Residual Potential and Nucleon Correlation in the Shell Model. I. E2 Transition in ⁶Li

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The effect of a class of residual potentials in the Hamiltonian and nucleon-nucleon correlation on calculations in the independent-particle shell-model wave function of ⁶Li has been investigated. A method has been developed to give minimum energies of various states of a nuclear system with a somewhat realistic Hamiltonian and wave function. The results on energy calculations are in good agreement with the observed data. The E2 transition rate and other relevant observables pertaining to this transition using this wave function and several others have been calculated. Comparison of the results of these calculations with experimental data and other theoretical predictions shows a definite preference for the correlated wave function of ⁶Li developed here. The method is convenient for application to other nuclear systems.

1. INTRODUCTION

The usual independent-particle shell model (IPSM) has been used in explaining nuclear properties more than any other model. This may be partly due to its simplicity, but the main quality of this model is its wide range of success. Nevertheless, the failure of IPSM in the case of ⁶Li has been well known for some time. Many calculations pertaining to the ground state of ⁶Li have been found to give unsatisfactory results. The model is even worse for the excited states. Other models have been tried, but the situation was not improved as a whole.¹⁻⁹ Several attempts at modifying the IPSM wave function of ⁶Li and other finite-nucleus-model approaches have also been made with very little success.¹⁰⁻¹⁷ In this paper a simple nonperturbative method is developed which promises to predict some interesting results in a quick way. It is not, certainly, being claimed that this procedure would be able to compete with other highly developed finite-nuclei theories like Brueckner's. As an application of this approach we shall calculate the quadrupole transition of ⁶Li which involves its first excited state and the ground state. Since the decay of atomic nuclei is determined by the spatial overlap of the initial and final wave functions, fine details of the nuclear wave functions become apparent. In particular, the study of such transitions demonstrates more effectively the usefulness of nuclear models. In this transition, it is the p proton of the nucleus which contributes nonzero terms to the matrix element of the quadrupole operator. The IPSM wave function of the p proton in ⁶Li, as derived from the harmonic oscillator, does not describe the electromagnetic behavior of ⁶Li successfully. Some modifications are, therefore, proposed here.

It may also be timely to remark that electromagnetic properties of a nucleon inside a nucleus may be seriously affected by the presence of other nucleons in its vicinity.¹⁸ It is quite appropriate that the p nucleons should be treated rather more explicitly, since only these nucleons are involved in this transition. It seems quite plausible to modify the independent behavior of p nucleons by some nucleon-nucleon correlation function. Such correlations appearing in a wave function are the Pauli correlations and the dynamical correlations. The former are due to the particle statistics and can be incorporated by properly antisymmetrizing the nuclear wave function. The latter correlations arise from the behavior of the nucleon-nucleon interaction. The use of such correlation in the IPSM wave function has been found somewhat helpful in explaining some of the anomalous features^{16, 17} of ⁶Li and of some other nuclei¹⁹⁻²⁵ which could not be explained otherwise. The variational approach developed by Brink and Grypeos²⁴ for finite-nuclei calculations is similar to what was described a few years ago by Da Providencia and Shakin²⁵ following the effective-Hamiltonian formalism by the use of a unitary operator suggested by Villars.²⁶

In case of ⁶Li the basic assumption of the IPSM - that the two-body nucleon-nucleon forces can be completely represented by an average central potential - is unlikely to be valid. We expect to have a substantial residual two-body interaction in it^{13,14} which may be simulated to cause some dynamical correlation among the particles moving independently. It should, therefore, be necessary in general to add some form of the two-body nucleonnucleon interaction as a residual potential in the IPSM Hamiltonian. It is desirable to evaluate by the variational principle the extra parameters introduced in the wave functions through the corre-

lation terms. The variational principle can be applied to all those states which are orthogonal to each other. The other parameters involved in the residual potential may be adjusted to give the minimum energy for each desired level and to give the correct spacings between them. This method may be regarded as somewhere between the simplest uncorrelated single-particle model and the threebody model of Wackman and Austern.³ The treatment of the core is rather different from that of Wackman and Austern but the treatment of the two valence nucleons is similar. However, this method gives energy spacings in good agreement with the observed values; whereas the above-mentioned three-body model displaces all the energy levels upwards in energy on an absolute scale by about 3-5 MeV, and, contrary to experiments, the isospin-triplet level J = 0 lies below the J = 3 level.

2. CORRELATED WAVE FUNCTION OF ⁶Li

The Hamiltonian of the nuclear wave function is given by¹⁹

$$H = H_0 + \sum_{i < j}^{A} V_{ij} , \qquad (1)$$

where H_0 is the harmonic-oscillator Hamiltonian and V_{ij} is the residual nucleon-nucleon interaction within the nucleus. Although the summation in (1)is taken over all pairs of nucleons, in this scheme we shall study the effect of V_{ij} explicitly only on the two valence nucleons of ⁶Li. It will be seen in Sec. 5 that the residual potential V_{ii} affects the nuclear wave function implicitly through the correlation coefficient. This coefficient depends on the parameters involved in the potential. One may take a realistic nucleon-nucleon interaction and derive the effective central and the residual potentials and proceed with the scheme outlined here. The purpose of this paper is to develop a simple method for studying the nuclear system with a doubly closed shell plus two particles (holes) and not to study the salient features of the so-called realistic two-body nucleon-nucleon potential. The realistic nucleon-nucleon interaction appearing in the literature in several forms is quite complicated. Its finer and detailed features are not of gross importance in this formalism. We therefore choose a simple form of the two-body interaction of the phenomenological type^{13, 14}:

$$V_{12} = \left(\frac{3}{4}V_t + \frac{1}{4}V_s\right) + \left(\frac{1}{4}V_t - \frac{1}{4}V_s\right)\vec{\sigma}_1 \cdot \vec{\sigma}_2$$
(2)
with¹⁹

$$V_{t,s} = -V_{0t,0s} [a - b(r/r_{0t,0s})^{2\nu}] e^{-r^2/r_{0t,0s}^2}, \quad (3)$$

where $r = r_{ij} = |\vec{\mathbf{r}}_i - \vec{\mathbf{r}}_j|$ and V_{0i} or V_{0s} are adjustable parameters not exceeding the free values for given a, b, ν , and r_0 . The usual IPSM wave function of a closed-shell nucleus is the Slater determinant of single-particle functions determined by a central-field model. Here in the Hamiltonian (1), apart from a central field we have a twobody interaction V_{ij} which makes the admixture of higher configurations important in the shell model.^{13, 14, 27-29} It is always questionable where to stop adding higher configurations. To get out of this dilemma on the one hand and to incorporate the effect due to the residual potential in the wave function on the other, we propose here a correlation function which is simulated to replace the admixture of an infinite number of higher configurations. In the harmonic-oscillator well, the radial wave functions of particles in various states differ only in their polynomial parts depending on the quantum numbers n and l. Their corresponding exponential parts are mathematically identical. In particular, in a two-particle system the radial wave function of the admixture for a given system would look like

$$R(r_1, r_2) [1 + \sum_{h} G_h(r_1, r_2)], \qquad (4)$$

where R is the radial wave function in the lowest configuration, and G_h is the polynomial of the order k, say, arising from the admixture of higher configurations. The polynomial G_h in (4) is replaced by a suitable dynamical correlation function whose argument is the relative distance between r_1 and r_2 . Let such a function be $(1 \pm Cr_{12}/r_0)$ in which the correlation coefficient C is state dependent and is evaluated by the variational principle. The range parameter r_0 is introduced to make C dimensionless. The term Cr_{12}/r_0 can be expanded in the Legendre polynomials as

$$\frac{Cr_{12}}{r_0} = \frac{C}{r_0} \sum_{k=0}^{\infty} U_k(r_<, r_>) P_k(\cos\omega_{12}), \qquad (5)$$

where $r_{<}(r_{>})$ is the smaller (greater) of r_1 and r_2 , and ω_{12} is the angle between $\mathbf{\bar{r}}_1$ and $\mathbf{\bar{r}}_2$. The expansion of U_k is given explicitly by

$$U_{k}(r_{1}, r_{2}) = \frac{r_{1}^{k+2}}{(2k+3)r_{2}^{k+2}} - \frac{r_{1}^{k}}{(1-2k)r_{2}^{k-1}}.$$
 (6)

Accordingly, here U_k is a polynomial function of r_1 and r_2 . Although it is not identical to G_h it is similar enough in character to replace it by Cr/r_0 in (4) in order to account in some way for the effect on the IPSM wave function due to the residual interaction. The correlation wave function can be written as

$$\Psi = (1/N)\psi^0 (1 \pm Cr_{12}/r_0) |0\rangle, \qquad (7)$$

where ψ^0 is the coupled wave function of the two extracore particles, and $|0\rangle$ stands for the four 1s particles representing the core. We shall drop the minus sign from the correlation function and develop our discussion on the basis of the plus sign. The effects of different signs of C will be discussed in Sec. 8. Since the inclusion of the correlation function f_{12} destroys the normalization of ψ^0 , as obtained from the normalized single-particle harmonic-oscillator (SPHO) wave functions, it is necessary to renormalize the correlated wave function. The quantity N in (7) is defined such that the total wave function Ψ is normalized to unity. It may also be pointed out that the modified wave function (7) when multiplied by the appropriate spin and isospin functions still maintains its antisymmetric properties and is an eigenfunction of L^2 , L_z , S^2 , and S_z .¹⁹ Thus the wave function (7) being antisymmetrized includes the Pauli correlation in addition to the dynamical correlation.

3. RENORMALIZATION

The expectation value of a unit operator with normalized wave function (7) is readily given by

$$\langle \Psi | \Psi \rangle = 1$$
$$= \frac{1}{N^2} \left\langle \psi^0 \right| 1 + 2 \frac{Cr}{r_0} + \frac{C^2 r^2}{r_0^2} \left| \psi^0 \right\rangle, \qquad (8)$$

where r is the same as r_{12} . The renormalization can be written in operator form as

$$\tilde{N} = 1 + 2C(r/r_0) + C^2(r^2/r_0^2), \qquad (9)$$

whose expectation value is the renormalization constant N^2 given by (8). Since the expectation values of the last two terms in the operator (9) depend on the state of the wave function used and since *C* is also state dependent, we shall designate the renormalization constant *N* as

$$N_L^2 = 1 + 2C_L \langle r/r_0 \rangle_L + C_L^2 \langle r^2/r_0^2 \rangle_L , \qquad (10)$$

where L denotes the state of the wave function used to evaluate the matrix elements of the operators r/r_0 and r^2/r_0^2 . The matrix elements in (10), and in the rest of this paper, are evaluated with the wave function $\psi(0)$. The matrix elements are obtained after laborious integrations as

$$N_i^2 = \left[1 + \frac{26\sqrt{2}}{5\sqrt{\pi}} \frac{C_i}{\lambda} + 5\frac{C_i^2}{\lambda^2}\right] \langle 210M_J \mid 3M_J \rangle^2 \qquad (11)$$

and

$$N_f^2 = 1 + \frac{5\sqrt{2}}{\sqrt{\pi}} \frac{C_f}{\lambda} + 5 \frac{C_f^2}{\lambda^2},$$
 (12)

where $\lambda = \alpha r_0$, and α is the harmonic-oscillator length parameter. The suffixes *i* and *f* refer to the relevant values of *L* in the initial and final states, respectively.

4. EFFECTIVE HAMILTONIAN

In order to facilitate the discussion of this work, we shall transpose the correlation function $f(r_{12})$ from the wave function to the Hamiltonian. The energy of a two-particle system in an arbitrary state given by wave function (7) can be readily obtained by the Hamiltonian (1) as

$$W = \langle \tilde{H} \rangle / N^2 , \qquad (13)$$

where

$$H = (1 + Cr/r_0)H(1 + Cr/r_0)$$

= $H + (C/r_0)(rH + Hr) + (C^2/r_0^2)(rHr)$, (14)

called the "effective Hamiltonian." The Hamiltonian (1) for a two-particle system can be written as

$$H = H_{01} + H_{02} + V_{12} , (15)$$

where H_{oi} is the Hamiltonian for the *i*th particle in a central field U_i and where V_{12} is the residual interaction. This U_i should not be confused with $U_k(r_1, r_2)$ introduced in (4). The zeroth-order calculation consists of a product of individual particle wave functions $\phi_{nlm}(\mathbf{\tilde{r}}_i)$ which are the eigenfunction of H_{0i} ; i.e.,

$$H_{0i} | \phi_{nlm}(\mathbf{\tilde{r}}_i) = \epsilon_{nlm}^0 | \phi_{nlm}(\mathbf{\tilde{r}}_i) , \qquad (16)$$

where

$$\phi_{nlm}(\vec{\mathbf{r}}_i) = R_{nl}(\mathbf{r}_i) Y_l^m(\theta_i \phi_i) \tag{17}$$

and ϵ_{nlm}^0 is the eigenvalue of the *i*th particle in the state nlm. The radial wave function $R_{nl}(r_i)$ is of the harmonic-oscillator type.

Since we shall be concerned primarily with a system of two equivalent particles, it follows readily from the Appendix A that

$$\langle \boldsymbol{r}_{12}\boldsymbol{H} + \boldsymbol{H}\boldsymbol{r}_{12} \rangle = 4\epsilon \langle \boldsymbol{r}_{12} \rangle + 2 \langle \boldsymbol{r}_{12} \boldsymbol{V}_{12} \rangle , \qquad (18)$$

where ϵ is the same as ϵ_{nim}° . The suffixes will be dropped from now on. Also from (A22)

$$\langle r_{12}Hr_{12} \rangle = 2\epsilon \langle r_{12}^{2} \rangle + \hbar^{2}/m + \langle r_{12}^{2}V_{12} \rangle.$$
 (19)

These matrix elements are taken with the SPHO wave functions defined by (16) and (17). By means of (14), (18), and (19), the matrix element $\langle \tilde{H} \rangle$ can be written as

$$\langle \tilde{H} \rangle = 2\epsilon N^2 + \langle V_{12} \rangle + \frac{2C}{r_0} \langle r_{12} V_{12} \rangle + \frac{C^2}{r_0^2} \left(\frac{\hbar^2}{m} + \langle r_{12}^2 V_{12} \rangle \right).$$
(20)

5. ENERGIES

We shall evaluate the energies of the ground and the first excited states of ⁶Li using the correlated wave function (7) and the total Hamiltonian (1). In the *L*-S coupling scheme, which is quite appropriate for ${}^{6}Li$, ${}^{13, 14}$ the two states of this nucleus are specified as follows³⁰:

ground state, Ψ_f :

$$J^{\pi} = 1^{+}, \quad T = 0, \quad L = 0, \quad S = 1;$$
 (21)

first excited state, Ψ_i :

$$J^{\pi} = 3^+, \quad T = 0, \quad L = 2, \quad S = 1.$$
 (22)

The total energy in the state L can be written symbolically as

$$W_{L} = \langle \tilde{H}_{L} \rangle / \langle \tilde{N}_{L} \rangle , \qquad (23)$$

where L corresponds to either the wave function (21) or (22). Substituting the expressions given by (8) and (20) in (23) and dropping the suffixes of V_{12} and r_{12} for brevity, we obtain

$$W_{L}(C) = \epsilon_{s} + 2\epsilon + \left(1 + 2\frac{C_{L}}{r_{0}}\langle r \rangle_{L} + \frac{C_{L}^{2}}{r_{0}^{2}}\langle r^{2} \rangle_{L}\right)^{-2} \times \left[\langle V \rangle_{L} + 2\frac{C_{L}}{r_{0}}\langle r V \rangle_{L} + \frac{C_{L}^{2}}{r_{0}^{2}}\left(\frac{\hbar^{2}}{m} + \langle r^{2} V \rangle_{L}\right)\right],$$
(24)

where ϵ_s is the energy belonging to the core consisting of four 1s particles. The total energy in (24) essentially consists of two parts, namely, the degenerate energy ($\epsilon_s + 2\epsilon$), which is the same for

$$(24) \qquad (22) for all a gradients and the second se$$

ing on L and S. We shall write (24) for computational purposes as

all L and S, and the perturbation energy depend-

$$W_L(C) = \epsilon_s + 2\epsilon + W_{L_{s, Lt}}, \qquad (25)$$

where

$$W_{Ls,Lt} = \left[\frac{a_1^{(L)} + a_2^{(L)}C_L + a_3^{(L)}C_L^2}{1 + a_4^{(L)}C_L + a_5^{(L)}C_L^2} \right]_{s,t},$$
(26)

and

$$\alpha_1^{(L)} = \langle V \rangle, \tag{27a}$$

$$q_2^{(L)} = 2\langle (r/r_0) V \rangle , \qquad (27b)$$

$$a_{3}^{(L)} = \hbar^{2} / m r_{0}^{2} + \langle (r^{2} / r_{0}^{2}) V \rangle, \qquad (27c)$$

$$a_4^{(L)} = 2\langle r/r_0 \rangle , \qquad (27d)$$

$$a_5^{(L)} = \langle r^2 / r_0^2 \rangle$$
. (27e)

The subscripts s and t in $W_{Ls, Lt}$ denote the singlet and triplet states, respectively. The energy in each of the two states can be obtained by using the appropriate uncorrelated wave functions (21) and (22) for a given L as the basis. With the condition

$$\partial W_L / \partial C_L = 0 , \qquad (28)$$

the value of C is determined in terms of the a's defined by (27). From the condition (28), it readily follows that

$$C_{L\pm} = \frac{-(a_3 - a_1a_5) \pm \left[(a_3 - a_1a_5)^2 - (a_3a_4 - a_2a_5)(a_2 - a_1a_4)\right]^{1/2}}{a_3a_4 - a_2a_5}.$$
(29)

Of the two values of $C_{L\pm}$, that value is selected which gives the corresponding energy minimum. It may be observed that C is specified entirely by matrix elements (27) which in turn, when evaluated, are functions of the parameters involved in the residual potential (3) and in the wave function (17). We therefore select only those sets of parameters which give the correct level spacings and reproduce other experimental data. Since we are concerned with the triplet state in both ground and excited states, we shall drop the subscript Ls from (26) and designate the coefficients C as C_{0t} and C_{2t} , in the state L=0 and L=2, respectively. The spin dependence of the matrix elements a and coefficients C is determined by potential (2) which is spin dependent.

6. QUADRUPOLE TRANSITION

Electromagnetic moments are good means of measuring the nuclear deformation. In general, because of the experimental difficulties, measured quadrupole moments are not of high accuracy, but nonetheless they do give valuable evidence as to the magnitude of nuclear charge deformation. Un-

fortunately, the quadrupole moment of ⁶Li vanishes in pure LS coupling, although this is the coupling scheme which leads to the best description of ⁶Li on the basis of theoretical predictions and experimental measurements. A small admixture of other states such as ${}^{3}P_{1}$, ${}^{1}P_{1}$, and ${}^{3}D_{1}$ to the predominantly ${}^{3}S_{1}$ state (which gives the quadrupole moment zero) yields a nonvanishing value of the quadrupole moment. However, this approach is rather unrealistic, since no simultaneous fit of any other data is possible.³¹ On the other hand, the quadrupole moment predicted by *jj* coupling is definitely too large and gives the wrong sign. It is desirable to evaluate the electric quadrupole (E2)transition rate which measures the off-diagonal matrix elements of the same operator whose diagonal element is the ground-state quadrupole moment. The quadrupole transition matrix elements can be determined for a system even with spin zero (or $\frac{1}{2}$), whereas their corresponding quadrupole moments vanish. Therefore, in particular, the deformation of ⁶He, which is the isobaric analog of ⁶Li, can be determined. Also, in general, the available data on the quadrupole transition rate

are more extensive and their accuracy of measurement is relatively greater. The electromagnetic transitions in ⁶Li have been examined with wave functions having a harmonic-oscillator radial dependence.³² The authors showed qualitatively that the *M*1 transition from the J=0 state to the ground state was overwhelming in comparison with the E2transition from the J=3 state to the ground state. This was in qualitative agreement with experiment.³³ However, their further calculations³² proved much less satisfactory with that potential. It seems proper to study the situation for various types of nucleon-nucleon interaction in the case of ⁶Li. Such a study was also suggested independently on the basis of the calculations on some p- and d-shell nuclei.³⁴ In the present work we have a class of potentials which have a Gaussian radial dependence with a variety of polynomials of the relative coordinate giving a simple Gaussian or Gaussian tail with a soft or hard core. Of course, this potential is introduced to yield the second-order effects. The central potential is of the isotropic harmonic-oscillator type.

A. IPSM and Nucleon-Nucleon Correlation

The transition probability from an excited state *i* to the ground state *f* in a nucleus with emission of a quantum of quadrupole radiation, $E_{\gamma} = \kappa \hbar c$, is given by³⁵

$$T(E2) = \frac{1}{2I_i + 1} \sum_{M} \frac{4\pi}{75} \frac{\kappa^5}{\hbar} \langle Q_2^M \rangle^2 , \qquad (30)$$

where

$$\langle Q_2^M \rangle = \frac{1}{2} e \sum_{i=1}^{Z} \int [1 + \tau_3(i)] \gamma_i^2 Y_2^{M*}(\Omega_i) \rho_{ij}^{MM'} dV, \quad (31)$$

and where e is the charge on the *i*th proton, I_i is the total spin in the state *i*, and the summation is taken over all protons involved. $\rho_{if}^{MM'}$ is the transition density, which is the matrix element taken between the initial state of the nucleus JM and the final state J'M'. Using the correlated wave functions given by (7), we have $\rho_{if}^{MM'}$ for ⁶Li

$$\rho_{if}^{MM'}(\mathbf{\tilde{r}}_{i}) = \int \Psi_{L=0}^{M'*}(\mathbf{\tilde{r}}_{1}, \dots, \mathbf{\tilde{r}}_{A}) \Psi_{L=2}^{M}(\mathbf{\tilde{r}}_{1}, \dots, \mathbf{\tilde{r}}_{A})$$
$$\times d\mathbf{\tilde{r}}_{1} \cdots d\mathbf{\tilde{r}}_{i-1} d\mathbf{\tilde{r}}_{1+1} \cdots d\mathbf{\tilde{r}}_{A}.$$
(32)

Because of the spherical harmonic of second order in (31), only the p proton contributes a nonvanishing term to $\langle Q_2^M \rangle_C$; since there is only one proton in the p state, the summation will be dropped from (31). Expressing the matrix elements evaluated with the correlated wave functions as $\langle Q_2^M \rangle_C$, we obtain

$$\langle Q_q^M \rangle_C = \frac{e}{N_i N_f} [Q_0 + (C_i + C_f) Q_1 + C_i C_f Q_2],$$
 (33)

where

 $Q_0 = \langle Y_2^{M*}(1) \gamma_1^2 \rangle_{if}$

$$Q_1 = \langle Y_2^{M*}(1) r_1^2 r / r_0 \rangle_{if}, \qquad (34b)$$

and

$$Q_2 = \langle Y_2^{M*}(1) r_1^2 r^2 / r_0^2 \rangle_{if}, \qquad (34c)$$

where 1 and 2 denote the 1p-shell proton and neutron, respectively. The matrix elements in (33) do not involve the residual potential directly. However, the coefficients C_i and C_f do depend on the residual interactions. Finally,

$$\begin{split} \langle Q_2^{\mathbf{M}} \rangle_{C} &= -\left(\frac{5}{2\pi}\right)^{1/2} \frac{e}{N_i N_f \alpha^2} \left[\frac{1}{2} + \frac{11}{4\sqrt{2\pi}} \frac{C_i + C_f}{\lambda} + 3 \frac{C_i C_f}{\lambda^2} \right] \\ &\times \langle 210 M_J \mid 3M_J \rangle \;. \end{split} \tag{35}$$

By setting $C_i = C_f = 0$ in (35), we get $\langle Q_2^{M} \rangle$ for the uncorrelated simple harmonic-oscillator wave functions, in which case

$$\langle Q_2^{M} \rangle_0 = -\left(\frac{5}{2\pi}\right)^{1/2} \frac{e}{2\alpha^2} \,. \tag{36}$$

If we consider the total charge e on the p proton to be distributed evenly on both of the p nucleons so that the matrix element (35) for the transition from the state i to the state f may be evaluated entirely by the uncorrelated wave functions, we have

$$\langle Q_2^M \rangle_{\mathcal{C}} = 2 \left[-\left(\frac{5}{2\pi}\right)^{1/2} \frac{qe}{2\alpha^2} \right] = 2 \langle Q_2^M \rangle_0 q, \qquad (37)$$

where qe is the effective charge on the p nucleons. The mean lifetime and level width for this transition are given by

$$\tau = 1/T(E2), \qquad (38)$$

$$\Gamma = \hbar T(E2) . \tag{39}$$

The matrix element for the transition from the state *i* to *f*, the mean lifetime, width, and effective charge are given in Table I along with the so-called reduced transition probability B(2; 1-3). We were interested in the radiative transition in ⁶Li from the first excited state I=3, T=0 to the ground state I=1, T=0. We are, however, reporting the so-called reduced matrix element for the transition from the ground to the first excited state in order to compare with other calculations and the experimental data which were reported in this form. The so-called reduced matrix element from the state *a* to the state *b* is defined³⁶:

$$B(\lambda; I_a \rightarrow I_b) = (2I_a + 1)^{-1} \sum_{M_a, M_b} |\langle b | O_{\lambda, \mu} | a \rangle|^2, \quad (40)$$

where $O_{\lambda,\mu}$ stands for the Q_2^M operator in our case.

B. Single-Particle Model

It will be of interest to see how the E2 transition is predicted by other models for this nucleus. On the basis of the single-particle model, the electric multipole so-called reduced transition is given by³⁷

$$B_{\rm sp}(\lambda) = (2\lambda + 1)\frac{e^2}{4\pi} \left(\frac{3}{3+\lambda}\right)^2 R^{2\lambda}, \qquad (41)$$

where R is given by

$$R = R_0 A^{1/3} \, \text{fm} \,, \tag{42}$$

and $1.18 \le R_0 \le 1.42$ for all nuclei except for ⁶Li for which it is 1.92 fm.³⁸ For the quadrupole transition in a nucleus with A = 6, (41) becomes

$$B_{\rm sp}(2) = 1.562 R_0^4 e^2 \, {\rm fm}^4 \,. \tag{43}$$

The electric transition probability for singleparticle transition is given by^{36}

$$T_{W}(E\lambda) = \frac{2(\lambda+1)}{\lambda[(2\lambda+1)!!]^{2}} \left(\frac{3}{\lambda+3}\right)^{2} \frac{e^{2}}{\hbar c} \left(\frac{\omega R}{c}\right)^{2\lambda} \omega \operatorname{sec}^{-1},$$
(44)

where the subscript *W* refers to Weisskopf who introduced these units, and ω is the frequency of the electric multipole radiation of order λ . For $\lambda = 2$, (44) is reduced to

$$T_{w}(E2) = 3.511 \times 10^{7} E^{5} R^{4} \text{ sec}^{-1}, \qquad (45)$$

where *E* is the energy in MeV and *R* $(=R_0A^{1/3})$ is the nuclear radius in fm. In the case of ⁶Li, we get

$$T_{W}(E2) = 3.827 \times 10^{6} E^{5} R_{0}^{2} \text{ sec}^{-1}.$$
(46)

The width for γ decay as defined by (39) is predicted by the single-particle model as

$$\Gamma_{W} = 2.311 \times 10^{-8} E^{5} A^{4/3}, \qquad (47)$$

where E is in MeV and Γ_{W} is in eV. In the case of

⁶Li, the width is given by

$$\Gamma_{W} = 2.519 \times 10^{-7} E^{5} R_{0}^{4} \,. \tag{48}$$

The relevant results pertinent to the E2 transition in ⁶Li discussed under the single-particle model are given in Fig. 9 in the following section.

C. Configuration Mixing

We shall calculate the quadrupole transition matrix element in the IPSM with the admixture of higher configurations in the harmonic-oscillator well due to the residual potential (2). The basis wave function used here is the same as that used for the calculations in Sec. 6 A. The residual potential is only of the Gaussian type. The higher configuration mixing that we allow in these calculations are those oscillator states which are above the lowest states by $2\hbar\omega$. As usual, $\omega = \hbar \alpha^2/M$ and M is the mass of a nucleon. In this way we obtain the wave functions of ⁶Li in the states 1⁺ and 3⁺ with L-S coupling as^{13, 14}

$$\Psi_{I=1} = \{ [(1p)_{0}^{2}]_{0} + g_{p} [(1p2p)_{0}]_{0} + g_{d} [(1p)_{2}^{2}(1s)^{-1}1d]_{0} + g_{s} [(1p)_{0}^{2}(1s)^{-1}2s]_{0} \} | 0 \rangle$$
(49)

and

$$\Psi_{I=3} = \{ [(1p)_{2}^{2}]_{2} + e_{p}[(1p2p)_{2}]_{2} + e_{f}[(1p1f)_{2}]_{2} + e_{d}[(1p)_{0}^{2}(1s)^{-1}1d]_{2} \} | 0 \rangle .$$
(50)

The admixture coefficients g and e are evaluated to first order in perturbation theory using the method of second quantization.

The reduced transition probability B(E2; I + I')can be derived readily from the inelastic form factor $|F_{in}(q)|^2$ as obtained from electron scattering according to the relation

$$B(E2\uparrow) = \frac{225}{4\pi} Z^2 \lim_{q \to 0} \frac{|F_{in}(q)|^2}{q^4},$$
(51)

TABLE I. Potential parameters and the correlation coefficients C_{0t} and C_{2t} (as obtained from the variation principle) for the ground state and the first excited state in ⁶Li, respectively, using a $(1 + Cr/r_0)$ -type correlation function. These parameters give the excitation energy of the first excited state as $2.189 \pm 10\%$ MeV. The value of r_{0t} is 1.36 fm.

Type of potential	V ₀	Ь	λ	$-C_{0t}$	-C _{2t}	$-\langle Q \rangle$ (fm ²)	$10^{-11}T$ (sec ⁻¹)	$10^{11}\tau$ (sec)	Г (µeV)	$B(E2\dagger)$ (fm ⁴)	q
(55b)	20		0.70	0.150	0.092	1.535	1.193	0.838	78.499	5.500	0.456
(55c)	30		0.75	0.151	0.102	1.354	1.128	0.887	74.222	4.276	0.462
(55d)	40		0.70	0.150	0.111	1.791	1.648	0.607	108.438	7.484	0.459
(55e)	40		0.75	0.149	0.119	1.366	0.713	1.403	46.915	4.356	0.466
(55f)	40	0.20	0.75	0.142	0.098	1.364	0.583	1.714	38.648	4.341	0.465
	50	0.25	0.75	0.150	0.107	1.359	1.099	0.910	72.444	4.306	0.463
	60	0.30	0.70	0.147	0.107	1.552	1.462	0.684	93.376	5.619	0.461
	70	0.35	0.75	0.150	0.113	1.361	1.262	0.792	83.180	4.322	0.464
	80	0.40	0.75	0.144	0.111	1.367	0.806	1.240	53.149	4.362	0.466

where q is the momentum transfer here and should not be confused with the effective charge. Using the expression for $|F_{in}(q)|^2$ obtained from the wave functions (49) and (50),¹³ we get

$$B(E2; 1 \rightarrow 3) = \frac{35}{24\pi} \alpha^{-4} \left\{ 1 - 2 \left[\sqrt{0.4} \left(g_p + e_p \right) + \sqrt{2.1} e_f + 1.5 \left(g_d + e_d \right) \right] \right\}.$$
(52)

The admixture coefficients in (52) are evaluated from those parameters which fit the elastic electron scattering data for not too large momentum transfer.¹³ They are given in Table II in Sec. 7.

7. RESULTS

Since we are dealing with the triplet states of 6 Li, the form factor (3) is expressed as

$$V = -V_0 [a - b(r/r_0)^{2\nu}] X, \qquad (53)$$

where

$$X = e^{-r^2/r_0^2} . (54)$$

The matrix elements (27a) through (27c) are evaluated with the following sets of parameters in the form factors (53):



FIG. 1. The depth parameter V_0 for triplet cases as functions of the repulsive core parameters b of the potential of the (55f) type for $\lambda = 0.5$ to 0.8. The curves are indistinguishable for $\lambda = 0.65$ and above. For this reason no further figures are possible in similar cases where a correlation function of the type $(1 + Cr/r_0)$ is used. These parameters give the excitation energy of the first excited state of ⁶Li as 2.189 MeV $\pm 10\%$.

$$a = 0$$
, $\nu = 1$, $b = -1$; $-V_0(r_0/r)^2 X$; (55a)

$$u = 0, \quad \nu = -\frac{1}{2}, \quad \delta = -1; \quad -\nu_0(r_0/r)X; \quad (550)$$

$$a=0, \nu=0, b=-1; -V_0X;$$
 (55c)

$$a = 0$$
, $\nu = \frac{1}{2}$, $b = -1$; $-V_0(r/r_0)X$; (55d)

$$a=0$$
, $\nu=1$, $b=-1$; $-V_0(r/r_0)^2 X$; (55e)

a=1, $\nu = -\frac{1}{2}$, and b as adjustable parameter;

$$-V_0[1 - b(r_0/r)]X; (55f)$$

a=1, $\nu=1$, and b as adjustable parameter;

$$-V_0[1 - b(r/r_0)^2]X.$$
 (55g)

The results are expressed as



FIG. 2. The dimensionless parameter λ is given versus V_0 (triplet) for potentials of the types (55b)-(55e) using $(1 - Cr/r_0)$ so that $\Delta W = 2.189$ MeV $\pm 10\%$.

(56b)

$$a_{1}^{(L)} = \langle V \rangle = a(\langle V \rangle_{k=0}^{\nu=0} + \theta_{L} \langle V \rangle_{k=2}^{\nu=0}) - b(\langle V \rangle_{k=0}^{\nu} + \theta_{L} \langle V \rangle_{k=2}^{\nu}),$$

$$(56a)$$

$$a_{2}^{(L)} = 2\langle r/r_{0}V \rangle = 2a(\langle V \rangle_{k=0}^{\nu=1/2} + \theta_{L} \langle V \rangle_{k=2}^{\nu=1/2})$$

$$-2b(\langle V \rangle_{k=0}^{\nu=\nu+1/2} + \theta_L \langle V \rangle_{k=2}^{\nu=\nu+1/2}),$$

and

$$a_{3}^{(L)} = \frac{\hbar^{2}}{mr_{0}^{2}} + a(\langle V \rangle_{k=0}^{\nu=1} + \theta_{L} \langle V \rangle_{k=2}^{\nu=1}) - b(\langle V \rangle_{k=0}^{\nu=\nu+1} + \theta_{L} \langle V \rangle_{k=2}^{\nu=\nu+1}), \qquad (56c)$$

where

$$\langle V \rangle_{k=0}^{\nu} = \frac{1}{24\sqrt{2}} \left(5I_{0}^{\nu} + I_{1}^{\nu} + \frac{5}{4}I_{2}^{\nu} \right), \qquad (57)$$

$$\langle V \rangle_{k=2}^{\nu} = \frac{25}{24\sqrt{2}} \left(I_0^{\nu} - I_1^{\nu} + \frac{1}{4} I_2^{\nu} \right), \qquad (58)$$

and

$$I_{l}^{\nu} = -V_{0} \frac{(2l+2\nu+1)!}{(2l+1)!!} \left(\frac{1}{2+\lambda^{2}}\right)^{\nu} \left(\frac{2\lambda^{2}}{2+\lambda^{2}}\right)^{l+3/2}.$$
 (59)

With the use of appropriate matrix elements, the values of C_L given by (29) are determined which give the minimum energies in the two states of ⁶Li. Such values of C_l contain a set of parameters



FIG. 3. The depth parameter V_0 is given versus *b* for the potential of the type (55f) for $\lambda = 0.50$ to 0.75 using $(1 - Cr/r_0)$ so that $\Delta W = 2.189$ MeV $\pm 10\%$.

belonging to the class of potentials (55). Those parameters are adjusted so that the correct value of the excitation energy of the first excited state of ⁶Li is obtained, which is 2.189 MeV.^{39, 40} For computational purposes, the results given in the tables and figures are such that the excitation energy ΔW is allowed to vary in the range $2.0 \leq \Delta W$ ≤ 2.4 MeV. The coefficients *C* are evaluated with the parameters thus obtained. The potential parameters have been varied within the following ranges:

$$\begin{array}{ll} 0.5 \leqslant \lambda \leqslant 1.2 \ , & \Delta \lambda = 0.05 \\ & \text{for all potentials;} \\ 10 \leqslant V_0 \leqslant 200 \ , & \Delta V_0 = 10 \ \text{MeV} \\ & \text{for potentials (55a)-(55e);} \end{array}$$



FIG. 4. Solid lines represent C_{0t} and broken lines represent C_{2t} . They are the correlation coefficients for L = 0 and L = 2 triplet states, respectively. The coefficients are evaluated with $(1 - Cr/r_0)$ so as to give the minimum energies for the ground and first excited states, respectively, and $\Delta W = 2.189 \text{ MeV} \pm 10\%$, using potentials (55b)-(55e). For a given value of V_0 the corresponding value of λ can be obtained from Fig. 3.

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 $10 \le V_0 \le 1000$, $\Delta V_0 = 10 \text{ MeV}$

for potentials (55f) and (55g);

 $0.05 \le b \le 0.50$, $\Delta b = 0.05$

for potentials (55f) and (55g).

The numerical analysis was carried out on the IBM 360/50 computer. The results belonging to the correlation function of the type $(1 + Cr/r_0)$ are presented in Table I and Fig. 1, and those belonging to $(1 - Cr/r_0)$ are given in Figs. 2 to 9. In the former case most of the acceptable values for the excitation energies ΔW and B or Γ correspond to unphysical values of the parameters. We therefore report in Table I only those observables which correspond to some admissible values of the parameters selected for each type of potential. The parameters, in Table I and Figs. 1-5, obtained from the variational principle giving the minimum energy and the correct excitation energy within the 10% error for the 3⁺ state of ⁶Li, belong to potentials (55b)-(55f). Within the allowed range of the parameters, potentials (55a) and (55g) could not satisfy the above stated stringent conditions with either sign in the correlation

Cnt

0.9

0.8

functions. Thus, those two potentials were eliminated. The observables reported in Figs. 6-8 have been evaluated using only those parameters which meet the criteria of appearing in Figs. 2-5. Summarizing the results reported in Table I and Figs. 6 and 8 in terms of the reduced transition probability B(E24), we note that:

 $0.766 \le B_0(E2\dagger) \le 25.409$

with no correlation but the same α as in the corresponding $(1 + Cr/r_0)$ cases;

$$0.683 \le B_C(E2\dagger) \le 20.642$$

with correlation of the $(1 + Cr/r_0)$ type;

 $2.421 \leq B_0(E2\uparrow) \leq 25.409$

with no correlation but the same α as in the corresponding $(1 - Cr/r_0)$ cases;

 $4.343 \leq B_C(E2\uparrow) \leq 53.536$

0.9

0.8

with correlation of the $(1 - Cr/r_0)$ type.

Obviously the correlation of the type $(1 + Cr/r_0)$ has cut down the transition rate when compared with the results obtained from the uncorrelated wave function, whereas the correlation of the type $(1 - Cr/r_0)$ has enhanced it.



FIG. 5. C_{0t} and C_{2t} are given versus b for the potential (55f) for $\lambda = 0.55$, 0.60, 0.65, 0.70, 0.75 in ascending order. The corresponding values of V_0 for given b's can be read from Fig. 3. The conditions of minimum energies and ΔW are the same as those of Fig. 4.

On the basis of the single-particle model, the reduced transition probability B(E24) and the level width Γ_W of the 3⁺ state of ⁶Li have been calculated (see Fig. 9), in order to search for any reasonable value of R_0 which would give B(E2) or Γ comparable to any observed data or theoretical results. For the value of $R_0 = 1.92$ fm quoted in Ref. 38, we get B(E2) = 21.227 fm⁴, which is less than any observed value but comparable with other theoretical ones.

As cited earlier, the admixture of higher configuration enhanced the E2 transition in other nuclei. We have examined the effect due to the many particle states in the case of ⁶Li. With admixture co-



FIG. 6. The solid curves are for $B(E2^{\dagger})$ when $(1-Cr/r_0)$ is used with potentials (55b)-(55e), whereas the broken curve represents $B(E2^{\dagger})$ with no correlation. The dot-dashed lines represent the effective charge parameters q scaled on the right.

efficients tabulated below, we get $B(E24) = 5.3 \text{ fm}^4$, which is about the same as predicted by the oscillator wave function in the lowest configuration with the same spring constant. One could perhaps get a larger magnitude of B(E24) than evaluated by this set of parameters in the configuration-mixture calculations. However, the change would not be expected to be large enough to make the magnitude of B(E24) anywhere near the observed ones. Besides, any set of parameters other than those quoted in Table II are not likely to give the correct excitation energy of the 3^+ state of ⁶Li.

8. DISCUSSION

The purpose of these calculations has been to study the effect of the residual potential on the



FIG. 7. The solid curves represent Γ_{γ} when $(1 - Cr/r_0)$ is used with potentials (55b)–(55f), whereas the broken curve shows the same with no correlation.

50

10 50

Hamiltonian and thereby the effect of the nucleonnucleon correlation on the IPSM wave function of ⁶Li. This work has been motivated by the general assumption that the two-body nucleon-nucleon interaction cannot be replaced completely by an average central potential. The foregoing statement is of particular interest in the case of ⁶Li. While constructing the IPSM wave function of ⁶Li, the central potential chosen to replace the actual twobody interaction is either overestimated or underestimated. Such an erroneous estimate of the central potential is bound to give a wave function which is incapable of representing the actual behavior of ⁶Li. The over- or underestimated central potential is likely to yield an over- or undercorrected IPSM wave function for the system concerned. As pointed out earlier, the effect of the residual potential is manifested in the wave function through the nucleon-nucleon correlation function. Moreover, this correlation function should be added to or subtracted from the IPSM wave function according to the under- or overestimation of the wave function in the first approximation because of the wrong assumption of the cen-



FIG. 8. The solid lines represent $B(E2\dagger)$ when $(1-Cr/r_0)$ is used with the potential (55f). The curves are for $\lambda=0.55$, 0.60, 0.65, 0.70, 0.75 (from top to bottom). The energy conditions are satisfied as before.

TABLE II. Reduced transition probability B(E2t) of ⁶Li with configuration mixing, and admixture coefficients g and e. These coefficients were evaluated in the first-order perturbation theory using a Gaussian-type potential with parameters $r_{0t} = 1.36$ fm, $r_{0s} = 1.76$ fm, $V_{0t} = 47.6$ MeV, and $V_{0s} = 32.0$ MeV. The harmonic-oscillator length parameter $\alpha = 0.55$ fm⁻¹.

$B(E2\uparrow)$ (fm ⁴)	g _þ	<i>E</i> _d	e _p	e_f	e _d
5.3	0.078	0.071	0.052	-0.065	-0.043

tral potential. Accordingly, we have studied both aspects in this work.

Using the correlation function $(1 \pm Cr_{ij}/r_0)$ in either case, the energies in the ground state and in the first excited state are corrected and an exact amount of excitation energy ΔW can be obtained with a certain set of parameters belonging to the potentials (55). (See Table I and Figs. 1-5.) Nevertheless, the use of the plus and minus signs has opposite effects on the E2 transitions and other related observables. (See Table I and Figs. 6 and 7.) Using the plus sign with f(r) reduces the quadrupole transition and enhances the mean lifetime for the E2 transition compared with what one



FIG. 9. The solid curve shows the reduced transition probability B(E2), whereas the broken curve gives the level width Γ_{γ} of the first excited state of ⁶Li in the single-particle model.

gets with the uncorrelated simple harmonic wave function of ⁶Li. A similar effect has been found in the E2 transition of $^{7}_{\Lambda}$ He.⁴¹ The use of the same correlation function in those calculations enhances the decay time of ${}^{7}_{\Lambda}$ He^{*} to the point of establishing its $\frac{5}{2}$ state as isomeric. Alternatively, by the admixture of higher configurations in the wave function of ⁶He, the same conclusion about $^{7}_{\Lambda}$ He^{*} was reached.^{42,43} In the present calculations, the use of correlation term +f(r) has not enhanced the lifetime of ⁶Li enough in going from the 3⁺ to the 1^+ state to lead to its 3^+ state being isomeric. Such a conclusion would not be physically correct. The use of this correlation function gives the correct excitation energy of the first excited state (see Table I). It cuts down the E2 transition rate and the so-called effective charge - by an amount depending upon the type of the potential used - obtained from the calculations using the basis wave function with no correlation (see Table I and Figs. 6 and 7). Using the $(1 + Cr/r_0)$ -type correlation, many unphysical values of the parameters are obtained, which we have not entered in Table I. In Fig. 1 we also observe that there is a functional relationship between V_0 and b for unphysical values of λ (0.5 to 0.6), but for higher values of λ (which may be more readily acceptable) the values of V_0 are indistinguishable for all values of

 λ and b.

Before we discuss these results and compare them with the other theoretical and experimental work, we would like to make one observation regarding the use of the correlation term preceded by the minus sign. The evaluation of the correlation energy terms in (26) and the correlation coefficients C_{+} such as (29) from the variational principle using the correlation function $(1 - Cr/r_0)$ in (7) have been done *ab initio*. However, it is found (as shown in Appendix C) that the effect of this correlation function is the same as that of $(1 + Cr/r_0)$ except for its effect in the C values. The relevant formulas and expressions obtained with the function $(1 + Cr/r_0)$ can be used in case of $(1 - Cr/r_0)$ if the values of C_{\pm} evaluated with (1) $+Cr/r_0$) are replaced by C_{\pm} while using the function $(1 - Cr/r_0)$. More explicitly, the variational principle admits both values of C given by (29) to yield the minimum energy. The choice of either of the two values of C depends on the sign of the correlation function used in the wave function (7). The use of $(1 - Cr/r_0)$ gives the correct excitation energy for the 3⁺ state of ⁶Li on one hand, and enhances the E2 transition and effective charge on the other. Alternatively, such an enhancement in the quadrupole transition has been obtained by the admixture of higher configurations in other p-

$B(E2\dagger)$ (fm ⁴)								
	Other wo	ork		This work				
Reference	Method	Value	s.p. model	CM model	Correl. model			
	,	Experimental						
33	${}^{9}\mathrm{Be}(p,\gamma\alpha)$ reaction	Very little compared with $B(M1)$. No quantitative data given.						
49	⁶ Li(γ , d) reaction	1.75	yes ^a	no	yes ^b			
50	6 Li(e, e') reaction	23.59	yes ^a	no	yes ^b			
48	(Li, αd) reaction	95	no	no	Ū			
39	6 Li(e, e') reaction	30 ± 3	no	no	yes ^b			
40	6 Li(e, e') reaction	32 ± 3	no	no	yes ^b			
52	⁶ Li(e, e') reaction	25.1±2	no	no	yes ^b			
		Theoretical						
32	Variational method with Yukawa potential	Very little. No quan- titative data given.						
46,48	Single-particle model	3.3	yes ^a	5.3	ves ^b			
46,48	α -d cluster model	85	no	no	no			
9	Shell model	3.36	yes ^a	5.3	ves ^{b, c}			
9	Projected HF method with Volkov potential	10.96	yes ^a	no	yes ^b			
9	Projected HF method with Brink potential	12.98	yes ^a	no	yes ^b			

TABLE III. The observed and calculated values of the reduced transition probability $B(E2^{\dagger})$ in ⁶Li. CM is abbreviated for configuration mixing.

^aSee Fig. 10.

^bFor the actual values of $B(E2^{\dagger})$ and the relevant parameters see Figs. 2-9.

^cSee Table I.

shell^{27-29,44} as well as s-d-shell nuclei.^{44,45} The inclusion of $(1 - Cr/r_0)$ in the wave function (7) and the residual potential (2) in the Hamiltonian (1) yields the minimum energy and correct excitation energy for the 3⁺ state of ⁶Li as does the $(1 + Cr/r_0)$ type correlation function. In addition, it provides a range of values of the so-called reduced transition probability $B(E2; 1 \rightarrow 3)$ and other related quantities which are reasonably acceptable in relation to other theoretical results^{9, 32, 46, 47} and observed data.^{33, 39, 45, 48-55} Since all the theoretical and experimental values of B(E2) differ from each other and also among themselves so drastically, it is difficult to decide which to prefer (see Tables III and IV). For this reason, we are giving the entire range of transition probabilities and other related quantities for a class of potentials (55) with those sets of parameters which give the minimum energy states and correct excitation energy of the first excited state of ⁶Li. Here we may emphasize the need for a decisive experiment giving some definite observables pertaining to the E2 transition of ⁶Li.

On comparing the results of these calculations with the existing data and other similar theoretical work, we notice that an agreement of the values of B(E24) and Γ for the 3⁺ state in ⁶Li as reported in Table I and Figs. 6-9 is found with the experimentally observed and other theoretically predicted values. There is, however, one exception, for the values reported in Refs. 46 and 47, which we could not produce within the range of parameters used in our computational work. It is usual practice to report a set of parameters for any potential or wave function. Since there is a large uncertainty involved (although the results of Refs. 39, 50-55 tend to agree with each other but differ with those of Ref. 56), it is difficult to determine a unique set of parameters for potentials (55) for these experiments. Nevertheless, we are reporting sets of unique parameters in Table V which give the quantities agreeing with other work. However, at this stage, it seems wisest to regard this question as an unsettled problem until more reliable values of observables belonging to this transition are accepted for ⁶Li.

9. SUMMARY AND CONCLUSIONS

In this work it has been shown that the residual nucleon-nucleon two-body interaction is important if IPSM calculations are performed for ⁶Li. As a consequence of the residual potential, a nucleonnucleon correlation exists in the IPSM wave function of ⁶Li. The two aforesaid effects have been studied by considering a class of potentials (55) and correlation functions of the type $(1 \pm Cr_{12})$. A method has been developed employing the variational principle which corrects the over- or underestimated independent-particle harmonic-oscillator wave function. We have calculated the groundstate and the first-excited-state energies of ⁶Li and obtained the correct difference in the energies for these two states. In this procedure the correlation functions apparently affect the extracore nucleons; in fact, they cause the readjustment of

		Γ				
	Other w	ork	This	This work		
eference	Method	Value	s.p. model	Correl. model		
		Experimental				
49	⁶ Li(γ , d) reaction	30 ± 15	yes ^a	yes ^{b,c}		
50	6 Li(e, e') reaction	410^{+300}_{-150}	no	yes ^c		
39	6 Li(e, e') reaction	519 ± 52	no	yes ^c		
51	⁶ Li(γ, γ') reaction	140	yes ^a	yes ^c		
52	6 Li(e, e') reaction	431 ± 34	no	yes ^c		
53	${}^{4}\text{He}(d,\gamma){}^{6}\text{Li reaction}$	450 ± 130		yes		
54	6 Li(e, e') reaction	440 ± 34		yes ^c		
55	6 Li(e, e') reaction	390 ± 50	no	yes ^c		
		Theoretical				
56	Intermediate coupling	30	yes ^a	yes ^c		
46	$^{6}Li \rightarrow \alpha + d$	1460 ± 730	no	no		
9	Projected HF method with Volkov's inter- action	190	yes ^a	yes ^c		

TABLE IV. The observed and calculated values of the level width Γ_r of the first excited state 3⁺ in ⁶Li.

TABLE V. Some typical values of potential parameters which give $\Delta W = 2.189 \text{ MeV} \pm 10\%$ and also the $B_C(E2\dagger)$ values of interest by using the $(1 - Cr/r_0)$ type of correlation function. The values of λ are 0.59 and 0.55 for $B(E2\dagger) = 13.0$ and 25.0 fm⁴, respectively. There is no $B_0 = 32.0 \text{ fm}^4$ for any λ within the range considered.

$B_{C}(E2\dagger)$	Type of		V_0		
(fm ⁴)	potential	λ	(MeV)	$-C_{0t}$	$-C_{2t}$
13.0	b	0.680	88.0	0.54	0.49
	Ċ	0.695	136.0	0.68	0.49
	d	0.700	166.0	0.64	0.50
	е	0.715	•••	•••	•••
25.0	b	0.580	66.0	0.57	0.37
	с	0.600	102.0	0.59	0.40
	d	0.600	108.0	0.51	0.39
	е	0.600	96.0	0.49	0.38
32.0	b	0.560	62.0	0.53	0.35
	с	0.565	84.0	0.50	0.34
	d	0.565	92.0	0.47	0.36
	e	0.565	78.0	0.44	0.34

the inner core particles also. The so-called effective-Hamiltonian prescription used in these calculations has retained the simplicity of the simple harmonic-oscillator-type shell-model calculations despite the inclusion of the relative coordinates in the total wave function. The phenomenological Jastrow-type correlation⁵⁷ function makes the calculations rather tedious.

The correlated wave functions have been used to calculate the E2 transition. The transition is enhanced or cut down according to the under- or overestimation of the uncorrelated wave function. This seems to be an advantage of this method over other procedures such as the one of mixing the higher configurations or the three-body model. The E2 transition has been estimated in this work by other methods, namely the single-particle model, configuration mixing, and simple harmonicoscillator-type IPSM. On comparison with each other and with other theoretical and experimental values of the relevant quantities involved in the E2transition of ⁶Li, it is evident that the correlated wave function is the most plausible one. As a byproduct of these calculations, a comparison of the reduced transition probabilities obtained by the single-particle method and other work provides a value for the parameter R_0 for ⁶Li. Table I and Fig. 6 provide the parameter q for the so-called effective charge for the p nucleons in ⁶Li which would avoid lengthy calculations in the future and permit evaluation of the transition matrix element Q by means of the relation $Q = 2Q_0q$.

To sum up, this method should be applicable to other nuclear systems, particularly to those which have a doubly closed shell and two particles or holes. The residual two-body interaction leads to some clustering of the valence nucleons. The combined effect of the residual potential and the nucleon-nucleon correlation in ⁶Li provides (i) the minimum energy for each level, (ii) the correct ground-state and first-excited-state energies, (iii) a considerable improvement in the *E*2 transition rate in comparison with other models, and (iv) correlated wave functions which are relatively simple and realistic. Finally it is capable of expediently yielding interesting results when applied to other nuclear problems as demonstrated by the excellent agreement⁵⁸ with the electron scattering data⁵⁹ from ⁶Li.

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APPENDIX A

Effective-Hamiltonian Formalism

The effective Hamiltonian \tilde{H} has been written for a two-particle system outside a doubly closed shell in (14). In this Appendix we shall deduce the results for a general system of any number of particles and use their particular form in the main text. The so-called effective Hamiltonian \tilde{H} for an *n*-particle system is given by

$$\tilde{H} = H + \frac{C}{r_0} (r_{ij}H + Hr_{ij}) + \frac{C^2}{r_0^2} r_{ij}Hr_{ij}, \qquad (A1)$$

where

$$H = H_0 + V, \tag{A2}$$

and

$$H_{0} = \sum_{i=1}^{n} H_{0i} = \sum_{i=1}^{n} \left(-\frac{\hbar^{2}}{2m} \nabla_{i}^{2} + U_{i} \right), \qquad (A3)$$

$$V = \sum_{i < j}^{n} V_{ij} . \tag{A4}$$

The subscripts of r_{ij} will be dropped from now on unless it is necessary to specify them in order to avoid confusion. It is desirable to evaluate the matrix element of \tilde{H} with uncorrelated harmonic-oscillator wave functions such as (20). We have then

$$\langle \tilde{H} \rangle = \langle H \rangle + \frac{C}{r_0} \langle (rH + Hr) \rangle + \frac{C^2}{r_0^2} \langle rHr \rangle .$$
 (A5)

We have

$$rH + Hr = r(\sum H_{0i}) + (\sum H_{0i})r + 2r\sum_{i < j} V_{ij}.$$
 (A6)

The last term in the above expression has been used for rV + Vr. However, since V commutes with r, it may be written as in (A6). Since it follows that the eigenfunctions of H_{oi} are used as the basis, we may write

$$\begin{aligned} \langle \phi_{nl\,m}(i)\phi_{n\,\prime l\,\prime m\,\prime}(j) \,|\, rH_{0i} \,|\, \phi_{nl\,m}(i)\phi_{n\,\prime l\,\prime m\,\prime}(j) \rangle \\ &= \langle \phi_{nl\,m}(i)\phi_{n\,\prime l\,\prime m\,\prime}(j) \,|\, r\epsilon_{nl\,m}(i) \,|\, \phi_{nl\,m}(i)\phi_{n\,\prime l\,\prime m\,\prime}(j) \rangle \\ &= \epsilon_{nl\,m}(i)\langle r \rangle \,. \end{aligned}$$
(A7)

Also,

 $\langle \phi_{nlm}(i)\phi_{n'l'm'}(j)|H_{0l}r|\phi_{nlm}(i)\phi_{n'l'm'}(j)\rangle$

$$= \langle \phi_{nlm}(i)\phi_{n'l'm'}(j) | \epsilon_{nlm}(i)r | \phi_{nlm}(i)\phi_{n'l'm'}(j) \rangle$$

$$=\epsilon_{nlm}(i)\langle r\rangle. \tag{A8}$$

So that

$$\langle rH_{0i} \rangle = \langle H_{0i}r \rangle = \epsilon_{nlm}(i)\langle r \rangle . \tag{A9}$$

By means of (A6) and (A9), we get for an n-particle system

$$\langle rH + Hr \rangle = 2 \langle r \rangle \sum_{i=1}^{n} \epsilon_i + 2 \langle r \sum_{i < j}^{n} V_{ij} \rangle.$$
 (A10)

We next consider

$$rHr = r(\sum H_{0i} + V)r$$
$$= r(\sum H_{0i})r + r^2 V.$$
(A11)

For a single *i*th particle and a given function ϕ , we can write

$$rH_{0i}r\phi = r\left(-\frac{\hbar^2}{2m}\nabla_i^2 + U_i\right)r\phi .$$
 (A12)

From the properties of the Laplacian operator,

$$-\frac{\hbar^2}{2m}(r\nabla_i^2 r\phi) = -\frac{\hbar^2}{2m} [r^2 \nabla_i^2 \phi + r\phi \nabla_i^2 r + 2r \vec{\nabla}_i r \cdot \vec{\nabla}_i \phi].$$
(A13)

In the Cartesian expansion, we can write

$$\nabla_i^2 \gamma = \left(\frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2}\right) \\ \times \left[(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2\right]^{1/2}.$$
(A14)

Since

$$\frac{\partial}{\partial x_i} \gamma_{ij} = \frac{x_i - x_j}{\gamma_{ij}}$$

and

$$\frac{\partial^2}{\partial x_i^2} r_{ij} = \frac{1}{r_{ij}} - \frac{(x_i - x_j)^2}{r_{ij}^3}, \text{ etc.},$$
(A15)

(A14) and (A15) readily give

$$\nabla_i^2 r = (3/r - r^2/r^3) = 2/r.$$
 (A16)

Hence,

$$\gamma \nabla_i^2 \gamma = 2$$

or

$$\langle r \nabla_i^2 r \rangle = 2 . \tag{A17}$$

Considering the last term in (A13),

. .

$$\begin{aligned} r_{ij} \vec{\nabla}_{i} r_{ij} \cdot \vec{\nabla}_{i} &= \frac{1}{2} \vec{\nabla}_{i} r_{ij}^{2} \cdot \vec{\nabla}_{i} \\ &= \frac{1}{2} \vec{\nabla}_{i} (r_{i}^{2} + r_{j}^{2} - 2r_{i} r_{j} \cos \omega_{ij}) \cdot \vec{\nabla}_{i} . \end{aligned}$$
(A18)

The term containing $\cos \omega_{12}$ will vanish on integration over the angular coordinates of particles *i* and *j* while actually evaluating the matrix element of this operator. We shall, therefore, drop this term from now on. It follows then that

$$\langle r \nabla_{i} r \cdot \nabla_{i} \rangle = \langle \frac{1}{2} \nabla_{i} r_{ij}^{2} \cdot \nabla_{i} \rangle$$

$$= \left\langle r_{i} \frac{\partial}{\partial r_{i}} \right\rangle$$

$$= \int_{0}^{\infty} R_{nl}(r_{i}) r_{i} \frac{\partial}{\partial r_{i}} [R_{nl}(r_{i})] r_{i}^{2} dr$$

$$= \frac{1}{2} \int_{0}^{\infty} \left(\frac{\partial}{\partial r_{i}} \{ r_{i}^{3} [R_{nl}(r_{i})]^{2} \}$$

$$- 3r_{i}^{2} [R_{nl}(r_{i})]^{2} \right) dr_{i} .$$
(A19)

For a well-behaved wave function such as R_{nl} as defined by (17), the first term in the above integral vanishes on integration and the second term is reduced to -3 by the normalization condition. Hence

$$\langle \vec{r} \nabla_i \vec{r} \cdot \nabla_i \rangle = -\frac{3}{2}. \tag{A20}$$

The diagonal matrix element of (A12) can be immediately written using the results (A13), (A17), and (A20) as

$$\langle \boldsymbol{r}H_{0i}\boldsymbol{r}\rangle = \left\langle \boldsymbol{r}^{2}\left(-\frac{\hbar^{2}}{2m}\nabla_{i}^{2}+U_{i}\right)\right\rangle - \frac{\hbar^{2}}{2m}\left[2+2\left(-\frac{3}{2}\right)\right]$$
$$= \left\langle \boldsymbol{r}^{2}H_{0i}\right\rangle + \hbar^{2}/2m$$
$$= \left\langle \boldsymbol{r}^{2}\right\rangle \boldsymbol{\epsilon}_{i} + \hbar^{2}/2m .$$
(A21)

By means of (A11) and (A21), we get

$$\langle rHr \rangle = \langle r^2 \rangle \sum_{i=1}^n \epsilon_i + n \frac{\hbar^2}{2m} + \langle r_{ij}^2 \sum_{i (A22)$$

Substitution of (A10) and (A22) in (A5) yields

$$\langle \tilde{H} \rangle = \sum_{i=1}^{n} \epsilon_{i} + \left\langle \sum_{i=1}^{n} V_{ij} \right\rangle + \frac{C}{r_{0}} \left(2 \langle r \rangle \sum_{i=1}^{n} \epsilon_{i} + 2 \left\langle r \sum_{i

$$+ \frac{C^{2}}{r_{0}^{2}} \left(\langle r^{2} \rangle \sum_{i=1}^{n} \epsilon_{i} + \frac{n\hbar^{2}}{2m} + \left\langle r_{ij}^{2} \sum_{i

$$= \sum_{i=1}^{n} \epsilon_{i} \left(1 + 2 \frac{C}{r_{0}} \langle r \rangle + \frac{C^{2}}{r_{0}^{2}} \langle r^{2} \rangle \right)$$

$$+ \langle V \rangle + 2 \frac{C}{r_{0}} \langle r V \rangle + \frac{C^{2}}{r_{0}^{2}} \left(\frac{n\hbar^{2}}{2m} + \langle r^{2}V \rangle \right). \qquad (A24)$$$$$$

Using (10) and (A24), we get

$$\langle \tilde{H} \rangle = W_0 N^2 + \langle V \rangle + 2 \frac{C}{r_0} \langle r V \rangle + \frac{C^2}{r_0^2} \left(\frac{n\hbar^2}{2m} + \langle r^2 V \rangle \right),$$
(A25)

where W_0 is the total energy of the system belonging to the Hamiltonian H_0 . Finally, the total energy of the system belonging to the complete Hamiltonian H with a correlated wave function like (7) is given by

$$W = \langle \tilde{H} \rangle / N^{2}$$

= $\epsilon_{0} + \left[\langle V \rangle + 2 \frac{C}{r_{0}} \langle r V \rangle + \frac{C^{2}}{r_{0}^{2}} \left(\frac{n\hbar^{2}}{2m} + \langle r^{2} V \rangle \right) \right] / N^{2}.$
(A26)

APPENDIX B

Infinite Integrals

In this Appendix we shall discuss the integrals that arise while evaluating the various matrix elements of the operators \tilde{N} , \tilde{H} , and Q. These terms involve harmonic-oscillator wave functions for two p particles, an operator of the form $r_i^2 Y_2^M(i)$, and an expansion of r_{ij} or r_{ij}^2 . Using the standard method of Racah algebra, the angular part can be evaluated. Whenever the Talmi method⁶⁰ is applicable, the radial part is also readily obtained. However, some integrals are of the type

$$\int_{0}^{\infty} \int_{0}^{\infty} e^{-\alpha (r_{1}^{2} + r_{2}^{2})} r_{1}^{p} r_{2}^{p} x_{2}^{p} \times \left(\frac{r_{<}^{k+2}}{(2k+3)r_{>}^{k-1}} - \frac{r_{<}^{k}}{(2k-1)r_{>}^{k-1}} \right) dr_{1} dr_{2},$$
(B1)

which lead to the integrals of the type

$$\int_{0}^{\infty} e^{-\alpha^{2}r_{1}^{2}} r_{1}^{p} dr_{1} \int_{0}^{r_{1}} e^{-\alpha^{2}r_{2}^{2}} r_{2}^{q} dr_{2} .$$
 (B2)

If q is odd, the finite integral can be evaluated easily in closed form. If q is even, the finite integral when evaluated by parts results in an error function of the argument αr_1 . As a result the infinite integral is reduced to the form

$$\int_0^\infty e^{-\alpha^2 r_1^2} r_1^{\,\rho} \operatorname{erf}(\alpha r_1) \,, \tag{B3}$$

where⁶¹

$$\operatorname{erf}(\alpha r_{1}) = \int_{0}^{r_{1}} e^{-\alpha^{2}r^{2}} dr$$
$$= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{2^{n} (\alpha r_{1})^{2n+1}}{1.3 \cdots (2n+1)} e^{-\alpha^{2}r^{2}}.$$
(B4)

When (B4) is substituted in (B3) and integrated, it yields a series of the type

$$\sum_{n=0}^{\infty} \frac{n^l}{2^n},\tag{B5}$$

where l is a given integer. The infinite series (B5) can easily be summed in a closed form for finite l.

APPENDIX C

Correlation Coefficient

The correlation function introduced into the wave function (7) has the form

$$f(r) = (1 + Cr/r_0)$$
(C1)

and leads to the two values of C (from the variational principle) as given by (29). It turned out that in our calculations for the minimum energy state that C_+ was selected with the form of the correlation function (C1). However, if the form of the correlation function were chosen as

$$g(r) = (1 - Cr/r_0),$$
 (C2)

the other value of C, i.e., C_{-} belonging to (C1) would be identical to $-C_{+}$ belonging to (C2). This can be shown as follows.

Using the correlation functions (C1) or (C2), we have the total energy given by (25)

$$W = \epsilon_s + 2\epsilon + \frac{a_1 \pm a_2 C + a_3 C^2}{1 \pm a_4 C + a_5 C^2},$$
 (C3)

where the plus or minus signs correspond to the correlation functions (C1) or (C2), respectively. Using the variational principle, the value of C is obtained as given by (29) if the plus sign is used in (C3). When the minus sign is maintained in (C3) and the same procedure is followed, the two values of C are found to be

$$C'_{\pm} = \frac{(a_3 - a_1a_5) \pm [(a_3 - a_1a_5)^2 - (a_3a_4 - a_2a_5)(a_2 - a_1a_4)]^{1/2}}{a_3a_4 - a_2a_5}$$
(C4)

The prime is used on C in (C4) to distinguish it from C which belongs to (C1). Comparing (29) and (C4), one readily finds

$$C'_{+} = -C_{-}$$

and

 $C'_{-} = -C_{+} .$ (C5)

This is what one would naively expect. The two values of C or C' correspond to the two situations

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whether the correlation term $(Cr/r_0)\psi_0$ is added to or subtracted from the uncorrelated basis wave function ψ_0 . This fact leads to an interesting physical situation discussed in the text of this article.

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