J. Chem. Phys. 42, 309 (1965).

[11]Assuming a diffusion-controlled process one may write $\kappa = (\frac{1}{3})v z \sigma$. $\sigma \approx 2.5 \times 10^{-15}$ cm^2 is the geometric cross section of an anthracene molecule. The factor $\frac{1}{3}$ is needed because only encounters where the total spin is $\frac{1}{2}$ (atomic units) can lead to triplet destruction. z, which we may assume to be 8, is the number of configurations of two neighboring molecules (one occupied by a triplet exciton, the other by an electron) which allow reaction. Insertion yields a thermal electron velocity $v \approx 1 \times 10^6$ cm sec^{-1}. This agrees well with the theoretical value.[9]

[12]W. Helfrich and F. R. Lipsett, J. Chem. Phys. 43, 4368 (1965).

FOUNDATIONS FOR HARTREE-FOCK CALCULATIONS WITH SINGULAR POTENTIALS*

Carl Shakin and Yeshwant R. Waghmare

Department of Physics and Laboratory for Nuclear Science,
Massachusetts Institute of Technology, Cambridge, Massachusetts

(Received 10 February 1966)

It has been clear for some time that the application of the Hartree-Fock method to the problems of nuclear structure would provide a natural foundation for the discussion of most nuclear properties. The fact that two-body forces which fit the scattering data are strongly repulsive at short distances has made a direct application of the Hartree-Fock method impossible and thus various groups have tried to construct velocity-dependent or nonlocal potentials for which the Hartree-Fock method may be applied. These potentials have only had a qualitative success when applied to nuclear structure problems. Also, calculations using reaction matrices taken from infinite nuclear matter calculations have had rather limited success and are also computationally difficult.

Recently, investigations of the effective interaction in finite nuclei using realistic forces have been performed using a unitary model-operator approach.[1] Using this approach we, in this paper, try to provide a theoretical foundation for the application of effective interaction in the nuclear Hartree-Fock calculations. Two important advantages of this method over a reaction-matrix approach are (1) the fundamentally Hermitian character of the effective Hamiltonian generated and (2) the absence of rearrangement terms in the calculational procedure.

It has been shown previously[1] that the application of a unitary operator, e^{iS}, to a set of uncorrelated basis states leads to an effective Hamiltonian of the form

$$\tilde{H} = e^{-iS} H e^{iS} = \sum t_{\alpha\beta} a_\alpha^\dagger a_\beta + \tfrac{1}{2} \sum a_\alpha^\dagger a_\beta (\alpha\beta | e^{-iS} (t_1 + t_2 + v_{12}) e^{iS} - (t_1 + t_2) | \gamma\delta) a_\delta a_\gamma + \cdots . \quad (1)$$

The highest order terms in the cluster expansion implied in Eq. (1) can be shown to be quite small if the correlations induced by e^{iS} are of sufficiently short range. Indeed, the requirement of convergence of the cluster expansion leads directly to the introduction of a generalized separation method[2] approach for defining the short-range correlation structure.

It is useful at this point to add the following expression[1] to the matrix element in Eq. (1):

$$(\alpha\beta | e^{-iS} (U_1 + U_2) e^{iS} - (U_1 + U_2) | \gamma\delta). \quad (2)$$

It is easily seen that for the short-range correlations we define below, the added term makes a negligibly small contribution to the energy. We require the single-particle potentials U_1 and U_2 to have the harmonic-oscillator form: $U_1 = \frac{1}{2} k r_1^2$, $U_2 = \frac{1}{2} k r_2^2$.

We introduce the solutions of the following problem:

$$(t_1 + t_2 + U_1 + U_2 + v_{12}^S) \Psi_{n_1 n_2}(\vec{r}_1, \vec{r}_2) = (\epsilon_{n_1} + \epsilon_{n_2}) \Psi_{n_1 n_2}(\vec{r}_1, \vec{r}_2),$$

$$(t_1 + t_2 + U_1 + U_2) \Phi_{n_1 n_2}(\vec{r}_1, \vec{r}_2) = (\epsilon_{n_1} + \epsilon_{n_2}) \Phi_{n_1 n_2}(\vec{r}_1, \vec{r}_2), \quad (3)$$

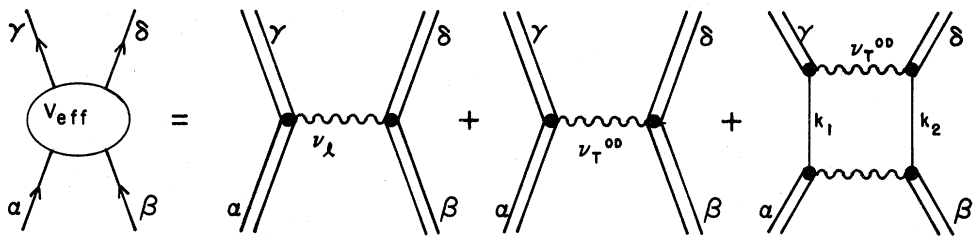

FIG. 1. Diagrammatic representation of the effective interaction.

where the subscripts n_1 and n_2 refer to the quantities $\{n,l,j,m\}$ necessary to specify the orbitals for particle motion in a harmonic-oscillator potential. Here v_{12}^S is the short-range part of v_{12}, defined so as to give no energy shift in $\Psi_{n_1n_2}$ relative to $\varphi_{n_1n_2}$.

Now we define the operator e^{iS} in the space of two-body wave functions by the equation

$$e^{iS}\Phi_{n_in_j}=\Psi_{n_in_j} \tag{4}$$

for all n_i and n_j.

We note that this definition is independent of any self-consistency problem.

If we expand the orbitals in (1) in a harmonic-oscillator basis, i.e.,

$$\varphi_\alpha(r)=\sum_{n_i}C_{\alpha n_i}\varphi_{n_i}(r), \tag{5}$$

we may rewrite (1) as

$$\tilde{H}=\sum_{\alpha\beta}t_{n_1n_2}a_\alpha^\dagger a_\beta C_{\alpha n_1}C_{\beta n_2}+\sum_{\alpha\beta\gamma\delta}a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma C_{\alpha n_1}C_{\beta n_2}C_{\gamma n_3}C_{\delta n_4}\times(\Psi_{n_1n_2}|v_{12}^{\,l}|\Psi_{n_3n_4}), \tag{6}$$

or

$$\tilde{H}=\sum t_{n_1n_2}a_{n_1}^\dagger a_{n_2}+\tfrac{1}{2}\sum a_{n_1}^\dagger a_{n_2}^\dagger a_{n_3}a_{n_4}(\Psi_{n_1n_2}|v_{12}^{\,l}|\Psi_{n_4n_3}),$$

where all quantities now refer to the harmonic-oscillator basis. In Eqs. (3) we neglect the coupling between states of different l that arises due to the tensor force, i.e., e^{iS} induces only central correlations. Thus Eq. (6) should be written more generally as

$$\tilde{H}=\sum t_{n_1n_2}a_{n_1}^\dagger a_{n_2}+\tfrac{1}{2}\sum a_{n_1}^\dagger a_{n_2}^\dagger a_{n_3}a_{n_4}\times(\varphi_{n_1n_2}|v_{12}^{\,l}+v_T^{\,\mathrm{OD}}|\Psi_{n_4n_3}), \tag{7}$$

where v_T^{OD} refers to that part of the complete tensor force nondiagonal in the orbital angular momentum. The Hamiltonian defined in Eq. (7) can now be readily used for the Hartree-Fock calculations. However, it must be remembered that there are large second-order contributions from the tensor force.

We, therefore, suggest that this effect can be taken into account by slightly modifying the Hamiltonian (7) as

$$\tilde{H}=\sum t_{n_1n_2}a_{n_1}^\dagger a_{n_2}+\tfrac{1}{2}\sum a_{n_1}^\dagger a_{n_2}^\dagger a_{n_3}a_{n_4}(\Psi_{n_1n_2}|[v_{12}^{\,l}+v_T^{\,\mathrm{OD}}+v_T^{\,\mathrm{OD}}(Q/e)v_T^{\,\mathrm{OD}}]|\Psi_{n_4n_3}), \tag{8}$$

where Q is the Pauli-principle operator that projects out of the space in which we will expand our orbitals. Diagramatically, the effective interaction appears as in Fig. 1. In this figure a double line is an indication that we are using correlated (central correlations only) basis functions in the evaluation of the matrix elements. In general, the calculations for the second-order terms in v_T^{OD} are difficult and one could use the prescription of Kuo and Brown[3] in the treatment of the intermediate states.

Hartree-Fock calculations using Eq. (8) are under way. However, the results we obtained with each orbital approximated by a single harmonic-oscillator function are reported below.

In Table I we present the results of our preliminary calculation. We have used an oscillator size parameter $b=1.76$ $[b=(\hbar/M\omega)^{1/2}]$. The second-order terms have been calculated only for the $^3S_1$ state where they are known to make a large contribution.

The matrix elements are given for the various states of relative motion which contribute after one makes the Moshinsky transformation. The weight factors necessary for the calculation of the potential energy are taken from MacKellar's thesis.[4] We obtain a binding energy of

Table I. Potential energy of O^{16} for Yale potential.

State	nl	NL	Matrix element First order (MeV)	Second order (MeV)	Weight factor	Contribution to the potential energy (MeV)
$^3S_1$	00	00	−2.02	−6.98	3	−27.0
$^3S_1$	00	01	−2.02	−6.74	9	−78.8
$^3S_1$	00	02	−2.02	−6.53	15/2	−64.1
$^3S_1$	00	10	−2.02	−6.57	$\frac{3}{2}$	−12.9
$^3S_1$	10	00	−0.66	−6.97	$\frac{3}{2}$	−11.4
$^1S_0$	00	00	−8.03	···	3	−24.1
$^1S_0$	00	01	−8.03	···	9	−72.3
$^1S_0$	00	02	−8.03	···	15/2	−60.2
$^1S_0$	00	10	−8.03	···	$\frac{3}{2}$	−12.0
$^1S_0$	10	00	−7.24	···	$\frac{3}{2}$	−10.8
$^1P_1$	01	00	4.86	···	6	+24.2
$^3P_0$	01	00	−1.63	···	6	−9.8
$^3P_1$	01	00	2.70	···	18	48.6
$^3P_2$	01	00	−0.84	···	30	−25.2
$^1D_2$	02	00	−0.50	···	15/2	−3.8
$^3D_1$	02	00	1.08	···	$\frac{3}{2}$	1.6
$^3D_2$	02	00	−2.01	···	$\frac{5}{2}$	−5.0
$^3D_3$	02	00	0.07	···	$\frac{7}{2}$	0.2
					Total =	−337.8

about 6.5 MeV per particle after correcting for the Coulomb energy and the center-of-mass motion. Results of Hartree-Fock calculations using the harmonic-oscillator basis will be reported shortly as well as further calculational details. We want to emphasize at this stage that in the framework of our theory we have already obtained reasonable values for the binding energy, spin-orbit splittings, and the p-shell effective interaction.

We are grateful to Professor F. Villars for stimulating discussions and comments during this work and to M. Tomaselli for preliminary calculations of the second-order terms.

*This work is supported in part through funds provided by the Atomic Energy Commission under Contract No. AT(30-1)-2098.

[1]F. Villars, in Proceedings of the Enrico Fermi International School of Physics, Course XXIII, 1961 (Academic Press, Inc., New York, 1963); J. Da Providencia and C. M. Shakin, Ann. Phys. (N.Y.) 30, 95 (1964).

[2]S. A. Moszkowski and B. L. Scott, Ann. Phys. (N.Y.) 11, 65 (1960); M. H. Hull, Jr., and C. M. Shakin, Phys. Letters 19, 506 (1965).

[3]T. T. S. Kuo and G. E. Brown, Phys. Letters 18, 54 (1965).

[4]A. D. MacKellar, thesis, Texas A. & M. University, January 1966 (unpublished).

COSMIC BACKGROUND RADIATION AT 3.2 cm—SUPPORT FOR COSMIC BLACK-BODY RADIATION*

P. G. Roll† and David T. Wilkinson

Palmer Physical Laboratory, Princeton University, Princeton, New Jersey

(Received 27 January 1966)

Dicke et al.[1] have suggested that the universe may be filled with black-body radiation which originated at a time when the matter and radiation were in a hot, highly contracted, state—the primordial fireball. As the universe expanded, the cosmological red shift would have cooled the cosmic black-body radiation to the extent that one should now look for it in the microwave band. Concurrent with this suggestion, Penzias and Wilson[2] reported the discovery of an excess background radiation at a wavelength of 7.35 cm. The measurement of the spectrum of this new microwave background provides a severe test of the cosmic black-body-radiation hypothesis. This Letter reports a measurement of the microwave background at a wavelength of 3.2 cm; the flux found is that which would be emitted by a black body at 3.0 ± 0.5°K. A more complete description of the experiment will appear elsewhere.

Figure 1 shows a schematic diagram of the instrument. It is a Dicke-type radiometer[3] in which the receiver input is periodically switched between a horn antenna and a reference source (cold load). The output of the receiver at the switching frequency is synchronously detected and recorded. The record is a measure of the difference between the temperature of the reference source and the apparent temperature of the radiation collected by the antenna. The horn antenna is shielded to exclude radiation from the ground and has a main lobe half-angle (10 dB down) of 10°. The cold-load termination is immersed in liquid helium to es-