Microscopic Calculation of Rearrangement Energies in ^{16}O†

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The second- and third-order rearrangement contributions to the single-particle energies in ^{16}O are calculated microscopically using the Sprung-de Tourreil force. The s-state second-order rearrangement has been evaluated by an energy-averaging procedure proposed by Engelbrecht and Weidenmüller. The second order is as big as the third for p states and much bigger for the s state. Thus it should be included before comparison to experiment. The average rearrangement energy per particle is 10.5 MeV and the s-state spreading width 13 MeV.

In the present work we compute the rearrangement energy in ^{16}O entirely microscopically, starting from a two-body interaction and calculating explicitly the second- and third-order contributions to the single-particle energies [Figs. 1(a) and 1(b)].

The first calculations of rearrangement corrections in nuclear matter by Brueckner *et al.*[1,2] and by Köhler[3,4] indicated the importance of these corrections to the single-particle energies. Brueckner, Gammel, and Kubis[2] obtained for the contribution of diagram 1(a) 26.8 MeV at the bottom and 4.4 MeV at the top of the Fermi sea. Calculations using nonlocal density-dependent single-particle potentials in nuclear matter by Brueckner, Meldner, and Perez[5,6] and in finite nuclei by Meldner and Shakin[7] again indicated large rearrangement contributions to the separation energies. A similar conclusion may be drawn from the recent density-dependent Hartree-Fock calculations of various authors.[8-11] We note here that in ^{16}O all separation energies are known experimentally[12]; they lead to an experimental estimate of the average rearrangement energy of approximately 8 MeV per particle.[13]

Regarding evaluations of rearrangement energies in finite nuclei by explicit computation of diagrams with finite-nucleus wave functions (without making use of nuclear-matter results), we note that while the third-order rearrangement contribution [Fig. 1(b)] has been treated in the framework of renormalized Brueckner-Hartree-Fock theory by various authors,[14,15] there is for the second-order term apparently only one microscopic result calculated with a G matrix, that of Becker and Patterson.[16] Bassichis and Strayer[17] have also considered a second-order rearrangement, calculated with the bare Tabakin interaction.

We first compute the single-particle energies taking into account the third-order rearrangement diagram 1(b). Thus

$$\epsilon_i = \epsilon_i^0 + \Delta_i^3 , \tag{1}$$

where

$$\epsilon_i^0 = t_i + \sum_{k\,\mathrm{occ}} \langle ik|G|ik\rangle , \tag{2}$$

and

$$\Delta_i^3 = \sum_{k\,\mathrm{occ}} \langle ik|G|ik\rangle \rho_{kk}^1 \tag{3}$$

is the third-order correction. Here

$$\rho_{kk}^1 = -\frac{1}{2} \sum_{\substack{j\ \mathrm{occ} \\ m,n\ \mathrm{unocc}}} \frac{|\langle kj|G|mn\rangle|^2}{(\epsilon_k^0 + \epsilon_j^0 - \epsilon_m^0 - \epsilon_n^0)^2} \tag{4}$$

represents the occupation-probability correction.[18] The total energy is computed according to Bran-

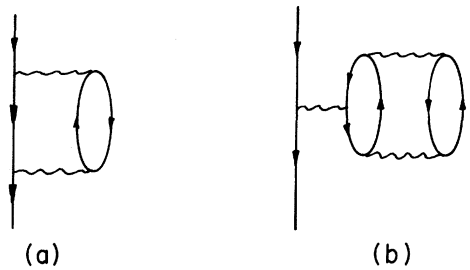

FIG. 1. Second-order (a) and third-order (b) rearrangement contributions to the single-particle energies of occupied states.

dow's prescription,[18] which we express as[19]

$$E = E^0 + E^{\text{corr}}, \tag{5}$$

with

$$E^0 = \sum_{i\ \text{occ}} t_i + \frac{1}{2} \sum_{i,k\ \text{occ}} \langle ik|G|ik\rangle \tag{6}$$

and

$$E^{\text{corr}} = \frac{1}{2} \sum_{i,k\ \text{occ}} \rho^1_{ii} \langle ik|G|ik\rangle \rho^1_{kk} . \tag{7}$$

E^{corr} is the four-body-cluster energy corresponding to the diagram of Fig. 2(a).

In the next step the single-particle energies (1) and the occupation-probability corrections (4) are used to compute the diagonal part of the second-order diagram 1(a). This diagram represents the lowest-order off-shell contribution to the self-energy operator M and is energy dependent:

$$M^{\text{off}}_{ii}(\omega) = \sum_{\substack{j,k\ \text{occ} \\ m\ \text{unocc}}} \frac{|\langle im|G|jk\rangle|^2 (1+\rho^1_{jj})(1+\rho^1_{kk})}{\omega + \epsilon_m - \epsilon_j - \epsilon_k - i\delta} \tag{8}$$

where δ is a positive infinitesimal. The matrix elements appearing in all these equations are antisymmetrized. The G matrix is to be evaluated on shell as shown in Ref. 6.

The single-particle energies corrected for the second-order process 1(a) appear as the solutions of the self-consistency equation

$$\omega = \epsilon_i + M^{\text{off}}_{ii}(\omega) . \tag{9}$$

In our calculation, $M^{\text{off}}_{pp}(\omega)$ for the p states is a smooth function of ω in the relevant energy interval and was computed without energy averaging. In contrast, the s-state self-energy operator $M^{\text{off}}_{ss}(\omega)$ has poles on the real axis corresponding to the 2h-1p excitations and is a strongly varying function of ω. Following the suggestion of Engelbrecht and Weidenmüller[20] we have performed an averaging of $M^{\text{off}}(\omega)$ over an energy interval $\tau > d$, where d is the average spacing between the energies of 2h-1p configurations:

$$\langle M^{\text{off}}(\omega)\rangle_\tau = M^{\text{off}}(\omega + i\tau) . \tag{10}$$

The expressions for the real and imaginary parts of $\langle M^{\text{off}}(\omega)\rangle$ are:

$$\text{Re}\langle M^{\text{off}}_{ii}(\omega)\rangle = \sum_{\substack{j,k\ \text{occ} \\ m\ \text{unocc}}} \frac{(\omega + \epsilon_m - \epsilon_j - \epsilon_k)|\langle im|G|jk\rangle|^2 (1+\rho^1_{jj})(1+\rho^1_{kk})}{(\omega + \epsilon_m - \epsilon_j - \epsilon_k)^2 + \tau^2} , \tag{11}$$

$$\text{Im}\langle M^{\text{off}}_{ii}(\omega)\rangle = -\sum_{\substack{j,k\ \text{occ} \\ m\ \text{unocc}}} \frac{\tau|\langle im|G|jk\rangle|^2 (1+\rho^1_{jj})(1+\rho^1_{kk})}{(\omega + \epsilon_m - \epsilon_j - \epsilon_k)^2 + \tau^2} . \tag{12}$$

The s-state quasiparticle pole ω_s is again given by the solution of the self-consistency equation

$$\omega = \epsilon_i + \text{Re}\langle M^{\text{off}}_{ii}(\omega)\rangle . \tag{13}$$

The spreading width of the s-state quasiparticle and the residue of the quasiparticle pole are given by

$$\Gamma_s = 2\text{Im}\langle M^{\text{off}}_{ss}(\omega_s)\rangle \tag{14}$$

and

$$\text{Res}\langle M^{\text{off}}_{ss}(\omega_s)\rangle = \left(1 - \frac{\partial\, \text{Re}\langle M_{ss}(\omega)\rangle}{\partial\omega}\bigg|_{\omega=\omega_s}\right)^{-1} . \tag{15}$$

The present calculation has been performed with a recent realistic soft-core two-body force of de Tourreil and Sprung[21] (their potential C) which fits the two-body data very well. The tensor component is fairly strong, giving a deuteron d-state probability of 5.5%. Nuclear-matter calculations with this potential, performed in second-order perturbation theory and in Brueckner theory, agree closely with each other, saturation occurring at $k_F \approx 1.6$–1.7 fm^{-1} with $E/A \approx -17$ MeV. The wound integral is $K \approx 0.075$ at saturation.

These results seem to justify the use of this force in second-order perturbation in nuclei. Thus for our effective G matrix we have renormalized the bare interaction up to second-order ladder diagrams. Furthermore, we have followed the prescription of Kerman and Pal,[22] which uses plane waves for the intermediate states. For the parameters appearing in the renormalization we

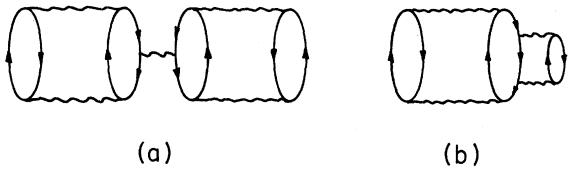

FIG. 2. Two four-body cluster contributions to the ground-state energy, corresponding to third-order (a) and second-order (b) rearrangement contributions.

TABLE I. Effective G-matrix single-particle energies ϵ^0, occupation-probability corrections ρ^1, third- and second-order rearrangement corrections (Δ^3 and Re $\langle M^{\rm off}\rangle$, respectively), and final theoretical (e_p) and experimental ($e_p^{\rm exp}$) proton single-particle energies. $\Delta^{\rm Coul}$ and $\Delta^{\rm c.m.}$ are Coulomb and center-of-mass corrections.

	$0s_{1/2}$	$0p_{3/2}$	$0p_{1/2}$
ϵ^0	−54.8	−26.3	−21.4
ρ^1	−0.055	−0.081	−0.100
Δ^3	4.9	3.6	3.2
$\Delta^{\rm Coul}$	3.9	3.6	3.6
$\mathrm{Re}\langle M^{\rm off}\rangle$	17.1	3.0	3.8
$e_p = \epsilon^0 + \Delta^3 + \mathrm{Re}\langle M^{\rm off}\rangle + \Delta^{\rm Coul} + \Delta^{\rm c.m.}$	−30.5	−16.1	−10.8
$e_p^{\rm exp}$	−44 ± 5	−19.0 ± 1	−12.4 ± 1

have chosen the values $k_F = 1$ fm^{-1} and $\Delta = 20$ MeV.

The diagrams of Fig. 1 were evaluated in the oscillator basis with an oscillator parameter $\gamma = \hbar/m\omega = 2.6$ fm^2. The unoccupied (particle) states in Fig. 1 run through four major shells, from the $1s$-$0d$ shell up to the $2p$-$1f$-$0h$ shell.

The total binding energy E [Eq. (5)], with Coulomb and center-of-mass corrections included, is 113.7 MeV, which is quite satisfactory for a single-oscillator calculation. The four-body-cluster correction $E^{\rm corr}$ [Eq. (7)] contributes 2.3 MeV to E.

In Table I we first show the single-particle energies ϵ^0 and the rearrangement corrections Δ^3. Our occupation-probability corrections are somewhat smaller than those found by McCarthy and Davies[14] using the Hamada-Johnston potential. This difference probably reflects the softness of the de Tourreil-Sprung force. Our rearrangement corrections Δ^3 are also slightly smaller.

Table I also shows the second-order corrections $\mathrm{Re}M^{\rm off}$ and the final single-particle energies for protons as well as the experimental values of Tyrén *et al.*[12] The second-order correction for the s state was obtained using the energy averaging explained earlier. In Fig. 3 we show the curves of $\mathrm{Re}\langle M_{ss}^{\rm off}(\omega)\rangle_\tau$ for several values of the parameter τ. The average spacing d between successive 2h-1p configurations is in our case of the order of 3 MeV. For $\tau = 3$ MeV we see that there are slight oscillations in the curve. The values of 3.5 or 4 MeV for τ are just large enough to smooth out the curve $M_{ss}(\omega)$. The results shown in Table I correspond to $\tau = 4$ MeV. The $\mathrm{Re}M^{\rm off}$ values again represent a sizable rearrangement. In fact, for the more deeply bound state this term is much more important than Δ^3.

The results obtained for $\mathrm{Re}M^{\rm off}(\omega)$ are in very good agreement with nuclear-matter calculations

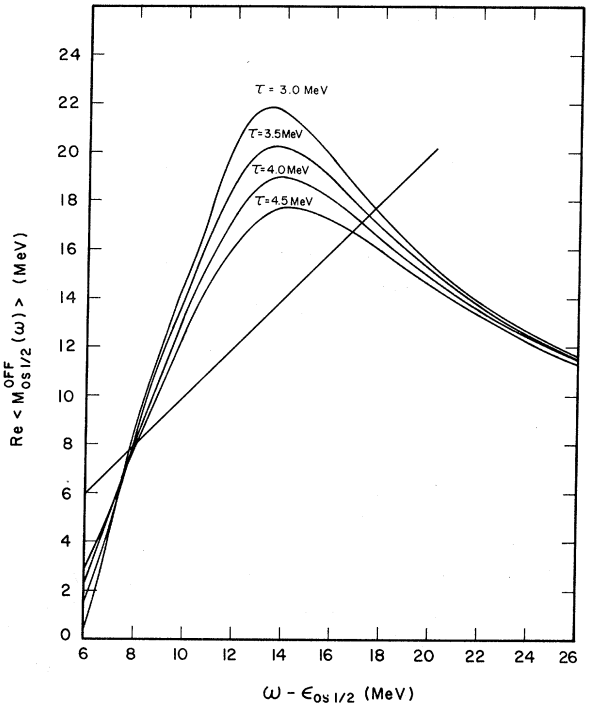

FIG. 3. The curves $< M_{ss}^{\rm off}(\omega) >_\tau$ plotted for four different values of the parameter τ. The intersection points with the 45° straight line give the positions of the quasiparticle pole [Eq. (9)].

of Refs. 2 and 3. Introducing the ratio

$$R_i = \frac{\mathrm{Re}\langle M_{ii}^{\rm off}(\omega)\rangle}{U_{i\,\rm HF}},$$

where

$$U_{i\,\rm HF} = \sum_{k\ \rm occ}\langle ik|G|ik\rangle,$$

we find it to be roughly −0.24 at $k_i/k_F = 0.1$, −0.22 at $k_i/k_F = 0.8$, and −0.06 at $k_i/k_F = 1.0$ in the nuclear-matter calculations. Our calculation in ^{16}O gives: for the deepest bound ($s_{1/2}$) state, $R = -0.26$; for the states at the top of the Fermi sea ($p_{3/2}$ and $p_{1/2}$), $R = -0.07$ and −0.09, respectively. Since the ratio R essentially depends on finite geometry only through the energy denominators[23] in the expression for $\mathrm{Re}M^{\rm off}$, and the energy range of these denominators is roughly the same in nuclear matter and in finite nuclei, R should be quite insensitive to finite geometry. The above-mentioned numbers verify this feature of R.

To compare to the proton separation energies from $(p, 2p)$ experiments, we must also add Coulomb and center-of-mass corrections $\Delta^{\rm Coul}$ and $\Delta^{\rm c.m.}$[24] to the single-particle energies. For the p states the final energies (Table I) are in good

agreement with experiment. For the s state our separation energy is smaller than the Tyrén *et al.*[12] value.[25] We note that a full calculation on a Hartree-Brueckner basis would be of benefit here, since the single-particle energies ϵ_i^0 would be lower (more negative) and therefore the final s-state separation energy would be in closer agreement with experiment. Also, if the interaction used were artificially modified to give more binding, the separation energies would be larger. However, it is also clear that even in a Hartree-Brueckner calculation the binding energy should be smaller than the experimental energy, since various terms (e.g. Bethe-Faddeyev three-body clusters) are not included.

Our final single-particle energies are in rough agreement with those of various density-dependent Hartree-Fock calculations.[8-11] The calculation of Ref. 9 is completely phenomenological and it is difficult to see its diagram content; however, both diagrams that we have explicitly evaluated *are* wholly *included* in calculations such as those of Refs. 8, 10, and 11 for states near the Fermi surface, while for more deeply bound states Refs. 8, 10, and 11 contain only part of the second-order rearrangement.[26]

The average rearrangement energy including both corrections is 10.5 MeV per particle, which is somewhat greater than the experimental estimate.

As for the residue of the s-state quasiparticle [Eq. (15)] it is evaluated as ≈ 0.6, which is quite reasonable. The p-state residues are found to be very close to 1.

When the parameter τ takes the value of 4 MeV, the calculated s-state spreading width Γ_s [Eq. (14)] is 13 MeV, in very good agreement with the experimental value ≈ 14 MeV.[12] The calculated width also agrees closely with a previous theoretical result, 13.7 MeV, of Köhler, obtained using nuclear-matter results and an averaging procedure.[13] Actually, we note that the width Γ_s varies sensitively with τ. For $\tau = 3.5$, $\Gamma_s \approx 11.5$ MeV and for $\tau = 4.5$, $\Gamma_s \approx 14.8$ MeV, so that the value of τ chosen is of some consequence in this respect. We have seen that τ cannot be smaller than d if there are to be no oscillations in $\langle M_{ss}^{\rm off}(\omega)\rangle_\tau$, while too large values of τ are unrealistic, due to the considerable suppression of the correlations.

From the curves $\mathrm{Re}M_i^{\rm off}(\omega)$ for large off-shell values of ω plotted in Fig. 4 it is possible to estimate the contribution of the diagram of Fig. 1(a) to the total energy. This contribution is shown in Fig. 2(b). Here the diagram corresponding to Fig. 1(a) can be treated approximately as an insertion[2] taken at an average 2p-1h energy:

$$\Delta E = \sum_i M_{ii}(\omega = \omega_{2\mathrm{p}-1\mathrm{h}}^{\rm av})\rho_{ii}^1 .$$

For $\omega_{2\mathrm{p}-1\mathrm{h}}^{\rm av} = 70$ MeV we obtain $\Delta E \approx -2$ MeV. This contribution is of the same order of magnitude as $E^{\rm corr} \approx 2.3$ MeV. Of course our value for ΔE is only a rough estimate. A recent careful evaluation of ΔE and $E^{\rm corr}$ in nuclear matter by Köhler[27] indicates that $\Delta E \ll E^{\rm corr}$.

This calculation confirms that the second- and third-order rearrangement corrections in nuclei are indeed important and both should be properly

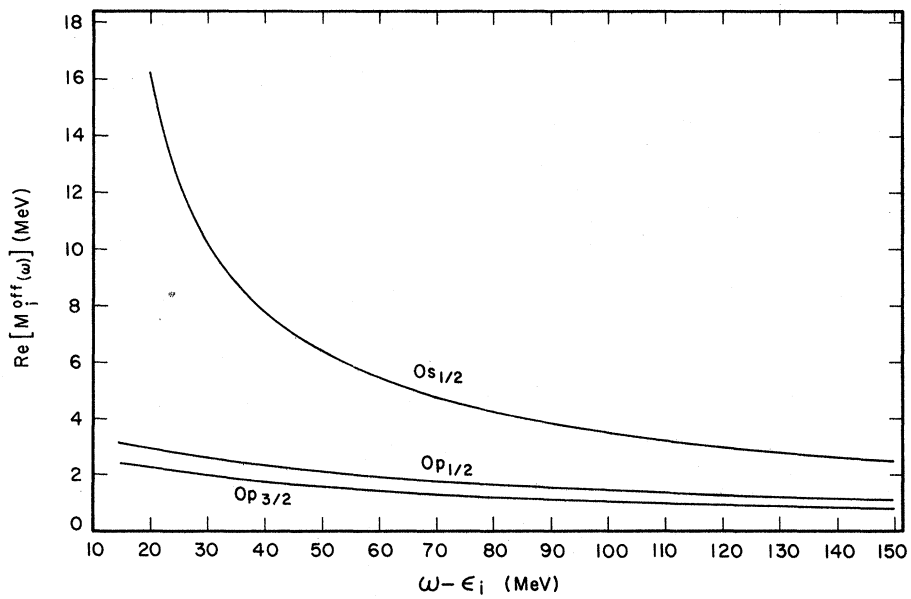

FIG. 4. The nonaveraged curves $M_{ii}^{\rm off}(\omega)$ plotted in the off-shell range of ω.

taken into account when comparing to experimental separation energies. Since the main contribution to the off-shell diagram 1(a) comes from the long-range part of the interaction,[3] any reasonable force should give a non-negligible M^{off}.

In view of the results of this single-oscillator calculation, it would be of interest to perform a complete Brueckner-Hartree-Fock calculation including both rearrangement terms, and with G matrices evaluated from various hard-core and soft-core forces. Furthermore, the inclusion of the nondiagonal terms $M_{ij}^{\text{off}}(\omega)$ in the framework of such a Brueckner-Hartree-Fock calculation should improve saturation in finite nuclei for those forces which tend to give too small a radius.

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