrak{q}_{N+1}).\qquad(6)$$

Multiplying (4) by Φ_{A}^*, integrating over the space coordinates $\mathfrak{r}_1\dots\mathfrak{r}_N$ and summing over all the spin coordinates, we get

$$\left[\Delta_{N+1}+2\left(\frac{Z}{r_{N+1}}-\sum_{i=1}^{N}\int \mathrm{d}^3\mathfrak{r}_1\int \mathrm{d}^3\mathfrak{r}_2\dots\right.\right.\qquad(7)$$
$$\left.\left.\cdot\int \mathrm{d}^3\mathfrak{r}_N\,\frac{|\Phi(\mathfrak{r}_1\dots\mathfrak{r}_N)|^2}{|\mathfrak{r}_{N+1}-\mathfrak{r}_i|}\right)\right]F(\mathfrak{r}_{N+1})=-2\,E_k\,F(\mathfrak{r}_{N+1})$$

where the normalisation condition

$$\int \mathrm{d}^3\mathfrak{r}_1\int \mathrm{d}^3\mathfrak{r}_2\dots\int \mathrm{d}^3\mathfrak{r}_N\,|\Phi(\mathfrak{r}_1\dots\mathfrak{r}_N)|^2=1$$

has been used, and $E_k=E-E_{\mathrm{A}}$

is the energy parameter for $(N+1)^{\mathrm{st}}$ particle.

We may note that to be more accurate one has to antisymmetrize the right hand side of (6) properly. If one makes allowance in this way for the exchange between $(N+1)^{\mathrm{st}}$ particle and each of the N particles, one will obtain an integro-differential equation instead of (7). The exchange between the N atomic electrons has been in principle taken into account.

The second term on the left hand side of (7) is a function of $\mathfrak{r}_{N+1}$ alone and may be looked upon to be the effective potential acting on $F(\mathfrak{r}_{N+1})$; it is in fact what HARTREE denotes Z_{p}/r_{N+1}. So (7) may be formally written as (dropping the suffix)

$$[\Delta-2\,V(r)]\,F(\mathfrak{r})=-2\,E_k\,F(\mathfrak{r}).\qquad(8)$$

We expand

$$F(\mathfrak{r})=\sum_{l,m}a_{l,m}\,\frac{\chi_l(r)}{r}\,Y_{l,m}(\Theta,\varphi)\qquad(9)$$

where $Y_{l,m}(\Theta,\varphi)$ is a normalised spherical harmonic. By multiplication of (8) with $Y^*_{l,m}(\Theta,\varphi)$ and integration over the angles we get our final equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+k^2-\frac{l(l+1)}{r^2}-2\,V(r)\right]\chi_l(r)=0\qquad(10)$$

where $k^2=2\,E_k$.

This is precisely the equation of a particle scattered by the potential

$$V(r)=-\frac{Z}{r}+\sum_{i=1}^{N}\int \mathrm{d}^3\mathfrak{r}_1\int \mathrm{d}^3\mathfrak{r}_2\dots$$
$$\cdot\int \mathrm{d}^3\mathfrak{r}_N\,\frac{|\Phi(\mathfrak{r}_1\dots\mathfrak{r}_N)|^2}{|\mathfrak{r}-\mathfrak{r}_i|}.$$

The function $V(r)$ in (7) will take a different form depending on the approximation used for Φ. Although (7) is the HARTREE equation for $F(\mathfrak{r}_{N+1})$; the essential idea of self consistency is dropped out in deducing (7). In calculating Φ through (5) the presence of $F(\mathfrak{r})$ is neglected. This corresponds to the physical picture that the atom remains unperturbed even at the presence of the scattered particle. An improvement to this may be done by introducing a so-called polarisation potential.

For $V(r)$ in (8) one may use the charge density as given by HARTREE or HARTREE–FOCK wave functions for the bound electrons. This can be very well approximated by a series of exponential functions as done by HOLTSMARK [10], RUARK [11], and BYATT [12].

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[10] J. HOLTSMARK, Z. Phys. **66**, 49 [1930].

[11] A. E. RUARK, Phys. Rev. **57**, 62 [1940].

[12] W. O. BYATT, Phys. Rev. **104**, 1298 [1956].

For $N=Z$, i. e. neutral atom

$$V(r) = -\frac{Z}{r}\sum_n A_n \exp(-\gamma_n r) \tag{11}$$

where A_n and γ_n are constants depending on Z. A polarization potential $V_{\text{pol}}(r)$ might be added to the expression (11) for $V(r)$. $V_{\text{pol}}(r)$ is usually taken as an approximation to a second order perturbation calculation in the so-called static model, i. e. a model where the atom is polarized by the scattered electron which is assumed to be fixed. The polarization potential is an attractive potential, which behaves for large r as r^{-4}.

If (10) represents the equation for the scattering, with the asymptotic conditions

$$\chi_l(r) \xrightarrow[r\to\infty]{} \text{const} \sin\left(k r - \frac{\pi l}{2} + \lambda_l\right),$$
$$\chi_l(r) \xrightarrow[r\to 0]{} 0 \tag{12}$$

where λ_l is the phase shift for the l-th partial wave, the scattering amplitude $f(\Theta)$ is given by

$$f(\Theta) = \frac{1}{2ik}\sum_l (2l+1)\, P_l(\cos\Theta)[\exp(2i\lambda_l) - 1]$$

where $P_l(\cos\Theta)$ is the l-th LEGENDRE polynomial. The differential cross section for the scattering into the solid angle $d\Omega$ in direction Θ is

$$I(\Theta)\, d\Omega = |f(\Theta)|^2\, d\Omega$$

and the total cross section

$$Q = 2\pi \int_0^\pi I(\Theta) \sin\Theta\, d\Theta = \frac{4\pi}{k^2}\sum_{l=0}^\infty (2l+1)\sin^2\lambda_l = \sum_{l=0}^\infty Q_l . \tag{13}$$

II. Relation between the phase shift and the existence of negative ions

Apart from the obvious simplicity of the eq. (10) [together with (11)], one can now use the different theorems connected with the potential scattering theory. Studying the behaviour of the analytical extension of the phase shift in the complex energy plane, one will get information on the bound states given by the potential in (10). LEVINSON[13] has proved a theorem connecting the number of bound states and the phase shift λ. This may be stated as follows:

If the scattering potential $V(r)$ is a continuous (or at least piecewise continuous) function of r and if

$$\int_0^1 r\,|V(r)|\, dr + \int_1^\infty r^2\,|V(r)|\, dr < \infty , \tag{14}$$

then either

$$|\lambda(k=\infty) - \lambda(k=0)| = m\pi$$

or

$$|\lambda(k=\infty) - \lambda(k=0)| = (m+\tfrac{1}{2})\,\pi$$

where m is the number of eigenvalues on the positive imaginary axis of the k-plane. In our case the first of the two equations holds.

Since from the physical point it is clear that a particle with infinite energy will not see the finite potential at all, $\lambda(k=\infty)=0$.

Studying the behaviour of the phase shift near the zero energy scattering, one can get information on the number of bound states available for a potential satisfying (14).

The potential in (10) as given by (11) satisfies (14) obviously. From the value of $\lambda(k=0)$ it should be possible to say if a negative ion of an atom whose corresponding potential is used in (11) exists and if so, the number of available bound states of this ion can be known. The physical atom for which exchange and the polarisation effects must be included, differs certainly from the HARTREE atom, that will be used here. The experience shows that usually the polarisation and exchange potential will make the attractive potential deeper, so that one might expect that the number of bound states occurring in the HARTREE atom will also accur in the actual ion *. So this model may serve to study the existence of different negative ions as well as the number of their bound states.

III. Variational solution

In order to find a suitable solution of eq. (10), we have applied here the variational methods of HULTHÉN[14], KOHN[15] and a related one[16]. We have used the different relations connecting them in order to check the consistency of the results obtained. Let L_l be equal

$$L_l \equiv \int \chi_l(r)\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2V(r) + k^2\right]\chi_l(r)\, dr \tag{15}$$

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* There is however a conjecture due to SWAN that if PAULI principle is included, LEVINSON's theorem would be $\lambda(0)=(n+m)\,\pi$ where n is the number of extra nodes coming in due to PAULI principle.

[13] N. LEVINSON, Mat. Fys. Medd. Dan. Vid. Selsk. **25**, No. 9 [1949].

[14] L. HULTHÉN, K. Fys. Sällsk. Lund Förk. **14**, Nr. 21 [1944].

[15] W. KOHN, Phys. Rev. **74**, 1763 [1948].

[16] F. B. MALIK, Z. Naturforschg. **14 a**, 172 [1959].

with the asymptotic conditions

$$\lim_{r\to\infty} \chi_l(r) \to \sin k\,r + (-1)^l\, a \cos k\,r\,,$$

$$\lim_{r\to 0} \chi_l(r) = 0\,.$$

Variation of (15) with respect to χ_l gives [14]

$$\delta L_l = -k\,\delta a \quad \text{or} \quad \delta(L_l + k\,a) = 0\,. \tag{16}$$

For the correct solution is

$$a = \tan\lambda\,.$$

Henceforth we are omitting the index l from L_l.

If a suitable trial function for $\chi_l(r)$ is now chosen containing $n+1$ independent parameters $c_1 \dots c_n$, a according to **Hulthén**'s method these parameters are determined by

$$L = 0 \tag{17 a}$$

and
$$\partial L/\partial c_i = 0, \quad i = 1, \dots, n \tag{17 b}$$

where
$$\lambda = \operatorname{arc\,tan} a\,.$$

On the other hand **Kohn** [15] uses the following equations to determine the $(n+1)$ unknowns

$$\left(\frac{\partial L}{\partial a}\right)_{a=a_{\mathrm{K}}} = -k\,, \qquad \frac{\partial L}{\partial c_i} = 0\,. \tag{18 a, b}$$

The phase shift is then given in first approximation by

$$\lambda_{\mathrm{K}} = \operatorname{arc\,tan}(L_{\mathrm{K}}/k + a_{\mathrm{K}})\,.$$

The subscript K refers to **Kohn**'s method.

Another possibility to determine the parameters and the phase shift are the equations [16]

$$\int_0^\infty \chi_l\, 2\,V(r)\, j_l(k\,r)\,\mathrm{d}r = -a\,k\,, \qquad \frac{\partial L}{\partial c_i} = 0 \tag{19 a, b}$$

and
$$\lambda_{\mathrm{t}} = \operatorname{arc\,tan}(a_{\mathrm{t}} + L_{\mathrm{t}}/k)$$

where the subscript „t" refers to the parameters determined by (19 a) and (19 b) and $j_l(k\,r)$ is the spherical **Bessel** function regular at the origin. The three methods are interrelated by the equations [16]

$$L = \frac{a}{2}\,\frac{\partial L}{\partial a} - \frac{a\,k}{2} - \int_0^\infty \chi_l\, 2\,V(r)\, j_l(k\,r)\,\mathrm{d}r \tag{20}$$

if
$$\partial L/\partial c_i = 0\,.$$

A good criterion for the correctness of **Hulthén**'s method will be an approximate fulfillment of (19 a) and the reliability of the results calculated by (19 a) and (19 b) will depend on the approximate fulfillment of the equation $L_{\mathrm{t}} = 0$. On the other hand if L_{K} is quite small against $a_{\mathrm{K}}\,k$, one may expect a good result from **Kohn**'s method. The equation (20) indicates that if any two of conditions (17 a), (18 a), and (19 a) are fulfilled the third is automatically fulfilled. This seems to indicate that one may determine one unknown parameter c_0 by putting $(20) = 0$, after either the set (18 a) and (18 b) or the set (19 a) and (19 b) has been used to determine the rest of the parameters (not using $\partial L/\partial c_0 = 0$). This procedure means an amalgamation of all three methods and simultaneous fulfillment of the respective reliability condition.

In the following we have used the potential scattering model of part I and the variational methods of part III to treat low energy s-wave [i. e. $l=0$ in (11)] scattering by neutral He, C and N atoms where we have taken pure **Hartree**-field (i. e. no exchange in Φ). The parameters A_n and γ_n are taken from the table given by **Byatt** [12]. The ansatz for the trial wave function [17] is

$$\chi_0 = \sin k\,r + (a + b\,e^{-c\,r})\,(1 - e^{-d\,r})\cos k\,r\,. \tag{21}$$

In the calculation for these three cases we have put $c = d$ and have determined this parameter in such a way that $(20) \approx 0$ approximately for all energies, and the rest of the parameters are determined either by (18 a) and (18 b) or (19 a) and (19 b).

IV. Results and Discussions

a) *Scattering by helium atoms:* Table I a gives the s-wave phase shifts and low energy electron scattering (0 to 54 eV) by He-atoms. The subscripts H, K and t correspond to the results obtained by **Hulthén**, **Kohn** and equations (19 a), (19 b) respectively. Q_{t} represents the cross section for $l=0$, using the λ_{t} values. The column, "numerical integration" means the use of numerically tabulated ground state He **Hartree** wave function for Φ in the integral of equation (7) and solving the corresponding differential equation for $\chi_0(r)$ numerically, to get the phase shifts. The column "**Moiseiwitsch**'s value" refers to the values obtained by **Moiseiwitsch** [18] using **Hulthén**'s method to solve the corresponding equation for $\chi_0(r)$, if one uses simple **Slater** type wave func-

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[17] Massey-Moiseiwitsch, Proc. Roy. Soc., Lond. A **205**, 483 [1951].

[18] B. L. Moiseiwitsch, Proc. Roy. Soc., Lond. A **219**, 102 [1953].

a) *The phase shifts*

Wave No. k	Energy k^2 in a.u.	Numerical integration N	MOISEIWITSCH's values (HULTHÉN)	λ_K	λ_H	λ_t (Pot. I)	λ_t (Pot. II)	$Q_t/\pi a_0^2$
0.136	0.0184	2.570	2.340	2,312	2.417	2.454	2,028	87,569
0.272	0.0739	2.110	1.960	2.023	2.023	2.060	1.729	42,175
1.000	1.000	—	—	1.371	1.370	1.388	1.252	3.868
1.053	1.1088	1.360	1.340	1.347	1.346	1.345	1.232	3.427
1.359	1.8468	1.260	1.220	1.229	1.228	1.238	1.134	1.935
1.922	3.694	1.090	1.070	1.073	1.073	1.069	0.999	0.832
2.000	4.000	—	—	1.056	1.055	1.050	0.984	0.752

b) *The parameters and the reliability conditions* $c=1,6875$

k^2 in a.u.	a_K	a_H	a_t (Pot. I)	b_K	b_H	b_t (Pot. I)	L_K/k	Integration for tan λ_H	L_t/k
0.0184	− 0.866	− 0.885	− 0,822	− 1.045	− 1.088	− 1.948	− 0.020	− 0.914	− 0.061
0.0739	− 2.009	− 2.059	− 1.878	− 2.460	− 2.564	− 2.189	− 0.052	− 2.130	− 0.170
1.0000	4.628	4.918	5.417	6.884	6.973	7.125	0.301	5.108	− 0.001
1.053	4.106	4.376	4.744	6.204	—	—	0.280	—	—
1.8468	2.626	2.805	2.891	4.200	4.113	4.071	0.182	2.864	0.000
3.694	1.957	1.838	1.821	2.708	2.810	2.824	− 0.118	1.824	0.000
2.000	1.940	1.765	1.743	2.566	2.718	2.737	− 0.173	1.745	0.000

Table I. Elastic scattering of low energy electrons by the neutral Helium atom (for *s*-wave).

tions for the ground state of the He-atom. For the rest of the columns, but for the column under λ_t (Pot. II), we have used the two term exponential series of BYATT [12] to approximate the HARTREE field, and λ_t (Pot. II) gives the result if only one exponential term is used to approximate the HARTREE field. The reasonably good agreement between λ_N, and each of λ_H, λ_K and λ_t (Pot. I) certainly indicates that the analytical potential is a good approximation to the HARTREE potential. λ_t (Pot. I) agrees on the whole best with λ_N, the derivation lying between 0.8% to 6% of λ_N. The result of λ_t (Pot. II) where only one exponential term has been used to approximate the HARTREE field, shows the need for a good

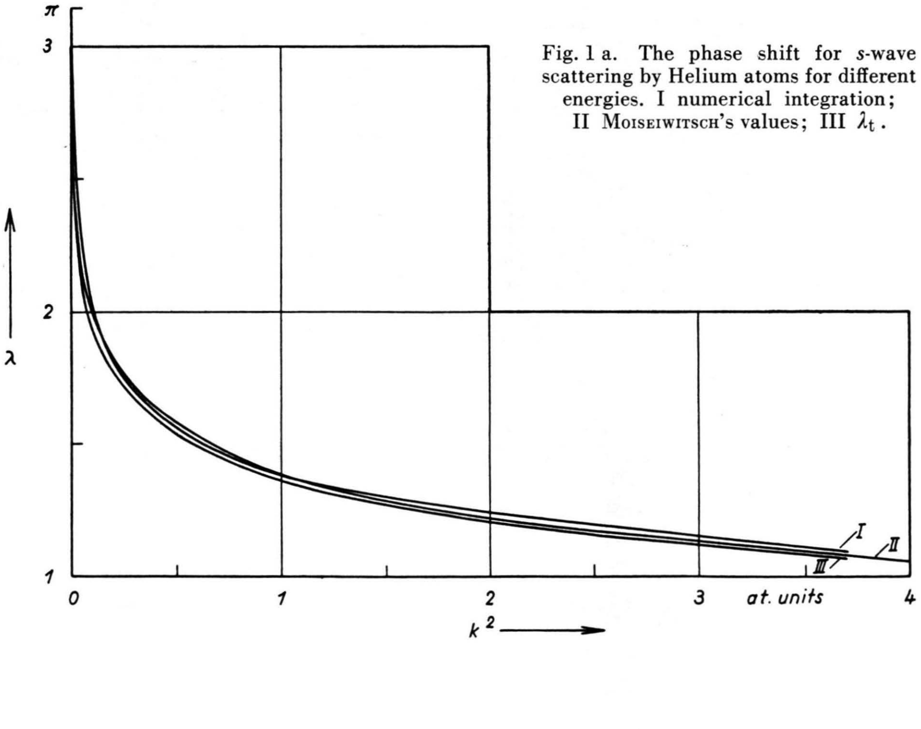

Fig. 1 a. The phase shift for *s*-wave scattering by Helium atoms for different energies. I numerical integration; II MOISEIWITSCH's values; III λ_t.

approximation of the atomic field; the deviation of MOISEIWITSCH's results from λ_N confirms this point too. Table I b gives the values of the parameters a and b. The column "integration for tan λ_H" means the integration of the left hand side integral of (19 a) (divided by k), using HULTHÉN's parameters for the wave function. It is a check for HULTHÉN's method, and should be equal to a_H. L_K/k and L_t/k are given as check of KOHN's and the last method respectively.

Fig. 1 a gives the phase shifts λ_N, λ_M (i. e. MOISEIWITSCH's value) and λ_t (Pot. I) against energy in atomic units ($k^2=1$ corresponds to $E=13.6$ eV). Fig. 1 b plots Q_t against k^2 and Fig. 1 c shows the difference of the phase shifts between λ_N and λ_H, λ_N and λ_K, and λ_N and λ_t (Pot. I) showing that λ_t gives the best variational result over the whole energy range for this case.

It seems that the two term exponential potential is a good approximation of the HARTREE field and since this potential satisfies the condition (14) and the zero energy phase shift tends to π, one may conclude from § II, that the two term exponential potential corresponding to HARTREE field is strong enough to have a bound state. Since the net effect of the exchange and polarisation terms is expected from experience to make the potential more attractive, this makes the existence of He$^-$ ion plausible; contrary to the usual belief. It may of course be very loosely bound. But if it does exist and has an energy of the order of -0.5 eV, this will certainly have influence on the continuum of the photosphere spectrum of the sun, where there is indeed still some discrepancy between the theory and the observation. The free-free and the bound-free transitions of He$^-$ will give contribution to this continuum spectrum.

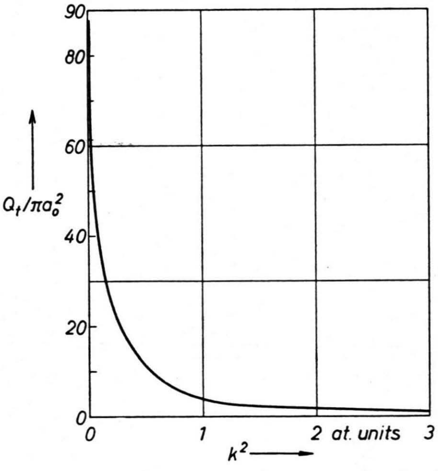

Fig. 1 b. The total cross section for scattering by Helium using the s-wave contribution only.

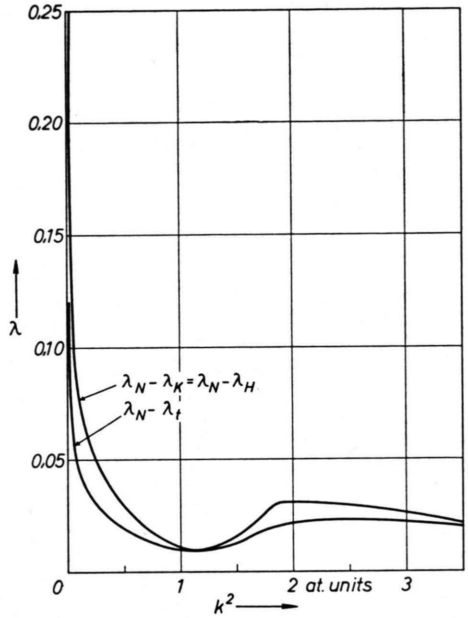

Fig. 1 c. The difference curves between the numerical result and the results obtained by the three different variational methods for different energies.

b) *The scattering by carbon atoms:* An approximation of the HARTREE field by three exponential functions has been used to calculate the s-wave scattering in this case (s refers here only to the angular momentum of the scattered particle, the total angular momentum is different). The parameter c has been chosen in such a way that the three methods give the same result and varies slightly from higher to the lower energy, where it becomes constant.

Table II a gives the phase shift, and the total cross section. Table II b gives the values of the parameters together with L_k/k, integration for tan λ_H and L_t/k. Fig. 2 a plots the phase shift against the energy, and Fig. 2 b gives the total cross section as a function of energy. The zero energy phase shift $\lambda=\pi$ confirms the existence of the already established C$^-$ ion. The HARTREE field seems to be strong enough only for a single bound s-state. The supposition [19, 20] that there may be an excited state of C$^-$ ion is left open

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[19] H. R. JOHNSON and F. ROHRLICH, J. Chem. Phys. **30**, 1608 [1959].

[20] D. R. BATES and B. L. MOISEIWITSCH, Proc. Phys. Soc., Lond. A **68**, 540 [1955].

a) *The phase shifts*

Energy k^2 in a.u.	c-value	λ_K	λ_H	λ_t	$Q_t/\pi a_0^2$
0.005	2,60	2.816	2.816	2.816	81.853
0.01	2.60	2.688	2.688	2.688	76.808
0.05	2.60	2.224	2.224	2.224	50.453
0.10	2.60	1.956	1.956	1.956	34.352
0.50	2.60	—	1.243	—	—
0.80	2.60	1.017	1.017	1.017	3.617
1.00	2.55	0.905	0.905	0.905	2.474
1.20	2.55	0.814	0.813	0.813	1.759
1.50	2.45	0.693	0.692	0.692	1.086

b) *The parameters and the reliability conditions*

k^2 in a.u.	a_K	a_H	a_t	b_K	b_H	b_t	L_K/k	Integration for tan λ_H	L_t/k
0.005	– 0.337	– 0.338	– 0.334	0.824	0.828	0.816	– 0.001	– 0.340	– 0.004
0.01	– 0.486	– 0.488	– 0.482	1.193	1.198	1.182	– 0.002	– 0.490	– 0.006
0.05	– 1.305	– 1.307	– 1.299	3.280	3.287	3.262	– 0.002	– 1.311	– 0.006
0.10	– 2.471	– 2.470	– 2.477	6.395	6.391	6.411	0.001	– 2.468	0.007
0.50	2.994	2.940	2.832	—	—	—	—	—	—
0.80	1.658	1.618	1.590	– 6.222	– 6.119	– 6.045	– 0.039	1.602	0.028
1.00	1.346	1.273	1.243	– 5.490	– 5.308	– 5.232	– 0.071	1.252	0.029
1.20	1.105	1.058	1.045	– 5.010	– 4.893	– 4.861	– 0.047	1.046	0.013
1.50	0.931	0.829	0.817	– 4.710	– 4.475	– 4.446	– 0.100	– 0.819	0.012

Table II. Elastic scattering of low energy electrons by the neutral Carbon atom (for s-wave).

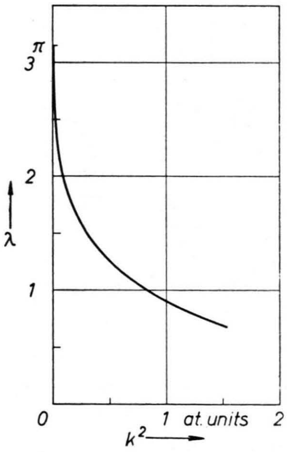

Fig. 2 a. The phase shift for s-wave scattering by Carbon atoms for different energies.

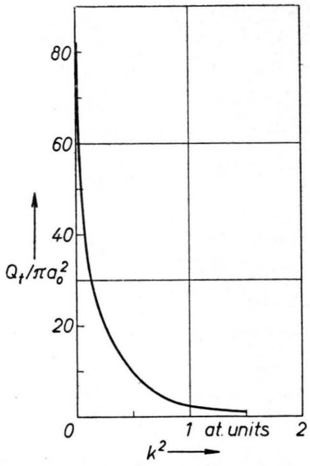

Fig. 2 b. The total cross section for scattering by Carbon taking s-wave contribution only.

since this will certainly require inclusion of the exchange and polarisation term in the wave function for the negative ion.

c) *The scattering by nitrogen atoms:* Here too we have used three exponential functions to reproduce the HARTREE field. The parameter c is chosen just as in the case of Carbon and is constant but for $k^2 = 2$.

In Table III a the phase shifts calculated by the three methods and the total cross section using λ_t are tabulated. Table III b lists the parameters and L_k/k, integration for tan λ_H and L_t/k. Fig. 3 a gives the phase shift as a function of energy. Fig. 3 b represents Q_t as a function of k^2.

The value of zero energy phase shift indicates that the existence of N^- ion is possible, which confirms the result of JOHNSON and ROHRLICH[19] who

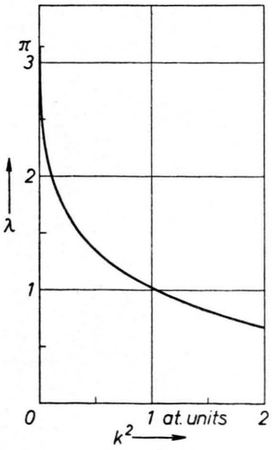

Fig. 3 a. The phase shift for s-wave scattering by Nitrogen atoms for various energies.

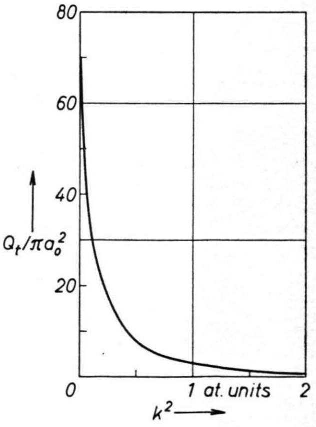

Fig. 3 b. The total cross section for scattering by Nitrogen taking s-wave contribution only.

a) *The phase shifts*

Energy k^2 in a.u.	c-value	λ_K	λ_H	λ_t	$Q_t/\pi a_0^2$
0.005	3.00	2.841	2.841	2.841	70.135
0.05	3.00	2.286	2.286	2.286	45.597
0.10	3.00	2.030	2.030	2.030	32.142
0.50	3.00	—	—	1.344	7.595
0.80	3.00	1.128	1.128	1.128	4.082
1.00	3.00	1.022	1.022	1.022	2.911
1.50	3.00	0.825	0.825	0.825	1.439
2.00	2.90	0.676	0.676	0.676	0.783

b) *The parameters and the reliability conditions*

k^2 in a.u.	a_K	a_H	a_t	b_K	b_H	b_t	L_K/k	Integration for tan λ_H	L_t/k
0.005	− 0.308	− 0.311	− 0.303	0.763	0.770	0.748	− 0.002	− 0.314	− 0.008
0.05	− 1.146	− 1.153	− 1.127	2.896	2.916	2.839	− 0.007	− 1.163	− 0.026
0.10	− 2.017	− 2.026	− 1.984	5.213	5.239	5.118	− 0.009	− 2.038	− 0.041
0.50	4.375	4.342	4.219	—	—	—	—	—	—
0.80	2.137	2.108	2.072	− 7.388	− 7.309	− 7.312	− 0.029	2.092	0.035
1.00	1.660	1.636	1.617	− 6.209	− 6.147	− 6.097	− 0.024	1.626	0.018
1.50	1.072	1.082	1.085	− 4.925	− 4.951	− 4.960	0.010	1.085	− 0.003
2.00	0.795	0.802	0.803	− 4.430	− 4.447	− 4.450	0.007	0.803	0.001

Table III. Elastic scattering of low energy electrons by the neutral Nitrogen atom (for s-wave).

obtain a dissociation energy of 0.5 eV for N^- whereas Bates and Moiseiwitsch [20] come to the conclusion that N^- ion is unlikely to exist. While Branscomb's [21] experiment is uncertain about the existence of N^-, the experiment of Boldt [22] on the spectrum of gas discharge in N shows a continuum which he could explain by the bound-free transition of N^-. The existence of the N^- ion will be of interest in connection with upper atmosphere physics.

In conclusion, we may mention that a general computation program for the electronic computer G 2 has been set up to calculate the scattering by any neutral atom having atomic number $Z < 80$ with the trial function (21) for $c \neq d$ but $c + d < 8$ in the energy range 0 to 54 eV and for a potential represented by at the most three exponential functions. This program is available for any particular interest. The functional L given by (15) and the expression for $a\,k$ given by (19 a) are noted in the appendix.

For details, we may note that the scattering by oxygen, fluorine and potassium has been tried under this scheme but from the criteria of reliability of the variational methods it seems that the results obtained are unreliable and c varies very much if one wants to choose it in such a way that all variational methods give the same result. This may be due to the fact that in all these cases more than one bound state exist and the ansatz (21) is not good; one may have to use some more exponential functions in (21).

All calculations are done on the electronic computer G 2 at the Max-Planck-Institut für Physik und Astrophysik.

We thank Professor Heisenberg and Professor Biermann for their interest, the calculating group here for their helps, and Mr. Vaidya for some discussion on § II.

Appendix

Introducing the expression (11) into eq. (15), one obtains for $l = 0$:

$$L = \int_0^\infty \chi_0 \left[\frac{d^2}{dr^2} + k^2 + \frac{2\,Z}{r} \sum A_n\, e^{-\gamma_n r}\right] \chi_0\, dr$$

$$= \int_0^\infty \chi_0 \left[\frac{d^2}{dr^2} + k^2\right] \chi_0\, dr + \int_0^\infty \chi_0\, \frac{2\,Z}{r} \sum_n A_n\, e^{-\gamma_n r}\, \chi_0\, dr\,.$$

Substituting (21) for χ_0

$$L \equiv C_1^{KE}\, a^2 + C_2^{KE}\, b^2 + C_3^{KE}\; a\, b + C_4^{KE}\, a + C_5^{KE}\, b$$
$$+ C_1^{PE}\, a^2 + C_2^{PE}\, b^2 + C_3^{PE}\, a\, b + C_4^{PE}\, a + C_5^{PE}\, b + C_0^{PE}$$

where the C's are functions of c and d. The explicit

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[21] L. M. Branscomb, Advances in Electronics and Electron Physics. Vol. IX [1957].

[22] G. Boldt, Z. Phys. **154**, 330 [1959].

forms of the C's are

$$C_1^{KE}=d^2\sum_{\nu=0}^{2}\left\{(-1)^\nu\binom{2}{\nu}\frac{\nu}{2}\,\frac{(\nu\,d)^2+2\,k^2}{\nu\,d[(\nu\,d)^2+4\,k^2]}\right\}$$

$$+2\,k^2\,d\sum_{\nu=0}^{2}\left\{(-1)^\nu\binom{2}{\nu}\frac{\nu}{2}\,\frac{1}{(\nu\,d)^2+4\,k^2}\right\},$$

$$C_2^{KE}=\sum_{\nu=0}^{2}(-1)^\nu\binom{2}{\nu}\left\{\left(c^2+\frac{\nu}{2}\,(2\,c\,d+d^2)\right)\right.$$

$$\left.\cdot\frac{(2\,c+\nu\,d)^2+2\,k^2}{(2\,c+\nu\,d)\,[(2\,c+\nu\,d)^2+4\,k^2]}+\frac{k^2(2\,c+\nu\,d)}{(2\,c+\nu\,d)^2+4\,k^2}\right\},$$

$$C_3^{KE}=\sum_{\nu=0}^{2}(-1)^\nu\binom{2}{\nu}\left\{[c^2+\nu(c\,d+d^2)]\right.$$

$$\left.\cdot\frac{(c+\nu\,d)^2+2\,k^2}{(c+\nu\,d)\,[(c+\nu\,d)^2+4\,k^2]}+\frac{2\,k^2(c+\nu\,d)}{(c+\nu\,d)^2+4\,k^2}\right\},$$

$$C_4^{KE}=-k\,,\qquad C_5^{KE}=0\,,$$

$$C_1^{PE}=Z\sum_n\sum_{\nu=0}^{2}(-1)^{\nu+1}\binom{2}{\nu}2^{-1}A_n$$

$$\cdot[\ln((\gamma_n+\nu\,d)^2+4\,k^2)+2\ln(\gamma_n+\nu\,d)],$$

$$C_2^{PE}=Z\sum_n\sum_{\nu=0}^{2}(-1)^{\nu+1}\binom{2}{\nu}2^{-1}A_n$$

$$\cdot[\ln((\gamma_n+2\,c+\nu\,d)^2+4\,k^2)+2\ln(\gamma_n+2\,c+\nu\,d)],$$

$$C_3^{PE}=2\,Z\sum_n\sum_{\nu=0}^{2}(-1)^{\nu+1}\binom{2}{\nu}2^{-1}A_n$$

$$\cdot[\ln((\gamma_n+c+\nu\,d)^2+4\,k^2)+2\ln(\gamma_n+2\,c+\nu\,d)],$$

$$C_4^{PE}=Z\sum_n A_n\arctan\frac{2\,k\,d}{\gamma_n(\gamma_n+d)+4\,k^2},$$

$$C_5^{PE}=Z\sum_n A_n\arctan\frac{2\,k\,d}{(\gamma_n+c)\,(\gamma_n+c+d)+4\,k^2},$$

$$C_0^{PE}=-Z\sum_n 2^{-1}A_n\ln\frac{\gamma_n^2}{\gamma_n^2+4\,k^2},$$

The equation (19 a) gives [15]

$$a\,k=(C_4^{KE}+C_4^{PE})\,a+(C_5^{KE}+C_5^{PE})\,b+2\,C_0\,.$$

Elastic Scattering of Low Energy Positrons by Atoms

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(Z. Naturforschg. 16 a, 500—505 [1961]; eingegangen am 1. Dezember 1960)

Elastic scattering cross sections of low energy positrons (0 to about 40 eV) by Helium, Carbon, Nitrogen, Oxygen, Fluorine, Neon and Argon atoms are calculated by variational methods. The scattering potentials are taken to be the analytical approximations of different HARTREE potentials. Only s-wave is included. Comparisons with the available experimental datas of positron scattering by He, Ne and A reveal that either a considerable strong polarisation potential will be required to bring the theoretical results at par with experiments or the formation of virtual positronium play a dominant role for this kind of elastic scattering.

Lately some experimental results are available for the elastic scattering of positrons by atoms and this has revived naturally some interest to treat this problem theoretically. This problem is theoretically simpler than electron scattering since there is no exchange between the scattered positrons and the bound electrons. MASSEY and MOUSSA [1] treated theoretically the positron scattering by He, Ne, A and H atoms in HARTREE-approximation where the total wave functions of the system is written as a product of atomic wave function and the scattered wave function; they solved the derived differential equation for the scattered wave function numerically using HARTREE wave functions for the atomic electrons of Ne and HARTREE–FOCK wave functions for He and H. Their results indicate that for positron scattering the polarisation is of fundamental importance [2]. On the other hand it seems that the comparison of the experimental datas with the theoretical calculations of no-polarisation approximation may serve as a possible mean to determine the polarisation effect so long as one tends to take this effect in a potential form. The already theoretically available calculations of polarisation potential by perturbation methods have more validity for positron scattering since in most of the cases, the ex-

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* Now at Princeton University and with Pakistan Atomic Energy Commission.

[1] H. S. W. MASSEY and A. H. A. MOUSSA, Proc. Phys. Soc., Lond. **71**, 38 [1958].

[2] cp. also A. H. A. MOUSSA, Proc. Phys. Soc., Lond. **74**, 101 [1959].