Effect of short-range correlations on Coulomb matrix elements*

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Correlated wave functions obtained by solving the Bethe-Goldstone equation with the Hamada-Johnston potential are used to calculate Coulomb matrix elements for use in the nuclear $1p$ shell. When proper attention is given to the Pauli operator we find that Coulomb matrix elements are not appreciably larger than those obtained using uncorrelated wave functions, in contrast to conclusions reached by previous investigators.

INTRODUCTION

In order to investigate the possibility of a charge-symmetry breaking term in the specifically nuclear force, one must first eliminate from the data all purely electromagnetic effects. In nuclear-structure studies this subtraction of Coulomb effects is usually accomplished by adopting model nuclear wave functions and treating the Coulomb interaction in first-order perturbation theory. Because of the approximate knowledge of nuclear wave functions such complications as configuration mixing and the Thomas-Ehrman shift make it exceedingly difficult to present clear evidence of the need for a charge-symmetry breaking term in the nuclear Hamiltonian. There do exist intriguing situations, however, where it is not immediately obvious that the complications mentioned above will suffice to explain the data. Two interesting examples are (1) the ^{6}Be($2^+ - 0^+$ g.s.) energy difference (1.5 MeV) compared to the ^{6}He and ^{6}Li ($T=1$) ($2^+ - 0^+$) energy difference (1.8 MeV)[1] and (2) the apparent considerable isospin impurity in certain ($T=0,1$) $1^+, 2^+, 3^+$ states in the 16–20-MeV region in ^{8}Be.[2]

It has recently been suggested by Anderson, Wilson, and Goldhammer[3,4] (AWG) that including short-range correlations in the nuclear wave function can significantly improve the agreement between theory and experiment, particularly in the mass-6 and -8 systems mentioned above. Because of the general importance of such an effect, we have repeated the calculations of AWG using the Hamada-Johnston potential and including Pauli corrections in the Bethe-Goldstone (BG) wave functions. In contrast to AWG, we do not find large changes from results obtained with uncorrelated wave functions.

THEORY

The simplest way to investigate the effects of short-range correlations is to treat the Coulomb interaction as a perturbation and calculate Coulomb matrix elements between correlated nuclear wave functions. Even this simple picture is complicated, however, because of the difficulty of defining a correlated many-body wave function.

In the calculations presented here we treat the ^{4}He core as inert and simply introduce correlations in the relative coordinates of the p-shell nucleons. This procedure is similar to a low-order Jastrow-type calculation but is also closely related to the linked-cluster expansion since we replace uncorrelated (oscillator) wave functions by relative BG wave functions. It is very important to include the Pauli operator when calculating the BG wave functions since this conserves orthogonality between core and valence wave functions. We also choose to renormalize the relative BG wave function but find that this has little effect on our results once the Pauli operator has been included.

It is not immediately obvious that our relative BG wave functions should be renormalized. In the linked-cluster expansion for the energy, the normalization term is used to eliminate unlinked clusters, and it is not customary to renormalize the BG wave function. It is possible, however, to arrange the linked-cluster expansion for the wave function in a form consistent with wave-function renormalization.

The lowest-order diagrams in our perturbation expansion (neglecting single-particle excitations) are shown in Figs. 1 and 2. Replacing matrix elements of V_c between oscillator wave functions by matrix elements between conventionally normalized BG wave functions corresponds to summing the diagrams shown in Fig. 1. When renormalized BG wave functions are used, one also sums the diagrams shown in Fig. 2, plus higher-order diagrams. This approach would not be appropriate if we were including the Coulomb interaction to all orders in calculating binding energies, but seems to be reasonable in our first-order perturbation treatment.

We use an approximate Pauli operator, Q, which

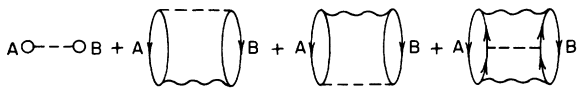

FIG. 1. Linked-cluster diagrams included when conventionally normalized BG wave functions are used. The dashed lines correspond to the Coulomb potential V_c, while wiggly lines represent G-matrix interactions.

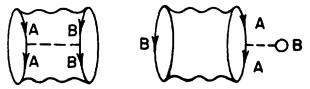

FIG. 2. Lowest-order diagrams included by renormalizing the BG wave functions.

forbids scattering into intermediate states with unperturbed energy less than or equal to two p-state nucleons. This definition of Q enables us to insure the orthogonality of core and valence wave functions and still carry out all calculations in the relative coordinate system. The relative BG wave functions can now be expanded in terms of relative harmonic-oscillator (HO) wave functions using the formalism of Barrett, Hewitt, and McCarthy.[5]

First the BG wave function is expanded in terms of eigenstates ψ_i of the equation

$$(H_{\rm osc} + V)\psi_i = E_i\psi_i \tag{1}$$

and the eigenstates ψ_i are themselves expanded in terms of relative HO wave functions, φ. The potential V we use is the Hamada-Johnston potential. From Ref. 5, we express the BG wave function as

$$\begin{aligned}\Psi_\alpha(\omega_r) &= \sum_i a_{i\alpha}(\omega_r)\psi_i \\ &= \sum_i a_{i\alpha}(\omega_r)\sum_\gamma b_{i\gamma}\varphi_\gamma \\ &= \sum_\gamma \left((\epsilon_\alpha - \omega_r)\sum_i \frac{b_{i\alpha}b_{i\gamma}}{E_i - \omega_r} \right. \\ &\quad \left. + \sum_\mu (1 - Q_\mu)G_{\mu\alpha}\sum_i \frac{b_{i\mu}b_{i\gamma}}{E_i - \omega_r}\right)\varphi_\gamma .\end{aligned} \tag{2}$$

Here $b_{i\gamma} = \langle\varphi_r | \psi_i\rangle$, ϵ_α is a relative HO energy, $Q_\mu = 0$ (1) if $2n_\mu + l_\mu + 2N + L \leq (>)\ 6$, and ω_r is the starting energy referred to the relative coordinate system. For two p-state nucleons we define

$$\omega_r = \omega - E_{NL} = 2E_p + 2C - E_{NL}, \tag{3}$$

where C controls the gap between occupied and unoccupied states and thus determines the intermediate-state spectrum. It turns out that our results are quite insensitive to shifts of the intermediate-state spectrum.

Coulomb matrix elements can now be expressed as

$$\begin{aligned}\langle\Psi_\alpha(\omega_r)|V_c|\Psi_\alpha(\omega_r)\rangle &= \sum_{\beta,\gamma} C_{\alpha\beta}(\omega_r)C_{\alpha\gamma}(\omega_r) \\ &\quad \times\langle\varphi_\beta|V_c|\varphi_\gamma\rangle ,\end{aligned} \tag{4}$$

where

$$C_{\alpha\gamma}(\omega_r) = (\epsilon_\alpha - \omega_r)B_{\alpha\gamma}(\omega_r) + \sum_\mu (1 - Q_\mu)G_{\mu\alpha}B_{\mu\gamma}(\omega_r) \tag{5}$$

and

$$B_{\alpha\gamma}(\omega_r) = \sum_i \frac{b_{i\alpha}b_{i\gamma}}{E_i - \omega_r} . \tag{6}$$

Renormalized matrix elements are given by

$$\langle\alpha|V_c|\alpha\rangle = \frac{\sum_{\beta\gamma}C_{\alpha\beta}(\omega_r)C_{\alpha\gamma}(\omega_r)\langle\varphi_\beta|V_c|\varphi_\gamma\rangle}{\sum_\beta C^2_{\alpha\beta}(\omega_r)} . \tag{7}$$

The effect of including Pauli corrections is quite interesting. If we neglect the Pauli operator ($Q_\mu = 1$ for all μ),

$$C_{\alpha\gamma}(\omega_r) = (\epsilon_\alpha - \omega_r)B_{\alpha\gamma}(\omega_r) . \tag{8}$$

However, two distinct situations arise when we include this particular approximate Pauli operator. First, for cases where α represents relative $1s$ (and c.m. $1d$ or $2s$), relative $1p$ (and c.m. $1p$), or relative $1d$ (and c.m. $1s$) states then only a single term survives in the sum over μ states in Eq. (5), that is

$$C_{\alpha\gamma}(\omega) = (\epsilon_\alpha - \omega_r + G_{\alpha\alpha})B_{\alpha\gamma}(\omega_r) . \tag{9}$$

This simple relationship occurs because we are considering only the relative center-of-mass states, α, arising from two $1p$-state protons ($T = 1$ channels), and our Pauli operator is diagonal in the center-of-mass states. Thus, for these cases, the effect of including Q is simply to renormalize the BG wave function.

The second situation is more complicated. When α represents relative $2s$ (and c.m. $1s$) the sum over μ in Eq. (5) has two terms; one a relative $1s$ and the other a relative $2s$. Only for this case will the Pauli contribution make a difference in renormalized results.

RESULTS

In order to compare with AWG we calculate the Coulomb integrals L, K_{SD}, and K_{SP} which are

TABLE I. Relative Coulomb matrix elements in keV. The column labeled with * is not Pauli corrected. $\hbar\omega = 16.2$ MeV.

	$\langle 1s \mid V_c \mid 1s\rangle$	$\langle 1p_0 \mid V_c \mid 1p_0\rangle$	$\langle 1p_1 \mid V_c \mid 1p_1\rangle$	$\langle 1p_2 \mid V_c \mid 1p_2\rangle$	$\langle 1p \mid V_c \mid 1p\rangle$	$\langle 1d \mid V_c \mid 1d\rangle$	$\langle 2s \mid V_c \mid 2s\rangle$	$\langle 2s \mid V_c \mid 2s\rangle^*$
Uncorrelated	717	478	478	478	478	383	598	598
Correlated ω_r (MeV)								
−54.3	713	476	464	487	478	385	551	585
−44.3	717	476	464	488	479	385	552	594
−34.3	723	477	463	489	479	385	554	605
−24.3	729	477	462	490	479	385	555	622
−14.3	737	477	461	491	479	386	557	649
−4.3	748	478	459	493	480	386	560	699

TABLE II. Coulomb integrals in keV. $\hbar\omega = 16.2$ MeV. Numbers in parentheses are obtained using conventionally normalized wave functions.

	L	K_{SD}	K_{SP}
Uncorrelated	586	36	36
AWG	690	49	61
No Pauli corrections			
$\omega = 0$	589	39	37
$\omega = 20$	605	52	46
Pauli corrected			
$\omega = 0$	578 (584)	28 (30)	31 (33)
$\omega = 20$	581 (588)	29 (30)	32 (35)

defined as[6]

$$
\begin{aligned}
L &= \tfrac{1}{3}(\langle p^2\,{}^1S_0 \mid V_c \mid p^2\,{}^1S_0\rangle \\
&\quad + 2\langle p^2\,{}^1D_2 \mid V_c \mid p^2\,{}^1D_2\rangle), \\
K_{SD} &= \tfrac{1}{3}(\langle p^2\,{}^1S_0 \mid V_c \mid p^2\,{}^1S_0\rangle \\
&\quad - \langle p^2\,{}^1D_2 \mid V_c \mid p^2\,{}^1D_2\rangle), \\
K_{SP} &= \tfrac{1}{5}(\langle p^2\,{}^1S_0 \mid V_c \mid p^2\,{}^1S_0\rangle \\
&\quad - \langle p^2\,{}^3P \mid V_c \mid p^2\,{}^3P\rangle),
\end{aligned} \tag{10}
$$

where the averaged ^3P matrix element is given by

$$
\langle p^2\,{}^3P \mid V_c \mid p^2\,{}^3P\rangle = \frac{\sum_J (2J+1)\langle p^2\,{}^3P_J \mid V_c \mid p^2\,{}^3P_J\rangle}{\sum_J (2J+1)}. \tag{11}
$$

It is convenient here to redefine L, K_{SD}, and K_{SP} in terms of relative matrix elements:

$$
\begin{aligned}
L &= \tfrac{1}{2}\langle 1s \mid V_c \mid 1s\rangle + \tfrac{1}{6}\langle 2s \mid V_c \mid 2s\rangle \\
&\quad + \tfrac{1}{3}\langle 1d \mid V_c \mid 1d\rangle, \\
K_{SD} &= \tfrac{1}{6}\langle 2s \mid V_c \mid 2s\rangle - \tfrac{1}{6}\langle 1d \mid V_c \mid 1d\rangle, \\
K_{SP} &= \tfrac{1}{10}\langle 1s \mid V_c \mid 1s\rangle + \tfrac{1}{10}\langle 2s \mid V_c \mid 2s\rangle \\
&\quad - \tfrac{1}{5}\langle 1p \mid V_c \mid 1p\rangle.
\end{aligned} \tag{12}
$$

In Table I we list the uncorrelated and correlated relative matrix elements needed in the calculations as a function of relative starting energy, ω_r. The last two columns show the effect of including Pauli corrections in the $\langle 2s \mid V_c \mid 2s\rangle$ matrix element.

The effect of short-range correlations is largest and most strongly ω-dependent for the relative s states, as would be expected. The relative d-state matrix elements are almost unaffected, and the averaged p-state matrix elements are also unaffected due to cancellations between effects in the $^3p_1$ and $^3p_2$-$^3f_2$ partial waves.

Table II lists the Coulomb integrals L, K_{SD}, and K_{SP}. The first two rows contain uncorrelated values and the results of AWG. Rows 3–6 show

results we obtained using two different ω values and the effect of including the Pauli operator. We find that it is quite important to include Pauli corrections—especially for the smaller off-diagonal K's. Including these corrections wipes out most of the large effects in Coulomb shifts and isospin mixing found by AWG.

The numbers in parentheses are calculated using conventionally normalized BG wave functions. It is seen that renormalization has little effect on our final results. We would obtain large results, however, if we neglected both the Pauli operator and wave-function renormalization. For example, the $\omega = 0$ results for L and K_{SD} using no Pauli operator and no wave-function renormalization are $L = 698$ keV and $K_{SD} = 55$ keV, respectively.

The largest change in the Coulomb integrals is a 15–20% *decrease* in the magnitude of K_{SD}. Thus while AWG find a Coulomb shift in the ^{6}He-^{6}Be system of ~147 keV (for the Hamada-Johnston potential), we find a Coulomb shift of ~85 keV. Comparing these results with the uncorrelated shift of ~108 keV and the experimentally measured value of ~300 keV, we find that using correlated wave functions tends to reduce the agreement with experiment.

We have also calculated the off-diagonal Coulomb matrix elements which contribute to the isospin mixing in the appropriate 1^+, 2^+, and 3^+ states of ^{8}Be. The net effect of correlation corrections —which in this case involve both K_{SD} and K_{SP} —is to decrease the off-diagonal matrix elements by about 10% from results obtained using oscillator wave functions.

Thus, while we cannot say with certitude that the effect of short-range correlations is never important in calculating nuclear Coulomb matrix elements, it is obvious that short-range correlations cannot be used to explain the discrepancies in the mass-6 and mass-8 systems.

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