FORMULA FOR CALCULATION OF PHASE SHIFTS IN CASE OF THOMAS-FERMI AND HARTREE POTENTIALS

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A formula for phase shifts is deduced for small orbital momentum values. The formula is useful in practical calculations.

IT is known that in the case of small quantum numbers the Born approximation does not permit the phase shifts to be calculated with sufficient accuracy. The Pais method [1] gives in this case better results than the Born method, but if $l = 0$ the Pais method is inapplicable. In addition, the Pais method has that shortcoming that the transcendental equation obtained for the phase shift is not convenient in practical calculations. In the present communication we give a simple and convenient formula for the phase shifts in the case of Thomas-Fermi and Hartree potentials.

Let us write out the Schrödinger equation for the Thomas-Fermi and Hartree potentials in the form

$$\frac{d^2R_l}{dr^2} + \left[2E + \frac{2Z}{r}\frac{Z_p}{Z} - \frac{l(l+1)}{r^2}\right] R_l = 0. \qquad (1)$$

We use atomic units, $e = m = \hbar = 1$; the energy unit is e^2/a_H, which is equal to double the ionization energy of the hydrogen atom in the normal state (numerically equal to 27.23 eV). The factor Z_p/Z represents the screening of the nucleus on the part of the orbital electrons. According to Ruark [2] [1)]

$$Z_p/Z = \sum_i c_i \exp(-b_i x); \quad x = \frac{r}{\mu},$$
$$\mu = 0.88534 Z^{-1/3}; \qquad (2)$$

Z is the nuclear charge and the constants c_i and b_i [4] are listed in Table I. We write out the Pais formula for the phase shift δ_l in the form

$$\frac{2l+1-2\delta_l/\pi}{2l+1-4\delta_l/\pi}\,\delta_l = \pi Z \int_0^\infty (Z_p/Z)\, J^2_{l+1/2-2\delta_l/\pi}(\sqrt{2E}\, r)\, dr, \qquad (3)$$

[1)] See also the work by Gombas [3] on the statistical theory of the atom.

Table I. Values of the constants c_i and b_i in Eq. (2), after Byatt [4] *

Element	c_1	c_2	b_1	b_2
He	1	—	1.60	—
Ne	1	—	0.95	—
Cr	1	—	0.731	—
Br	0.360	0.640	0.366	1.483

*The values of c_i and b_i for other elements can be found in the paper by Byatt. [4]

where E is the energy of the incident electron. For large quantum numbers this formula goes over into the well known Born formula for the phase shifts $\delta_l^{(1)}$.

We represent the Pais shift δ_l in the form

$$\delta_l = \delta_l^{(1)} + \delta_l^{(2)} + \ldots \quad . \qquad (4)$$

If δ_l is small, then the correction $\delta_l^{(2)}$ to the Born shift $\delta_l^{(1)}$ can be calculated from the formula

$$\delta_l^{(2)} = \frac{2}{\pi}\left(a_l - \frac{\delta_l^{(1)}}{2l+1}\right)\delta_l^{(1)}; \qquad a_l = -\left(\frac{\partial \delta_p^{(1)}}{\partial p}\right)_{p=l+1/2}. \qquad (5)$$

In our case the Born phase shift is

$$\delta_l^{(1)} = \frac{Z}{\sqrt{2E}} \sum_i c_i Q_l \left(1 + \frac{1}{2}\left(\frac{b_i}{\mu\sqrt{2E}}\right)^2\right), \qquad (6)$$

where Q_l are Legendre polynomials of the second kind. After simple calculations we obtain for the a_l in (5)

$$a_l = -\frac{4Z}{\pi}\sum_i c_i \int_0^{\pi/2} \frac{\varphi \cos(2l+1)\varphi}{\sqrt{(b_i/\mu)^2 + 8E\sin^2\varphi}} \times \ln \frac{\sqrt{(b_i/\mu)^2 + 8E\sin^2\varphi} + 2\sqrt{2E}\sin\varphi}{\sqrt{(b_i/\mu)^2 + 8E\sin^2\varphi} - 2\sqrt{2E}\sin\varphi}\, d\varphi. \qquad (7)$$

The index i in (2), (3), (6), and (7) runs through values that are never outside the range from one

Table II. Comparison of phase shift for He ($c_1 = 1$, $b_1 = 1.60$), calculated from formulas (4)—(6), with the numerical calculations [5]

E, eV	$\delta_l^{(1)}$ (after Born)	$\delta_l = \delta_l^{(1)} + \delta_l^{(2)}$ present work	Numerical calculation [5]	E, eV	$\delta_l^{(1)}$ (after Born)	$\delta_l = \delta_l^{(1)} + \delta_l^{(2)}$ present work	Numerical calculation [5]
16	$\delta_1^{(1)} = 0.05356$	$\delta_1 = 0.0731$	0.070	121	$\delta_1^{(1)} = 0.2276$	$\delta_1 = 0.2796$	0.272
49	$\delta_1^{(1)} = 0.1340$	$\delta_1 = 0.1875$	0.186		$\delta_2^{(1)} = 0.0892$	$\delta_2 = 0.0924$	0.0946
					$\delta_3^{(1)} = 0.0492$	$\delta_3 = 0.04917$	—

to three, depending on the charge of the nucleus Z. Detailed values of the index i can be found in the table by Byatt [4].

Formula (7) is more convenient for practical calculations than (3). Knowing a_l (7) we can find δ_l (4) with the aid of (5) and (6). Table II gives a numerical example for Z = 2. It is seen from this table that in the case when $l = 1$ or 2 our formula gives much better results compared with the phase shift $\delta_l^{(1)}$ obtained by the Born method.

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