

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

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Several years ago KUPPERMANN, KARPLUS and ISAACSON¹ 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

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

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

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

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

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

(d) Equation (25) reads

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

and it should read

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

(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

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

and it should read as follows

$$L = \frac{1+(-1)^{\sigma-s}}{\sigma-s+1} \lim_{a \rightarrow 0} \dots = \frac{1+(-1)^{\sigma-F}}{\sigma-F+1} \frac{F!}{(\zeta + \zeta')^{F+1}} \delta_{F,s}.$$

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 $\langle \psi(R' \partial' \varphi') | X^\alpha Y^\beta Z^\gamma | \psi(R \partial \varphi) \rangle$ 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

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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 num-

ber 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

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

with the following kernel, which is similar to those used in calculations of elastic nucleon-nucleus scattering¹:

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



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$$\begin{aligned}
K(\mathbf{r}, \mathbf{r}') &= U_N \left(\frac{1}{2} [r + r'] \right) \delta_\beta(\mathbf{r} - \mathbf{r}') \\
&\quad + U_C(r) \left(\frac{1}{2} - t_3 \right) \delta_0(\mathbf{r} - \mathbf{r}'), \\
\delta_\beta(\mathbf{r}) &= \pi^{-3/2} \beta^{-3} \exp[-(\mathbf{r}/\beta)^2], \\
\Theta_a(r) &= [1 + \exp(-r/a)]^{-1}, \\
U_N(r) &= -V \left(1 - \frac{\tau}{A} \frac{N-Z-2t_3}{2} t_3 \right) \\
&\quad \cdot \left[1 + \sigma \frac{1}{2} \left(j(j+1) - l(l+1) - \frac{3}{4} \right) \frac{r_0^2}{r} \frac{\partial}{\partial r} \right] \\
&\quad \cdot \Theta_a(r_0 A^{1/3} - r)
\end{aligned}$$

where the parameter β is the range of nonlocality and the parameters V , r_0 , a , τ and σ are respectively the depth, radius constant, surface thickness, isospin and spin-orbit dependence of the single particle potential. The spin-orbit interaction is the simplest invariant (with respect to rotations and inversions) proportional to $\mathbf{p} \cdot \mathbf{s}$ and ∇U , namely $\nabla U(\mathbf{p} \times \mathbf{s})$. It happens to be similar to the "THOMAS term" but is apparently of independent origin and therefore we do not use factors m and c . The factor r_0^2 is introduced for dimensional reasons; due to the approximate $r_0^2 U$ -invariance this will give a rather constant σ parameter for different fits. The expression $\frac{1}{2}(N-Z-2t_3)t_3$ is derived from the eigenvalues of the isospin-operator $\mathbf{t} \cdot \mathbf{T}$, which operates on the total wave function². U_C is the COULOMB-potential of $Z-1$ protons for which a FERMI distribution is assumed:

$$\begin{aligned}
\varrho(r) &= \varrho_0 \Theta_{a'}(r_0' A^{1/3} - r), \\
a' &= 0.55 \text{ fm}, \quad r_0' = 1.07 \text{ fm}^3. \quad (2)
\end{aligned}$$

For the numerical solution of the integro-differential equation (1) PEREY and SAXON⁴ have developed a very accurate local energy approximation (LEA), where one has to solve

$$A\chi - \left[U_N g + \frac{2m}{\hbar^2} (U_C - E) - \right. \quad (3)$$

$$\left. \frac{g'}{4(1+U_N g)^2} \left(g'(\nabla U_N)^2 - \Delta U_N (1+U_N g') \right) \right] \chi = 0$$

$$\text{with } \psi(\mathbf{r}) = \chi(\mathbf{r}) f(r), \quad f(r) = (1 + U_N g')^{-1/2},$$

$$g(\kappa^2) = (2m/\hbar^2) \exp[-(\beta\kappa/2)^2],$$

$$g' \equiv \partial g / \partial (\kappa^2), \quad \kappa^2 = (2m/\hbar) (E - U_C) - U_N g(\kappa^2).$$

In order to be consistent with the measurements of HOFSTADTER et al.³ we required the \bar{r}^2 calculated from the distribution $\Sigma |\psi_p|^2$ of protons to coincide with the \bar{r}^2 of the input charge distribution (2) within three percent. The parameters turned out to be very close to those used in earlier calculations⁵ of extreme single particle levels where the potential was taken from fits of elastic neutron scattering¹. A comparison of proton-nucleus scattering fits⁶ with the present potential (in the local energy approximation, neglecting surface terms) shows again the parameters to be in satisfactory agreement. Thus this unified potential for nucleons appears to be

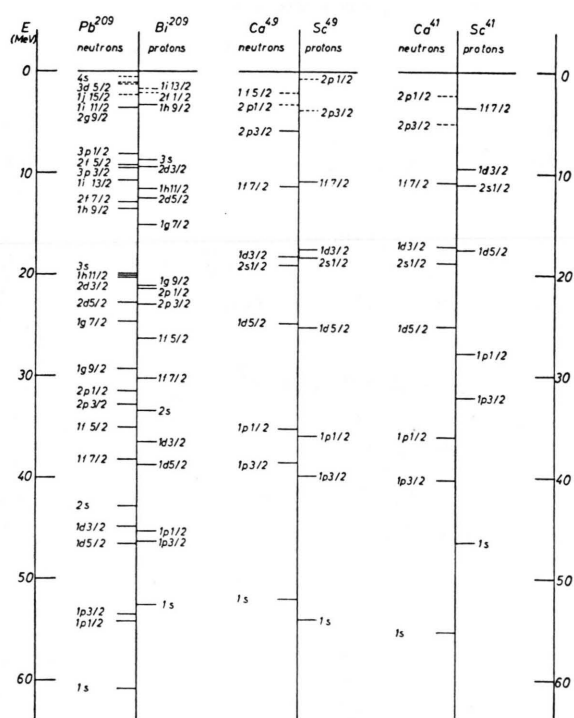


Fig. 1. Neutron and proton levels in double closed shell nuclei plus one nucleon. The extreme single particle levels are rather deep but this effect which originates from the nonlocality has already been observed experimentally in high energy (e,e'p)⁷ and (p,p) scattering and was estimated in another theoretical investigation⁸. For a comparison with levels near the FERMI energy, as observed in stripping and pick-up reactions, it appears necessary to take into account residual interactions and rearrangement effects⁹. The parameters for all calculations were: $\beta=0.9$ fm, $V=76$ MeV, $r_0=1.2$ fm, $a=0.65$ fm, $\sigma=0.47$, $\tau=2$.

² A. M. LANE, Nucl. Phys. **35**, 676 [1962].

³ e. g. M. CROISIAUX, R. HOFSTADTER, A. E. WALKER, M. R. YEARIAN, D. G. RAVENHALL, B. C. CLARK, and R. HERMAN, Phys. Rev. **137**, B 865 [1965].

⁴ F. G. PEREY and D. S. SAXON, to be published and e. g. W. E. FRAHN, Nucl. Phys. **66**, 358 [1965].

⁵ H. MELDNER and G. SÜSSMANN, Phys. Letters **6**, 353 [1963].

⁶ F. G. PEREY, Phys. Rev. **131**, 745 [1963].

Nucleus	N	State	Binding energy in MeV	
			experimental	calculated
Ca ³⁹	20-1	1 d 3/2	15.63	16.9
Ca ⁴¹	20+1	1 f 7/2	8.36	10.5
Ca ⁴⁷	28-1	1 f 7/2	10.07	11.1
Ca ⁴⁹	28+1	2 p 3/2	5.00	5.8
Ti ⁵¹			6.36	7.2
Cr ⁵³			7.94	8.6
Fe ⁵⁵			9.30	9.9
Kr ⁸⁵	50-1	1 g 9/2	9.76	11.4
Sr ⁸⁷			11.12	12.4
Mo ⁹¹			13.13	14.5
Sr ⁸⁹	50+1	2 d 5/2	6.77	6.1
Zr ⁹¹			7.21	6.9
Mo ⁹³			7.85	7.8
Ba ¹³⁹	82+1	2 f 7/2	4.72	4.3
Ce ¹⁴¹			5.53	4.8
Nd ¹⁴³			5.46	5.4
Sm ¹⁴⁵			6.82	6.0
Pb ²⁰⁷	126-1	3 p 1/2	7.38	8.0
Po ²⁰⁹			7.69	8.4
Rn ²¹¹			7.96	8.8
Pb ²⁰⁹	126+1	2 g 9/2	3.93	3.6
Po ²¹¹			4.55	4.0

Table 1. Ground states of some nuclei with a closed neutron shell plus or minus 1 neutron ¹⁰.

well compatible with scattering data. Further details about this investigation will be published elsewhere.

⁷ U. AMALDI, G. CAMPOS VENUTI, G. CORTELESSA, C. FRONTEROTTA, E. REALE, P. SALVADORI, and P. HILLMAN, Phys. Rev. Letters **8**, 171 [1964], and private communication by Dr. G. CORTELESSA on experiments with Ca⁴⁰.

⁸ D. M. BRINK and N. SHERMAN, Phys. Rev. Letters **14**, 393 [1965].

On the Relation between Experimentally Observed Single Particle Energies and Levels of the Extreme Single Particle Model

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Comparison of experimental levels with the distances between eigenvalues in realistic single particle potentials shows the latter to be usually somewhat larger. Especially in nonlocal potentials¹ the spacings are wider by a factor of about 1.5. As a

Nucleus	Z	State	Binding energy in MeV	
			experimental	calculated
K ³⁹	20-1	1 d 3/2	8.34	9.9
Sc ⁴¹	20+1	1 f 7/2	1.08	3.5
Sc ⁴³			4.93	5.5
Sc ⁴⁵			6.89	7.3
Sc ⁴⁷			8.49	9.1
Sc ⁴⁹			9.47	10.8
Cu ⁵⁹	28+1	2 p 3/2	3.42	3.2
Cu ⁶¹			4.81	4.5
Cu ⁶³			6.13	5.7
Cu ⁶⁵			7.45	6.9
Cu ⁶⁷			8.52	8.1
Sb ¹²¹	50+1	2 d 5/2	5.78	4.5
Tl ²⁰³	82-1	3 s 1/2	6.60	8.3
Tl ²⁰⁵			7.29	8.8
Tl ²⁰⁷			8.04	9.2
Tl ²⁰⁹			8.33	9.7
Bi ²⁰⁷	82+1	1 h 9/2	3.55	2.8
Bi ²⁰⁹			3.77	3.3
Bi ²¹¹			4.38	3.9

Table 2. Ground states of some nuclei with a closed proton shell plus or minus 1 proton ¹⁰.

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⁹ H. MELDNER and G. SÜSSMANN, Z. Naturforsch. **20 a**, 1219 [1965].

¹⁰ The experimental data on the binding energies are taken from L. A. KÖNIG, J. H. E. MATTAUCH, and A. H. WAPSTRA, Nucl. Phys. **31**, 18 [1962].

matter of fact, one was forced in the last few years by other experimental evidence^{2,3} to increase the potential depths while the radius constants were decreased from about 1.4 to 1.2 fm.

The purpose of this note is to sketch some possible reasons with which deviations of order 1 MeV

¹ H. MELDNER, G. SÜSSMANN, and W. ULRICH, Z. Naturforsch. **20 a**, 1217 [1965].

² F. PEREY and B. BUCK, Nucl. Phys. **32**, 353 [1962]. — U. AMALDI, G. CAMPOS VENUTI, G. CORTELESSA, C. FRONTEROTTA, A. REALE, P. SALVADORI, and P. HILLMAN, Phys. Rev. Letters **8**, 171 [1964]. — In addition see the results of various (p,2p) experiments.

³ For radius constants see the results of scattering experiments by HOFSTADTER et al.