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A system of A particles has 3A degrees of freedom of which 3(A-1) associated with the intrinsic motion (the motion of the particles with respect to their c.m.) and 3 associated with the c.m. motion. The intrinsic wave function depends only on the 3(A-1) intrinsic coordinates. For fermions it must be antisymmetric, and complete sets of antisymmetric wave functions can be easily obtained only by keeping all the 3A coordinates. Wave functions depending on all the 3A coordinates are acceptable as intrinsic wave functions provided their dependence on the c.m. coordinate is factorized /1/

$$\Psi_n = \Psi_{In}\ \chi(\boldsymbol{R}),\ \langle\chi|\chi\rangle = 1,\ \boldsymbol{R} = \frac{1}{A}\sum_{i}^{A} \boldsymbol{r}_i\,,\quad \Psi_{In}\ \text{independent of}\ \boldsymbol{R}\,, \tag{1}$$

with the same factor χ for every state n. Indeed the factor χ is irrelevant to intrinsic motion, while it is possible to describe effects involving the physical c.m. motion by properly correcting /2/ for the unphysical factor χ. Since factorized wave functions are the unique known shell model wave functions useful for the description of intrinsic states, a wave function is said spurious unless it is factorized, and the factor depending on R is the one assigned in the definition (1).

In the Bloch-Horowitz theory /3/ a complete basis is needed, and complete factorized bases are not explicitly available. It is the scope of this note to provide a simple tool for obtaining factorized eigen-functions in the framework of the Bloch-Horowitz theory using a non factorized basis.

2. Let us consider the exact nuclear eigenvalue equation

$$(H_I - E_n)\Psi_{In} = 0, \quad H_I = \sum_i^A \frac{p_i^2}{2m} - \frac{P^2}{2Am} + \sum_{i<j}^A v_{ij}, \quad P = \sum_i^A p_i, \tag{2}$$

and see how eigenfunctions of the form (1) can be obtained by using as a basis Slater determinants of single particle wave-functions.

Let us replace /4/ H_I by $H_I + H_{CM}$, with

$$H_{CM} = \beta\left(\frac{P^2}{2Am} + \frac{1}{2} A k_0 R^2 - \frac{3}{2}\hbar\sqrt{\frac{k_0}{m}}\right),$$

k_0 and β arbitrary parameters. Since H_I and H_{CM} commute with each other the eigenfunctions Ψ_n of

$$(H_I + H_{CM} - E_n)\Psi_n = 0, \tag{3}$$

belonging to eigenvalues E_n satisfying the inequality

$$|E_n - E_0| < \beta\hbar\sqrt{\frac{k_0}{m}},$$

are factorized and have as a factor the ground state harmonic oscillator wave function which we denote by $\chi_0(R)$

$$\Psi_n = \Psi_{In} \ \chi_0 (R). \tag{4}$$

By choosing conveniently the constant $\beta\hbar\sqrt{\frac{k_0}{m}}$ we can obtain factorized eigenfunctions in the region of the energy spectrum we are interested in.

In terms of the relative and c.m. coordinates and momenta

$$r_{il} = \frac{1}{\sqrt{2}}(r_i - r_l), \quad R_{il} = \frac{1}{\sqrt{2}}(r_i + r_l),$$

$$p_{il} = \frac{1}{\sqrt{2}}(p_i - p_l), \quad P_{il} = \frac{1}{\sqrt{2}}(p_i + p_l),$$

H_{CM} has the following expression

$$H_{CM} = \frac{\beta}{A-1}\left\{\sum_{i<l}^{A}\left(\frac{P_{il}^2}{2m} + \frac{k_0}{2} R_{il}^2 - \frac{3}{2}\hbar\sqrt{\frac{k_0}{m}}\right) - \frac{A-2}{A}\sum_{i<l}^{A}\left(\frac{p_{il}^2}{2m} + \frac{k_0}{2} r_{il}^2 - \frac{3}{2}\hbar\sqrt{\frac{k_0}{m}}\right)\right\}. \tag{5}$$

To impose the form (4) to the eigenfunctions Ψ_n means to impose that their expansion in harmonic oscillator wave functions contains about the same number of excitations of the c.m. as of the relative motion of the pairs.

We can now apply /5/ the Bloch-Horowitz theory /3/ to eq. (3), which gives

$$(H_0 + V_{E_n} - E_n) P \Psi_n = 0, \tag{6a}$$

$$V_{E_n} = V\left(1 + \frac{Q}{E_n - H_0} V_{E_n}\right), \tag{6b}$$

where

$$H_0 = \sum_i^A \left(\frac{p_i^2}{2m} + U_i\right), \quad V = \sum_{i<l}^A v_{il} - \frac{P^2}{2Am} - \sum_i^A U_i + H_{CM} = \sum_{i<l}^A v'_{il}, \tag{7}$$

U_1 is a single particle potential, and P and Q are projection operators defined with the eigenfunctions of H_0

$$(H_0 - \epsilon_\nu)\Phi_\nu = 0, \quad P = \sum_1^N |\Phi_\nu\rangle\langle\Phi_\nu| , \quad Q = 1 - P . \tag{8}$$

The space P is called the model space. Eqs. (6) with (7) and (8) are equivalent to eq. (3) in the sense that the eigenvalues of eq.(6a) are eigenvalues of eq. (3) and the corresponding eigenfunctions are projections of the eigenfunctions of eq. (3) on P. We see that in order to evaluate the effective interaction V_{En} we need the complete basis Φ_ν.

Eqs. (6) are generally further transformed /6/, but the forms they can be given do not affect the problem at hand.

Let us observe that in principle lack of factorization in the exact eigenfunctions Ψ_n can introduce errors only in transition amplitudes. In practice, due to the approximations introduced in the evaluation of V_{En}, errors of order $\frac{1}{A}$ will appear also in energy. The errors in transition amplitudes can be much greater than order $\frac{1}{A}$ if either coherent spurious effects are present /7/ (1^- excited states) or high momentum transfers are involved. So taking into account the c.m. coordinate is important in order to prevent these effects in transition amplitudes and prevent errors of order $\frac{1}{A}$ in the energy of light nuclei.

Some spurious components can be eliminated from P if it is possible to construct in it exact excited states of H_{CM} (this happens in practice only with harmonic oscillator single particle wave functions). Let us call Θ_a all these excited states and construct the operator $P' = \sum_a |\Theta_a\rangle\langle\Theta_a| \in P$. Since Ψ_n is orthogonal to P' we can expand it into an arbitrary basis in $P_0 = P - P'$ and solve eq.(6a) in P_0. This does not eliminate completely spurious components in P because in general P_0 has components both on the ground state and on the excited states of H_{CM} . If the single particle wave functions are harmonic oscillator wave functions and P encloses all and only the configurations with excitation energy less or equal to $\nu\hbar\omega$ (ν integer, ω the oscillator frequency), then P_0 is orthogonal to the excited states of H_{CM} , and spurious components can be exactly prevented in P solving eq. (6a) in the factorized basis of P_0 . In any case spurious components are left in Q unless H_{CM} is taken into account.

Let us see which is the effect of H_{CM} on energies. In order to do this let us consider eqs. (6) with $V' = V - H_{CM}$ instead of V . Let us define the wave operators Ω_{E_n} and Ω'_{E_n}

$$V_{E_n} = V\,\Omega_{E_n} \,, \qquad (9)$$
$$V'_{E_n} = V'\Omega'_{E_n} \,.$$

These operators satisfy the equations

$$\Omega_{E_n} = 1 + \frac{Q}{E_n - H_0} V\,\Omega_{E_n} \,, \qquad (10)$$
$$\Omega'_{E_n} = 1 + \frac{Q}{E_n - H_0} V'\Omega'_{E_n} \,.$$

From eqs. (6), (9) and (10) it follows /8/ .

$$V_{E_n} = V'_{E_n} + \Omega'^{+}_{E_n} H_{CM}\Omega_{E_n} \,, \qquad (11)$$

which in first approximation becomes

$$V_{E_n} \approx V'_{E_n} + \Omega'^{+}_{E_n} H_{CM}\,\Omega'_{E_n} \,. \qquad (12)$$

Since the second term in eq. (12) is positive semi-definite, it will decrease in general the binding energy.

Let us consider now the case in which $P' \neq 0$ and P_0 is orthogonal to the excited states of H_{CM}, so that spurious components can be exactly prevented in P using the factorized basis of P_0. However if we use the effective interaction V'_{E_n} spurious components will remain in Q. In order to see their effect let us write eq. (11) more explicitly

$$V_{E_n} = V'_{E_n} + \Omega'^{+}_{E_n} H_{CM} \Omega_{E_n} = V'_{E_n} + H_{CM} +$$

$$+ \Omega'^{+}_{E_n} V' \frac{Q}{E_n - H_0} H_{CM} \frac{Q}{E_n - H_0} V \Omega_{E_n} + \tag{13}$$

$$+ \Omega'^{+}_{E_n} V' \frac{Q}{E_n - H_0} H_{CM} + H_{CM} \frac{Q}{E_n - H_0} V \Omega_{E_n} .$$

Since the basis wave functions in the model space P_0 contain χ_0 as a factor, and $H_{CM}\, \chi_0 = 0$, the matrix elements of V_{E_n} are

$$< V_{E_n} > = < V'_{E_n} > + < V'_{E_n} \frac{Q}{E_n - H_0} H_{CM} \frac{Q}{E_n - H_0} V_{E_n} >, \tag{14}$$

which in first approximation become

$$< V_{E_n} > \approx < V'_{E_n} > = + < V'_{E_n} \frac{Q}{E_n - H_0} H_{CM} \frac{Q}{E_n - H_0} V'_{E_n} > . \tag{15}$$

This shows what corrections still can arise from the space Q. These corrections still will decrease in general the binding energy since the second term of eq. (15) is positive semi-definite.

In standard calculations using V' the term $\frac{P^2}{2Am}$ is usually neglected, and the constant $\frac{1}{2} \frac{3}{2} \hbar \sqrt{\frac{k_0}{m}}$ which should represent the kinetic energy of the c.m. is substracted from the eigenvalues. This is exactly equivalent to replace in the present scheme H_{CM} by $\frac{P^2}{2Am} - \frac{1}{2}\frac{3}{2}\hbar\sqrt{\frac{k_0}{m}}$. Due to the fact that in these calculations the c.m. state is not qualitatively different from χ_0 and $\langle \chi_0 \frac{P^2}{2Am} \chi_0 \rangle = \langle \chi_0 \frac{1}{2} A k_0 R^2 \chi_0 \rangle$, we must expect effects similar to those described by eqs. (12) and (15). If fact these effects show up in the calculation on He^4 by Kuo and Mc Grory /9/. They use harmonic oscillator single particle potentials and the effective interaction derived from the Hamada-Johnston potential. The model space encloses all and only the configurations with excitation energy less or equal to $2\hbar\omega$ i.e. $(0s)^4$, $(0s)^2(0p)^2$, $(0s)^3(1s)$ and $(0s)^3(0d)$, so that spurious components in the model space can be exactly prevented using the factorized basis in it. The calculation with the factorized basis (i.e. taking into acoount a part of the correction of e.q. (12)) gives a binding energy of 21.3 MeV, while with the non factorized basis gives a binding energy of 27.4 MeV. The difference is of order 1/A. The result must still be corrected for the second term of eq. (15), which would presumably reduce the binding energy still further.

3. Calculations in the framework of the Bloch-Horowitz theory are expansions /6/ involving the two-body reaction matrix G. The equation defining G can be put into the form

$$G(\omega) = v' + v' \frac{q}{\omega - h_0} G(\omega), \tag{16}$$

where q is the two-body projection operator out of the model space, h_0 is the two-particle Hamiltonian $\frac{p_1^2}{2m} + \frac{p_2^2}{2m} + U_1 + U_2$, v' is defined by eq. (7), and the energy parameter ω depends on the problem at hand. Eq. (16) is generally solved in terms of the Bethe-

-Goldstone wave function ψ which satisfies the equations

$$G\phi = v'\psi \quad , \quad \psi = \phi + \frac{q}{\omega - h_0} v'\psi \; , \tag{17}$$

where ϕ is an eigenfunction of h_0 .

Errors due to lack of factorization are connected with the unaccurate treatment of the Pauli operator q which is not diagonal in relative and c.m. coordinates. The most accurate way to treat q in the Bethe-Goldstone equation, seems the method recently proposed by Truelove and Nicholls /10/.

It remains to investigate numerically the dependence of energies on β and k_0 /11/, (exact energies do not depend on them). Increasing β -reduces the spurious admixtures /7/, but increases the effects of the left spuriousity.

If we use harmonic oscillator single-particle potentials

$$V = \sum_{i<j}^{A} v'_{ij} = \sum_{i<j}^{A} v_{ij} - \sum_{i}^{A} \frac{1}{2} k_0 r_i^2 - \frac{P^2}{2Am} + H_{CM} =$$

$$= \sum_{i<j}^{A} v_{ij} + \frac{\beta-1}{A-1} \sum_{i<j}^{A} \left(\frac{P_{ij}^2}{2m} + \frac{1}{2} k_0 R_{ij}^2 - \frac{\beta}{\beta-1} \frac{3}{2} \hbar \sqrt{\frac{k_0}{m}} \right) +$$

$$- \sum_{i<j}^{A} \left[\frac{(\beta-1)(A-2)}{A(A-1)} \frac{p_{ij}^2}{2m} + \frac{\beta(A-2)+A}{A(A-1)} \frac{k_0}{2} r_{ij}^2 - \frac{\beta(A-2)}{A(A-1)} \frac{3}{2} \hbar \sqrt{\frac{k_0}{m}} \right].$$

For $\beta = 1$

$$v'_{ij} = v_{ij} - \frac{2}{A} \frac{k_0}{2} r_{ij}^2 - \frac{2}{A(A-1)} \frac{3}{2} \hbar \sqrt{\frac{k_0}{m}} .$$

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11. As it has been discussed in ref. (4), in practice k_0 is not a free parameter. In fact the space P contains only a few linearly independent states of the c.m., so that k_0 must be of order $m \epsilon^2 / h^2$, where ϵ is the average difference of single particle energy from shell to shell.

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