Submitted to the International Conference on Nuclear Physics, Gatlinburg,
Tenn. (Sept. 1966).

MIT-2098 -255

CONF-660906-6

CPST VANCE

AUG 3 1966

H.C. \$ 1.00; MN .50

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GENERALIZED HARTREE-FOCK CALCULATION FOR Zr^{90} USING
AN EFFECTIVE INTERACTION*

Y. R. Waghmare, C. M. Shakin and J. P. Svenne
Department of Physics and Laboratory of Nuclear Science
Massachusetts Institute of Technology
Cambridge, Massachusetts

RELEASED FOR ANNOUNCEMENT
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*This work is supported in part through funds provided by the Atomic
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ABSTRACT

Hartree-fock calculations have been performed for Zr^{90} using an effective interaction derived from the Yale potential. Results are presented for the binding energy r.m.s. radius, and single-particle energies. Comparison is made with similar calculations using the non-local Tabakin potential.

Recently, an effective Hamiltonian method¹ has been developed which allows one to calculate the properties of finite nuclei starting from singular potentials which fit the nucleon-nucleon scattering data. Hartree-Fock calculations based on this method were carried out for ^{16}O and ^{40}Ca and the results were found to be in satisfactory agreement with experiment². In this paper similar calculations for ^{90}Zr are reported. Here we are interested in testing the theory for a heavier nucleus than has been considered previously.

The effective interaction suggested in reference (1) is,

$$H_{\text{eff}} = e^{-iS} H_{\text{He}} e^{iS}$$

$$= \sum_{\alpha\beta} t_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta}$$

$$+ \frac{1}{e} \sum_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} \langle \Psi_{\alpha\beta} | v_{\ell} - VP + v_t^{\text{OD}} + v_t^{\text{OD}} \frac{Q}{e} v_t^{\text{OD}} | \Psi_{\gamma\delta} \rangle a_{\delta} a_{\gamma}$$

where e^{iS} is a unitary operator which induces short-range correlations in the wave functions, $t_{\alpha\beta}$ is the kinetic-energy operator, v_{ℓ} is the "long-range" part of the nucleon-nucleon potential, VP is a pseudopotential introduced in certain states of relative motion, v_t^{OD} is that part of the tensor interaction off-diagonal in the relative orbital angular momentum, Q is a Pauli-Principle operator, and e is an appropriate energy denominator. The details of the construction of H_{eff} are discussed in references (1) and (2).

In order to use this interaction for nuclear structure calculations, we expand the orbitals in harmonic-oscillator functions as,

$$\psi_{\alpha} = \sum_n c_{\alpha n} \phi_n,$$

and self-consistency is achieved by appropriate choice of the expansion coefficients, $c_{\alpha n}$. For the Zr^{90} calculation the s, p and d states are expanded in three orbitals ($n = 0, 1, 2$) and the f and g states are expanded in two orbitals ($n = 0, 1$). The binding energy is calculated using the Yale potential³ as a function of the oscillator parameter, $b = \sqrt{\hbar/M\omega}$ and a minimum is obtained (Fig. 1). From the figure we see that in order to obtain a straight line for the binding energy vs b we would require a few more orbitals than the number used. Experience with calculations of this type indicates that an increase in the number of orbitals would not make a significant change in the binding energy.

In Table I, we present our results for $b = 2.09$ Fermis, appropriate for the minimum of the binding energy curve. In this table the results of Waghmare et al⁴ who have used the Tabakin⁵ potential are also given. We note that the results for the Tabakin potential do not include any second-order corrections.

The coulomb and center-of-mass correction terms to the binding energy are estimated using the following expressions:

$$E_{\text{coul}} = \frac{3}{5} \frac{Z(Z-1)e^2}{R}$$

$$E_{\text{CM}} = 3/2 \hbar \omega, \quad \hbar \omega = 41.6/b^2$$

In Table II the single-particle energies and the expansion coefficients for the occupied orbitals are presented.

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Table I

Comparison of calculated and experimental results for Zr^{90} .

	Waghmare et al ⁴⁾	Present calculations	Experimental
B.E./A (without C.M. and coulomb) in Mev.	-6.03	-11.70	-
B.E./A (including C.M. only) in Mev.	-6.18	-11.85	-
B.E./A (including C.M. and coulomb) in Mev.	-3.60	-9.27	-8.71
R.M.S. radius in fermis.	3.50	3.70	3.91
$\text{Op}_{1/2} - \text{Op}_{3/2}$ splitting in Mev	8.29	2.44	-
$\text{Od}_{3/2} - \text{Od}_{5/2}$ splitting in Mev.	11.58	3.78	-
$\text{Of}_{5/2} - \text{Of}_{7/2}$ splitting in Mev.	14.28	5.17	-
$\text{lp}_{1/2} - \text{lp}_{3/2}$ splitting in Mev.	5.85	7.83	-

TABLE II

Single particle energies (E in Mev) and expansion coefficients (C_n) obtained for Zr^{90} using the Yale potential.

State	Energy	Expansion Coefficients		
nlj	E(Mev)	C_0	C_1	C_2
Os _{1/2}	-114.28	0.992337	0.122109	0.189122
Op _{3/2}	-88.00	-0.978065	-0.208255	0.004383
Op _{1/2}	-85.56	-0.978710	-0.205082	0.008264
Od _{5/2}	-61.78	0.959075	0.282053	0.024918
ls _{1/2}	-56.14	0.108840	-0.936248	-0.334056
Od _{3/2}	-58.00	0.958288	0.284443	0.027880
Of _{7/2}	-35.91	0.950266	0.311438	- -
lp _{3/2}	-28.59	-0.191128	0.905596	0.378637
Of _{5/2}	-30.74	0.943727	0.330727	- -
lp _{1/2}	-25.66	-0.187758	0.910849	0.367560
Og _{9/2}	-12.52	0.950371	0.311119	- -

FIG. 1