Pauli corrections for correlated wave functions

Paul Goldhammer and James A. Pintar*
Department of Physics, University of Kansas, Lawrence, Kansas 66045
(Received 5 November 1973)

An exact prescription is given for taking reference spectrum wave functions, and deriving correlated wave functions which properly adhere to the Pauli exclusion principle.

The reference spectrum method[1] is widely used in nuclear structure studies to obtain solutions of the Bethe-Goldstone equation:

$$\psi_0 = \varphi_0 + \frac{Q}{e} v\psi_0 . \tag{1}$$

The starting point is generally to replace Q in Eq. (1) by unity:

$$\psi_0^R = \varphi_0 + \frac{1}{e} v\psi_0^R , \tag{2}$$

thus neglecting the effect of the Pauli exclusion principle. It is well known that this is a poor approximation in finite nuclei. It is acceptable, however, because the exact g matrix

$$g = v + v\frac{Q}{e} g \tag{3}$$

can then be accurately determined from the reference spectrum g matrix

$$g_R = v + v\frac{1}{e} g_R \tag{4}$$

through the relationship[2]:

$$g = g_R + g\left(\frac{Q-1}{e}\right) g_R . \tag{5}$$

Corrections to the reference spectrum wave function ψ^R are the subject of this paper. Let us begin by defining the defect functions:

$$\chi_0 = \psi_0 - \varphi_0 = \frac{Q}{e} g\varphi_0 \tag{6}$$

and

$$\chi_0^R = \psi_0^R - \varphi_0 = \frac{1}{e} g_R\varphi_0 . \tag{7}$$

Combining Eqs. (5)–(7) one obtains:

$$\begin{aligned}\chi_0 &= \frac{Q}{e} g_R\varphi_0 + \frac{Q}{e} g\left(\frac{Q-1}{e}\right) g_R\varphi_0 \\ &= Q\chi_0^R + \frac{Q}{e} g(Q-1)\chi_0^R .\end{aligned} \tag{8}$$

Now consider the operator $P \equiv 1 - Q$, which can be written as

$$P = \sum_d |\varphi_d\rangle\langle\varphi_d| . \tag{9}$$

The Brueckner form of the Pauli operator prohibits any nucleon from being scattered into an occupied state, including those states defining φ_0. We designate all such forbidden states by d in Eq. (9). One then has

$$P\chi_0^R = \sum_d \langle\varphi_d|\chi_0^R\rangle\varphi_d . \tag{10}$$

Substituting Eq. (10) into Eq. (8) we obtain:

$$\begin{aligned}\chi_0 &= \chi_0^R - \sum_d \langle\varphi_d|\chi_0^R\rangle\varphi_d - \frac{Q}{e} g \sum_d \langle\varphi_d|\chi_0^R\rangle\varphi_d \\ &= \chi_0^R - \sum_d \langle\varphi_d|\chi_0^R\rangle\psi_d ,\end{aligned} \tag{11}$$

where ψ_d is the correlated wave function corresponding to φ_d:

$$\psi_d = \varphi_d + \chi_d = \varphi_d + \frac{Q}{e} v\psi_d . \tag{12}$$

Eq. (11) can be arranged into a more compact form:

$$\begin{aligned}\psi_0^R &= \psi_0 + \sum_d \langle\varphi_d|\chi_0^R\rangle\psi_d \\ &= \sum_d (\langle\varphi_d|\varphi_0\rangle + \langle\varphi_d|\chi_0^R\rangle)\psi_d \\ &= \sum_d \langle\varphi_d|\psi_0^R\rangle\psi_d .\end{aligned} \tag{13}$$

To extract ψ_0 out of Eq. (13) one must calculate reference spectrum wave functions[3] in the space d

$$\psi_d^R \equiv \varphi_d + \frac{1}{e} v\psi_d^R , \tag{14}$$

so that Eq. (13) is generalized into

$$\psi_{d'}^R = \sum_d \langle\varphi_d|\psi_{d'}^R\rangle\psi_d . \tag{15}$$

Then one simply solves Eq. (15) for ψ_0 by matrix inversion. Note that the transformation matrix is not unitary. ψ_d and the ψ_d^R form sets of functions which are neither normalized nor orthogonal, nor is either set complete. Equation (15) is, however, very easy to set up and solve numerically with modern electronic computers. In practical applications the space defined by d will be of infinite dimension, and thus must be truncated as an approximation. The same problem is present in Pauli correcting the g matrix elements through Eq. (5). In most calculations on finite nuclei it is found that retaining less than 20 functions in d yields acceptable accuracy.[4,5]

A fair approximation for Eq. (15) can frequently be obtained merely by limiting the space d to one function, φ_0. In this case one obtains

$$\psi_0 \cong (\langle\varphi_0|\psi_0^R\rangle)^{-1}\psi_0^R , \tag{16}$$

which can be rewritten

$$\chi_0 \cong (1+\langle\varphi_0|\chi_0^R\rangle)^{-1}(\chi_0^R - \langle\varphi_0|\chi_0^R\rangle\varphi_0). \tag{16'}$$

The approximation often attempted (but seldom published[6]) in place of Eq. (16′) is

$$\chi_0' \approx \chi_0^R - \langle\varphi_0|\chi_0^R\rangle\varphi_0 . \tag{16''}$$

Equation (16′) is just as easy to calculate as Eq. (16″), and by far superior. In particular if one is working with a hard core potential, one should have within the core radius

$$\chi_0 = \chi_0^R \equiv -\varphi_0 .$$

This condition is violated for χ_0'. On the other hand Eq. (15) retains all boundary conditions on χ at any order of approximation.

To illustrate the procedure we calculate the Pauli correction appropriate for two nucleons in the $0p$ shell coupled to the $^1S_0$ state, using the Reid soft core interaction. This example is chosen because the $^1S_0$ component of modern nuclear interactions is the strongest partial wave which does not involve any channel coupling. The needed overlap integrals, truncated at the $0s2s$ configuration, are displayed in Table I. One simply inserts these into Eq. (15) and solves for $\psi(0p^2)$ by matrix inversion (all states must obviously be coupled to $^1S_0$ so we omit that designation).

TABLE I. Overlap integrals $\langle\varphi(n_1l_1n_2l_2)|\psi^R(n_1'l_1'n_2'l_2'$ needed in the $^1S_0$ state, with $\hbar\omega = 16$ MeV and $W = -30$ MeV.

Φ \ Ψ	$0p^2$	$0s^2$	$0s1s$	$0s2s$
$0p^2$	1.082	−0.046	0.029	0.030
$0s^2$	−0.080	1.151	0.080	0.024
$0s1s$	0.029	0.046	1.082	0.045
$0s2s$	0.019	0.010	0.030	1.033

$$\psi(0p^2) = 0.928\psi^R(0p^2) + 0.066\psi^R(0s^2) - 0.027\psi^R(0s1s) - 0.017\psi^R(0s2s) + \cdots . \tag{17}$$

Coefficients for the remaining components ($0s3s$, $0s4s$, ...) converge quite rapidly because the appropriate Moshinsky-Brody brackets:

$$|n_1l_1n_2l_2L\rangle = \sum \langle nlN\mathfrak{L}L|n_1l_1n_2l_2L\rangle\,|nlN\mathfrak{L}L\rangle , \tag{18}$$

needed to calculate the two-body overlap integral:

$$\langle\varphi(n_1l_1n_2l_2L)|\psi^R(n_1'l_1'n_2'l_2'L\rangle = \sum_{nln'l'N\mathfrak{L}} \langle n_1l_1n_2l_2L|nlN\mathfrak{L}L\rangle\langle n'l'N\mathfrak{L}L|n_1'l_1'n_2'l_2'L\rangle \times\langle\varphi(nl)|\psi(n'l')\rangle \tag{19}$$

will force the terms $\langle\varphi(0sns)|\psi^R(0p^2)\rangle$ rapidly toward zero for increasing values of n. Since only one of the Pauli corrected wave functions given by inversion of Eq. (15) has significance in this case [$\psi(0p^2)$] convergence should be adequate. Of course, the actual number of terms needed will depend on the sensitivity of any dynamical variable to be calculated to the higher configurations. At any rate, this convergence will offer the same difficulty in any method for correcting ψ^R.

Previously published methods[7,8,10] for calculating Pauli corrected correlated wave functions normally start by including some approximation for Q directly in the Bethe-Goldstone equation, rather than making the Pauli correction afterward. The procedure most closely resembling the one presented here is that of Becker, MacKeller, and Morris,[9] who start by setting $Q = 1 - P$ [as in Eq. (9) of this paper]. This yields the Bethe-Goldstone equation in the form:

$$(e - v)\psi_0 = e\varphi_0 - \sum_d \varphi_d\langle\varphi_d|v|\psi_0\rangle . \tag{20}$$

The effect of the Pauli operator (the last term on the right) is to change the character of the original inhomogenous differential equation into an inhomogenous integrodifferential equation. Becker, MacKeller, and Morris find that Eq. (20) is not too hard to solve, however, so long as the number of states included in d is not very large.

The procedure presented in this paper has a twofold advantage. First of all, it is extremely easy to calculate the overlap integrals and reference spectrum wave functions needed in Eq. (15). More important is the fact that calculations for the Pauli corrected wave functions can now be done directly in the appropriate two-particle space. It is, there-

fore, very easy to avoid the approximation that Q commutes with the center of mass motion for two nucleons. We see from Eq. (19) that it is very natural to do the calculation in two-particle space $(n_1 l_1 n_2 l_2)$; since one must use the Moshinsky-Brody in either case the usual approximation, where one assumes that Q commutes with the center of mass motion and performs the correction in relative coordinates, would be a nuisance.

Applications of the reference spectrum method to finite nuclei sometimes include a modified spectrum of particle states (e') as well as initial suppression of the Pauli principle. In this case one must also make a spectral correction, which is not included in Eq. (15).

---

*Supported by a research grant from the University of Kansas.

[1]H. A. Bethe, B. Brandow, and A. G. Petschek, Phys. Rev. 129, 225 (1963).

[2]Both g and g_R are taken to be Hermitian. In Ref. 1 it is demonstrated that this will be the case so long as the starting energy (W) is the propagator

$$e^{-1} \equiv (W - H_0)^{-1}$$

is regarded as a constant.

[3]It is important to emphasize that all the ψ_d^R in Eq. (14) are computed with the same starting energy. Thus only one of the $\psi_d(\psi_0)$ usually has physical significance. The others are derived with an inappropriate value of W, and are computed strictly for the purposes of making the Pauli correction.

[4]H. S. Kohler and R. J. McCarthy, Nucl. Phys. 86, 611 (1966); A99, 65 (1967); A106, 313 (1967).

[5]R. K. Tripathi and P. Goldhammer, Phys. Rev. C 6, 101 (1972).

[6]M. C. Bruels, Ph.D. thesis, University of Kansas, 1969 (unpublished).

[7]M. Baranger, in *Nuclear Structure and Nuclear Reactions, Proceedings of the International School of Physics, "Enrico Fermi," Course XL,* edited by M. Jean and R. Ricci (Academic, N. Y., 1969), p. 511.

[8]G. F. Bertsch, *The Practitioner's Shell Model* (North-Holland, Amsterdam, 1972).

[9]R. L. Becker, A. D. MacKeller, and B. M. Morris, Phys. Rev. 174, 1264 (1968).

[10]B. R. Barret, R. G. L. Hewitt, and R. J. McCarthy, Phys. Rev. C 3, 1137 (1971).