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Irregular scattering functions

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Abstract. By scattering in a central potential $V(r)$ the state function is split into irregular parts, $\Psi = \Phi + X$, where Φ satisfies the Schrödinger equation with a modified potential $V + W$. The non-Hermitian term W vanishes in $\boldsymbol{r}$ space except on the incident (z) axis, where it is singular and non-local. On the energy shell in $\boldsymbol{p}$ space W compensates the potential V. In $\boldsymbol{r}$ space Φ and X become logarithmically singular on the z axis, and the asymptotic difference between Φ and a plane wave is assumed to be of $O(V)$. The scattering amplitude can be expressed by an integral containing Ψ, Φ and W. Half-shell F matrices are defined, which are closely related to the T matrix. The formalism is valid also for Coulomb scattering, where Φ and X become equal to the usual irregular solutions. The Coulomb F matrix is found explicitly, and gives the scattering amplitude on the energy shell, without any 'anomalies'. The classical limits of the phases of Coulomb's Φ and X are found, and they coincide with the incoming and scattering part of the action function respectively. This property of the irregular functions is believed to be of general validity. The theory is also applied to the Yukawa case, where Ψ and Φ are given to all orders. General orthonormality relations for Φ are established by means of reciprocal functions.

1. Introduction

In the standard theory for scattering in short-range potentials V the wavefunction is split into two parts

$$\Psi(\boldsymbol{r}) = \Psi^0(\boldsymbol{r}) + \Psi'(\boldsymbol{r}) = \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}) + \Psi'(\boldsymbol{r}) \tag{1.1}$$

$$\xrightarrow[r\to\infty]{} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}) + f(\hat{\boldsymbol{r}})[\exp(\mathrm{i}kr)/r] + O(1/r^2). \tag{1.2}$$

The scattering amplitude f can be expressed by an integral containing the total Ψ and the free Ψ^0 (and V). f is also proportional to the on-shell value of the transition matrix T, etc.

If this formalism is applied to the Coulomb case, well-known on-shell 'anomalies' appear: infinite phases, and incorrect absolute values. The last anomaly can be avoided, however, by using a screening (of the potential), which is removed only after having passed on to the energy shells (Kolsrud 1978). But the infinite phases—i.e. infrared divergencies—still remain.

A new approach was initiated by Dollard (1964, 1966, 1968), who added some time- and momentum-dependent terms to the Hamiltonian, which in a sense compensated the awkward long-range effects of the Coulomb potential.

An equivalent way of avoiding the Coulomb anomalies was given by van Haeringen (1976a, b). He replaced the free states by the so-called 'asymptotic states' of Nutt

(1968), which are expressed by means of generalised distributions in momentum space. However, these states are difficult to formulate explicitly in coordinate space.

Recently Hamza (1979) showed how one could avoid explicit calculations of the asymptotic states by employing certain modified 'long-range' Green functions (Kolsrud 1977).

The present paper was initiated by the observation that the Coulomb scattering amplitude could be expressed by an integral which contained a quantity closely connected with the irregular Coulomb functions Φ^c and X^c, say, where $\Psi^c = \Phi^c + X^c$. By means of these functions certain (half-shell) F^c matrices can be defined, which have the correct on-shell value, i.e. they become proportional to the Coulomb scattering amplitude f^c without any anomalies.

The functions Φ^c and X^c satisfy the Schrödinger equation in all space except on the positive part of the incident (z)axis, where they are logarithmically singular. At large distances Φ^c behaves like a modified plane wave, while X^c behaves like a modified scattered wave.

In the present paper we shall give a general treatment of such irregular scattering functions for arbitrary central potentials $V(r)$. By means of a non-Hermitian potential-like quantity W, we define a splitting of the scattering wavefunction

$$\Psi(\boldsymbol{r}) = \Phi(\boldsymbol{r}) + X(\boldsymbol{r}). \tag{1.3}$$

Here Φ and X satisfy the Schrödinger equation in all space except on the z axis, where they are logarithmically singular. With short-range $V(r)$ their asymptotic forms become

$$\Phi(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) + O[V(r)], \tag{1.4}$$

$$X(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} f(\hat{\boldsymbol{r}})[\exp(\mathrm{i}kr)/r] + O(1/r^2). \tag{1.5}$$

The term $O(V)$ in (1.4), rather than $O(r^{-2})$, is a conjecture in the present paper.

Note the difference between (1.1), (1.2) and (1.3), (1.4), where Ψ^0 satisfies the free and Φ the total equation. In spite of their irregular character it seems natural to call Φ and X the incident and scattered wave respectively. The radial functions of Φ and X satisfy modified Schrödinger equations. In the Coulomb case these partial waves and their equations have been given by van Haeringen (1976b). But he assumes that his results cannot be generalised to other potential cases.

A special reason for characterising Φ and X as the incident and scattered wave is the fact that the classical limits of the phases (times $\hbar$) of Φ^c and X^c are equal to the Coulomb action functions for the incident and scattered particle orbits, respectively. We assume that this property is valid for any central-potential scattering.

2. Irregular scattering states

In order to define the 'irregular splitting' of the scattering state

$$|\Psi_{\boldsymbol{k}}\rangle = |\Phi_{\boldsymbol{k}}\rangle + |X_{\boldsymbol{k}}\rangle \tag{2.1}$$

for central potentials $V(r)$, we introduce a potential-like quantity $W_{\boldsymbol{k}}$ with the following properties ($\hbar = 1$):

$$(a) \qquad \langle \boldsymbol{r}'| W_k = 0 \qquad \text{for } \boldsymbol{r}'_\perp \equiv \boldsymbol{r}' - z'\hat{\boldsymbol{k}} \neq 0, \tag{2.2}$$

$$(b) \qquad \langle \boldsymbol{p}'| W_k = -\langle \overline{\boldsymbol{p}'}| V \qquad \text{for } p' = k, \tag{2.3}$$

where

$$\langle \overline{\boldsymbol{p}'}| = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\phi' \langle p'_\perp, p'_z, \phi'|. \tag{2.4}$$

Our solution is

$$W_k = -Q_k J_k V, \tag{2.5}$$

where

$$Q_k = |\boldsymbol{r}'_\perp = 0\rangle\langle \boldsymbol{p}'_\perp = 0|, \tag{2.6}$$

$$J_k = J_0[r_\perp (k_+^2 - p_z^2)^{1/2}]. \tag{2.7}$$

Here $k_+ = k + \mathrm{i}\epsilon$, and J_0 is the Bessel function

$$J_0(q) = \sum_{n=0}^{\infty} \frac{1}{n!^2} \left(-\frac{q^2}{4} \right)^n. \tag{2.8}$$

We shall often use the formula

$$J_0(q) = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\psi \exp(\mathrm{i}q \cos \psi). \tag{2.9}$$

Our normalisation is shown by

$$\langle p'_x | p''_x \rangle = \delta(p'_x - p''_x), \qquad \langle x' | x'' \rangle = 2\pi\delta(x' - x''). \tag{2.10}$$

Note that

$$|x' = 0\rangle = \int \mathrm{d}p'_x |p'_x\rangle, \qquad \langle p'_x = 0| = \int \frac{\mathrm{d}x'}{2\pi} \langle x'|, \tag{2.11}$$

because

$$\langle p'_x | x' \rangle = \exp(-\mathrm{i}p'_x x'). \tag{2.12}$$

Condition (a) in (2.2) is satisfied by (2.5), (2.6) because

$$\langle \boldsymbol{r}'| Q_k = (2\pi)^2 \delta(\boldsymbol{r}'_\perp) \langle z'| \langle \boldsymbol{p}'_\perp = 0|. \tag{2.13}$$

By means of (2.9) we write (2.4) as

$$\langle \overline{\boldsymbol{p}'}| = \frac{1}{(2\pi)^3} \int \mathrm{d}^3\boldsymbol{r}' \langle \overline{\boldsymbol{p}'} | \boldsymbol{r}' \rangle \langle \boldsymbol{r}'| = \frac{1}{(2\pi)^3} \int \mathrm{d}^3\boldsymbol{r}' \exp(-\mathrm{i}p'_z z') J_0(p'_\perp r'_\perp) \langle \boldsymbol{r}'|. \tag{2.14}$$

According to (2.3) and (2.5) this should be compared with

$$\begin{aligned} \langle \boldsymbol{p}'| Q_k J_k &= \langle p'_z | \langle \boldsymbol{p}''_\perp = 0 | J_0[r_\perp (k_+^2 - p_z'^2)^{1/2}] \\ &= \frac{1}{(2\pi)^3} \int \mathrm{d}^3\boldsymbol{r}' \langle p'_z | z' \rangle \langle \boldsymbol{r}' | J_0[r'_\perp (k_+^2 - p_z'^2)^{1/2}]. \end{aligned} \tag{2.15}$$

As $p_\perp'^2 = p'^2 - p_z'^2$, we see that the second condition (2.3) is fulfilled. Note that

$$\langle \boldsymbol{p}'| W_k + \langle \overline{\boldsymbol{p}'}| V = \mathrm{O}(k^2 - p'^2). \tag{2.16}$$

With short-range potentials $V(r)$ the 'irregular' vectors $|\Phi_k\rangle$ and $|\mathrm{X}_k\rangle$ are defined by the equations

$$\left.\begin{matrix}|\Phi_k\rangle\\|\mathrm{X}_k\rangle\end{matrix}\right\} = \left\{\begin{matrix}|\boldsymbol{k}\rangle\\0\end{matrix}\right. + \frac{1}{E_k+\mathrm{i}\epsilon-H_0}\times\left\{\begin{matrix}(V|\Phi_k\rangle+W_k|\Phi_k\rangle)\\(V|\mathrm{X}_k\rangle-W_k|\Phi_k\rangle)\end{matrix}\right. . \tag{2.17}$$

Hence $|\Psi_k\rangle$ in (2.1) satisfies the usual

$$|\Psi_k\rangle=|\boldsymbol{k}\rangle+\frac{1}{E_k+\mathrm{i}\epsilon-H_0}V|\Psi_k\rangle. \tag{2.18}$$

With $H=H_0+V$ we may also write

$$\left.\begin{matrix}|\Phi_k\rangle\\|\mathrm{X}_k\rangle\end{matrix}\right\} = \left\{\begin{matrix}|\Psi_k\rangle\\0\end{matrix}\right. \pm\frac{1}{E_k+\mathrm{i}\epsilon-H}W_k|\Phi_k\rangle, \tag{2.19}$$

where

$$|\Psi_k\rangle=|\boldsymbol{k}\rangle+\frac{1}{E_k+\mathrm{i}\epsilon-H}V|\boldsymbol{k}\rangle, \tag{2.20}$$

and with $H_k=H+W_k$

$$|\Phi_k\rangle=|\boldsymbol{k}\rangle+\frac{1}{E_k+\mathrm{i}\epsilon-H_k}(V+W_k)|\boldsymbol{k}\rangle. \tag{2.21}$$

These equations correspond to the modified Schrödinger equation

$$(E_k-H_k)|\Phi_k\rangle=0, \tag{2.22}$$

or

$$(E_k-H)\times\left\{\begin{matrix}|\Phi_k\rangle\\|\mathrm{X}_k\rangle\end{matrix}\right.=\pm|w_k\rangle, \tag{2.23}$$

where

$$|w_k\rangle=W_k|\Phi_k\rangle. \tag{2.24}$$

As shown in appendix 3 the orthonormalisation of $|\Phi\rangle$ can be expressed by means of reciprocal vector sets.

3. Momentum and coordinate representations

As $[L_z, V]=0$ and $[L_z, W_k]=0$, the solutions of (2.17)–(2.21) are symmetric about the $\boldsymbol{k}$ axis. Hence $V(\boldsymbol{p}', \boldsymbol{p}'')=\langle\boldsymbol{p}'|V|\boldsymbol{p}''\rangle$ may be replaced by

$$\begin{aligned}\langle\overline{\boldsymbol{p}'}|V|\boldsymbol{p}''\rangle&=\frac{1}{(2\pi)^3}\int \mathrm{d}^3\boldsymbol{r}'\exp(-\mathrm{i}p_z'z')J_0(p_\perp'r_\perp')\exp(\mathrm{i}\boldsymbol{p}''\cdot\boldsymbol{r}')V(r')\\&\equiv\bar{V}(p_\perp'^2, p_z';\boldsymbol{p}''),\end{aligned} \tag{3.1}$$

according to (2.14). Equations (2.5) and (2.15) then show that

$$\langle\boldsymbol{p}'|W_k|\boldsymbol{p}''\rangle=-\bar{V}(k_+^2-p_z'^2, p_z';\boldsymbol{p}'')\equiv W_k(p_z', \boldsymbol{p}''). \tag{3.2}$$

The momentum representations of (2.17) are

$$\Phi_k(\boldsymbol{p}) = \delta(\boldsymbol{p}-\boldsymbol{k}) + \frac{2m}{k_+^2 - p^2}\int \mathrm{d}^3p'[V(\boldsymbol{p},\boldsymbol{p}') + W_k(p_z,\boldsymbol{p}')]\Phi_k(\boldsymbol{p}') \tag{3.3}$$

$$= \delta(\boldsymbol{p}-\boldsymbol{k}) + \frac{2m}{k_+^2 - p^2}\left(\int \mathrm{d}^3p' \; V(\boldsymbol{p},\boldsymbol{p}')\Phi_k(\boldsymbol{p}') + \frac{1}{(2\pi)^2} w_k(p_z)\right), \tag{3.4}$$

$$\mathrm{X}_k(\boldsymbol{p}) = \frac{2m}{k_+^2 - p^2}\left(\int \mathrm{d}^3p' \; V(\boldsymbol{p},\boldsymbol{p}')\mathrm{X}_k(\boldsymbol{p}') - \frac{1}{(2\pi)^2} w_k(p_z)\right), \tag{3.5}$$

where

$$w_k(p_z) = (2\pi)^2 \int \mathrm{d}^3p' \; W_k(p_z,\boldsymbol{p}')\Phi_k(\boldsymbol{p}'). \tag{3.6}$$

Note that $\Phi_k(\boldsymbol{p})$ is finite on the energy shell, according to (3.2) and (2.16). Because of the axial symmetry, equation (3.3) leads to (with $P \equiv p_\perp^2$)

$$\Phi_k(P, p_z)_{p=k} = \frac{1}{\pi}\delta(P)\delta(p_z - k)_{p=k} - 2m\pi \int_0^\infty \mathrm{d}P' \int_{-\infty}^{\infty} \mathrm{d}p_z' \left(\frac{\partial}{\partial P}\bar{V}(P, p_z; P', p_z')\right)_{p=k} \Phi_k(P', p_z'). \tag{3.7}$$

We recall that $\Psi_k(\boldsymbol{p})$ is singular on the energy shell, where it gives the scattering amplitude:

$$\lim_{p\to k}(k^2 - p^2)\Psi_k(\boldsymbol{p}) = 2m\int \mathrm{d}^3p' \; V(\boldsymbol{p},\boldsymbol{p}')_{p=k}\Psi_k(\boldsymbol{p}') = -\frac{1}{2\pi^2} f_k(\hat{\boldsymbol{p}}). \tag{3.8}$$

Hence $\Phi_k(\boldsymbol{p})$ has no scattering part.

In coordinate space (2.5) and (2.13) lead to

$$\begin{aligned} W_k(\boldsymbol{r}', \boldsymbol{r}'') &= -\frac{1}{(2\pi)^3}\langle \boldsymbol{r}'|Q_k J_k V|\boldsymbol{r}''\rangle \\ &= -\frac{1}{2\pi}\delta(\boldsymbol{r}_\perp')\langle z'|\langle \boldsymbol{p}_\perp' = 0|J_0[r_\perp(k_+^2 - p_z^2)^{1/2}]\int \mathrm{d}p_z' |p_z'\rangle\langle p_z'|z''\rangle|\boldsymbol{r}_\perp''\rangle V(r'') \\ &= -\delta(x')\delta(y')D_k(z'-z'', r_\perp'')V(r''), \end{aligned} \tag{3.9}$$

where

$$D_k(z'-z'', r_\perp'') = \frac{1}{2\pi}\int \mathrm{d}p_z' \exp[\mathrm{i}(z'-z'')p_z']J_0[r_\perp''(k_+^2 - p_z'^2)^{1/2}]. \tag{3.10}$$

D_k is a (divergent) generalised function, which is always multiplied by the 'test function' $V\phi$ in an integral. The potential-like quantity W_k thus vanishes in $\boldsymbol{r}$ space except on the z axis, where it is singular and non-local. (Note: $W_k(\boldsymbol{r}', \boldsymbol{r}'') = -V(\boldsymbol{r}', \boldsymbol{r}'')$ for $r_\perp'' = 0$.)

The modified Schrödinger equations (2.22), (2.23) become

$$\left(\frac{1}{2m}(k^2 + \nabla^2) - V(r)\right)\Phi_k(\boldsymbol{r}) - \int \mathrm{d}^3r' \; W_k(\boldsymbol{r}, \boldsymbol{r}')\Phi_k(\boldsymbol{r}') = 0, \tag{3.11}$$

$$\left(\frac{1}{2m}(k^2 + \nabla^2) - V(r)\right) \times \begin{Bmatrix}\Phi_k(\boldsymbol{r}) \\ \mathrm{X}_k(\boldsymbol{r})\end{Bmatrix} = \pm\delta(x)\delta(y)w_k(z), \tag{3.12}$$

where (3.6) and (3.9) yield

$$w_k(z) = -\int d^3r'\, D_k(z - z', r'_\perp) V(r') \Phi_k(\boldsymbol{r}') \tag{3.13}$$

$$= \int dp_z \exp(izp_z) w_k(p_z). \tag{3.14}$$

Equations (2.17), or rather (3.4), (3.5), correspond to

$$\left.\begin{matrix}\Phi_k(\boldsymbol{r})\\ X_k(\boldsymbol{r})\end{matrix}\right\} = \left\{\begin{matrix}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})\\ 0\end{matrix}\right. + \int d^3r'\, G_k^0(\boldsymbol{r}, \boldsymbol{r}') V(r') \times \left\{\begin{matrix}\Phi_k(\boldsymbol{r}')\\ X_k(\boldsymbol{r}')\end{matrix}\right. \pm \int dz'\, G_k^0(\boldsymbol{r}, z'\hat{\boldsymbol{k}}) w_k(z'). \tag{3.15}$$

They are equivalent to the representation of (2.19)

$$\left.\begin{matrix}\Phi_k(\boldsymbol{r})\\ X_k(\boldsymbol{r})\end{matrix}\right\} = \left\{\begin{matrix}\Psi_k(\boldsymbol{r})\\ 0\end{matrix}\right. \pm \int dz'\, G_k(\boldsymbol{r}, z'\hat{\boldsymbol{k}}) w_k(z'). \tag{3.16}$$

From (3.15) we get the asymptotic forms

$$\left.\begin{matrix}\Phi_k(\boldsymbol{r})\\ X_k(\boldsymbol{r})\end{matrix}\right\} \xrightarrow[r\to\infty]{} \left\{\begin{matrix}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})\\ 0\end{matrix}\right. - \frac{\exp(ikr)}{r}\frac{m}{2\pi}\left(\int d^3r' \exp(-ik\hat{\boldsymbol{r}}\cdot\boldsymbol{r}') V(r') \left\{\begin{matrix}\Phi_k(\boldsymbol{r}')\\ X_k(\boldsymbol{r}')\end{matrix}\right.\right.$$

$$\left. \pm \int dz' \exp(-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}z') w_k(z')\right). \tag{3.17}$$

Alternatively, the asymptotic value of G_k in (3.16) (cf Rodberg and Thaler 1967) and of Ψ_k yields

$$\Phi_k(\boldsymbol{r}) \xrightarrow[r\to\infty]{} \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) + \frac{\exp(ikr)}{r}\left(f_k(\hat{\boldsymbol{r}}) - \frac{m}{2\pi}\int dz'\, \Psi_{-k\hat{r}}(z'\hat{\boldsymbol{k}}) w_k(z')\right), \tag{3.18}$$

$$X_k(\boldsymbol{r}) \xrightarrow[r\to\infty]{} \frac{\exp(ikr)}{r}\frac{m}{2\pi}\int dz'\, \Psi_{-k\hat{r}}(z'\hat{\boldsymbol{k}}) w_k(z'). \tag{3.19}$$

We will show that the term in the large parentheses in (3.17) for Φ_k vanishes. With $\boldsymbol{p} \equiv k\hat{\boldsymbol{r}}$ it can be written

$$\left(\ldots\right) = \int d^3r' \exp(-i\boldsymbol{p}\cdot\boldsymbol{r}') V(r') \Phi_k(\boldsymbol{r}') + \int dz' \exp(-ip_z z') w_k(z')$$

$$= (2\pi)^3 \int d^3p' [V(\boldsymbol{p}, \boldsymbol{p}') + W_k(p_z, \boldsymbol{p}')]_{p=k} \Phi_k(\boldsymbol{p}') = 0, \tag{3.20}$$

according to (3.2) (and $V \to \bar{V}$). Hence $\Phi_k(\boldsymbol{r})$ contains no scattering part, as noted earlier for $\Phi_k(\boldsymbol{p})$. (The currents associated with $\Phi_k(\boldsymbol{r})$ and $X_k(\boldsymbol{r})$ have a sink and a source, respectively, on the z axis.)

Using (3.20) in (3.18), we get the following new formula for the scattering amplitude:

$$f_k(\hat{\boldsymbol{p}}) = \frac{m}{2\pi}\int dz\, \Psi_{-\boldsymbol{p}}(z\hat{\boldsymbol{k}}) w_k(z), \qquad p = k. \tag{3.21}$$

By means of (3.9) and (3.13) this can also be written

$$f_k(\hat{p}) = \frac{m}{2\pi} \iint d^3r\, d^3r'\, \Psi_{-p}(r) W_k(r, r') \Phi_k(r') \tag{3.22}$$

$$= 4\pi^2 m \langle \Psi_p^{(-)} | W_k | \Phi_k^{(+)} \rangle \tag{3.23'}$$

$$= 4\pi^2 m \langle \Psi_p^{(-)} | w_k^{(+)} \rangle, \tag{3.23''}$$

(recall (2.24)), because

$$\Phi_k(r) \equiv \Phi_k^{(+)}(r), \qquad \Psi_{-p}(r) \equiv \Psi_{-p}^{(+)}(r) = \Psi_p^{(-)}(r)^*. \tag{3.24}$$

Note that the (general) micro-reversibility property

$$f_k(\hat{p}) = f_{-p}(-\hat{k}), \qquad p = k, \tag{3.25}$$

yields variants of these formulae.

Concerning the behaviour of $\Phi_k(r)$ near the z axis, we see that the last term in (3.15) (and (3.16)) is singular for $r = z\hat{k}$. (G behaves like $|r - r'|^{-1}$ when $r \approx r'$, like G^0.) We therefore consider the corresponding term in (3.4)

$$\Phi_k^w(p) \equiv \frac{2m}{k_+^2 - p^2} \frac{1}{(2\pi)^2} w_k(p_z). \tag{3.26}$$

The Fourier transform can be written

$$\Phi_k^w(r) = \frac{m}{2\pi} \int dp_z \exp(izp_z) w_k(p_z) g(r_\perp, p_z), \tag{3.27}$$

where (2.9) gives

$$g(r_\perp, p_z) = \int_0^\infty d(p_\perp^2) J_0(r_\perp p_\perp) \frac{1}{k_+^2 - p_\perp^2 - p_z^2}. \tag{3.28}$$

By partial integration we see that

$$r_\perp \frac{\partial g}{\partial r_\perp} = -\int_0^\infty d(p_\perp^2) J_0(r_\perp p_\perp) \frac{\partial}{\partial(p_\perp^2)} \frac{2p_\perp^2}{k_+^2 - p_\perp^2 - p_z^2} \xrightarrow[r_\perp \to 0]{} 2. \tag{3.29}$$

Hence

$$g(r_\perp, p_z) \xrightarrow[r_\perp \approx 0]{} 2 \ln(kr_\perp), \tag{3.30}$$

and (3.27) with (3.14) yields

$$\left.\begin{matrix} \Phi_k(r) \\ X_k(r) \end{matrix}\right\} \xrightarrow[r_\perp \approx 0]{} \pm \frac{m}{\pi} w_k(z) \ln(kr_\perp). \tag{3.31}$$

We note that $\int_v d^3r |\Phi_k(r)|^2$ exists for finite volumes v.

4. Radial functions

We expand in partial waves

$$\left.\begin{matrix} \Psi_k(r) \\ \Phi_k(r) \\ X_k(r) \end{matrix}\right\} = \sum_l P_l(\hat{r} \cdot \hat{k})(2l+1) i^l \times \left\{\begin{matrix} \psi_l(r, k) \\ \phi_l(r, k), \\ \chi_l(r, k) \end{matrix}\right. \tag{4.1}$$

i.e.

$$\psi_l(r, k) = \phi_l(r, k) + \chi_l(r, k). \tag{4.2}$$

With $\zeta \equiv \cos\theta$ equation (3.12) is written

$$[\nabla^2 + k^2 - 2mV(r)] \times \begin{cases} \Phi_k(\boldsymbol{r}) \\ \mathrm{X}_k(\boldsymbol{r}) \end{cases} = \pm \frac{2m}{\pi r^2} \delta(\zeta^2 - 1) w_k(r\zeta), \tag{4.3}$$

which leads to the radial equations

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2} + k^2 - 2mV(r)\right) \times \begin{cases} \phi_l(r, k) \\ \chi_l(r, k) \end{cases} = \pm \frac{m}{2\pi r^2}[(-\mathrm{i})^l w_k(r) + \mathrm{i}^l w_k(-r)]. \tag{4.4}$$

Equations (1.4), (1.5) indicate that

$$\phi_l(r, k) \xrightarrow[r\to\infty]{} \frac{1}{kr} \sin\left(kr - l\frac{\pi}{2}\right) + \mathrm{O}[V(r)], \tag{4.5}$$

$$\chi_l(r, k) \xrightarrow[r\to\infty]{} f_l(k) \frac{1}{r} \exp\left[\mathrm{i}\left(kr - l\frac{\pi}{2}\right)\right] + \mathrm{O}\left(\frac{1}{r^2}\right), \tag{4.6}$$

where

$$f_l(k) = (1/2\mathrm{i}k)[\exp(2\mathrm{i}\delta_l) - 1]. \tag{4.7}$$

However, $\phi_l(r, k)$ may contain terms which asymptotically are of lower order than $V(r)$, but which do not contribute to (1.4). If, for example, $\mathrm{i}^l \phi_l$ is independent of l when $r \to \infty$, the sum (4.1) will asymptotically be proportional to

$$\sum_l P_l(\zeta)(2l+1) = 2\delta(\zeta - 1) = 0 \qquad \text{for } \theta > 0.$$

5. *F* matrices

We get off-shell extensions of (3.21)–(3.23) by introducing two 'half-shell' matrices for arbitrary $\boldsymbol{p}$:

$$F_k(\boldsymbol{p}, \boldsymbol{k}) = -\langle \Psi_p^{(-)} | W_k | \Phi_k^{(+)} \rangle = -\langle \Psi_p^{(-)} | w_k^{(+)} \rangle, \tag{5.1}$$

$$F_p(\boldsymbol{p}, \boldsymbol{k}) = -\langle \Phi_p^{(-)} | W_p^\dagger | \Psi_k^{(+)} \rangle = -\langle w_p^{(-)} | \Psi_k^{(+)} \rangle. \tag{5.2}$$

The W operators may be eliminated by means of (2.22), which gives

$$F_k(\boldsymbol{p}, \boldsymbol{k}) = (E_p - E_k) \langle \Psi_p^{(-)} | \Phi_k^{(+)} \rangle, \tag{5.3}$$

$$F_p(\boldsymbol{p}, \boldsymbol{k}) = (E_k - E_p) \langle \Phi_p^{(-)} | \Psi_k^{(+)} \rangle. \tag{5.4}$$

Recalling (3.24), and noting $W_{-p} = W_p$, etc, we see that $F_k(\boldsymbol{p}, \boldsymbol{k}) = F_p(-\boldsymbol{k}, -\boldsymbol{p})$.

For short-range cases (5.3), (5.4) are equivalent to

$$F_k(\boldsymbol{p}, \boldsymbol{k}) = \langle \Psi_p^{(-)} | V | \boldsymbol{k} \rangle + (E_p - E_k)(\langle \Psi_p^{(-)} | \Phi_k^{(+)} \rangle - \langle \Psi_p^{(-)} | \boldsymbol{k} \rangle), \tag{5.5}$$

$$F_p(\boldsymbol{p}, \boldsymbol{k}) = \langle \boldsymbol{p} | V | \Psi_k^{(+)} \rangle + (E_k - E_p)(\langle \Phi_p^{(-)} | \Psi_k^{(+)} \rangle - \langle \boldsymbol{p} | \Psi_k^{(+)} \rangle). \tag{5.6}$$

As the differences in the last parentheses in (5.5), (5.6) are finite for $p=k$ (recall (1.4)), we get on the energy shell

$$F_k(\boldsymbol{p},\boldsymbol{k}) \xrightarrow[p\to k]{} \langle \Psi_{\boldsymbol{p}}^{(-)}|V|\boldsymbol{k}\rangle = -f_k(\hat{\boldsymbol{p}})/4\pi^2 m, \tag{5.7}$$

$$F_p(\boldsymbol{p},\boldsymbol{k}) \xrightarrow[p\to k]{} \langle \boldsymbol{p}|V|\Psi_{\boldsymbol{k}}^{(+)}\rangle = -\delta_k(\hat{\boldsymbol{p}})/4\pi^2 m. \tag{5.8}$$

Equations (5.5), (5.6) show the connection between the F matrices and the half-shell T matrices, where

$$T_p(\boldsymbol{p},\boldsymbol{k}) = \langle \boldsymbol{p}|T_p|\boldsymbol{k}\rangle = \langle \Psi_{\boldsymbol{p}}^{(-)}|V|\boldsymbol{k}\rangle, \tag{5.9}$$

$$T_k(\boldsymbol{p},\boldsymbol{k}) = \langle \boldsymbol{p}|T_k|\boldsymbol{k}\rangle = \langle \boldsymbol{p}|V|\Psi_{\boldsymbol{k}}^{(+)}\rangle, \tag{5.10}$$

with

$$T_k = V + V\frac{1}{E_k + \mathrm{i}\epsilon - H}V, \text{ etc.} \tag{5.11}$$

The first-order forms of (5.1), (5.2) are easily obtained. Recalling (3.2) and writing $V(\boldsymbol{p}',\boldsymbol{p}'') = V(|\boldsymbol{p}'-\boldsymbol{p}''|^2)$, we get

$$F_{\boldsymbol{k}}^{(1)}(\boldsymbol{p},\boldsymbol{k}) = V(2k^2-2kp_z), \qquad F_{\boldsymbol{p}}^{(1)}(\boldsymbol{p},\boldsymbol{k}) = V(2p^2-2kp_z), \tag{5.12}$$

$$T_k^{(1)}(\boldsymbol{p}',\boldsymbol{p}'') = T_p^{(1)}(\boldsymbol{p}',\boldsymbol{p}'') = V(\boldsymbol{p}',\boldsymbol{p}'') = V(p'^2+p''^2-2\boldsymbol{p}'\cdot\boldsymbol{p}''). \tag{5.13}$$

They have the common on-shell limit

$$-f_k^{(1)}(\hat{\boldsymbol{p}})/4\pi^2 m = V(|\boldsymbol{p}-\boldsymbol{k}|^2)_{p=k} = V(2k^2-2k^2\cos\theta). \tag{5.14}$$

6. Coulomb functions

The Coulomb potential is written (with $\hbar = 1$)

$$V(r) = -\frac{\nu k}{m}\frac{1}{r}, \qquad \nu = \frac{Zme^2}{k}(=\nu_k). \tag{6.1}$$

The scattering wave function is split like (1.3) with the following modified version of (1.4), (1.5) when $kr - \boldsymbol{k}\cdot\boldsymbol{r} \to \infty$:

$$\Phi_k(\boldsymbol{r}) \to \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\exp[-\mathrm{i}\nu\ln(kr-\boldsymbol{k}\cdot\boldsymbol{r})]\left[1+\mathrm{O}\left(\frac{1}{r}\right)\right], \tag{6.2}$$

$$\mathrm{X}_k(\boldsymbol{r}) \to f_k(\hat{\boldsymbol{r}})\frac{\exp(\mathrm{i}kr)}{r}\exp[\mathrm{i}\nu\ln(2kr)] + \mathrm{O}\left(\frac{1}{r^2}\right), \tag{6.3}$$

where

$$f_k(\hat{\boldsymbol{p}}) = \frac{\Gamma(1-\mathrm{i}\nu)}{\Gamma(1+\mathrm{i}\nu)}\frac{2k\nu}{(\boldsymbol{p}-\boldsymbol{k})^2}\left(\frac{4k^2}{(\boldsymbol{p}-\boldsymbol{k})^2}\right)^{-\mathrm{i}\nu}, \qquad p = k. \tag{6.4}$$

The singularities appear on the positive part of the z axis, and have the form (3.31)

$$\left.\begin{matrix}\Phi_k(\boldsymbol{r})\\ \mathrm{X}_k(\boldsymbol{r})\end{matrix}\right\} \xrightarrow[r-z\approx 0]{} \pm\frac{m}{2\pi}w_k(z)\ln[k(r-z)], \tag{6.5}$$

where

$$\frac{m}{2\pi} w_k(z) = -\frac{\exp(-\nu\pi/2)}{\Gamma(i\nu)}\theta(z)\exp(ikz), \tag{6.6}$$

with $\theta(z>0)=1$, $\theta(z<0)=0$. (With $r_\perp^2 = r^2 - z^2$ we see that the term $\ln[k(r+z)]$ is eliminated by θ.)

van Haeringen (1979) has shown that the irregular Coulomb functions satisfy equations like (3.12), with $w_k(z)$ given by (6.6). An alternative proof is given in appendix 1.

We now wish to show that (6.6) satisfies the relation (3.13), and consequently that (3.11) is valid for the Coulomb function $\Phi_k(\boldsymbol{r})$. With equation (3.10) and with $\Phi_k(\boldsymbol{r})$ from appendix 1 we evaluate the quantity

$$\frac{m}{2\pi}\omega(z) \equiv -\frac{m}{2\pi}\int d^3\boldsymbol{r}'\, D_k(z-z', r'_\perp)\left(-\frac{\nu k}{m}\frac{1}{r'}\right)\Phi_k(\boldsymbol{r}') \tag{6.7'}$$

$$= \exp\left(\nu\frac{\pi}{2}\right)\Gamma(1-i\nu)\frac{1}{2\pi i}\int_{co} dt\, t^{-1+i\nu}(t-1)^{-i\nu} I(z,t), \tag{6.7''}$$

where

$$\begin{aligned} I(z,t) &= \frac{\nu k}{2\pi}\int_{-\infty}^{\infty} dp_z \exp(izp_z)\frac{1}{2\pi}\int d^3\boldsymbol{r}' \exp(-ip_z z')J_0[r'_\perp(k_+^2 - p_z^2)^{1/2}] \\ &\quad \times \frac{1}{r'}\exp\{ik[tr' + (1-t)z']\} \\ &= \frac{\nu}{2\pi}\int_{-\infty}^{\infty} dp_z \exp(izp_z)\frac{1}{p_z - k_+}\frac{1}{t-1} \\ &= i\nu\theta(z)\exp(ikz)\frac{1}{t-1}. \end{aligned} \tag{6.8}$$

Here we have used formulae from Magnus *et al* (1966). Inserting (6.8) in (6.7″) we get

$$\frac{m}{2\pi}\omega(z) = -\theta(z)\exp(ikz)\exp\left(\nu\frac{\pi}{2}\right)\Gamma(1-i\nu)\frac{1}{2\pi i}\int_{co} dt\frac{d}{dt}[t^{i\nu}(t-1)^{-i\nu}], \tag{6.9}$$

which with well-known formulae becomes equal to (6.6). Hence ω in (6.7′) equals w_k in (6.6).

In spite of the fact that the Coulomb $\Psi_k(\boldsymbol{r})$ does not satisfy the usual integral equation (obtained from (3.15)), the irregular part $X_k(\boldsymbol{r})$ does satisfy (3.15). van Haeringen (1979) has shown this for the equivalent (lower) equation (3.16). With (3.19) modified to the Coulomb case we therefore expect that the formulae (3.21)–(3.23) are valid also for the Coulomb amplitude (6.4). The simplest method for testing this is to consider the following relation, obtained from the Schrödinger equations:

$$\left(\int_{\sigma_\infty} - \int_{\sigma_0}\right) d\boldsymbol{\sigma}\cdot X_k \overleftrightarrow{\nabla}\Psi_{-p} = 0, \qquad r\neq z, \quad p = k, \tag{6.10}$$

where $A\overleftrightarrow{\nabla}B \equiv A\nabla B - B\nabla A$. Here σ_0 is the limit of the paraboloid of rotation $r - z =$ constant $\to 0$ about the singular positive z axis, with $d\boldsymbol{\sigma}_0$ oriented outwards. By means of (6.2), (6.3) we evaluate the first integral:

$$\int_{\sigma_\infty} \mathrm{d}\boldsymbol{\sigma}\,.\,\mathrm{X}_k \overleftrightarrow{\nabla} \Psi_{-p} = \int_{\sigma_\infty} \mathrm{d}\boldsymbol{\sigma}\,.\,\mathrm{X}_k \overleftrightarrow{\nabla} \Psi_{-p} \tag{6.11}$$

$$= \lim_{r\to\infty} (-\mathrm{i}r) 2^{\mathrm{i}\nu} \exp(\mathrm{i}kr) \int \mathrm{d}\Omega_r \exp(-\mathrm{i}\boldsymbol{p}\,.\,\boldsymbol{r}) f_k(\hat{\boldsymbol{r}})(1+\hat{\boldsymbol{p}}\,.\,\hat{\boldsymbol{r}})^{-\mathrm{i}\nu}\left(\boldsymbol{p}\,.\,\hat{\boldsymbol{r}} + k + \frac{2\nu+\mathrm{i}}{r}\right)$$

$$= 4\pi f_k(\hat{\boldsymbol{p}}), \tag{6.12}$$

where we have used

$$\exp(\mathrm{i}\boldsymbol{q}\,.\,\boldsymbol{r}) \xrightarrow[r\to\infty]{} (2\pi/\mathrm{i}qr)[\exp(\mathrm{i}qr)\delta(\Omega_r - \Omega_q) - \exp(-\mathrm{i}qr)\delta(\Omega_r + \Omega_q)]. \tag{6.13}$$

Note that the asymptotic logarithmic phases in the second integral (6.11) cancel.

Equations (6.10) and (6.12) show that

$$f_k(\hat{\boldsymbol{p}}) = \frac{1}{4\pi} \int_{\sigma_0} \mathrm{d}\boldsymbol{\sigma}\,.\,\mathrm{X}_k \overleftrightarrow{\nabla} \Psi_{-p}. \tag{6.14}$$

The integration over σ_0 can be performed with parabolic coordinates ξ, $\eta = r \mp z$ and ϕ. With (6.5) we get

$$f_k(\hat{\boldsymbol{p}}) = \lim_{\xi\to 0} \frac{1}{2} \int_0^\infty \mathrm{d}\eta\ \Psi_{-p}(\xi, \eta) \xi \frac{\partial}{\partial \xi} \frac{m}{2\pi} w_k\left(\frac{\eta - \xi}{2}\right) \ln(k\xi)$$

$$= \frac{m}{2\pi} \int_0^\infty \mathrm{d}z\ \Psi_{-p}(z\hat{\boldsymbol{k}}) w_k(z), \qquad p = k, \tag{6.15}$$

i.e. equation (3.21). Starting with Ψ_k and Φ_{-p} we get alternatively (cf (3.25))

$$f_k(\hat{\boldsymbol{p}}) = \frac{m}{2\pi} \int_0^\infty \mathrm{d}r\ \Psi_k(-r\hat{\boldsymbol{p}}) w_{-p}(r). \tag{6.16}$$

For later comparison we give the first-order Coulomb functions

$$\Phi_k^{(1)}(\boldsymbol{r}) = -\mathrm{i}\nu \exp(\mathrm{i}\boldsymbol{k}\,.\,\boldsymbol{r}) \ln(kr - \boldsymbol{k}\,.\,\boldsymbol{r}), \tag{6.17}$$

$$\mathrm{X}_k^{(1)}(\boldsymbol{r}) = \mathrm{i}\nu \exp(\mathrm{i}\boldsymbol{k}\,.\,\boldsymbol{r})\,\mathrm{Ei}(\mathrm{i}kr - \mathrm{i}\boldsymbol{k}\,.\,\boldsymbol{r}), \tag{6.18}$$

where

$$\mathrm{Ei}(z) = \int_0^1 \mathrm{d}t \frac{\exp(zt) - 1}{t} + \ln(-z) + \gamma \tag{6.19'}$$

$$\xrightarrow[z\to\infty]{} \frac{\exp z}{z} \qquad (\gamma = \text{Euler's constant}). \tag{6.19''}$$

The off-shell extension of (6.15) (i.e. $p \neq k$) is evaluated with Ψ from appendix 1 and w from (6.6). Referring to (5.1) we get

$$-4\pi^2 m F_k(\boldsymbol{p}, \boldsymbol{k}) = -\exp\left((\nu_p - \nu_k)\frac{\pi}{2}\right) \frac{\Gamma(1 - \mathrm{i}\nu_p)}{\Gamma(\mathrm{i}\nu_k)} \lim_{\epsilon\to 0} \frac{1}{2\pi\mathrm{i}} \int_{c_{01}} \mathrm{d}t\, t^{-1+\mathrm{i}\nu_p}(t-1)^{-\mathrm{i}\nu_p} I(t), \tag{6.20}$$

where

$$I(t) = \int_0^\infty \mathrm{d}z \exp\{\mathrm{i}[k - p_z + t(p + p_z) + \mathrm{i}\epsilon]z\} = \frac{\mathrm{i}}{(p + p_z)t + k - p_z + \mathrm{i}\epsilon}. \tag{6.21}$$

The condition for (6.21) is that $\mathrm{Im}\, t > -\epsilon/(p+p_z)$. The path c_{01} of integration may then be deformed to an anticlockwise path around the pole $t_0 = (p_z - k - \mathrm{i}\epsilon)/(p+p_z)$, an infinite circle, and two lines from t_0 to ∞. The only contribution comes from the pole t_0, which gives

$$-4\pi^2 mF_k(\boldsymbol{p}, \boldsymbol{k}) = \exp\left((\nu_p - \nu_k)\frac{\pi}{2}\right)\frac{\Gamma(1-\mathrm{i}\nu_p)}{\Gamma(1+\mathrm{i}\nu_k)}\frac{2Zme^2}{(\boldsymbol{p}-\boldsymbol{k})^2+k^2-p^2}\left(\frac{2k(p+k)}{(\boldsymbol{p}-\boldsymbol{k})^2+k^2-p^2}\right)^{-\mathrm{i}\nu_p}. \tag{6.22}$$

When $p = k$, we get (6.4), as already shown in (6.15).

Referring to (5.5), we compare (6.22) with the following Coulomb result (Guth and Mullin 1951):

$$-4\pi^2 m\langle\Psi_p^{(-)}|\frac{Ze^2}{r}\exp(-\epsilon r)|\boldsymbol{k}\rangle = \exp\left(\nu_p\frac{\pi}{2}\right)\Gamma(1-\mathrm{i}\nu_p)\frac{2Zme^2}{(\boldsymbol{p}-\boldsymbol{k})^2+\epsilon^2}\left(\frac{k^2-(p+\mathrm{i}\epsilon)^2}{(\boldsymbol{p}-\boldsymbol{k})^2+\epsilon^2}\right)^{-\mathrm{i}\nu_p}. \tag{6.23}$$

Note the on-shell anomalies of (6.23) when $\epsilon \to 0$.

With a partial-wave expansion like (4.1) the Coulomb $F_l(p, k)$ is found by a technique similar to that for $F_k(\boldsymbol{p}, \boldsymbol{k})$. We give only the result:

$$\begin{aligned} -4\pi^2 mF_l(p, k) &= (-\mathrm{i})^l \frac{m}{2\pi}\lim_{\epsilon\to 0}\int_0^\infty \mathrm{d}r\, \psi_l(r, p) w_k(r)\exp(-\epsilon r) \\ &= (-1)^{l+1}\frac{1}{2\mathrm{i}p}\exp\left((\nu_p-\nu_k)\frac{\pi}{2}\right)\frac{\Gamma(-l-\mathrm{i}\nu_p)}{\Gamma(\mathrm{i}\nu_k)} \\ &\quad\times\left[\lim_{s\to 0}\frac{\partial^l}{\partial s^l}\left(1+\frac{k+p}{2p}s\right)^{l-\mathrm{i}\nu_p}\left(1+\frac{k-p}{2p}s\right)^{l+\mathrm{i}\nu_p}\right. \\ &\quad\left.-\lim_{\epsilon\to 0}\frac{\partial^l}{\partial t_\epsilon^l}t_\epsilon^{l-\mathrm{i}\nu_p}(t_\epsilon - 1)^{l+\mathrm{i}\nu_p}\right] \end{aligned} \tag{6.24}$$

$$\xrightarrow[p\to k]{} \frac{1}{2\mathrm{i}k}\frac{\Gamma(l+1-\mathrm{i}\nu)}{\Gamma(l+1+\mathrm{i}\nu)} - \lim_{\epsilon\to 0} C_\epsilon, \qquad t_\epsilon = \frac{k+p}{2p}+\mathrm{i}\epsilon. \tag{6.25}$$

The phase of C_ϵ goes to infinity when ϵ vanishes. But as $\lim C_\epsilon$ is independent of l, it does not contribute in the partial-wave sum (giving $\sim\delta(\cos\theta - 1)$). Hence (6.25) is equivalent to the usual Coulomb expression

$$f_l(k) = (1/2\mathrm{i}k)\exp(2\mathrm{i}\sigma_l) \qquad \text{or } (1/2\mathrm{i}k)[\exp(2\mathrm{i}\sigma_l) - 1]. \tag{6.26}$$

7. Classical Coulomb limit

To find the asymptotic forms of the irregular Coulomb functions $\Phi_k(\boldsymbol{r})$ and $\mathrm{X}_k(\boldsymbol{r})$ when $\hbar \to 0$, i.e. when

$$\nu = me^2/\hbar p_\infty \to \infty, \qquad \boldsymbol{p}_\infty = \hbar\boldsymbol{k}, \tag{7.1}$$

we shall use the method of steepest descent (Tollefsen 1975, Kolsrud 1975, unpublished). With

$$\xi = r - \boldsymbol{r}\cdot\hat{\boldsymbol{k}}, \qquad a = me^2/p_\infty^2, \tag{7.2}$$

the integrals in equation (A1.2) are written

$$\frac{1}{2\pi i}\int_{c_i} dt\frac{1}{t}\exp[i\nu\phi(t)], \qquad i=0,1, \tag{7.3}$$

where

$$\phi(t)=(\xi/a)t+\ln t-\ln(t-1). \tag{7.4}$$

The saddle points, where $\phi'(t)=0$, are

$$\left.\begin{matrix}t_0\\t_1\end{matrix}\right\}\equiv t_{0,1}=\tfrac{1}{2}\mp(\tfrac{1}{4}+a/\xi)^{1/2}, \tag{7.5}$$

which gives

$$\phi(t_{0,1})=\frac{\xi}{2a}\mp\left(\frac{\xi^2}{4a^2}+\frac{\xi}{a}\right)^{1/2}\mp\ln\left[1+\frac{\xi}{2a}+\left(\frac{\xi^2}{4a^2}+\frac{\xi}{a}\right)^{1/2}\right]. \tag{7.6}$$

Writing (A1.1) as

$$\left.\begin{matrix}\Phi_k(\boldsymbol{r})=A_0(\boldsymbol{r})\exp[(i/\hbar)S_0(\boldsymbol{r})]\\ X_k(\boldsymbol{r})=A_1(\boldsymbol{r})\exp[(i/\hbar)S_1(\boldsymbol{r})]\end{matrix}\right\}\equiv A_{0,1}\exp\left(\frac{i}{\hbar}S_{0,1}\right), \tag{7.7}$$

equation (7.6) shows—according to the method—that the classical limits of S_0 and S_1 are

$$\begin{aligned}S_{0,1}^{\mathrm{cl}}&=\lim_{\hbar\to 0}S_{0,1}\\&=p_\infty z+\tfrac{1}{2}p_\infty\xi\mp(\tfrac{1}{4}p_\infty^2\xi^2+me^2\xi)^{1/2}\\&\mp\frac{me^2}{p_\infty}\ln\left[\frac{p_\infty^2\xi}{2me^2}+1+\frac{p_\infty}{me^2}\left(\frac{p_\infty^2\xi^2}{4}+me^2\xi\right)^{1/2}\right]+C_\infty.\end{aligned} \tag{7.8}$$

(The constant C_∞ is divergent like $\ln\nu$.)

The functions (7.8) are solutions of the classical Hamilton–Jacobi equation for the action function $S^{\mathrm{cl}}(\xi,\eta)$, separated in ξ, $\eta=r\mp z$:

$$\xi\left(\frac{d}{d\xi}S_\xi^{\mathrm{cl}}\right)^2+\eta\left(\frac{d}{d\eta}S_\eta^{\mathrm{cl}}\right)^2-me^2-\frac{mE}{2}(\xi+\eta)=0. \tag{7.9}$$

The constant of separation a_η, given by

$$a_\eta=\eta\left(\frac{d}{d\eta}S_\eta^{\mathrm{cl}}\right)^2-\eta\frac{mE}{2} \tag{7.10}$$

(which is zero for (7.8)), can be shown to have the physical meaning

$$a_\eta=\tfrac{1}{2}m(e^2-A_z). \tag{7.11}$$

Here $\boldsymbol{A}$ is the Runge–Lenz vector

$$\boldsymbol{A}=\frac{1}{m}\boldsymbol{p}\times(\boldsymbol{r}\times\boldsymbol{p})-e^2\frac{\boldsymbol{r}}{r}, \tag{7.12}$$

which is constant for Coulomb motion:

$$\boldsymbol{A}=2E\boldsymbol{c}, \qquad A_z=2Ea=e^2. \tag{7.13}$$

a in (7.2) is the semi-major axis, and the impact parameter b is the semi-minor axis of one hyperbolic orbit. Then $\boldsymbol{c}$ is the vector from the origin to the crossing point of the hyperbola's asymptotes. The ensemble of orbits given by $S^{\mathrm{cl}}_{0,1}$, with all values of b, are thus characterised by the three constants of motion E, A_z and $L_z(=0)$.

The role of A_z as the third quantised operator by Coulomb scattering is perhaps not so well known. Applying the symmetrised A_z to Ψ_k in (A1.1), we get the eigenvalue $e^2 + \mathrm{i}\hbar^2 k/m$. The reason why it is complex is that Ψ_k does not belong to a Hilbert space (simple example: put $e = 0$).

The fields of classical momenta obtained from (7.8) are

$$\left.\begin{matrix} \boldsymbol{p}_0(\boldsymbol{r}) \\ \boldsymbol{p}_1(\boldsymbol{r}) \end{matrix}\right\} = \nabla S^{\mathrm{cl}}_{0,1} = \frac{p_\infty}{2}\left[\hat{\boldsymbol{r}} + \hat{\boldsymbol{k}} \mp (\hat{\boldsymbol{r}} - \hat{\boldsymbol{k}})\left(1 + \frac{4me^2/p_\infty^2}{r - z}\right)^{1/2}\right] \xrightarrow[r-z\to\infty]{} \begin{cases} p_\infty \hat{\boldsymbol{k}} \\ p_\infty \hat{\boldsymbol{r}} \end{cases}. \tag{7.14}$$

(Note: $\boldsymbol{p}^2_{0,1}/2m - e^2/r = p^2_\infty/2m$.) The transition from the incident $\boldsymbol{p}_0$ to the scattered $\boldsymbol{p}_1$ occurs on the z axis.

The introduction of a 'classical wavefunction', or '*strahlen-optische Wellenfunktion*', given by

$$\Psi^{\mathrm{cl}} = \rho_0^{1/2} \exp[(\mathrm{i}/\hbar)S_0^{\mathrm{cl}}] + \rho_1^{1/2} \exp[(\mathrm{i}/\hbar)S_1^{\mathrm{cl}}], \tag{7.15}$$

where $\rho_{0,1}(\boldsymbol{r})$ is the particle density, was made by Gordon (1928) in his treatment of Rutherford scattering. Later Birkhoff (1933), Keller (1958) and others assumed that a form like (7.15) was in general the classical limit of Ψ. (The calculations above for Coulomb scattering do not seem to have been published before.)

8. Yukawa functions

With an exponentially screened Coulomb potential ($\hbar = 1$)

$$V(r) = -\frac{\nu k}{m}\frac{1}{r}\exp(-\kappa r) \tag{8.1}$$

we get (cf § 3)

$$V(\boldsymbol{p}, \boldsymbol{p}') = \frac{1}{(2\pi)^3}\int \mathrm{d}^3\boldsymbol{r} \exp[\mathrm{i}(\boldsymbol{p}' - \boldsymbol{p}) \cdot \boldsymbol{r}]V(r) = \frac{1}{2\pi^2}\frac{-\nu k/m}{(\boldsymbol{p} - \boldsymbol{p}')^2 + \kappa^2}, \tag{8.2}$$

$$\overline{V(\boldsymbol{p}, \boldsymbol{p}')} = \frac{1}{2\pi^2}\frac{-\nu k/m}{[(p^2 + p'^2 - 2p_z p'_z + \kappa^2)^2 - 4p_\perp^2 p'^2_\perp]^{1/2}}, \tag{8.3}$$

$$W_k(p_z, \boldsymbol{p}') = -\bar{V}(p_\perp^2 = k_+^2 - p_z^2) = \frac{1}{2\pi^2}\frac{\nu k/m}{[(k_+^2 + p'^2 - 2p_z p'_z + \kappa^2)^2 - 4(k_+^2 - p_z^2)p'^2_\perp]^{1/2}}. \tag{8.4}$$

With expansions in powers of ν, the equations for Ψ_k and Φ_k (cf (3.3)) are satisfied if

$$\Psi_k^{(n+1)}(\boldsymbol{p}) = \frac{2m}{k_+^2 - p^2}\int \mathrm{d}^3\boldsymbol{p}'\ V(\boldsymbol{p}, \boldsymbol{p}')\Psi_k^{(n)}(\boldsymbol{p}'), \tag{8.5$'$}$$

$$\Phi_k^{(n+1)}(\boldsymbol{p}) = \frac{2m}{k_+^2 - p^2}\int \mathrm{d}^3\boldsymbol{p}'[V(\boldsymbol{p}, \boldsymbol{p}') + W_k(p_z, \boldsymbol{p}')]\Phi_k^{(n)}(\boldsymbol{p}'). \tag{8.5$''$}$$

Gorshkov (1961) has given solutions of (8.5′) in a form which it is possible to modify and use for the solution of (8.5″). With upper limits of integration equal to 1 for Ψ and equal to ∞ for Φ we will show that the solutions are

$$\left.\begin{matrix}\Psi_k^{(n)}(\boldsymbol{p})\\ \Phi_k^{(n)}(\boldsymbol{p})\end{matrix}\right\} = \frac{(\mathrm{i}\nu)^n}{\mathrm{i}\pi^2}k\int_{s_0}^{1,\infty} \mathrm{d}s_1 \frac{1}{(1-s_1)S_1}\int_{s_1}^{1,\infty} \mathrm{d}s_2 \frac{1}{(1-s_2)S_2}\cdots$$

$$\times\int_{s_{n-2}}^{1,\infty} \mathrm{d}s_{n-1}\frac{1}{(1-s_{n-1})S_{n-1}}\int_{s_{n-1}}^{1,\infty}\mathrm{d}s_n\frac{1}{(Q_n^0)^2}, \tag{8.6}$$

where

$$Q_n^0 = (\boldsymbol{p}-\boldsymbol{k}+s_n\boldsymbol{k})^2 - k^2S_n^2, \tag{8.7}$$

$$S_n^2 = s_n^2 + \sum_{m=0}^{n-1}\left(2\mathrm{i}\frac{\kappa}{k}S_m - \frac{\kappa^2}{k^2}\right)\frac{1-s_n}{1-s_m}, \tag{8.8}$$

$$s_0 = 0, \qquad S_0 = 0. \tag{8.9}$$

The integration with respect to s_n in (8.6) can be carried out. We introduce

$$Q_n = (\boldsymbol{p}-\boldsymbol{k}+s_n\boldsymbol{k})^2 - (kS_n + \mathrm{i}\kappa)^2, \tag{8.10}$$

$$P = k_+^2 - p^2, \tag{8.11}$$

which, from (8.7), (8.8), satisfy

$$Q_n^0 = (Q_{n-1}+P)\frac{1-s_n}{1-s_{n-1}} - P. \tag{8.12}$$

This leads to the alternative forms

$$\left.\begin{matrix}\Psi_k^{(n)}(\boldsymbol{p})\\ \Phi_k^{(n)}(\boldsymbol{p})\end{matrix}\right\} = \frac{(\mathrm{i}\nu)^n}{\mathrm{i}\pi^2}k\int_{s_0}^{1,\infty}\mathrm{d}s_1\frac{1}{(1-s_1)S_1}\cdots\int_{s_{n-2}}^{1,\infty}\mathrm{d}s_{n-1}\frac{1}{S_{n-1}}\times\left\{\begin{matrix}F_{n-1}^1\\ F_{n-1}^{\infty}\end{matrix}\right., \tag{8.13}$$

where

$$F_{n-1}^1 = \frac{-1}{PQ_{n-1}}, \tag{8.14}$$

$$F_{n-1}^{\infty} = \frac{-1}{Q_{n-1}(Q_{n-1}+P)} = \frac{-1}{PQ_{n-1}} + \frac{1}{P(Q_{n-1}+P)}. \tag{8.15}$$

From (8.6) and (8.13)–(8.15), with $n \to n+1$, it follows that (8.5′), (8.5″) are satisfied if

$$2m\int \mathrm{d}^3p'\; V(\boldsymbol{p},\boldsymbol{p}')\frac{1}{(Q_n^0)^2} = \frac{-\mathrm{i}\nu}{S_nQ_n}, \tag{8.16}$$

$$2m\int \mathrm{d}^3p'\; W_k(p_z,\boldsymbol{p}')\frac{-1}{(Q_n^0)^2} = \frac{\mathrm{i}\nu}{S_n(Q_n+P)}. \tag{8.17}$$

Equation (8.16) is established from the obvious relation

$$\frac{1}{\mathrm{i}}\frac{\partial}{\partial K}\int \mathrm{d}^3p'\langle\boldsymbol{p}|\frac{\exp(-\kappa r)}{r}|\boldsymbol{p}'\rangle\langle\boldsymbol{p}'|\frac{\exp(\mathrm{i}Kr)}{r}|\boldsymbol{q}\rangle = \langle\boldsymbol{p}|\frac{\exp[(\mathrm{i}K-\kappa)r]}{r}|\boldsymbol{q}\rangle, \tag{8.18}$$

i.e., with $\operatorname{Im} K > 0$,

$$\frac{1}{\mathrm{i}}\frac{\partial}{\partial K}\frac{1}{2\pi^2}\int \mathrm{d}^3p'\frac{1}{(\boldsymbol{p}-\boldsymbol{p}')^2+\kappa^2}\,\frac{1}{(\boldsymbol{p}'-\boldsymbol{q})^2-K^2} = \frac{1}{(\boldsymbol{p}-\boldsymbol{q})^2-(K+\mathrm{i}\kappa)^2}. \tag{8.19}$$

As $\boldsymbol{q}$ is proportional to $\boldsymbol{k}$ in (8.7) and (8.10), V may be averaged in (8.16):

$$2m\int \mathrm{d}^3\boldsymbol{p}'\,\overline{V(\boldsymbol{p},\boldsymbol{p}')}\frac{1}{(Q_n^0)^2}=\frac{-\mathrm{i}\nu}{S_nQ_n}. \tag{8.20}$$

Using (3.2) we obtain (8.17), because (8.10), (8.11) show that

$$Q_n(p_\perp^2=k_+^2-p_z^2)=Q_n+P. \tag{8.21}$$

The nth-order term of (3.6), namely

$$w_k^{(n)}(p_z)=4\pi^2\int \mathrm{d}^3\boldsymbol{p}'\;W_k(p_z,\boldsymbol{p}')\Phi_k^{(n-1)}(\boldsymbol{p}'), \tag{8.22}$$

can, according to (8.13), (8.15), (8.17), be written

$$w_k^{(n)}(p_z)=-(\mathrm{i}\nu)^n\frac{2\mathrm{i}k}{m}\int_{s_0}^{\infty}\mathrm{d}s_1\frac{1}{(1-s_1)S_1}\cdots\int_{s_{n-2}}^{\infty}\mathrm{d}s_{n-1}\frac{1}{S_{n-1}(Q_{n-1}+P)}. \tag{8.23}$$

The first-order expressions are

$$\Psi_k^{(1)}(\boldsymbol{p})=-\frac{\nu k}{\pi^2}\frac{1}{PQ_0}=-\frac{\nu k}{\pi^2}\frac{1}{k_+^2-p^2}\frac{1}{(\boldsymbol{p}-\boldsymbol{k})^2+\kappa^2}, \tag{8.24}$$

$$\Phi_k^{(1)}(\boldsymbol{p})=-\frac{\nu k}{\pi^2}\frac{1}{(P+Q_0)Q_0}=-\frac{\nu k}{\pi^2}\frac{1}{2k_+^2-2\boldsymbol{k}\cdot\boldsymbol{p}+\kappa^2}\frac{1}{(\boldsymbol{p}-\boldsymbol{k})^2+\kappa^2}, \tag{8.25}$$

$$\mathrm{X}_k^{(1)}(\boldsymbol{p})=\Psi_k^{(1)}(\boldsymbol{p})-\Phi_k^{(1)}(\boldsymbol{p})=-\frac{\nu k}{\pi^2}\frac{1}{P(Q_0+P)}=-\frac{\nu k}{\pi^2}\frac{1}{k_+^2-p^2}\frac{1}{2k_+^2-2\boldsymbol{k}\cdot\boldsymbol{p}+\kappa^2}, \tag{8.26}$$

$$w_k^{(1)}(p_z)=\frac{2\nu k}{m}\frac{1}{Q_0+P}=\frac{2\nu k}{m}\frac{1}{2k_+^2-2kp_z+\kappa^2}. \tag{8.27}$$

The coordinate space functions are obtained by Fourier-transforming (8.6). The paths of s_i integrations can be chosen such that $\operatorname{Im} S_n>0$, and we get

$$\left.\begin{matrix}\Psi_k^{(n)}(\boldsymbol{r})\\ \Phi_k^{(n)}(\boldsymbol{r})\end{matrix}\right\}=(\mathrm{i}\nu)^n\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\int_{s_0}^{1,\infty}\mathrm{d}s_1\frac{1}{(1-s_1)S_1}\int_{s_1}^{1,\infty}\mathrm{d}s_2\frac{1}{(1-s_s)S_2}\cdots$$

$$\times\int_{s_{n-1}}^{1,\infty}\mathrm{d}s_n\frac{1}{S_n}\exp[\mathrm{i}(S_nkr-s_n\boldsymbol{k}\cdot\boldsymbol{r})]. \tag{8.28}$$

In (8.23) we write

$$Q_{n-1}+P=-2k(1-s_{n-1})(p_z-k_++k\sigma_{n-1}), \tag{8.29}$$

where (8.8)–(8.11) show that

$$\sigma_{n-1}=\sum_{m=0}^{n-1}\left(\mathrm{i}\frac{\kappa}{k}S_m-\frac{\kappa^2}{2k^2}\right)\frac{1}{1-s_m}. \tag{8.30}$$

Equation (3.14) then gives

$$w_k^{(n)}(z)=-\frac{2\pi}{m}\theta(z)\exp(\mathrm{i}kz)(\mathrm{i}\nu)^n\int_{s_0}^{\infty}\mathrm{d}s_1\frac{1}{(1-s_1)S_1}\cdots$$

$$\times\int_{s_{n-2}}^{\infty}\mathrm{d}s_{n-1}\frac{1}{(1-s_{n-1})S_{n-1}}\exp(-\mathrm{i}kz\sigma_{n-1}). \tag{8.31}$$

An alternative expression for $\Phi_k^{(n)}(\boldsymbol{r})$ is obtained by inserting (8.29) in (8.13), (8.15) before the Fourier transformation, which leads to

$$\Phi_k^{(n)}(\boldsymbol{r}) = \exp(\mathrm{i}kz)\int_0^\infty \mathrm{d}z' \frac{\exp\{-\kappa[r_\perp^2+(z-z')^2]^{1/2}\}}{[r_\perp^2+(z-z')^2]^{1/2}}\phi_k^{(n)}(\boldsymbol{r}, z'), \tag{8.32}$$

where

$$\phi_k^{(n)}(\boldsymbol{r}, z') = (\mathrm{i}\nu)^n \int_{s_0}^\infty \mathrm{d}s_1 \frac{1}{(1-s_1)S_1}\cdots\int_{s_{n-2}}^\infty \mathrm{d}s_{n-1}\frac{1}{(1-s_{n-1})S_{n-1}} \times \exp[\![\mathrm{i}k\{S_{n-1}[r_\perp^2+(z-z')^2]^{1/2} - s_{n-1}(z-z') - \sigma_{n-1}z'\}]\!]. \tag{8.33}$$

This form indicates the asymptotic behaviour

$$\Phi_k(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} \exp(\mathrm{i}kz) + \mathrm{O}[\exp(-\kappa r)/r], \tag{8.34}$$

which is an example of our general conjecture in (1.4).

The Fourier transforms of (8.27) and (8.25) are

$$w_k^{(1)}(z) = -(2\pi\mathrm{i}\nu/m)\theta(z)\exp[\mathrm{i}(1+\kappa^2/2k^2)kz], \tag{8.35}$$

$$\Phi_k^{(1)}(\boldsymbol{r}) = \mathrm{i}\nu\exp(\mathrm{i}kz)\int_0^\infty \mathrm{d}z'\frac{\exp\{-\kappa[r_\perp^2+(z-z')^2]^{1/2}\}}{[r_\perp^2+(z-z')^2]^{1/2}}\exp\left(\mathrm{i}\frac{\kappa^2}{2k}z'\right) \underset{r\to\infty}{\longrightarrow} \mathrm{O}\left(\frac{\exp(-\kappa r)}{r}\right). \tag{8.36}$$

From (3.15) and (8.35) we get

$$\mathrm{X}_k^{(1)}(\boldsymbol{r}) = -\mathrm{i}\nu\int_0^\infty \mathrm{d}z'\frac{\exp\{\mathrm{i}k[r_\perp^2+(z-z')^2]^{1/2}\}}{[r_\perp^2+(z-z')^2]^{1/2}}\exp\left[\mathrm{i}\left(k+\frac{\kappa^2}{2k}\right)z'\right] \underset{r\to\infty}{\longrightarrow} \frac{\exp(\mathrm{i}kr)}{r}\,\frac{-2\nu k}{(k\hat{\boldsymbol{r}}-\boldsymbol{k})^2+\kappa^2} = \frac{\exp(\mathrm{i}kr)}{r}f_k^{(1)}(\hat{\boldsymbol{r}}). \tag{8.37}$$

Our Yukawa results can be used for describing scattering in potentials which can be written

$$V(r) = L_\kappa V_\kappa(r), \tag{8.38}$$

where L_κ represents a linear operation upon the parameter κ in the Yukawa potential (8.1). We define

$$|\Psi_k\rangle^{(n)}_{\kappa_1,\kappa_2\ldots\kappa_n} \equiv G^0V_{\kappa_1}G^0V_{\kappa_2}\ldots G^0V_{\kappa_n}|\boldsymbol{k}\rangle \tag{8.39}$$

and correspondingly for $|\Phi_k\rangle^{(n)}_{\kappa_1\ldots}$ with potential $V_\kappa + W_{k,\kappa}$. This gives

$$|\Psi_k\rangle^{(n)} \equiv (G^0V)^n|\boldsymbol{k}\rangle = \lim_{\kappa_1=\ldots=\kappa_n} L_{\kappa_1}\ldots L_{\kappa_n}|\Psi_k\rangle^{(n)}_{\kappa_1\ldots\kappa_n}, \tag{8.40}$$

and similarly for $|\Phi_k\rangle^{(n)}$, i.e. also for $|\mathrm{X}_k\rangle^{(n)}$ and $|w_k\rangle^{(n)}$. Examples of L_κ are

(*a*) $$V(r) = V_0\exp(-\kappa r) = \frac{V_0 m}{\nu k}\frac{\partial}{\partial\kappa}V_\kappa(r), \tag{8.41}$$

(*b*) $$V(r) = V_0\frac{b^2}{r^2+a^2} = \frac{V_0b^2m}{ak\nu}\int_0^\infty \mathrm{d}\kappa\,\sin(a\kappa)\frac{\partial}{\partial\kappa}V_\kappa(r). \tag{8.42}$$

Concerning the problems (anomalies) in connection with the transition from screened to unscreened Coulomb scattering quantities, we refer to other papers by the author (Kolsrud 1978, 1977). There we also present a modified integral equation, which is valid also for $\Psi_{\rm coul}(\boldsymbol{r})$.

Appendix 1

The Coulomb functions are defined by

$$\left.\begin{matrix}\Psi_{\boldsymbol{k}}(\boldsymbol{r})\\ \Phi_{\boldsymbol{k}}(\boldsymbol{r})\\ \mathrm{X}_{\boldsymbol{k}}(\boldsymbol{r})\end{matrix}\right\} = \exp\left(\nu\frac{\pi}{2}\right)\Gamma(1-\mathrm{i}\nu)\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\times\left\{\begin{matrix}F_{01}\\ F_0,\\ F_1\end{matrix}\right. \tag{A1.1}$$

where

$$F_i[\mathrm{i}\nu, 1, \mathrm{i}(kr-\boldsymbol{k}\cdot\boldsymbol{r})] = \frac{1}{2\pi\mathrm{i}}\int_{c_i}\mathrm{d}t\, t^{-1+\mathrm{i}\nu}(t-1)^{-\mathrm{i}\nu}\exp[\mathrm{i}t(kr-\boldsymbol{k}\cdot\boldsymbol{r})]. \tag{A1.2}$$

Here c_{01} is a contour around the branch points $t=0$ and $t=1$, while $c_0(c_1)$ is a path from $\mathrm{Im}\, t=\infty$, anticlockwise around $t=0$ $(t=1)$, and back to $\mathrm{Im}\, t=\infty$. Hence $F_{01}=F_0+F_1$ and $\Psi=\Phi+\mathrm{X}$. We get in fact (with $\boldsymbol{k}\cdot\boldsymbol{r}=kz$)

$$\left(\nabla^2+k^2+\frac{2\nu k}{r}\right)\times\left\{\begin{matrix}\Psi_{\boldsymbol{k}}\\ \Phi_{\boldsymbol{k}}\\ \mathrm{X}_{\boldsymbol{k}}\end{matrix}\right. = \exp\left(\nu\frac{\pi}{2}\right)\Gamma(1-\mathrm{i}\nu)\frac{k}{\pi}\frac{\exp(\mathrm{i}kz)}{r}$$

$$\times\int_{c_i}\mathrm{d}t\frac{\partial}{\partial t}\{t^{\mathrm{i}\nu}(t-1)^{1-\mathrm{i}\nu}\exp[\mathrm{i}k(r-z)t]\} = D_i. \tag{A1.3}$$

The contour c_{01} makes $D_{01}=0$ for all z, while c_0 and c_1 make $D_0=D_1=0$ when $z<r$ and $D_0=D_1=\infty$ when $z=r$. We show that D_0 and D_1 can be written

$$D_i = \pm 2m\delta(x)\delta(y)\theta(z)w_{\boldsymbol{k}}(z), \qquad i=0,1, \tag{A1.4}$$

i.e.

$$-2m\theta(z)w_{\boldsymbol{k}}(z) = \iint \mathrm{d}x\,\mathrm{d}y\, D_1. \tag{A1.5}$$

We get indeed from (A1.1)–(A1.3)

$$\iint \mathrm{d}x\,\mathrm{d}y\,D_1 = \exp\left(\nu\frac{\pi}{2}\right)\Gamma(1-\mathrm{i}\nu)\exp(\mathrm{i}kz)\frac{2}{\mathrm{i}}\int_{c_1}\mathrm{d}t\frac{\partial}{\partial t}\{t^{-1+\mathrm{i}\nu}(t-1)^{1-\mathrm{i}\nu}\exp[\mathrm{i}kt(|z|-z)]\}, \tag{A1.6}$$

which equals zero when $z<0$, like $\theta(z)$, and which for $z>0$ yields the finite term

$$-2mw_{\boldsymbol{k}}(z) = \exp\left(\nu\frac{\pi}{2}\right)\Gamma(1-\mathrm{i}\nu)\exp(\mathrm{i}kz)\frac{2}{\mathrm{i}}[\exp(-2\pi\nu)-1] = 4\pi\frac{\exp(-\nu\pi/2)}{\Gamma(\mathrm{i}\nu)}\exp(\mathrm{i}kz). \tag{A1.7}$$

Appendix 2

The behaviour near $\xi \equiv r - z = 0$ of Coulomb's $\Phi_k(\boldsymbol{r})$ and $X_k(\boldsymbol{r})$ is perhaps most easily shown in the following way. From (A1.2) we get by partial integration

$$\xi\frac{\partial F_1}{\partial \xi} = -\frac{1}{2\pi \mathrm{i}}\int_{c_1} \mathrm{d}t\, \exp(\mathrm{i}k\xi t)\frac{\mathrm{d}}{\mathrm{d}t}[t^{\mathrm{i}\nu}(t-1)^{-\mathrm{i}\nu}] \xrightarrow[\xi\to 0]{} \frac{1}{2\pi\mathrm{i}}[\exp(-2\pi\nu)-1]$$

$$= \frac{\exp(-\pi\nu)}{\Gamma(1-\mathrm{i}\nu)\Gamma(\mathrm{i}\nu)}. \tag{A2.1}$$

With (A1.1) and (A1.7) we thus get

$$\left.\begin{matrix}\Phi_k(\boldsymbol{r})\\ X_k(\boldsymbol{r})\end{matrix}\right\} \xrightarrow[r-z\approx 0]{} \pm\frac{m}{2\pi} w_k(z)\ln[k(r-z)]. \tag{A2.2}$$

Appendix 3

Write $H = H_0 + V$ and $H_k = H + W_k$. We define the following set of vectors:

$$|\Phi_{k,q}\rangle = |\boldsymbol{q}\rangle + \frac{1}{E_q + \mathrm{i}\epsilon - H_0}(V + W_k)|\Phi_{k,q}\rangle \tag{A3.1}$$

$$= \left(1 + \frac{1}{E_q + \mathrm{i}\epsilon - H_k}(V + W_k)\right)|\boldsymbol{q}\rangle. \tag{A3.2}$$

(Hence $|\Phi_k\rangle = |\Phi_{k,k}\rangle$.) The reciprocal set is defined by

$$|\Phi_k^q\rangle = \left(1 + \frac{1}{E_q + \mathrm{i}\epsilon - H_k^\dagger}(V + W_k^\dagger)\right)|\boldsymbol{q}\rangle.$$

The two sets obviously satisfy

$$(E_q - H_k)|\Phi_{k,q}\rangle = 0, \qquad (E_q - H_k^\dagger)|\Phi_k^q\rangle = 0. \tag{A3.3}$$

The orthonormality relations follow from

$$\langle \Phi_k^q | \Phi_{k,q'}\rangle = \langle \boldsymbol{q}|\left(1 + (V + W_k)\frac{1}{E_q - \mathrm{i}\epsilon - H_k}\right)|\Phi_{k,q'}\rangle$$

$$= \langle \boldsymbol{q}|\left(1 + (V + W_k)\frac{1}{E_q - \mathrm{i}\epsilon - E_{q'}}\right)|\Phi_{k,q'}\rangle$$

$$= \langle \boldsymbol{q}|\left(1 - \frac{1}{E_{q'} + \mathrm{i}\epsilon - H_0}(V + W_k)\right)|\Phi_{k,q'}\rangle$$

$$= \langle \boldsymbol{q}|\boldsymbol{q}'\rangle = \delta(\boldsymbol{q} - \boldsymbol{q}'). \tag{A3.4}$$

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