C H A P T E R - 2

Short range correlations in many nucleon system : Variational Approach

1. Variational Method :

Variational calculations based on the work of Jastrow[1] has been developed only recently to take care of the short range correlation although, historically, Jastrow wave function precedes the Bethe-Goldstone model. In principle, if no approximations are made one obtains a rigorous upper bound which is physically useful only if the trial function is sufficiently realistic. It is defined for an A body system -

$$\psi = F \Phi \qquad \ldots \quad 1.1$$

where Φ is the slater determinant for A nucleons. It contains all the statistics and symmetry. The correlation function, on the other hand, has all the dynamics of short range built into it. The energy of the system is obtained from the expectation value of the Hamiltonian consisting of the kinetic energy operator and the two body interaction energy :-

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \qquad \ldots \quad 1.2$$

E is now a function of F. To evaluate equation (1.2) an elaborate technology of approximation schemes has evolved.

Most of them use the correlation function satisfying the following ansatz :-

1) F is symmetric in all particles.

2) $F_A = F_m F_{A-m}$ when any set of m particles in spatially well separated from others (cluster property) ... 1.3

3) $F = \prod_{i<j} f(r_{ij})$ (the Jastrow ansatz[1]) ... 1.4

Where the two body correlation function f approaches unity faster than $1/r^2$, a requirement for h (= f^2-1) to be of short range by definition.

$$F_1 = 1 \text{ and } F_2 = f \qquad \ldots \quad 1.5$$

One of the approximation schemes is the cluster expansion of equation (2). The many body system is taken to be consisting of clusters of 2, 3 and n body. Energy expectation value is also expanded accordingly. But the series has to be truncated to make the calculation managable, hoping that the higher body terms will become small. This idea of cluster expansion has been borrowed from classical statistical mechanics where it has long been used to approximate the partition function.

Two types of cluster expansions [2,3] - Factorised Iwamoto and Yamada (FIY, based on a Van Kampen[4] or 'factor-cluster' decomposition Ansatz) and Aviles, Hartogh and Tolhoek (AHT) have been used in nuclear many-body theory. Basic idea is the same as that of hole line expansion. In the perturbative approach the short range effects are treated in all orders whereas here the two body correlation is restricted and treated as the variational function. As the energy expectation

expansion series is truncated, the variational principle is only approximately valid and it is important that f(r) should be varied within some restricted class of functions for which the approximate method is adequate. This is known as Emery difficulty[5].

It has been found[6] that free variation of the truncated energy functional suffers from two drawbacks : the functional may have an unphysically deep minimum; Secondly, the healing of the correlation function is extremely weak. In fact, the correlation function strongly overshoots in the attractive region of the potential giving a large amount of binding energy, which is not compromised by the increase of the kinetic energy due to particle correlation. It is, therefore, essential to impose on the variation of f(r) certain constraints which confine this function to a domain corresponding to reasonably fast convergence of the cluster expansion.

Restriction on 'f'

This can be of two types :-

Integral type consisting of (a) Pauli condition (b) Normalisation condition.

a) Pauli condition on the two body wave function :-

$$\langle \phi_{kl} | \psi_{mn} - \phi_{mn} \rangle = 0 \quad \ldots \quad 1.6$$

With klmn all Fermi-Sea orbitals. In otherwords, the defect wave function $\psi_{mn} - \phi_{mn}$ should have no components in

Fermi-Sea. This condition, with kl = mn, again may be imposed for an 'average' pair or it may be averaged over the Fermi-Sea. It is motivated from the desire for a close correspondence with Brueckner theory.

b) Normalisation condition on the correlated two-body wave function :-

$$\langle \psi_{mn} | \psi_{mn} \rangle = 1 \qquad \ldots \quad 1.7$$

This condition may be imposed for an average pair or it may be averaged over states of the Fermi-Sea.

2. Differential Type :

The differential equation for f is given by [7,8]

$$\left(-\frac{\hbar^2}{m} \nabla^2 + V - \nu \right) f = 0$$

With $f(r > d) = 1$ and $\frac{df}{dr}(r = d) = 0$ ... 1.8

Where V is the potential and ν is the parameter determined by requiring that f has a zero derivative at a distance d, taken to be the variational parameter for minimising the energy.

There exist numerous applications of the Jastrow variational scheme to finite nuclei [9]. Present work is restricted to the light nuclei system. Excitation will make the nucleus move as a whole. This centre of mass motion has

to be subtracted before the energy expectation value is ~~subtracted~~ subjected to any expansion scheme.

Beautiful work of I.R.Afnan [9] consists of Van-Kampen expansion of the energy expectation value and the consequent numerical application in the mass 3 and 4 system. The Hamiltoniam taken was

$$H = -\frac{\hbar^2}{2m}\sum_{i=1} \nabla_i^2 + \sum_{i<j} V_{ij} \quad \ldots 1.9$$

i.e. a one body kinetic energy operator and a two body interaction.

Centre of mass motion was subtracted by hand later on. In doing so, a two body term is dropped off. We adopt a more systematic approach which is to subtract the center of mass kinetic energy so that the Hamiltonian is now purely for relative motion and then perform the Van-Kampen expansion. An extra, two body gradient term arises in this process. From the very early days of Jastrow calculation one is aware that it is the gradient term which makes the kinetic energy evaluation ambiguous and difficult. The procedure for centre of mass subtraction and the consequent expansion has been given in the next section. To compare with the known results[9,10] some numerical calculations in the mass 3,4 and 16 system have been performed. Details of the calculations are given in Section 3. Results are also summarised in this section.

2. Formalism :

Kinetic energy for the relative motion is -

$$T_{rel} = \sum_{i=1}^{A} \frac{p_i^2}{2m} - \frac{(\sum_{i=1}^{A} p_i)^2}{2Am}$$

$$= -\frac{\hbar^2}{2m} \frac{(A-1)}{A} \sum_{i=1}^{A} \nabla_i^2 + \frac{\hbar^2}{Am} \sum_{i<j} \nabla_i . \nabla_j \quad ..2.1$$

So that the Hamiltonian for relative motion is -

$$H = T_{rel} + \sum_{i<j} V_{ij} \quad \ldots \quad 2.2$$

Where V_{ij} is the two body interaction energy.

Using the trial function given in the equation (1.1) where the correlation function F satisfies the relations given by (1.3- 1.5) we get (See Appendix 'A')

$$\langle T_{rel} \rangle = \int d\tau \ \phi^* F^2 \left[\sum_i T_i + \sum_{i<j} T_{ij} \right] \phi - \frac{\hbar^2}{2m}$$

$$\cdot \int d\tau \ |\phi|^2 F^2 \sum_{i<j} \nabla_r^2 \ln f(r_{ij}) \quad \ldots. \quad 2.3$$

Where, $$T_i \Phi = - \frac{1}{\Phi^*} \frac{\hbar^2}{2m} \frac{(A-1)}{A} \frac{1}{4} \left[\nabla_i^2 |\Phi|^2 - 4 \nabla_i \Phi . \nabla_i \Phi^* \right]$$

... 2.4a

and $$T_{ij} \Phi = \frac{1}{\Phi^*} \frac{\hbar^2}{Am} \frac{1}{4} \left[\nabla_i . \nabla_j |\Phi|^2 - 2 \nabla_i \Phi . \nabla_j \Phi^* - 2 \nabla_i \Phi^* . \nabla_j \Phi \right]$$

... 2.4b

Define $$W_{ij} = V_{ij} - \frac{\hbar^2}{2m} \nabla_r^2 \ln f(r_{ij}) \quad \ldots \quad 2.5$$

as the effective interaction. This amounts to use of Jackson-Feenberg form[11] for kinetic energy. Using (2.4 a-b) and (2.5) the energy expectation value (equation 1.2) is written as -

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\int d\tau \, \Phi^* \prod_{i<j} f^2(r_{ij}) \left[\sum_i T_i + \sum_{i<j} T_{ij} + \sum_{i<j} W_{ij} \right] \Phi}{\int d\tau \, \Phi^* \prod_{i<j} f^2(r_{ij}) \, \Phi}$$

... 2.6

Because of the centre of mass subtraction the energy (equation 2.6) now contains the extra term arising from T_{ij}; otherwise it is the same as I.R. Afnan[9] started with. To accommodate this operator the normalisation integrals are introduced in the same way i.e.,

$$I(\beta) = \int d\tau \quad \Phi^* \prod_{i<j} g(i,j;\beta) \quad \prod_i h(i;\beta)\, \Phi$$

$$= \left\langle \prod_{i<j} g(i,j;\beta) \quad \prod_i h(i;\beta) \right\rangle \quad \ldots\ 2.7$$

Where $\prod_i h(i;\beta) = \exp\left(\beta \sum_i T_i\right)$ is the same as in the reference (9) but -

$$\prod_{i<j} g(i,j;\beta) = \exp\Big(\sum_{i<j} \Big[\ln f^2(r_{ij}) + W_{ij} + T_{ij} \Big] \Big) \quad \ldots \quad 2.10$$

and $$E = \operatorname*{Lt}_{\beta \to 0} \left(\frac{\partial}{\partial \beta} \ln I(\beta) \right) \quad \ldots \quad 2.11$$

E is expanded in 2, 3 particle correlation effects, the one particle effect coming from -

$$I^{(1)}(A,\beta) = \prod_i h(i;\beta) \quad \ldots \quad 2.12$$

So that -

$$E^{(1)} = \operatorname*{Lt}_{\beta \to 0} \left(\frac{\partial}{\partial \beta} \ln I^{(1)}(A,\beta) \right) = \sum_{i=1}^{A} T_i \quad \ldots\ 2.13$$

Next dynamical correlations due to two particle effects are incorporated through -

$$I^{(2)}(A,\beta) = I^{(1)}(A,\beta) \prod_{i<j} \frac{\langle g(i,j;\beta)\, h(i;\beta)\, h(j;\beta)\rangle}{\langle h(i;\beta)\rangle \langle h(j;\beta)\rangle} \qquad 2.14$$

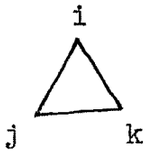
and $$E^{(2)} = \lim_{\beta\to 0} \left(\frac{\partial}{\partial\beta} \ln I^{(2)}(A,\beta) \right)$$

$$= E_1 + E_2 \qquad \ldots \qquad 2.15$$

$$E_1 = E^{(1)} = \sum_i \langle T_i \rangle \qquad \ldots \qquad 2.16$$

$$E_2 = \sum_{i<j} \left[\frac{\langle f^2(r_{ij})\,(W_{ij} + T_{ij} + T_i + T_j)\rangle}{\langle f^2(r_{ij})\rangle} - \langle T_i \rangle - \langle T_j \rangle \right] \qquad \ldots \qquad 2.17$$

Three particle correlation appears from the following type of interaction -



giving rise to 3 particle approximate -

$$I(A,\beta) \simeq I^{(3)}(A,\beta)$$

$$= I^{(2)}(A,\beta) \prod_{i<j<k} \frac{\langle g(i,j;\beta)\, g(i,k;\beta)\, g(j,k;\beta)\, h(i;\beta) h(j;\beta) h(k;\beta)\rangle}{I^{(2)}_{i,j,k}(A,\beta)}$$

Where,

$$I^{(2)}_{i,j,k}(A,\beta) = \frac{\langle g(i,j;\beta)\, h(i;\beta)\, h(j;\beta)\rangle \langle g(i,k;\beta)\, h(k;\beta)\, h(i;\beta)\rangle}{\langle h(i;\beta)\rangle \langle h(j;\beta)\rangle \langle h(k;\beta)\rangle}$$

$$\times \langle g(j,k;\beta)\, h(j;\beta)\, h(k;\beta)\rangle \quad \ldots \quad 2.18$$

and $E^{(3)} = \underset{\beta\to 0}{\mathrm{Lt}} \left[\frac{\partial}{\partial\beta} \ln I^{(3)}(A,\beta)\right] = E_1 + E_2 + E_3$

Where E_1 and E_2 are given by 2.16 and 2.17 and

$$E_3 = \sum_{i<j<k} \left[\frac{\langle f^2(ij) f^2(jk) f^2(ik) \{ W_{ij} + T_{ij} + W_{jk} + T_{jk} + W_{ik} + T_{ik} + T_i + T_j + T_k \}\rangle}{\langle f^2(ij) f^2(jk) f^2(ik)\rangle} \right.$$

$$- \frac{\langle f^2(ij)\left[W_{ij} + T_{ij} + T_i + T_j\right]\rangle}{\langle f^2(ij)\rangle}$$

$$- \frac{\langle f^2(jk)\left[W_{jk} + T_{jk} + T_j + T_k\right]\rangle}{\langle f^2(jk)\rangle}$$

$$- \frac{\langle f^2(ik)\left[W_{ik} + T_{ik} + T_i + T_k\right]\rangle}{\langle f^2(ik)\rangle}$$

$$+ \langle T_i\rangle + \langle T_j\rangle + \langle T_k\rangle \Big] \quad \ldots \quad 2.18$$

So that $E \simeq E^{(3)} = E_1 + E_2 + E_3$ ... 2.19

3. Numerical Results and Conclusion :

Mass 3 and 4 nuclei :

The ϕ of the trial function is chosen to be oscillators. Configurations of the mass A = 3 and 4 nuclei are therefore $(OS_{\frac{1}{2}})^3$ and $(OS_{\frac{1}{2}})^4$ respectively.

For S state orbital -

$$\langle T_i\rangle = \frac{3}{4}\,\frac{(A-1)}{A}\,\frac{h^2}{mb}2 \quad \text{(see Appendix 'B')} \quad \ldots \quad 3.1$$

Define $$J = \frac{\langle f^2\, W(12)\rangle}{\langle f^2\,(12)\rangle} = \frac{\int dr\; r^2 \exp(-r^2/2b^2) f^2\, W(r)}{\int dr\; r^2\, f^2 \exp(-r^2/2b^2)} \qquad \ldots \quad 3.2$$

and $$Z = \frac{\langle f^2\,(12)\, f^2\,(23)\, f^2\,(13)\, W\,(12)\rangle}{\langle f^2\,(12)\, f^2\,(23)\cdot f^2\,(13)\rangle}$$

$$= \frac{\int_0^\infty dr \int_0^\infty ds \int_{|r-s|}^{r+s} dt\; rst\; f^2(r) f^2(s) f^2(t)\, W(r) \exp\left[-(r^2+s^2+t^2)/3b^2\right]}{\int dr \int ds \int_{|r-s|}^{r+s} dt\; rst\; f^2(r) f^2(s) f^2(t) \exp\left[-(r^2+s^2+t^2)/3b^2\right]}$$

Therefore, for A = 4 nuclei

$$E_1 = \frac{9}{4}\,\frac{h^2}{mb^2}$$

$$E_2 = 6J \qquad \ldots \quad 3.4$$

$$E_3 = 12\,(Z - J)$$

and for A = 3 nuclei

$$E_1 = \frac{3}{2}\,\frac{h^2}{mb^2}$$

$$E_2 = 3J \qquad \ldots \quad 3.5$$

$$E_3 = 3\,(Z - J)$$

For S-orbital nuclei $T_{ij}\,\Phi = 0$ and as a consequence the above treatment becomes identical with I.R.Afnan [9]. So, instead of the differential type constraint as used by Afnan, the Pauli condition is put on the correlation function, so that one can compare the results with the same potential but different constraining condition.

Correlation function used is the standard Chakkalakal function[12] for hard core potential :-

$$f(r) = (1 - e^{-\mu(r-r_c)})\,(1 + g\,e^{-\mu(r-r_c)}) \quad \ldots \quad 3.6$$

where g is the overshoot obtained from the Pauli condition (equation 1.8), μ is the variational parameter and r_c is the hard core radius. The potential used is the Tang potential[13] which has exponential attraction in the triplet and singlet s-state :-

$$V_t(r) = \infty \qquad r < r_c$$

$$= -475.044 \exp(-2.5214\,(r-r_c)) \qquad r > r_c$$

$$V_s(r) = \infty \qquad r < r_c$$

$$= -235.414 \exp(-2.0344\,(r - r_c)) \qquad r > r_c$$

With r_c = .4 fm. ... 3.7

The optimised parameters and the ground state energy of A = 3, 4 nuclei are given in the table 1 and 2. Saturation curves are shown in the Figures 1 and 2.

T A B L E - 1

Optimum parameters of f(r) and energies from two body calculation given for three b values.

Mass No.	b (fm)	μ (fm^{-1})	g	E_1 (MeV)	E_2 (MeV)	E (MeV)
A = 4	1.1	1.77	1.60	77.11	-108.87	-31.76
	1.15	1.85	1.57	70.55	-102.54	-31.99
	1.25	1.98	1.52	59.72	- 90.67	-30.95
A = 3	1.25	1.98	1.52	39.81	- 45.33	- 5.52
	1.35	2.072	1.490	34.13	- 39.98	- 5.85
	1.45	2.145	1.467	30.59	- 35.24	- 5.25

T A B L E - 2

Optimum parameters of f(r) and energies from two-and-three body calculation given for three b values

Mass No.	b (fm)	μ (fm^{-1})	g	E_1 (MeV)	E_2 (MeV)	E_3 (MeV)	E (MeV)
A=4	1.15	2.07	1.55	70.55	-102.1	1.88	-29.63
	1.19	2.12	1.53	66.0	- 97.30	1.40	-29.90
	1.25	2.18	1.51	59.72	- 90.34	1.13	-29.50
A=3	1.23	2.046	1.526	41.12	- 46.44	0.40	- 4.92
	1.35	2.152	1.488	34.13	- 39.96	0.23	- 5.60
	1.45	2.216	1.466	29.59	- 35.22	0.15	- 5.48

As observed by Dey et al[14] it is seen from the tables 1 and 2 convergence is pretty good. Generally, differential type of constraintmakes the correlation function much shorter range. Here, it is found that the Pauli condition is just as good a constraint so far as the convergence problem is concerned.

$\langle f^2 T_{ij} \rangle$ (equation 2.7 and 2.8) starts contributing as soon as the S-state gets filled up, for example, in ^{16}O nucleus. It is well known[15] that with harmonic oscillator basis function and using the configuration $(0s)^4 (0p)^{12}$ for ^{16}O nucleus, kinetic

energy contributions with and without centre of mass correction (cmc) are -

$$E_{K.E.}(^{16}O) = 17.25 \times \frac{\hbar^2}{mb^2} \quad \text{(with cmc)} \quad \ldots \quad 3.8a$$

$$= 18 \times \frac{\hbar^2}{mb^2} \quad \text{(without cmc)} \quad \ldots \quad 3.8b$$

In this calculation, kinetic energy contribution coming from the two body energy term i.e. E_2, (equation 2.17) with $f^2 \longrightarrow 1$ should correspond with (3.8a). That it does can be shown easily. The one body energy E_1 is given by (equation B.2 and B.3)

$$E_1 = \frac{15 \times 18}{16} \times \frac{\hbar^2}{mb^2} \quad \ldots \quad 3.9$$

But kinetic energy contribution from $E_2^{KE}(f^2)$ as $f^2 \longrightarrow 1$ is

$$E_2^{KE} \quad (f^2 \longrightarrow 1) = \frac{3}{8} \frac{\hbar^2}{mb^2} \quad \ldots \quad 3.10$$

(See the equation B.9)

Equations (3.9) and (3.10) together give the uncorrelated kinetic energy, E_{KE} (uncorr).

$$E_{KE}(\text{uncorr}) = E_1 + E_2^{KE} \quad (f^2 \longrightarrow 1) = 17.25 \cdot \frac{\hbar^2}{mb^2} \quad \ldots \quad 3.11$$

Same as (3.8a). This may be different as soon as the correlation function is introduced even if the calculations are upto two body energy only. Kinetic energy calculated with the correlation function is termed as correlated kinetic energy, denoted by -

$$E_{KE}(corr) = E_1 + E_2^{KE}(f^2) \qquad \ldots \qquad 3.12$$

These two equations (3.11) and (3.12) have been compared with and given in the table 3. The correlation function used is the Chakkalakal function (3.6) constrained through average Pauli condition. The potential chosen is the OMY[16] interaction. This potential has exponential attraction in the even states and zero extra core contribution in the odd states :-

$$V_s = -A_s e^{-\beta_s (r-r_c)} ; \quad A_s = 397.307, \ \beta_s = 2.6272$$

and $$V_t = -A_t e^{-\beta_t (r-r_c)} ; \quad A_t = 947.023, \ \beta_t = 3.6765$$

$$\ldots \quad 3.13$$

where the hard core, r_c = .6 fm. Potential contribution in the two body energy E_2^{PE} along with the optimised parameters and the energy have been tabulated in the Table 3.

Table in the Next page

T A B L E - 3

Two body energy, kinetic and potential, and optimised parameters at different b values for ^{16}O nucleus.

b fm	E_{KE}(uncorr) MeV	E_{KE}(corr) MeV	E_2^{PE} MeV	μ fm^{-1}	g	E MeV
1.52	309.62	296.26	-391.88	2.1	1.46	-95.62
1.5	317.94	303.22	-399.05	2.1	1.47	-95.83
1.47	331.05	313.62	-409.30	2.05	1.47	-95.68

Two body cluster energy E (= E_{KE} (corr) + E_2^{PE}) yields - 95.83 MeV at b = 1.5 fm. The smallness parameter [10]

$$= \frac{1}{A} \sum_{i<j} \left\langle ij \left| f^2 - 1 \right| ij \right\rangle_a \quad \ldots \quad 3.14$$

comes out to be $\simeq .03$ at the saturation point.

If, on the other hand, one starts with the Hamiltonian (1.9), E_1 is given by (3.8b), the fraction $\frac{A-1}{A}$ in E_2^{KE} (s) (equation B.4) is unity, E_2^{KE} (D) (equation B.8) is, of course, zero. Two body energy saturates at b = 1.52 fm with -82.85 MeV binding (Table 4).

Table 4 is in the next page.

T A B L E - 4

Two body energy with the Hamiltonian (1.9) for ^{16}O

b fm	μ fm^{-1}	g	E_1 MeV	E_2^{PE} MeV	E MeV
1.54	2.1	1.46	314.75	-384.71	-82.63
1.52	2.1	1.46	323.09	-391.88	-82.85
1.50	2.1	1.47	331.76	-399.06	-82.77

If one arbitrarily assumes the centre of mass to be in the S state orbitals with the energy $\frac{3}{4}\frac{\hbar^2}{mb^2}$ and subracts it from the two body energy later on for the centre of mass motion correction

$$E\ (cmc) = -82.85 - \frac{3}{4}\frac{\hbar^2}{mb^2} = -96.32 \text{ MeV} \quad \ldots \quad 3.15$$

at $\hbar\omega = \dfrac{\hbar^2}{m \times (1.52)^2} = 17.95$ MeV.

Under the circumstances, the error due to not treating the centre of mass motion properly is ~.5 MeV as the binding in the other case is -95.83 MeV at $\hbar\omega \left(= \dfrac{\hbar^2}{m(1.5)^2}\right) = 18.43$ MeV (table 3).

Two body cluster contribution (roughly) in ^{16}O by Clark et al[10] shows -93.2 MeV at $\hbar\omega = 19$ MeV. Interaction used here is the KK[17] potential. This calculation is quite similar to that of Dabrowski many years ago[9]. Although the 3-body may shift the saturation point to a higher b/λ value as in the case

of mass 3 and 4 system (Figs. 1,2), small size of $\mathcal{S}$ (equation 3.14) encourages the belief that even two body cluster calculation should give much of the physics in finite system[18]. It must be admitted that the potentials used in these calculations are not realistic enough. Correlation functions must be state dependant[19] with realistic interactions. For realistic potentials, like Hamada Johnston (HJ), one finds that the Chakkalakal function does not give binding for A = 3,4 nuclei. It is, ofcourse, very natural as the potential falls off $\sim e^{-x}/x$, $(x = .7\ r)$ the wave function should also fall[20] $\sim e^{-x}/x$, but with the Chakkalakal function along with oscillator basis this is impossible to achieve. Apart from the practical problems of calculation the formalism developed here (following I.R.Afnan[9]) is quite general and applicable to finite nuclei.

- - -

Appendix - 'A'

Trial wave function $\psi = F\phi$ ..... A.1 and two body kinetic energy gives -

$$\int d\tau\ \phi^* F\ \ \nabla_i.\nabla_j\ \ \phi F = \frac{1}{2}\int d\tau\ \left[\phi^* F\ \nabla_i.\nabla_j\phi\ F + \phi\ F\ \nabla_i.\ \nabla_j\ \ \phi^* F\right]$$

$$= \int d\tau\ |\phi|^2 F\ \nabla_i.\nabla_j F + \frac{1}{2}\int d\tau\ \left[\phi^* F^2\ \nabla_i.\nabla_j\phi\ \ + \phi\ F^2\ \nabla_i\ \nabla_j\phi^*\right]$$

$$+ \frac{1}{2}\int d\tau\ \left[\phi^* F\ (\nabla_i\phi).(\nabla_j\ F) + \phi\ F\ (\nabla_i\phi^*).(\ \nabla_j\ F)\right]$$

$$+ \frac{1}{2}\int d\tau\ \left[\phi^* F\ (\nabla_j\phi).(\ \nabla_i F) + \phi\ F\ \ (\nabla_j\phi^*).(\ \nabla_i\ F)\right] \quad \ldots\ \text{A.2}$$

Now, $\frac{1}{2}\int d\tau\ \ \phi^* F\ (\nabla_i\phi)\ .\ (\ \nabla_j F)$

$$= -\frac{1}{2}\int d\tau\ \ \phi F\ \ \ \ \nabla_i\phi^*.\ \nabla_j F - \frac{1}{2}\int d\tau\ |\phi|^2 \nabla_i F\ .\ \nabla_j F - \frac{1}{2}\int\ d\tau$$

$$|\phi|^2 F\ \nabla_i\ .\ \ \nabla_j F \qquad \ldots\ldots \qquad \text{A.3}$$

So that the equation A.2 becomes -

$$\frac{1}{2}\int d\tau\ \ \left[\phi^*\ F^2\ \nabla_i.\nabla_j\phi + \phi\ F^2\ \nabla_i.\nabla_j\phi^*\right] - \int d\tau\ |\phi|^2\ \ \nabla_i.F\ \cdot\ \nabla_j\ F$$

$$= \frac{1}{2}\int d\tau\ F^2\left[\nabla_i\cdot\nabla_j|\phi|^2 - \nabla_i\phi^*.\nabla_j\phi\ \ - \nabla_i\phi\cdot\ \nabla_j\phi^*\right]$$

$$- \int d\tau\ |\phi|^2\ \nabla_i F\ .\ \ \nabla_j F \qquad \ldots \qquad \ldots \quad \text{A.4}$$

Again, $\int d\tau\ \ F^2\ \nabla_i\cdot\nabla_j|\phi|^2 \ = 2\int d\tau\ |\phi|^2\left[\nabla_i F\ .\ \nabla_j F + F\ \ \nabla_i.\nabla_j\ F\ \right]$

... A.5

Equations A.4 and A.5 give -

$$\int \phi^* F \nabla_i . \nabla_j F \phi \, d\tau = \frac{1}{4} \int d\tau \left[F^2 \left[\nabla_i . \nabla_j |\phi|^2 - 2 \nabla_i \phi . \nabla_j \phi^* - 2 \nabla_i \phi^* . \nabla_j \phi \right] \right.$$

$$\left. + \frac{1}{2} \int d\tau |\phi|^2 \left[F \nabla_i \nabla_j F - \nabla_i F . \nabla_j F \right] \right]$$

$$= \frac{1}{4} \int d\tau \, F^2 \left[\nabla_i . \nabla_j |\phi|^2 - 2 \nabla_i \phi . \nabla_j \phi^* - 2 \nabla_i \phi^* . \nabla_j \phi \right]$$

$$+ \frac{1}{2} \int d\tau \, |\phi|^2 \quad F^2 \nabla_i \nabla_j \ln F \qquad \ldots \qquad A.6$$

Similarly,

$$\int F \phi^* \nabla_i^2 \, F \phi \, d\tau = \frac{1}{4} \int d\tau \, F^2 \left[\nabla_i^2 |\phi|^2 - 4 \nabla_i \phi . \nabla_i \phi^* \right]$$

$$+ \frac{1}{2} \int d\tau |\phi|^2 \quad F^2 \nabla_i^2 \ln F \qquad \ldots \qquad A.7$$

Define -

$$T_i \phi = - \frac{1}{\phi^*} \frac{\hbar^2}{2m} \frac{(A-1)}{A} \frac{1}{4} \left(\nabla_i^2 |\phi|^2 - 4 \nabla_i \phi . \nabla_i \phi^* \right)$$

and $$T_{ij} \phi = \frac{1}{\phi^*} \frac{\hbar^2}{Am} \times \frac{1}{4} \left[\nabla_i . \nabla_j |\phi|^2 - 2 \nabla_i \phi^* . \nabla_j \phi \right.$$

$$\left. - 2 \nabla_i \phi . \nabla_j \phi^* \right] \qquad \ldots \qquad A.8$$

As $$T_{rel.} = - \frac{\hbar^2}{2m} \frac{(A-1)}{A} \sum_i \nabla_i^2 + \frac{\hbar^2}{Am} \sum_{i<j} \nabla_i . \nabla_j$$

Using equations A.6, A.7 with A.8

$$\langle T_{rel} \rangle = \int d\tau \; \phi^* F^2 \Big[\sum_i T_i + \sum_{i<j} T_{ij} \Big] \phi$$

$$+ \frac{1}{2} \int d\tau \, |\phi|^2 F^2 \Big[- \frac{\hbar^2}{2m} \frac{(A-1)}{A} \sum_i \nabla_i^2 + \frac{\hbar^2}{Am} \sum_{i<j} \nabla_i \cdot \nabla_j \Big] \ln F$$

... A.9

But $$\sum_i \nabla_i^2 \ln F = 2 \sum_{i<j} \nabla_{r_{ij}}^2 \ln f(r_{ij})$$

and $$\sum_{i<j} \nabla_i \cdot \nabla_j \ln F = - \sum_{i<j} \nabla_r^2 \ln f(r_{ij}) \quad \ldots \quad A.10$$

Where ∇_r corresponds to the relative momentum

$$\vec{p}_{rel} = (\vec{p}_i - \vec{p}_j)/2 \text{ with the relative coordinate}$$

$$\vec{r} = \vec{r}_i - \vec{r}_j$$

Use of A.10 finally yields

$$\langle T_{rel} \rangle = \int d\tau \; \phi^* \; F^2 \Big[\sum_i T_i + \sum_{i<j} T_{ij} \Big] \phi$$

$$- \frac{\hbar^2}{2m} \int d\tau \, |\phi|^2 F^2 \sum_{i<j} \nabla_r^2 \big(\ln f(r_{ij}) \big) \ldots \; A.11$$

Appendix - 'B'

Using the Oscillator wave function -

$$\phi_{n\ell}(\vec{r}_i) = R_{n\ell}(r_i) \cdot Y_{\ell m}(\hat{r}_i) \quad \ldots \quad B.1$$

One obtains $\phi_{oo}(r_i)\ T_i\ \phi_{oo}(r_i) = \frac{3}{4}\ \frac{(A-1)}{A}\ \frac{\hbar^2}{mb^2}\ |\phi_{oo}(r_i)|^2$

$\ldots$ B.2

and $\phi_{o1}(\vec{r}_i)\ T_i\ \phi_{o1}(\vec{r}_i) = \frac{\hbar^2}{mb^2}\ \frac{(A-1)}{A}\ \left[\frac{3}{4} \times |\phi_{o1}(\vec{r}_i)|^2 + \frac{1}{2} \times |\phi_{oo}(r_i)|^2\right]$ $\ldots$ B.3

Let us define

$$E_2^{KE}(s) = \sum_{i<j} \left[\frac{\langle f^2 (T_i + T_j)\rangle}{\langle f^2 (ij)\rangle} - \langle T_i + T_j \rangle\right] \ldots \text{B.4}$$

$E_2^{KE}(s) = 0$ when i,j belong to s orbitals $\ldots$ B.5

$$= 18\ \frac{\hbar^2}{mb^2}\ \frac{(A-1)}{A}\ \left[\frac{3}{4}\ \left(\frac{\int dr\ r^2\ f^2(r)\ R_{o1}^2(r)}{\int dr\ r^2\ f^2(r)\ R_{oo}^2(r)} - 1\right)\right]$$

$$+ \frac{30\ \hbar^2}{mb^2}\ \frac{(A-1)}{A}\ \left[\left(\frac{\int f^2(r)\ R_{oo}^2(r)\ r^2\ dr}{\int f^2(r)\ R_{o1}^2(r)\ r^2\ dr} - 1\right) \times \frac{5}{4}\right]$$

When i, j belong to s and p orbitals $\ldots$ B.6

$$= \frac{\hbar^2}{m b^2} \cdot \frac{(A-1)}{A} \cdot \left[\frac{6 \int f^2 r^2 dr \left(R_{00}^2 + R_{01}^2 \right) / 2}{\frac{1}{3} \int f^2 r^2 dr \left[(R_{00}^2 + R_{10}^2) / 2 + R_{00}^2 + R_{02}^2 \right]} \right.$$

$$+ \frac{6 \int f^2 r^2 dr \left(R_{00}^2 + R_{01}^2 \right) / 2}{\frac{1}{3} \int f^2 r^2 dr \left[(R_{00}^2 + R_{02}^2) / 2 + R_{00}^2 + R_{10}^2 \right]} + \frac{24 \int f^2 r^2 dr (R_{00}^2 + R_{01}^2)/2}{\int f^2 r^2 dr \left(R_{00}^2 + R_{02}^2 \right)/2}$$

$$\left. + \frac{30 \int f^2 r^2 dr \left(R_{00}^2 + R_{01}^2 \right)/2}{\int f^2 r^2 dr \; R_{01}^2} - 66 \right]$$

When i, j belong to p orbitals ... B.7

Define $E_2^{KE}(D) = \sum_{i<j} \left[\frac{\langle f^2 T_{ij} \rangle}{\langle f^2 \rangle} \right]$ ... B.8

So that $E_2^{KE}(f^2) = E_2^{KE}(s) + E_2^{KE}(D)$ B.9

$$E_2^{KE}(D) = \frac{3}{8} \frac{\hbar^2}{m b^2} \frac{\int f^2 R_{00}^2 r^2 dr}{\int f^2 R_{01}^2 r^2 dr} \quad \text{... for i,j in s,p orbitals}$$

$= 0$ for i,j in s,s and p,p orbitals ... B.10

Now, $f^2 W_{ij} = f^2 \left[V(r) - \frac{\hbar^2}{2m} \cdot \nabla_r^2 \ln f \right]$

$$= V(r) f^2 + \frac{\hbar^2}{2m} \left[\left(\frac{df}{dr} \right)^2 - f \frac{d^2 f}{dr^2} - \frac{2f}{r} \frac{df}{dr} \right] \quad \text{... B.11}$$

Assuming the correlation function to be state independent and as the potential itself is state dependent,

$\langle nL | f^2 W ({}^S L_J) | nL \rangle$ has been denoted by

$\langle nL | {}^S L_J | nL \rangle$ where n, L, S, are quantum numbers

for relative wave function. We find -

$$\sum_{i<j} \left[\frac{\langle f^2 W (ij) \rangle}{\langle f^2 (ij) \rangle} \right] = \frac{3 \langle 00 | {}^3S_1 + {}^1S_0 | 00 \rangle}{\int f^2 R_{00}^2 r^2 dr} \quad \text{for s state particles} \qquad \ldots \text{B.12}$$

$$= \frac{9 \langle 00 | {}^3S_1 + {}^1S_0 | 00 \rangle}{\int f^2 R_{00}^2 r^2 dr}$$

$$+ \frac{\langle 01 | (3\,{}^3P_0 + 9\,{}^3P_1 + 15\,{}^3P_2 + 3\,{}^1P_1) | 01 \rangle}{\int f^2 R_{01}^2 r^2 dr}$$

for s,p orbitals ... B.13

$$= \frac{\frac{3}{2}\langle 00 | {}^3S_1 + {}^1S_0 | 00 \rangle + \frac{1}{2}\langle 10 | {}^3S_1 + {}^1S_0 | 10 \rangle + \frac{1}{3}\langle 02 | \frac{7}{5}\,{}^3D_3 + {}^3D_2 + \frac{3}{5}\,{}^3D_1 + 3\,{}^1D_2 | 02 \rangle}{\frac{1}{3}\int f^2 r^2 dr \left[(R_{00}^2 + R_{10}^2)/2 + R_{00}^2 + R_{02}^2 \right]}$$

$$+ 4 \times \frac{\frac{3}{2}\langle 00|\,{}^3S_1 + {}^1S_0\,|00\rangle + \frac{1}{2}\langle 02|\,\frac{7}{5}\,{}^3D_3 + {}^3D_2 + \frac{3}{5}\,{}^3D_1 + 3\,{}^1D_2\,|02\rangle}{\frac{1}{2}\int f^2\, r^2 dr\,\left(R_{00}^2 + R_{02}^2\right)}$$

$$+ \frac{\frac{3}{2}\langle 00|\,{}^3S_1 + {}^1S_0\,|00\rangle + \langle 10|\,{}^3S_1 + {}^1S_0\,|10\rangle + \frac{1}{6}\langle 02|\,\frac{7}{5}\,{}^3D_3 + {}^3D_2 + \frac{3}{5}\,{}^3D_1 + 3\,{}^1D_2\,|02\rangle}{\frac{1}{3}\int f^2 r^2 dr\left[\left(R_{00}^2 + R_{02}^2\right)/2 + R_{00}^2 + R_{10}^2\right]}$$

$$+ 3 \frac{\langle 01\,|\,5\,{}^3P_2 + 3\,{}^3P_1 + {}^3P_0 + {}^1P_1\,|\,01\rangle}{\int dr\;\; f^2\, r^2\, R_{01}^2}$$

for p orbitals .. B.14

In lowest order shell model in Oxygen - 16, assuming pairwise interaction[15], one gets altogether $^{16}C_2 = 120$ interactions. Of these 42 are in relative (0S) state, 60 in (0P) state and 18 in (1S-0D) state. Interaction between ss particles gives 6-oS interactions, sp particles give 48 = [18 (oS) + 30 (oP)] and pp particles give 66 = [18 (oS) + 30 (oP) + 18 (1S-0D)]. When $f^2 \to 1$, f^2 W (ij) $\to$ V(ij) and we find equations (B.12- 14) check with these shell model numbers.

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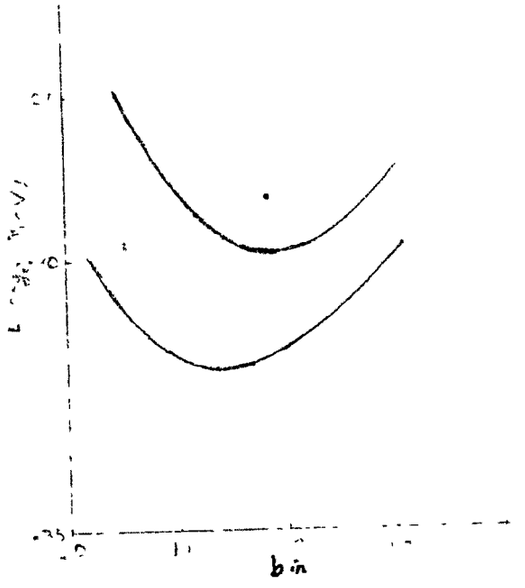
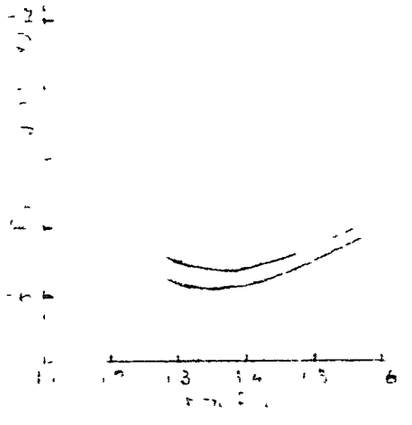


Binding Energy as a function of the size parameter b in A = 4. Lower curve gives the two body result while the upper curve includes three body contributions.



Same as in Fig. 1 for mass A = 3 nucleus