Corrections to "The Quantum-Mechanical Calculations of One-Electron-Properties II — One and Two-Center Integrals"

WALTER A. YERANOS and NICHOLAS W. WINTER

Department of Chemistry, Northern Illinois University, De Kalb, Illinois, U.S.A.

(Z. Naturforschg. **20 a**, 1217 [1965]; received 10 July 1965)

Several years ago KUPPERMANN, KARPLUS and ISAACSON [1] published a paper in this Journal which dealt with the general formulation of one and two center moment integrals. Unfortunately, however, a number of typographic errors have gone by unnoticed and after a thorough review, we would like to report the following corrections:

(a) In equation (18), the part that reads

$$P_l^m\left(\frac{1-\xi\eta}{\xi+\eta}\right) \quad \text{should read} \quad P_l^m\left(\frac{1-\xi\eta}{\xi-\eta}\right).$$

(b) In equation (20), the part at the very end that reads

$$p(\xi,\zeta) \quad \text{should read} \quad p(\xi,\eta).$$

(c) Equation (24) reads $I_\varphi = \dfrac{c_m\, c_{m'}}{2^{\alpha+\beta}}$

and it should read $I_\varphi = \dfrac{\pi\, c_m\, c_{m'}}{2^{\alpha+\beta}}$.

(d) Equation (25) reads

$$\varepsilon \equiv (\alpha+\beta-m-m')$$

and it should read

$$\varepsilon \equiv \tfrac{1}{2}\,(\alpha+\beta-m-m').$$

(e) In section 2.2, in the derivation of the equation for I_φ, the right hand sides of equations (34), (35), (36), (37), and (26) should be multiplied by π.

(f) The power series expansion for the integral $B_s(t)$, Section 4, equation (50), which reads

$$B_s(t) = (-1)^d \sum_{j=0}^{\infty} \frac{t^{2j+e}}{(2j+e)!\,(2j+e+1+s)!}$$

should read

$$B_s(t) = 2(-1)^s \sum_{j=0}^{\infty} \frac{t^{2j+e}}{(2j+e)!\,(2j+e+1+s)}\,.$$

(g) Equation (46) in Section 3 reads

$$L = \frac{1+(-1)^s}{s+1} \lim_{a\to 0} \ldots \quad = \frac{F!}{(\zeta+\zeta')^{F+1}}\,\delta_{F,s}$$

and it should read as follows

$$L = \frac{1+(-1)^{\sigma-s}}{\sigma-s+1} \lim_{a\to 0} \ldots$$

$$= \frac{1+(-1)^{\sigma-F}}{\sigma-F+1}\,\frac{F!}{(\zeta+\zeta')^{F+1}}\,\delta_{F,s}\,.$$

Furthermore, we have checked the validity of our corrections by comparing the results of long hand calculations of certain typical integrals with the results obtained from a program coded specifically for the IBM 1620 Model II of the Computer Center of Northern Illinois University. Copies of this program which calculates one and two center integrals of the type $<\psi(R'\vartheta'\varphi')\,|\,X^\alpha Y^\beta Z^\gamma\,|\,\psi(R\,\vartheta\,\varphi)>$ can be obtained from us.

[1] A. KUPPERMANN, M. KARPLUS, and L. M. ISAACSON, Z. Naturforschg. **14 a**, 311 [1959].

A Nonlocal Nuclear Single Particle Potential and Charge Independence of Short Range Forces

H. MELDNER, G. SÜSSMANN, and W. ULRICI

Institut für Theoretische Physik der Universität Frankfurt/M, Germany

(Z. Naturforschg. **20 a**, 1217—1218 [1965]; received 6 August 1965)

This letter reports some results obtained in an attempt to determine a nuclear single particle potential of the HARTREE–FOCK type that contains isospin dependent terms with the same parameters for both kinds of nucleons. Considering a large number of nuclei distributed over the entire periodic system we tried to find average potential parameters for the calculation of ground state energies. In our ansatz the equation for all single particle wave functions was assumed to have the form

$$\left(\frac{\boldsymbol{p}^2}{2m} - E\right)\psi(\boldsymbol{r}) + \int \mathrm{d}^3\boldsymbol{r}'\, K(\boldsymbol{r},\boldsymbol{r}')\,\psi(\boldsymbol{r}') = 0 \quad (1)$$

with the following kernel, which is similar to those used in calculations of elastic nucleon-nucleus scattering [1]:

[1] F. PEREY and B. BUCK, Nucl. Phys. **32**, 353 [1962].