

**SECOND EUROPEAN SUMMER SCHOOL on  
MICROSCOPIC QUANTUM MANY-BODY THEORIES  
and their APPLICATIONS**

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**THE COUPLED CLUSTER METHOD AND ITS APPLICATIONS**

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These are preliminary lecture notes, intended only for distribution to participants



# The Coupled Cluster Method and its applications

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# 1.1 Brief history of CCM

Invented in 1958 by Coester, Kümmel

Ground State energy of closed-shell nuclei

Rediscovered in 1966-70 by Čížek, Paldus

Realm of Quantum Chemistry

Revival in Nuclear Physics Bochum group

1974: calculations of GS properties of doubly magic nuclei  $^4\text{He}$ ,  $^{16}\text{O}$  and  $^{40}\text{Ca}$  using realistic interactions (HJ, Reid SSC)

From 1979 on large scale applications in atoms, molecules, electron gas, spin lattices, quantum optics, etc,

Standard accurate technique in Quantum Chemistry.

Ground and excited states

From 1990 on new revival in Nuclear Physics the Manchester - Valencia collaboration

Reformulation of CCM to take proper care of the Center-of-Mass motion in the description of finite nuclei

Recently, Quantum Liquids La Plata - Valencia collaboration

Drops of helium atoms

## 1.2 Basic references

- R.F. Bishop and K.H. Kümmel, Phys. Today **40**, 52 (1987)  
pedagogical introduction
- Proc. Workshop CCM, Cambridge, Mass. 1990  
Theor. Chim. Acta **80** (1991)  
formalism + reviews + lots of references
- 1st. Eur. School Microscopic Quantum Many-Body Theories and Their Applications, Valencia 1997  
Lecture Notes in Physics **510** (1998)  
R.F. Bishop *The Coupled Cluster Method*  
formalism + general overview
- H.G. Kümmel, K.H. Lührmann, and J.G. Zabolitzky,  
Phys. Rep. **36C**, 1 (1978)  
A classic: formalism + finite nuclei

## 2.1 The Exponential Form of the CCM Wave Function

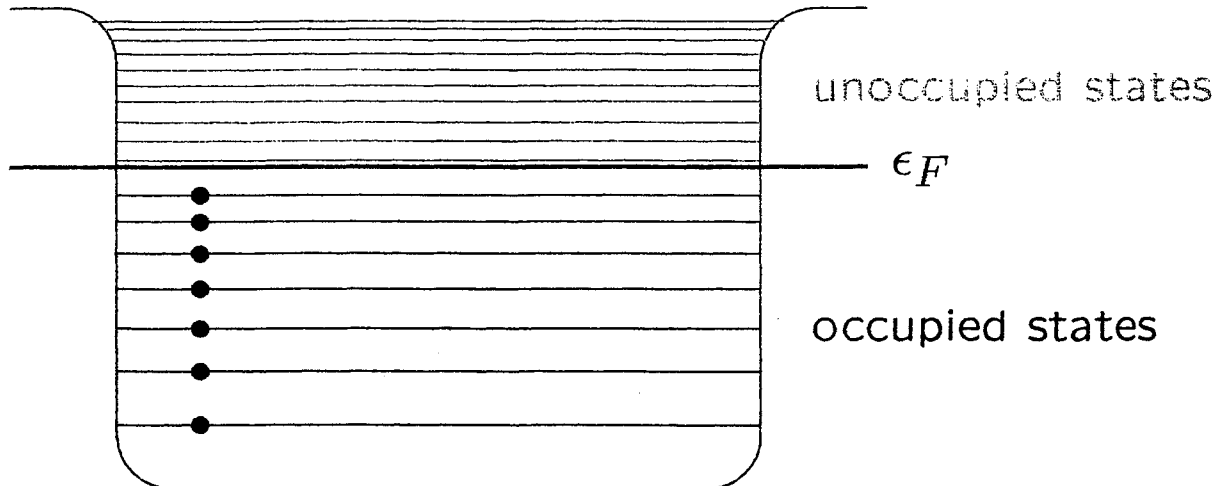
- First approach: Each nucleon moves independently in the mean field created by the other nucleons

Reference state:  $|\Phi\rangle = a_{\nu_A}^+ \dots a_{\nu_1}^+ |0\rangle$

Labels  $\nu \rightarrow$  occupied states in the Fermi sea

$\rho \rightarrow$  unoccupied states

$\alpha \rightarrow$  both occupied and unoccupied states



But all of this ignores interactions between nucleons

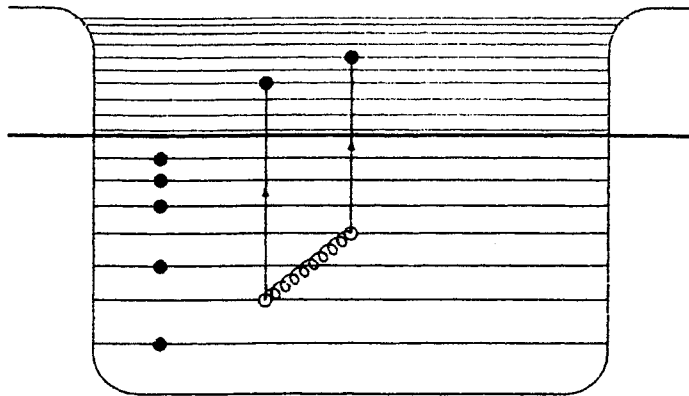
- Two particles may interact independently from all others and lift out of Fermi sea.

The process is described by an operator

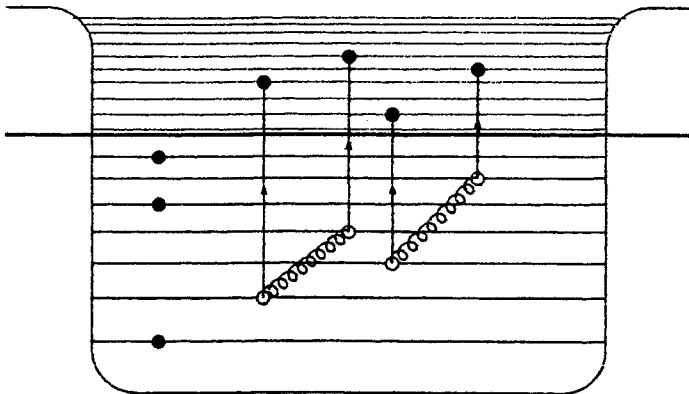
$$S_2 = \frac{1}{(2!)^2} \sum_{\nu_1, \nu_2, \rho_1, \rho_2} \langle \rho_1 \rho_2 | S_2 | \nu_1 \nu_2 \rangle_A a_{\rho_1}^+ a_{\rho_2}^+ a_{\nu_2} a_{\nu_1}$$

A  $\equiv$  antisymmetrisation  $\nu_1, \nu_2$

One-pair excitation:  $S_2 |\Phi\rangle$



Two independent pairs:  $\frac{1}{2!} S_2^2 |\Phi\rangle$



$m$  independent pairs:  $\frac{1}{m!} S_2^m |\Phi\rangle$

Sum of all terms involving independent excitations of pairs (including none)

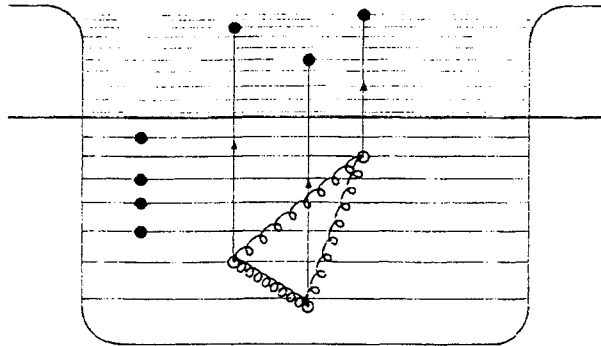
$$\sum_{m=0}^{\infty} \frac{1}{m!} S_2^m |\Phi\rangle \longrightarrow e^{S_2} |\Phi\rangle$$



- Three particles may interact independently from all others lifting out of Fermi sea.

The process is described by an operator

$$S_3 = \frac{1}{(3!)^2} \sum_{\nu_1, \nu_2, \nu_3, \rho_1, \rho_2, \rho_3} \langle \rho_1 \rho_2 \rho_3 | S_3 | \nu_1 \nu_2 \nu_3 \rangle_A a_{\rho_1}^+ a_{\rho_2}^+ a_{\rho_3}^+ a_{\nu_3} a_{\nu_2} a_{\nu_1}$$



Excitation of  $p$  independent triplets

$$\frac{1}{p!} S_3^p |\Phi\rangle$$

- $m$  pairs and  $p$  triplets may be excited independently

$$\frac{1}{m!} S_2^m \frac{1}{p!} S_3^p |\Phi\rangle$$

The operators  $S_2$  and  $S_3$  commute, as they are describing independent processes

Sum of all terms involving independent excitations of pairs and triplets (including none)

$$\sum_{m=0}^{\infty} \frac{1}{m!} S_2^m \sum_{p=0}^{\infty} \frac{1}{p!} S_3^p |\Phi\rangle \longrightarrow e^{S_2 + S_3} |\Phi\rangle$$

- $n$  cluster excitation described by an operator

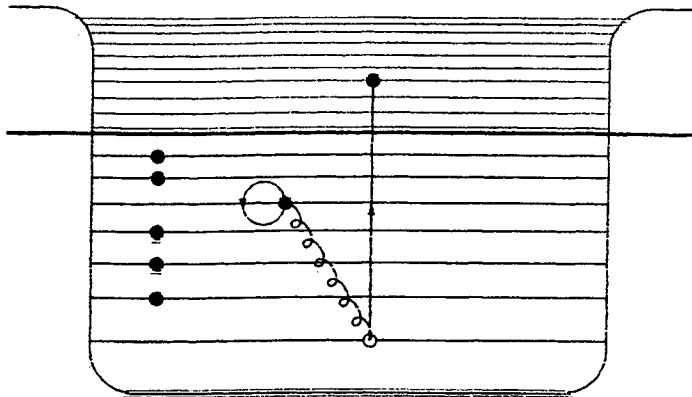
$$S_n = \frac{1}{(n!)^2} \sum_{\nu_1, \dots, \nu_n, \rho_1, \dots, \rho_n} \langle \rho_1 \dots \rho_n | S_n | \nu_1 \dots \nu_n \rangle_A a_{\rho_1}^+ \dots a_{\rho_n}^+ a_{\nu_n} \dots a_{\nu_1}$$

Sum of all terms involving independent excitations

$$e^{S_2 + S_3 + \dots + S_A} |\Phi\rangle$$

- Finally, it may also happen that in the interaction of any subset of particles, only one of them is lifted above the Fermi sea

$$S_1 = \sum_{\nu, \rho} \langle \rho | S_1 | \nu \rangle a_{\rho}^+ a_{\nu}$$



Sum of all independent 1p-1h excitations

$$e^{S_1} |\Phi\rangle$$

## CCM ansatz

$$|\Psi\rangle = e^S |\Phi\rangle$$

$$S = \sum_{n=1}^A S_n$$

$$S_n = \frac{1}{(n!)^2} \sum_{\nu_1 \dots \nu_n, \rho_1 \dots \rho_n} \langle \rho_1 \dots \rho_n | S_n | \nu_1 \dots \nu_n \rangle a_{\rho_1}^\dagger \dots a_{\rho_n}^\dagger a_{\nu_n} \dots a_{\nu_1}$$

- The exponentiated operatorial form is convenient in extended systems (Goldstone theorem)
- This is a *natural* decomposition of the wave function in clusters of excitations, where each independent excitation has been considered with its appropriate multiplicity
- Let the reference state  $|\Phi\rangle$  be a Slater determinant  
Each term in each cluster  $S_n$  produces a new Slater determinant  
The action of  $e^S$  on  $|\Phi\rangle$  is to generate in a specific way a complete set of many-particle states formed by Slater determinants  
Everything is exact up to now but not very practical for the moment

Formal writing of the wave function in coordinate space

- Single-particle wave functions

$$\langle x|\nu\rangle$$

- $n$ -ph amplitudes

$$\begin{aligned} & \langle x_1, x_2, \dots, x_n | S_n | \nu_1, \nu_2, \dots, \nu_n \rangle \\ &= \sum_{\rho_1, \dots, \rho_n} \langle x_1 | \rho_1 \rangle \dots \langle x_n | \rho_n \rangle \langle \rho_1, \dots, \rho_n | S_n | \nu_1, \dots, \nu_n \rangle \end{aligned}$$

These amplitudes are antisymmetric both in particle and state labels  $x_i, \nu_i$

$$\begin{aligned} & \langle x_1, \dots, x_A | \Psi \rangle \\ &= \mathcal{A}_\nu [\langle x_1 | \nu_1 \rangle \dots \langle x_A | \nu_A \rangle] \\ &+ \mathcal{S}_{\nu x} \mathcal{A}_\nu [\langle x_1 | S_1 | \nu_1 \rangle \langle x_2 | \nu_2 \rangle \dots \langle x_A | \nu_A \rangle] \\ &+ \mathcal{S}_{\nu x} \mathcal{A}_\nu [\langle x_1 x_2 | S_2 | \nu_1 \nu_2 \rangle \langle x_3 | \nu_3 \rangle \dots \langle x_A | \nu_A \rangle] \\ &+ \mathcal{S}_{\nu x} \mathcal{A} [\langle x_1 x_2 x_3 | S_3 | \nu_1 \nu_2 \nu_3 \rangle \langle x_4 | \nu_4 \rangle \dots \langle x_A | \nu_A \rangle] \\ &+ \dots \\ &+ \mathcal{S}_{\nu x} \mathcal{A} [\langle x_1 x_2 | S_2 | \nu_1 \nu_2 \rangle \langle x_3 x_4 | S_2 | \nu_3 \nu_4 \rangle \langle x_5 | \nu_5 \rangle \dots \langle x_A | \nu_A \rangle] + \\ & \dots \end{aligned}$$

The symbol  $\mathcal{A}$  means sum over all permutations of the single-particle state labels with the corresponding sign

The symbol  $\mathcal{S}$  means sum over all permutations of pairs of particle and single-particle state labels

This result leads to a unique definition of correlations

## 2.2 The Configuration Interaction Method (CIM)

Alternative way to obtain the  $np$ - $nh$  content of the wave function: project onto  $np$ - $nh$  state

$$a_{\rho_1}^+ \dots a_{\rho_n}^+ a_{\nu_1} \dots a_{\nu_n} |\Phi\rangle$$

The true wave function:

$$|\Psi\rangle = \left( 1 + \sum_{n=1}^N F_n \right) |\Phi\rangle$$

$$F_n = \frac{1}{(n!)^2} \sum_{\nu_1, \dots, \nu_n, \rho_1, \dots, \rho_n} \langle \rho_1 \dots \rho_n | F_n | \nu_1 \dots \nu_n \rangle_A a_{\rho_1}^+ \dots a_{\rho_n}^+ a_{\nu_1} \dots a_{\nu_n}$$

→ probability amplitude for the excitation of  $n$  nucleons from the occupied states  $(\nu_1, \dots, \nu_n)$  to the unoccupied states  $(\rho_1, \dots, \rho_n)$  in the reference state.

This is a generalized shell-model. Amplitudes and eigenvalues are determined by diagonalizing the hamiltonian matrix.

CCM  $\equiv$  CIM if no approximations are made

But there are conceptual differences ...

# Linked vs unlinked

Relations  $F_n \longleftrightarrow S_n$

$$F_1 = S_1$$

$$F_2 = S_2 + \frac{1}{2}S_1^2$$

$$F_3 = S_3 + S_2S_1 + \frac{1}{6}S_1^3$$

$$F_4 = S_4 + S_3S_1 + \frac{1}{2}S_2^2 + \frac{1}{2}S_2S_1^2 + \frac{1}{24}S_1^4$$

$S_n$  are linked by construction

$F_n$  contains unlinked pieces. They cancel out in the exact theory, but it is not true when truncations are made

## $n$ -particle subsystem amplitudes

$$\langle x_1 \dots x_n | \Psi_n | \nu_1 \dots \nu_n \rangle_A \equiv \langle \Phi | a_{\nu_1}^+ \dots a_{\nu_n}^+ a(x_1) \dots a(x_n) | \Psi \rangle$$

→ amplitude for  $1 \dots n$  particles moving freely (positions  $x_1 \dots x_n$ ) and the remaining  $N - n$  being in  $(\nu_{n+1} \dots \nu_N)$

$$\langle x_1 | \Psi_1 | \nu_1 \rangle = \langle x_1 | \nu_1 \rangle + \langle x_1 | S_1 | \nu_1 \rangle$$

$$= \langle x_1 | \nu_1 \rangle + \langle x_1 | F_1 | \nu_1 \rangle$$

$$\langle x_1 x_2 | \Psi_2 | \nu_1 \nu_2 \rangle_A = \{ \langle x_1 | \Psi_1 | \nu_1 \rangle \langle x_2 | \Psi_1 | \nu_2 \rangle \}_A + \langle x_1 x_2 | S_2 | \nu_1 \nu_2 \rangle_A$$

$$= \langle x_1 x_2 | \nu_1 \nu_2 \rangle_A + S_{12} \{ \langle x_1 | \nu_1 \rangle \langle x_2 | F_1 | \nu_2 \rangle \}_A$$

$$+ \langle x_1 x_2 | F_2 | \nu_1 \nu_2 \rangle_A$$

$\langle S_2 \rangle$  is that part of  $\langle \Psi_2 \rangle$  that cannot be described by  $\langle \Psi_1 \rangle$ . A similar interpretation does not exist for amplitudes  $\langle F_2 \rangle$

$$\langle x_1 x_2 x_3 | \Psi_3 | \nu_1 \nu_2 \nu_3 \rangle_A = \{ \langle x_1 | \Psi_1 | \nu_1 \rangle \langle x_2 | \Psi_1 | \nu_2 \rangle \langle x_3 | \Psi_1 | \nu_3 \rangle \}_A$$

$$+ S_{123} \{ \langle x_1 x_2 | S_2 | \nu_1 \nu_2 \rangle \langle x_3 | \Psi_1 | \nu_3 \rangle \}_A$$

$$+ \langle x_1 x_2 x_3 | S_3 | \nu_1 \nu_2 \nu_3 \rangle_A$$

$\langle S_n \rangle$  is that part of  $\langle \Psi_n \rangle$  which cannot be described in terms of one-, two, ...  $(n - 1)$ -body amplitudes. It describes correlations occurring within an  $n$ -body cluster

# Size-extensivity

Separate system with  $N$  particles into two subsystems  $A, B$  with  $N_A, N_B$  particles. Separation distance  $r_{AB}$ .

$$\begin{aligned} r_{AB} \rightarrow \infty \quad H &\rightarrow H^A + H^B, [H^A, H^B] = 0 \\ E_0 &\rightarrow E_0^A + E_0^B \\ |\Psi\rangle &\rightarrow |\Psi^A\rangle \otimes |\Psi^B\rangle \end{aligned}$$

A system is said to be size-extensive when it obeys the above separability properties. In such a case the energy has the (correct) linear dependence with the number of constituents

A common truncation: SUB( $n$ )

$$\begin{aligned} S &\rightarrow S_1 + S_2 + \dots + S_n \quad (S_m = 0, m > n) \\ F &\rightarrow F_1 + F_2 + \dots + F_n \quad (F_m = 0, m > n) \end{aligned}$$

CIM-SUB( $n$ )

$$\begin{aligned} (1 + F_1 + F_2 + \dots + F_n)|\Phi\rangle &\neq (r_{AB} \rightarrow \infty) \\ &(1 + F_1^{(A)} + F_2^{(A)} + \dots + F_n^{(A)})|\Phi^{(A)}\rangle \\ &\otimes (1 + F_1^{(B)} + F_2^{(B)} + \dots + F_n^{(B)})|\Phi^{(B)}\rangle \end{aligned}$$

does not have separability property: it would require excitations of up to  $2n$  excitations, which go beyond the assumed approximation

CCM-SUB( $n$ )

$$\begin{aligned} \exp(S_1 + S_2 + \dots + S_n)|\Phi\rangle &= (r_{AB} \rightarrow \infty) \\ \exp(S_1^{(A)} + S_1^{(B)} + S_2^{(A)} + S_2^{(B)} + \dots + S_n^{(A)} + S_n^{(B)})|\Phi\rangle \\ &\equiv \exp(S_1^{(A)} + S_2^{(A)} + \dots + S_n^{(A)})|\Phi^{(A)}\rangle \\ &\quad \otimes \exp(S_1^{(B)} + S_2^{(B)} + \dots + S_n^{(B)})|\Phi^{(B)}\rangle \end{aligned}$$

guarantees the separability relation, no matter how the cluster correlation operator  $S$  is truncated

## 2.3 The Coupled Cluster equations

Determine amplitudes  $\langle S_n \rangle$   
and ground state energy

Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle \longrightarrow He^S|\Phi\rangle = Ee^S|\Phi\rangle$$

Use  $\langle\Phi|\Psi\rangle = \langle\Phi|e^S|\Phi\rangle = 1$

$$\langle\Phi|He^S|\Phi\rangle = E\langle\Phi|e^S|\Phi\rangle \equiv E$$

Assume two-body interaction:

$$E = \sum_{\nu} \langle\nu|T\Psi_1|\nu\rangle + \frac{1}{2} \sum_{\nu\nu'} \langle\nu\nu'|V\Psi_2|\nu\nu'\rangle_A$$

Only one- and two-body amplitudes ( $\Psi_1, \Psi_2$  or  $S_1, S_2$ ) are needed to determine the ground state energy

Expanded expression:

$$E = \sum_{\nu\alpha} \langle\nu|T|\alpha\rangle \langle\alpha|\Psi_1|\nu\rangle + \frac{1}{2} \sum_{\nu\nu'\alpha\alpha'} \langle\nu\nu'|V|\alpha\alpha'\rangle \langle\alpha\alpha'|\Psi_2|\nu\nu'\rangle_A$$

Recall:

$$\langle x_1|\Psi_1|\nu_1\rangle = \langle x_1|\nu_1\rangle + \langle x_1|S_1|\nu_1\rangle$$

$$\begin{aligned} \langle x_1x_2|\Psi_2|\nu_1\nu_2\rangle_A &= \{\langle x_1|\Psi_1|\nu_1\rangle \langle x_2|\Psi_1|\nu_2\rangle\}_A \\ &\quad + \langle x_1x_2|S_2|\nu_1\nu_2\rangle_A \end{aligned}$$

Premultiply with  $\langle\Phi| \equiv$  Project onto 0ph state

Idea: Convert the Schrödinger equation into an equivalent set of coupled equations for amplitudes  $\langle S_n \rangle$  by projecting onto 0ph, 1ph, ...  $n$ ph states



Formal writing of cluster operator

$$S = \sum_{I \neq 0} S_I C_I^+ \quad , \quad C_I^+ \equiv a_{\rho_1}^+ \dots a_{\rho_n}^+ a_{\nu_n} \dots a_{\nu_1}$$

$np$ - $nh$  projection  $\longrightarrow \langle \Phi | C_I$

The Schrödinger equation transforms into

$$\langle \Phi | C_I H e^S | \Phi \rangle = E \langle \Phi | C_I e^S | \Phi \rangle \quad , \quad I \neq 0$$

with  $E = \langle \Phi | H e^S | \Phi \rangle$  if  $I = 0$

Warning:  $E$  is a macroscopic quantity. Problems in extended systems?

No: There are cancelations between unlinked terms in both sides of these equations

## Alternative CC equations

Transform the Schrödinger equation into

$$e^{-S} H e^S | \Phi \rangle = E | \Phi \rangle$$

0ph projection:

$$E = \langle \Phi | e^{-S} H e^S | \Phi \rangle \equiv \langle \Phi | H e^S | \Phi \rangle$$

$$\langle \Phi | C_I e^{-S} H e^S | \Phi \rangle = 0 \quad , \quad I \neq 0$$

No macroscopic quantity appears to determine  $S_I$

**$\longrightarrow$  EXERCISE 1**

Use the nested commutator expansion

$$e^{-S}He^S = H + [H, S] + \frac{1}{2!}[[H, S], S] + \frac{1}{3!}[[[H, S], S], S] \\ + \frac{1}{4!}[[[[H, S], S], S], S] + \dots$$

An infinite series for a general operator  $S$  is formed by creation operators  $C_I^+$  such that

$$[C_I^+, C_J^+] = 0$$

The only non-vanishing terms in the series comes from the contractions between the Hamiltonian and  $S$   
The operator  $e^{-S}He^S$  is a fully linked operator  
→ the series is finite

For an  $n$ -body hamiltonian the series will exactly terminate with the term involving  $2n$  cluster operators.

Two-body hamiltonian:

$$\langle \Phi | C_I H | \Phi \rangle + \sum_J S_J \langle \Phi | C_I [H, C_J^+] | \Phi \rangle \\ + \frac{1}{2!} \sum_{JK} S_J S_K \langle \Phi | C_I [[H, C_J^+], C_K^+] | \Phi \rangle \\ + \frac{1}{3!} \sum_{JKL} S_J S_K S_L \langle \Phi | C_I [[[H, C_J^+], C_K^+], C_L^+] | \Phi \rangle \\ + \frac{1}{4!} \sum_{JKLM} S_J S_K S_L S_M \langle \Phi | C_I [[[[H, C_J^+], C_K^+], C_L^+], C_M^+] | \Phi \rangle \\ = 0$$

A coupled set of non-linear equations in the amplitudes  $S_I$ , up to the fourth order.

## 2.4 The Reference state

In order to describe many-body correlations we always need a reference state with respect to which the correlations are defined. In some cases the choice of  $|\Phi\rangle$  may be determined by simple physical ideas, but it is important to realize that this choice may be not unique

System of bosons

Example: liquid  $^4\text{He}$

Obvious choice: the Bose condensate, in which all  $N$  particles condense into the lowest-energy single-particle state

Normalized reference state:

$$|\Phi\rangle = \frac{1}{\sqrt{N!}} (b_0^+)^N |0\rangle$$

Bosonic commutation relations:

$$[b_\alpha, b_\beta] = 0 = [b_\alpha^+, b_\beta^+] , [b_\alpha, b_\beta^+] = \delta_{\alpha,\beta}$$

s-p states in coordinate representation:  $\phi_\alpha(\mathbf{r})$

occupied states  $\alpha \rightarrow \nu \equiv 0$ , unoccupied states  $\alpha \rightarrow \rho$

Finite system:  $\{\alpha\} \leftarrow \text{HO}$

Homogeneous system: plane waves

Thermodynamical limit:

$N \rightarrow \infty, \Omega \rightarrow \infty, \rho = N/\Omega$  finite

## System of fermions

Examples: liquid  $^3\text{He}$ , finite nuclei, atoms, molecules, electron plasma

Obvious choice: an Slater determinant of single-particle states:

$$|\Phi\rangle = \prod_{i=1}^N a_{\nu_i}^+ |0\rangle$$

formed from some complete s-p basis  $\{|\alpha_i\rangle = a_{\alpha_i}^+ |0\rangle\}$   
Fermionic anticommutation relations

$$\{a_\alpha, a_\beta\} = 0 = \{a_\alpha^+, a_\beta^+\}, \{a_\alpha, a_\beta^+\} = \delta_{\alpha,\beta}$$

Finite systems

Atoms and molecules:  $\{\alpha\} \leftarrow \text{HF}$

Finite nuclei:  $\{\alpha\} \leftarrow \text{HF}$  (which may or not be consistent with the NN interaction), or  $\{\alpha\} \leftarrow \text{HO}$

Homogeneous system: plane waves

Thermodynamical limit:

$$N \rightarrow \infty, \Omega \rightarrow \infty, \rho = N/\Omega \text{ finite}$$

The choice of a Slater determinant for the reference state of a fermion system may seem obvious. However, it is worth noting that, depending on the type of physics one is interested in, other choices may be more convenient

- Open-shell systems

A multi-reference approach seems to be more reasonable. It results in a mixture of CCM and CIM

Atoms and molecules

- BCS state

The reference state is also an Slater determinant but formed from quasiparticle states. These quasiparticle states are linear combinations of the previous particle and hole states

Not considered here

- Quantum Spin Lattices

Spin-Half particles on a bipartite lattice: Néel state

Not considered here

...

- Systems with a very strong repulsion at short distances

It may be convenient to consider a correlated reference state. To be useful, these correlations have to be determined separately. It results in a mixture of Jastrow and CC correlations

Finite nuclei and drops of liquid He

→ **EXERCISE 2**

## 2.5 The Bra state

Up to this point we have only considered the ket state  $|\Psi\rangle$ . Ground state energy extracted from the Schrödinger equation projecting upon  $C_I$   $np$ - $nh$  excitations

Calculate  $E$  as an expectation value:

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Phi | e^{S^\dagger} H e^S | \Phi \rangle}{\langle \Phi | e^{S^\dagger} e^S | \Phi \rangle}$$

The resulting expression is generally of infinite order in the correlation operators  $S$  and  $S^\dagger$ , no matter how  $S$  is truncated

Cancellation of unlinked terms between the numerator and the denominator may be proven, but it is by no means transparent

Normal CCM and Extended CCM

parametrise independently the bra and the ket states

but the hermitian-adjoint relationship to one another is broken

## Parametrisation of the bra ground state

$$\langle \hat{\Psi} | = \frac{(|\Psi\rangle)^+}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi |}{\langle \Psi | \Psi \rangle}$$

$$\langle \hat{\Psi} | = \langle \Phi | \hat{S} e^{-S}$$

$$\hat{S} = 1 + \sum_{I \neq 0} \hat{S}_I C_I$$

Preserves the explicit normalisation

$$\langle \hat{\Psi} | \Psi \rangle = \langle \Phi | \Psi \rangle = \langle \Phi | \Phi \rangle = 1$$

The full set of independent variables  $\{S_I, \hat{S}_I\}$  provides a complete parametrisation of the ground state

## Expectation value of an arbitrary operator

$$\langle A \rangle = \langle \hat{\Psi} | A | \Psi \rangle = \langle \Phi | \hat{S} e^{-S} A e^S | \Phi \rangle \equiv A(S_I, \hat{S}_I)$$

It is fully linked even though the operator  $\hat{S}$  itself contains unlinked pieces

## NCCM equations

Schrödinger equation

$$\langle \hat{\Psi} | H = \langle \hat{\Psi} | E$$

Project onto states  $C_I^+ | \Phi \rangle$

$$\langle \Phi | \hat{S} (e^{-S} H e^S - E) C_I^+ | \Phi \rangle = 0, I \neq 0$$

Ground state energy ( $I = 0$ )

$$E = \langle \Phi | \hat{S} e^{-S} H e^S | \Phi \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Phi | e^{S^+} H e^S | \Phi \rangle}{\langle \Phi | e^{S^+} e^S | \Phi \rangle}$$

- Solve

$$\langle \Phi | C_I e^{-S} H e^S | \Phi \rangle = 0, I \neq 0$$

to obtain  $\{S_I\}$

- Use  $\{S_I\}$  as an input and solve the linear set of equations

$$\langle \Phi | \hat{S}_I e^{-S} [H, C_I^+] e^S | \Phi \rangle = 0, I \neq 0$$

to obtain  $\{\hat{S}_I\}$

The NCCM bra parametrisation is derivable from the Hellmann-Feynman theorem  $\rightarrow$  The expectation value of an arbitrary operator  $A$  may be calculated diagrammatically from the same set diagrams as for the energy: replace  $V$ -lines by  $A$ -lines

ECCM is a method to use fully linked basic amplitudes (NCCM  $\{\hat{S}_I\}$  contains unlinked terms)



# 3.1 The SUB(n) or CCn approximation

1p-1h projection

$$\begin{aligned} & \langle \alpha_1 | T \Psi_1 | \nu_1 \rangle + \sum_{\nu} \langle \alpha_1 \nu | T(2) S_2 | \nu_1 \nu \rangle_A + \sum_{\nu} \langle \alpha_1 \nu | V \Psi_2 | \nu_1 \nu \rangle_A \\ & + \frac{1}{2} \sum_{\nu, \nu'} \langle \alpha_1 \nu \nu' | V(23) \chi_3(1; 23) | \nu_1 \nu \nu' \rangle_A = \sum_{\nu} h_{\nu \nu_1} \langle \alpha_1 | \Psi_1 | \nu \rangle \end{aligned}$$

2p-2h projection

$$\begin{aligned} & \langle \rho_1 \rho_2 | [T(1) + T(2)] S_2 | \nu_1 \nu_2 \rangle_A + \sum_{\nu} \langle \rho_1 \rho_2 \nu | T(3) S_3 | \nu_1 \nu_2 \nu \rangle_A \\ & + \langle \rho_1 \rho_2 | V \Psi_2 | \nu_1 \nu_2 \rangle_A + \frac{1}{2} \sum_{\nu \nu'} \langle \rho_1 \rho_2 | S_2 | \nu \nu' \rangle_A \langle \nu \nu' | V \Psi_2 | \nu_1 \nu_2 \rangle_A \\ & + \sum_{\nu} \langle \rho_1 \rho_2 \nu | [V(13) \chi_3(2; 13) + V(23) \chi_3(1; 23)] | \nu_1 \nu_2 \nu \rangle_A \\ & + \frac{1}{2} \sum_{\nu \nu'} \langle \rho_1 \rho_2 \nu \nu' | V(34) \chi_4(12; 34) | \nu_1 \nu_2 \nu \nu' \rangle_A \\ & = \sum_{\nu} (h_{\nu \nu_1} \langle \rho_1 \rho_2 | S_2 | \nu \nu_2 \rangle_A + h_{\nu \nu_2} \langle \rho_1 \rho_2 | S_2 | \nu_1 \nu \rangle_A) \end{aligned}$$

$$\chi_3(1; 23) = S_2(13) \Psi_1(2) + S_2(12) \Psi_1(3) + S_3(123)$$

$$\chi_4(12; 34) = S_2(13) S_2(24) + S_2(14) S_2(23)$$

$$+ S_3(123) \Psi_1(4) + S_3(124) \Psi_1(3) + S_4(1234)$$

$$h_{\nu_1 \nu_2} = \langle \nu_1 | T \Psi_1 | \nu_2 \rangle + \sum_{\nu'} \langle \nu_1 \nu' | V \Psi_2 | \nu_2 \nu' \rangle_A$$

- Insert unit operators to derive explicit expressions

$np$ - $nh$  projection:

the amplitudes  $S_n$  coupled to  $S_{n+1}$  and  $S_{n+2}$ , as well as to all  $S_m$  with  $m < n$

The Schrödinger equation  $\rightarrow$  a set of non-linear coupled equations for the amplitudes

For the moment not too much progress has been obtained for practical purposes

Idea:

For relatively low density systems only comparatively rarely do more than a few particles come together to lift themselves simultaneously out of the Fermi sea

SUB( $n$ ) approximation hierarchy:

all clusters with more than  $n$  particles are neglected

Throwing away  $S_m, m > n$  still leaves us with a rich wave function

$$\exp(S_1 + S_2 + \dots + S_n)|\Phi\rangle$$

High-excitations, few-body effects, collective effects, ... are taken into account

SUB(1) approximation:  $S_n = 0, n > 1$

Equation for  $S_1$

$$\langle \alpha_1 | T \Psi_1 | \nu_1 \rangle + \sum_{\nu} \langle \alpha_1 \nu | V \Psi_1 \Psi_1 | \nu_1 \nu \rangle_A = \sum_{\nu} h_{\nu \nu_1} \langle \alpha_1 | \psi_1 | \nu \rangle$$

This is the Hartree Fock equation with a self-consistent potential

$$\langle \alpha_1 | U \Psi_1 | \nu_1 \rangle = \langle \alpha_1 \nu | V \Psi_1 \Psi_1 | \nu_1 \nu \rangle_A$$

A surprise?

SUB(1) wave function:

$$|\Psi\rangle = e^{S_1} |\Phi\rangle$$

$$S_1 = \sum_{\rho, \nu} \langle \rho | S_1 | \nu \rangle a_{\rho}^{\dagger} a_{\nu}$$

No: the Thouless theorem ensures that  $|\Psi\rangle$  is nothing more than a general Slater determinant non-orthogonal to the reference state  $|\Phi\rangle$

Usual choice:  $S_1 = 0$

- Use HF wave function as the reference state (with  $S_2 = 0, S_3 = 0$ )
- Solve the generalized HF equation (including couplings with  $S_2$  and  $S_3$ )
- Use a *reasonable* reference state, e.g. Harmonic Oscillator single-particle states. Converged results should be independent of the reference state  $\rightarrow$  our choice for finite nuclei and helium drops

## 3.2 Some examples from Quantum Chemistry

### CHEMICAL ACCURACY:

Ethylene molecule

- Total energy: -78.35451 hartrees
- Hartree-Fock energy: -78.04520 hartrees
- Correlation energy: 309.31 mh
- Reaction  $\text{H}_2 + \text{C}_2\text{H}_2 \rightarrow \text{C}_2\text{H}_4$

Experimental energy:  $66.99 \pm 0.40$  mh

- Equilibrium bond length:  $R_c = 1.339 \pm 0.001 \text{ \AA}$
- Transition from planar to twisted configuration at  $R_c \simeq 2 \text{ \AA}$
- 1% change in  $R_c \rightarrow 2$  mh change in energy

Typically a HF calculation provides  $\simeq 99\%$  of the energy, and very sophisticated methods are required to determine the correlation energy  $\rightarrow$  high-precision is needed ( $\leq 1$  mh)

## VOCABULARY

| Quantum Chemistry  |   | Physics                |
|--------------------|---|------------------------|
| Operators $T, T_n$ | → | Operators $S, S_n$     |
| CCS (singles)      | → | SUB(1), CC1            |
| CCSD (doubles)     | → | SUB(2), CC2            |
| CCSDT (triples)    | → | SUB(3), CC3            |
| CCSD(T)            | → | approximate $S_3$      |
| CCSD(T,Q)          | → | approximate $S_3, S_4$ |
| SR                 | → | single reference state |
| MR                 | → | multi reference state  |
| FCI                | → | full CI (converged CI) |

### Examples:

- Potential energy curves HF molecule (Paldus, RPMBT11)
- Vibrational levels  $N_2$  molecule (Paldus, RPMBT11)
- Spectroscopic parameters  $N_2$  molecule (Paldus, RPMBT11)
- Relativistic CCM: Excited states  $Sc^+$  atom (Kaldor, RPMBT11)
- Relativistic CCM: Excited states Xe atom (Kaldor, RPMBT11)

RPMBT11: 11th Conf. Recent Progress in Many-Body Theories, Manchester, July 2001

→ **S1, S2, S3, S4, S5**

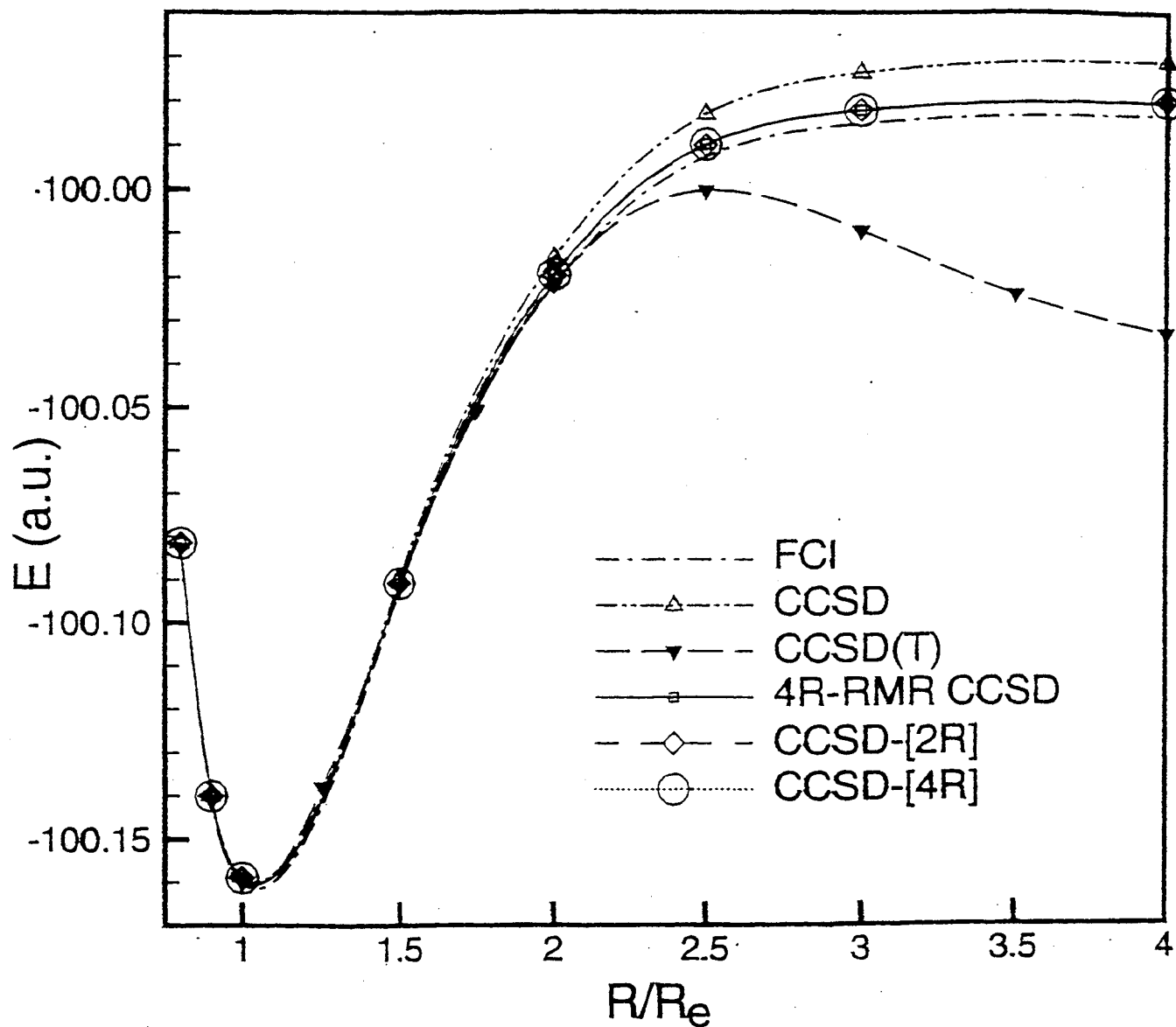


Figure 1. Potential energy curves for the HF molecule obtained with the FCI (dash-dot curve), CCSD (dash-dot-dot curve), CCSD(T) (long dash curve), 4R-RMR CCSD (solid curve), CCSD-[2R] (dashed curve), and CCSD-[4R] (dotted curve) methods and a DZ basis set.

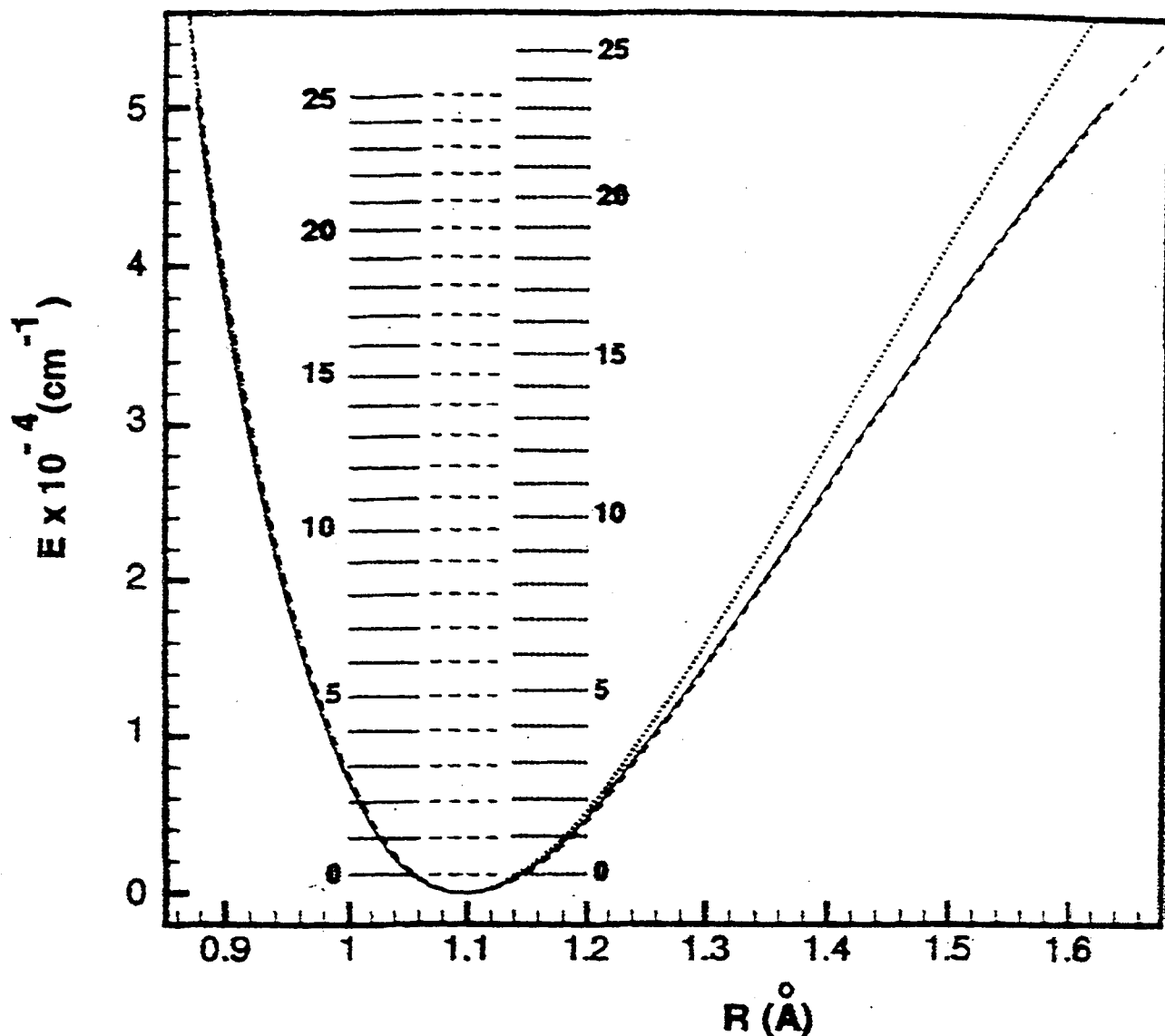


FIG. 1. The experimentally determined RKR PEC and the first 26 vibrational levels (Ref. 30) (solid curve and lines) and the corresponding *ab initio* data obtained with the SR CCSD (dotted curve and lines) and 8R RMR CCSD (dashed curve and lines) methods and cc-pVTZ basis set. The energy zero is chosen to coincide with the minimum of the PEC in each case.

A comparison of theoretical and experimental spectroscopic parameters for the  $N_2$  molecule

|                          | Expt.    | SR<br>CCSD | 4R RMR<br>CCSD |
|--------------------------|----------|------------|----------------|
| $R_e(\text{\AA})$        | 1.0977   | 1.0962     | 1.1012         |
| $\omega_e$               | 2358.54  | 2425.60    | 2365.2         |
| $-\omega_e x_e$          | -14.3058 | -12.9242   | -14.0058       |
| $\omega_e y_e / 10^{-3}$ | -5.07    | 5.92       | -7.62          |
| $\omega_e z_e / 10^{-4}$ | -1.10    | 0.57       | -0.53          |
| $B_e$                    | 1.9982   | 2.0040     | 1.9861         |
| $-\alpha_e / 10^{-2}$    | -1.7313  | -1.5969    | -1.6880        |
| $\gamma_e / 10^{-5}$     | -2.85    | -0.34      | -2.43          |
| $\delta_e / 10^{-7}$     |          | 0.199      | -4.241         |
| $-D_e / 10^{-6}$         | -5.74    | -5.46      | -5.56          |
| $\beta_e / 10^{-8}$      | -1.02    | -0.03      | -1.81          |



Pilot application: IP, EEs of  $\text{Sc}^+$  (eV, errors in meV):

FSCC: only  $4s, 3d$  can be included in  $P$ .

IH:  $P_m$ :  $4s, 3d, 4p$ ;  $P$ :  $5s, 6s, 5p, 6p, 4d, 5d, 4f$  added.

|                                  | State          | Expt.  | IH err | FS err |
|----------------------------------|----------------|--------|--------|--------|
| IP                               | $3d4s \ ^3D_1$ | 12.800 | 29     | 93     |
| EE                               | $\ ^3D_2$      | 0.009  | 1      | 1      |
|                                  | $\ ^3D_3$      | 0.022  | 3      | 3      |
|                                  | $\ ^1D_2$      | 0.315  | -16    | 29     |
|                                  | $3d^2 \ ^3F_2$ | 0.596  | 17     | -121   |
|                                  | $\ ^3F_3$      | 0.606  | 18     | -120   |
|                                  | $\ ^3F_4$      | 0.618  | 22     | -116   |
|                                  | $\ ^1D_2$      | 1.357  | 34     | -66    |
|                                  | $4s^2 \ ^1S_0$ | 1.455  | -56    | -82    |
|                                  | $3d^2 \ ^3P_0$ | 1.497  | 27     | -98    |
|                                  | $\ ^3P_1$      | 1.500  | 28     | -97    |
|                                  | $\ ^3P_2$      | 1.507  | 29     | -96    |
|                                  | $\ ^1G_4$      | 1.768  | 14     | -113   |
|                                  | $3d4p \ ^1D_2$ | 3.234  | 3      | NC     |
|                                  | $\ ^3F_2$      | 3.403  | 10     | NC     |
|                                  | $\ ^3F_3$      | 3.422  | 12     | NC     |
|                                  | $\ ^3F_2$      | 3.452  | 14     | NC     |
|                                  | many more      |        | good   | NC     |
| Average error, first 13 energies |                |        | 18     | 80     |

Accuracy quadrupled.

Many more states accessible.

Average error of first 20 states is 0.020 eV.

Excitation energies of Xe (cm<sup>-1</sup>).

| Configuration       | <i>J</i> | Expt. | Calculated |
|---------------------|----------|-------|------------|
| $5p^5(^2P_{3/2})6s$ | 2        | 67068 | 67466      |
|                     | 1        | 68046 | 68484      |
| $5p^5(^2P_{1/2})6s$ | 0        | 76197 | 76391      |
|                     | 1        | 77186 | 77457      |
| $5p^5(^2P_{3/2})6p$ | 1        | 77270 | 77735      |
|                     | 2        | 78120 | 78713      |
|                     | 3        | 78404 | 78983      |
|                     | 1        | 78957 | 79585      |
|                     | 2        | 79213 | 79913      |
|                     | 0        | 80119 | 80588      |
|                     | 1        | 88380 | 88985      |
| $5p^5(^2P_{1/2})6p$ | 2        | 89163 | 89810      |
|                     | 1        | 89279 | 89953      |
|                     | 0        | 89861 | 90395      |
|                     | 1        | 89861 | 90395      |
| $5p^5(^2P_{3/2})5d$ | 0        | 79772 | 80240      |
|                     | 1        | 79987 | 80441      |
|                     | 4        | 80197 | 80388      |
|                     | 3        | 80971 | 81275      |
|                     | 2        | 80323 | 80705      |
|                     | 1        | 83890 | 84495      |
|                     | 2        | 81926 | 82347      |
|                     | 3        | 82431 | 83008      |

Average error 0.060 eV or 0.6%

MVOs improve results by 0.03–0.05 eV.

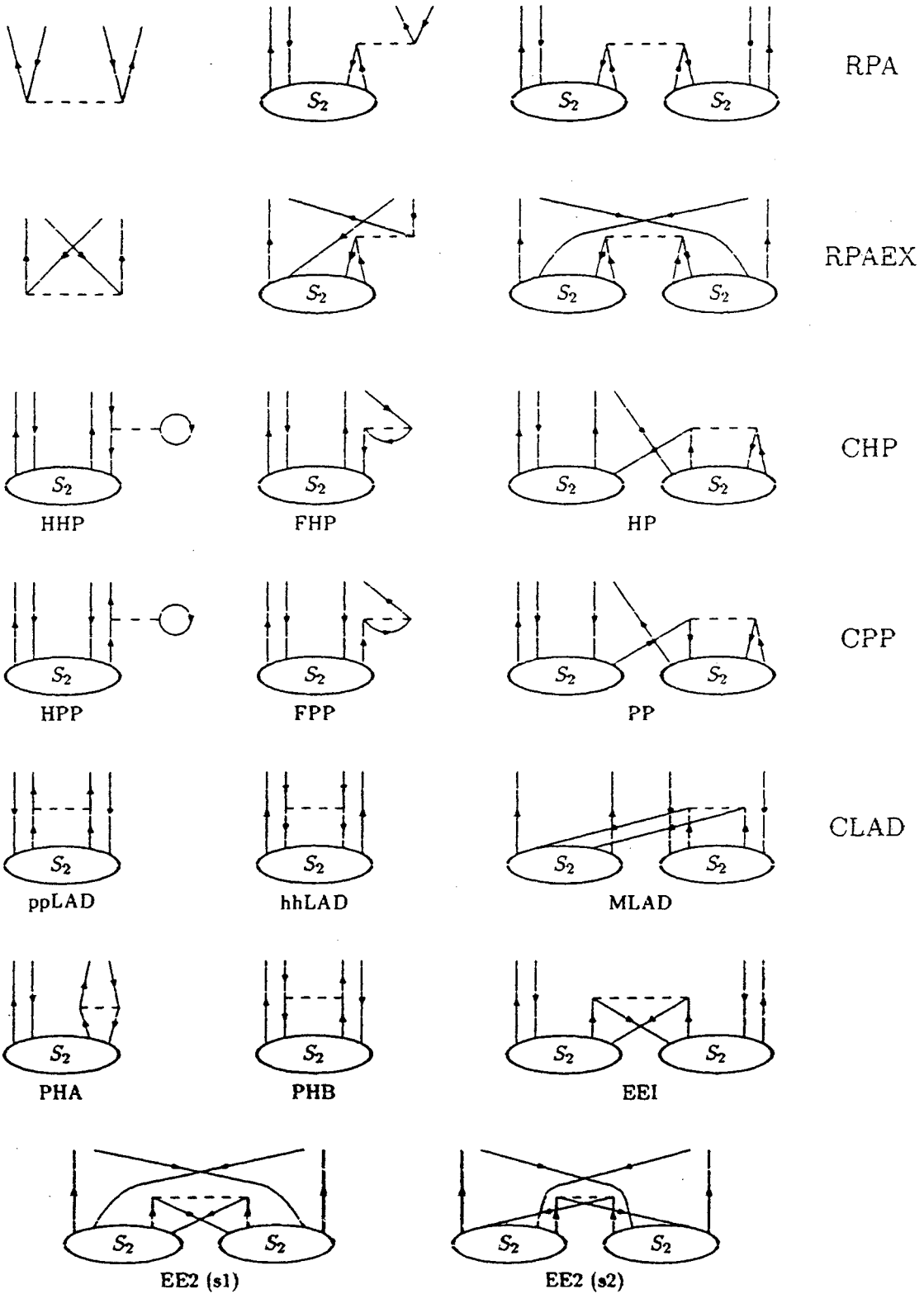
# 3.3 Diagrammatic representation of CC2 equations

2p-2h projection

$$S_1 = 0, S_{n>2} = 0$$

$$\begin{aligned}
 & - \langle \rho_1 \rho_2 | [T(1) + T(2)] S_2 | \nu_1 \nu_2 \rangle_A \\
 & \quad + \sum_{\nu} (h_{\nu \nu_1} \langle \rho_1 \rho_2 | S_2 | \nu \nu_2 \rangle_A + h_{\nu \nu_2} \langle \rho_1 \rho_2 | S_2 | \nu_1 \nu \rangle_A) \\
 = & \langle \rho_1 \rho_2 | V \Psi_2 | \nu_1 \nu_2 \rangle_A + \frac{1}{2} \sum_{\nu \nu'} \langle \rho_1 \rho_2 | S_2 | \nu \nu' \rangle_A \langle \nu \nu' | V \Psi_2 | \nu_1 \nu_2 \rangle_A \\
 & + 2 \sum_{\nu} \langle \rho_1 \rho_2 \nu | V(13) [S_2(12) + S_2(23)] | \nu_1 \nu_2 \nu \rangle_A \\
 & + \frac{1}{2} \sum_{\nu \nu'} \langle \rho_1 \rho_2 \nu \nu' | V(34) [S_2(13) S_2(24) \\
 & \quad + S_2(14) S_2(23)] | \nu_1 \nu_2 \nu \nu' \rangle_A
 \end{aligned}$$

- $h_{\nu_1 \nu_2} = \langle \nu_1 | T \Psi_1 | \nu_2 \rangle + \sum_{\nu'} \langle \nu_1 \nu' | V \Psi_2 | \nu_2 \nu' \rangle_A$
- Integers in parentheses after a particular operator refer that operator to those quantum labels in the associated bra or ket in the corresponding numerical positions (counting from the left)
- Insert unit operators to derive explicit expressions



## 3.4 Application to the Coulomb plasma

"Jellium": a model for electrons in metals

Ionic lattice  $\rightarrow$  uniform positive charge

Two-body interaction:

$$V(q) = \frac{4\pi e^2}{\Omega q^2} (1 - \delta_{q,0})$$

$\Omega$  = normalization volume

One-component Coulomb plasma

$N$  fermions (or bosons) of mass  $m$ , charge  $e$ , interacting via  $V(q)$

Thermodynamical limit:  $\rho = N/\Omega$ ,  $N \rightarrow \infty$ ,  $\Omega \rightarrow \infty$

Dimensionless coupling constant:  $r_s = r_0/a_0$

$r_0$  = average interparticle distance

$a_0 = \hbar^2/m_e^2$  Bohr radius

$$\rho = (4\pi r_s^3 a_0^3/3)^{-1} \equiv k_F^3/3\pi^2$$

Energy per particle in Rydberg units:

$$E/N = \epsilon \frac{e^2}{2a_0}$$

$$\epsilon = \epsilon_0 + \epsilon_c$$

$\epsilon_0$  = Hartree-Fock energy

$\epsilon_c$  = correlation energy

- Weak limit:

$$r_s \rightarrow 0 \text{ (plasma limit)}$$

- Intermediate coupling:

$$1 \leq r_s \leq 5 \text{ (metallic region)}$$

- Strong limit:

$$r_s \rightarrow \infty \text{ (Wigner crystal)}$$

$-\epsilon_c$  (in milliRydberg) for the unpolarized electron gas

| $r_s$ | 1   | 2    | 3      | 4      | 5    | 10    | 20    |
|-------|-----|------|--------|--------|------|-------|-------|
| RPA   | 158 | 124  | 106    | 93.6   | 84.9 | 61.3  | 42.8  |
| CC2   | 123 | 91.7 | 75.1   | 64.4   | 56.8 |       |       |
| CC[4] | 122 | 90.4 | 73.8   | 63.4   | 56.0 | 37.0  | 23.6  |
| GFMC  | 121 | 90.2 | (73.8) | (63.6) | 56.3 | 37.22 | 23.00 |

R.F. Bishop and K.H. Lührmann: PRB 17('78)3757

K. Emrich and J.G. Zabolitzky: PRB 30 ('84) 2049

GFMC: D.M. Ceperley and B.J. Alder: PRL 45 ('80)

566; ( S.H. Vosko et al: Can.J.Phys. 50 ('80) 1200 )

## 3.5 The HCSUB(n) approximation

Hard Core potential:

$$V(r) = \infty, r < r_c$$

SUB(1): Equation for  $S_1$

$$\langle \alpha_1 | T \Psi_1 | \nu_1 \rangle + \sum_{\nu} \langle \alpha_1 \nu | V \Psi_1 \Psi_1 | \nu_1 \nu \rangle_A = \sum_{\nu} h_{\nu \nu_1} \langle \alpha_1 | \Psi_1 | \nu \rangle$$

$$h_{\nu_1 \nu_2} = \langle \nu_1 | T \Psi_1 | \nu_2 \rangle + \sum_{\nu'} \langle \nu_1 \nu' | V \Psi_1 \Psi_1 | \nu_2 \nu' \rangle_A$$

$$E = \sum_{\nu} \langle \nu | T \Psi_1 | \nu \rangle + \frac{1}{2} \sum_{\nu, \nu'} \langle \nu \nu' | V \Psi_1 \Psi_1 | \nu \nu' \rangle_A$$

In the case the potential contains a hard core the description of the wave function in terms of solely single particle wave functions is not longer possible

Exact energy:

$$E = \sum_{\nu} \langle \nu | T \Psi_1 | \nu \rangle + \frac{1}{2} \sum_{\nu, \nu'} \langle \nu \nu' | V \Psi_2 | \nu \nu' \rangle_A$$

One has to include at least  
two-body correlations

## 1p-1h projection

$$\begin{aligned}
 & \langle \alpha_1 | T \Psi_1 | \nu_1 \rangle + \sum_{\nu} \langle \alpha_1 \nu | T(2) S_2 | \nu_1 \nu \rangle_A \\
 & + \sum_{\nu} \langle \alpha_1 \nu | V \Psi_2 | \nu_1 \nu \rangle_A \\
 & + \frac{1}{2} \sum_{\nu, \nu'} \langle \alpha_1 \nu \nu' | V(23) \chi_3(1; 23) | \nu_1 \nu \nu' \rangle_A \\
 & = \sum_{\nu} h_{\nu \nu_1} \langle \alpha_1 | \Psi_1 | \nu \rangle
 \end{aligned}$$

$\langle \alpha_1 \nu | V \Psi_2 | \nu_1 \nu \rangle_A$  finite if

$$\langle x_1 x_2 | \Psi_2 | \nu_1 \nu \rangle_A \equiv 0, |x_1 - x_2| < r_c$$

Since

$$\begin{aligned}
 \langle x_1 x_2 | \Psi_2 | \nu_1 \nu_2 \rangle_A & = \{ \langle x_1 | \Psi_1 | \nu_1 \rangle \langle x_2 | \Psi_1 | \nu_2 \rangle \}_A \\
 & + \langle x_1 x_2 | S_2 | \nu_1 \nu_2 \rangle_A
 \end{aligned}$$

this means that  $S_2$  inside the hard core is determined completely by the single particle wave functions

Consider the three-body amplitude

$$\langle \alpha_1 \nu \nu' | V(23) \chi_3(1; 23) | \nu_1 \nu \nu' \rangle_A$$

$$\chi_3(1; 23) = S_2(13) \Psi_1(2) + S_2(12) \Psi_1(3) + S_3(123)$$

Inside the hard core,  $S_3$  is completely determined by  $S_2$  and  $\Psi_1$

**SUB(2) approximation is meaningless in case of a HC potential** One has to neglect  $\chi_3$  altogether if one wants to calculate wave function with HC interactions including two-body and excluding higher correlations



SUB(2): Equation for  $S_2$  (Assume  $S_1 = 0$ )

$$\begin{aligned}
& \langle \rho_1 \rho_2 | [T(1) + T(2)] S_2 | \nu_1 \nu_2 \rangle_A \\
& + \langle \rho_1 \rho_2 | V \Psi_2 | \nu_1 \nu_2 \rangle_A + \frac{1}{2} \sum_{\nu \nu'} \langle \rho_1 \rho_2 | S_2 | \nu \nu' \rangle_A \langle \nu \nu' | V \Psi_2 | \nu_1 \nu_2 \rangle_A \\
& \left( + \sum_{\nu} \langle \rho_1 \rho_2 \nu | [V(13) \chi_3(2; 13) + V(23) \chi_3(1; 23)] | \nu_1 \nu_2 \nu \rangle_A \right) \\
& + \sum_{\nu} \langle \rho_1 \rho_2 \nu | V(13) [S_2(12) + S_2(23)] \\
& \quad + V(23) [S_2(12) + S_2(13)] | \nu_1 \nu_2 \nu \rangle_A \\
& \left( + \frac{1}{2} \sum_{\nu \nu'} \langle \rho_1 \rho_2 \nu \nu' | V(34) \chi_4(12; 34) | \nu_1 \nu_2 \nu \nu' \rangle_A \right) \\
& + \frac{1}{2} \sum_{\nu \nu'} \langle \rho_1 \rho_2 \nu \nu' | V(34) [S_2(13) S_2(24) \\
& \quad + S_2(14) S_2(23)] | \nu_1 \nu_2 \nu \nu' \rangle_A \\
& = \sum_{\nu} (h_{\nu \nu_1} \langle \rho_1 \rho_2 | S_2 | \nu \nu_2 \rangle_A + h_{\nu \nu_2} \langle \rho_1 \rho_2 | S_2 | \nu_1 \nu \rangle_A)
\end{aligned}$$

HCSUB(2): Equation for  $S_2$   
( $S_1 = 0, \chi_3 = 0, \chi_4 = 0, S_{n>2} = 0$ )

$$\begin{aligned}
& \langle \rho_1 \rho_2 | [T(1) + T(2)] S_2 | \nu_1 \nu_2 \rangle_A \\
& + \langle \rho_1 \rho_2 | V \Psi_2 | \nu_1 \nu_2 \rangle_A + \frac{1}{2} \sum_{\nu \nu'} \langle \rho_1 \rho_2 | S_2 | \nu \nu' \rangle_A \langle \nu \nu' | V \Psi_2 | \nu_1 \nu_2 \rangle_A \\
& = \sum_{\nu} (h_{\nu \nu_1} \langle \rho_1 \rho_2 | S_2 | \nu \nu_2 \rangle_A + h_{\nu \nu_2} \langle \rho_1 \rho_2 | S_2 | \nu_1 \nu \rangle_A)
\end{aligned}$$

→ EXERCISE 3

## 4. TICC2: Finite Nuclei

Previous CC calculations in finite nuclei:

- Kümmel, Lührmann, Zabolitzky (PRep 36 ('76) 1)  
 $^4\text{He}$ ,  $^{16}\text{O}$ ,  $^{40}\text{Ca}$ , CC(4), realistic interactions

→ S6

- Heisenber, Mihaila (PR C59 ('99) 1440)

$^{16}\text{O}$ , CC(3), configuration space up to  $50 \hbar\omega$

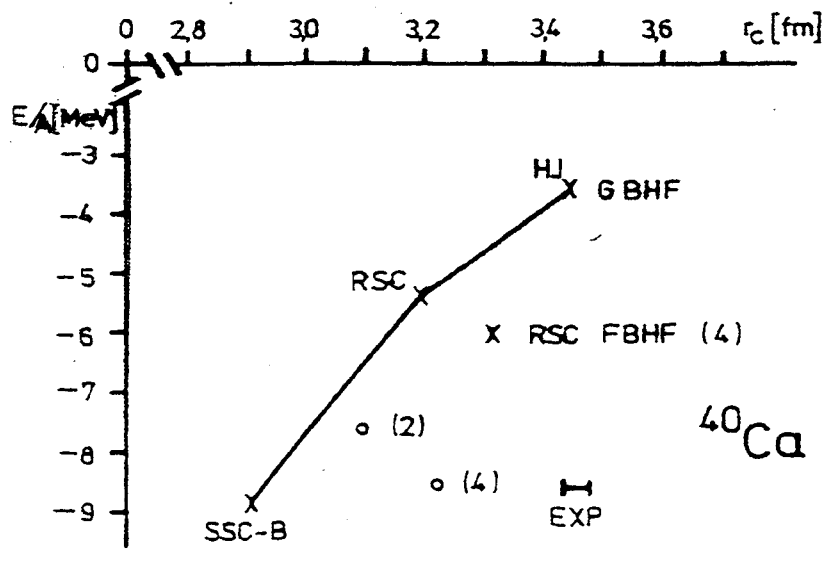
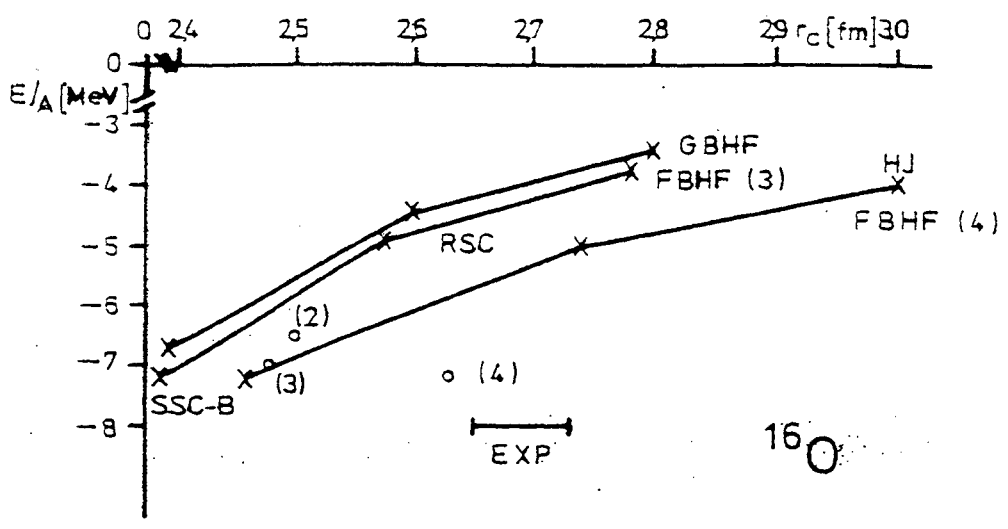
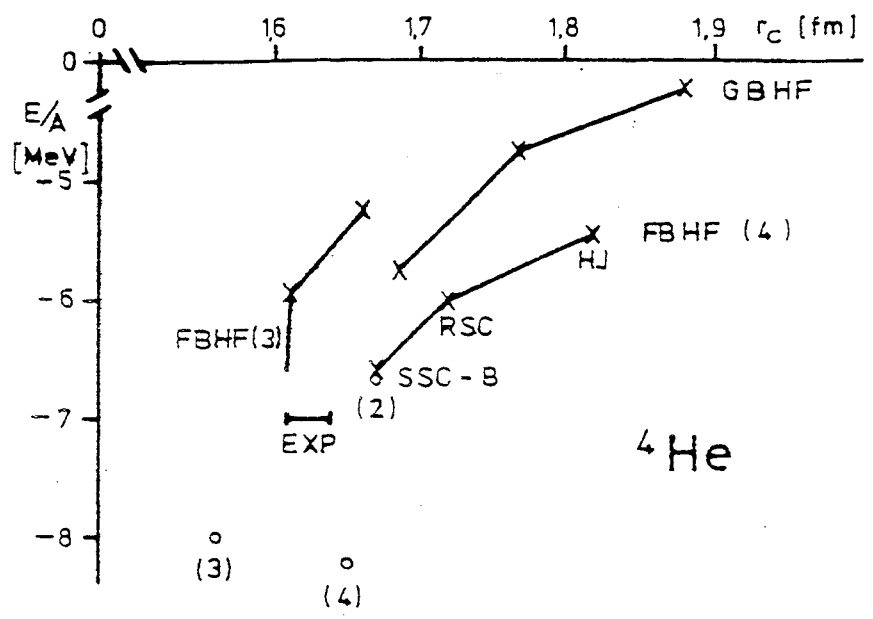
|      | $-E/A$ (MeV) | $r_c$ (fm)      |
|------|--------------|-----------------|
| AV14 | 6.1          | 2.86            |
| AV18 | 5.9          | 2.81            |
| Exp. | 8.0          | $2.73 \pm 0.03$ |

The Center-of-mass motion

→ Translational Invariance

- Approximation:  $T \rightarrow T - T_{\text{CM}}$  (only exact for HO)
- Use a TI reference state from the very beginning → TICCn

Kümmel, Lührmann, Zabolitzky  
 Phys. Rep. 36C (1978) 1



# 4.1 TICC2 in configuration representation

## N Boson system

Determine a wave function of the CCM form

$$|\Psi\rangle = e^S|\Phi\rangle$$

completely symmetric and translationally invariant

**Possibilities for the reference state:**

- Use a TI wave function (for instance, choose Jacobi coordinates or hyperspherical coordinates)
- Use the Harmonic Oscillator GS wave function

HO single-particle wave functions:

$$|nlm\rangle = a_{nlm}^+|0\rangle$$

N-boson wave function:

$$|\Phi\rangle = \frac{1}{\sqrt{N!}} \left(a_{000}^+\right)^N |0\rangle$$

Use coordinate representation:

$$\langle \mathbf{r}_1, \dots, \mathbf{r}_N | \Phi \rangle = \left( \frac{\alpha}{\sqrt{\pi}} \right)^{3N/2} \exp \left( -\frac{\alpha^2}{2N} \sum_{i < j} \mathbf{r}_{ij}^2 \right) \exp \left( -\frac{N\alpha^2}{2} \mathbf{R}^2 \right)$$

HO parameter:  $\alpha = (m\omega/\hbar)^{1/2}$

Although the wave function is not TI, this factorization allows us to eliminate the CMM unambiguously

A similar factorization also holds for a fermionic system, where the reference state is a Slater determinant build up from HO single particle wave functions

The correlation operator at the SUB(2) level

$$S = S_1 + S_2$$

$S_1$  and  $S_2$  are independent 1p-1h and 2p-2h operators  
Translational Invariance couples them

Example:

$$\begin{array}{rcl} (\mathbf{r}_i - \mathbf{r}_j)^2 & = & \mathbf{r}_i^2 + \mathbf{r}_j^2 - 2(\mathbf{r}_i \cdot \mathbf{r}_j) \\ \text{TI operator} & & \begin{array}{l} \text{1p - 1h operator} \quad \text{2p - 2h operator} \end{array} \end{array}$$

Neither the one-body operator  $\mathbf{r}_i^2$  nor the two-body operator  $\mathbf{r}_i \cdot \mathbf{r}_j$  are separately TI

$$\mathbf{TICC2} \quad S_1 + S_2 \longrightarrow S^{(1,2)}$$

Translational Invariance may be imposed by:

- Recoupling the product of sp HO states into sums of comparable products of HO states for the relative and center-of-mass coordinates of the pair
- Imposing that the CMM of the destroyed pair in the occupied subspace is the same as that of the created pair of particles in the unoccupied subspace

Since we are dealing with HO wave functions this is accomplished by using the Brody-Moshinsky brackets

# The Cluster Operator

$$\begin{aligned}
 \mathcal{S}^{(1,2)} &= \sum_{n=1}^{\infty} \mathcal{S}(n) \\
 &\quad \sum_{n_1, n_2, l} \langle n0, 00, 0 | n_1 l, n_2 l, 0 \rangle \\
 &\quad \left[ a_{n_1 l}^+ \times a_{n_2 l}^+ \right]^{(0,0)} a_{000}^2
 \end{aligned}$$

$\mathcal{S}_n$  is the amplitude to be determined

$\langle nl, NL, \lambda | n_1 l_1, n_2 l_1, \lambda \rangle$  is a Brody-Moshinsky coefficient  
 sp states  $n_1, l_1, n_2, l_2$  coupled to angular momentum  $\lambda$ .  
 BM coefficient gives its contents in terms of relative  
 state  $nl$  and CM state  $NL$  coupled to  $\lambda$

$a_{000}^2$  destroys two particles in occupied states

$\left[ a_{n_1 l}^+ \times a_{n_2 l}^+ \right]^{(\lambda, \mu)}$  creates two particles in occupied states,  
 coupling their angular momentum to  $(\lambda, \mu)$

- The term with both  $(n_1, l) = (0, 0)$  and  $(n_2, l) = (0, 0)$  is excluded, as it simply reproduces the uncorrelated reference state
- The terms with either  $(n_1, l) = (0, 0), n_2 \neq 0$  and  $n_1 \neq 0, (n_2, l) = (0, 0)$  must be included. These terms give precisely the required 1p-1h excitations in the admixture

Note the simplification implied by TI: the amplitudes to be determined are the c-numbers  $\mathcal{S}(n)$ , which depends on a single parameter  $n$ , which counts the number of oscillator quanta globally excited ( $2n\hbar\omega$ )

The use of a TI  $S^{(1,2)}$  does not imply that  $e^{S^{(1,2)}}$  is also TI

Simplified notation:

$$S^{(1,2)} = s(p)a_p^+ a_0^+ a_0^2 + s(p,q)a_p^+ a_q^+ a_0^2$$

sum over repeated indices is assumed,  $p \equiv (n_p, l_p, m_p)$ ,  $0 \equiv (0, 0, 0)$

$$\begin{aligned} s(p) &= \delta(l_p, 0)\delta(m_p, 0) 2 \langle n_p 0, 00, 0 | n_p 0, 00, 0 \rangle S(n_p) \\ s(p, q) &= C(l_p, l_q, 0; m_p, m_q, 0) \\ &\quad \langle n_p + n_q + l_p 0, 00, 0 | n_p l_p, n_q l_p, 0 \rangle S(n_p + n_q + l_p) \end{aligned}$$

Consider

$$\begin{aligned} S^{(1,2)} S^{(1,2)} &= [s(p_1)a_{p_1}^+ a_0^+ + s(p_1, q_1)a_{p_1}^+ a_{q_1}^+] \\ &\quad [s(p_2)a_{p_2}^+ a_0^+ + s(p_2, q_2)a_{p_2}^+ a_{q_2}^+] a_0^4 \\ &\quad + [s(p_1)a_{p_1}^+ a_0^+ + s(p_1, q_1)a_{p_1}^+ a_{q_1}^+] 2s(p_2)a_{p_2}^+ a_0^3 \end{aligned}$$

The red term is TI. The blue term is not TI.

The clue: the term in red is precisely the ordered form :  $S^{(1,2)} S^{(1,2)}$  :

The same device applies to all the powers of  $S^{(1,2)}$

## TICC2 Ansatz for the wave function

$$|\Psi\rangle = :e^{S^{(1,2)}}: |\Phi\rangle$$

## The TICC2 Equations

$$H : e^{S^{(1,2)}} : |\Phi\rangle = E : e^{S^{(1,2)}} : |\Phi\rangle$$

Op-0h projection:

$$E = \langle \Phi | H : e^{S^{(1,2)}} : |\Phi \rangle$$

Notation:

$$\begin{aligned} k(m, p) &= \langle n_m, l_m, m_m | K | n_p, l_p, m_p \rangle \\ v(n, m, p, q) &= \langle n_m, l_m, m_m; n_n, l_n, m_n | V | n_p, l_p, m_p; n_q, l_q, m_q \rangle \\ np_i &= N(N-1)\dots(N-i+1) \end{aligned}$$

Use REDUCE to obtain

$$\begin{aligned} E = & k(0,0)*np1 + v(0,0,0,0)*np2 \\ & + np2*( k(0,p)*s(p) + 2*(n-1)*v(0,0,p,0)*s(p) ) \\ & + np2*( 2*v(0,0,p,q)*s(p,q) ) \\ & + np4*( v(0,0,p,q)*s(p)*s(q) ) \end{aligned}$$

Recall:

$$E = \sum_{\nu} \langle \nu | T \Psi_1 | \nu \rangle + \frac{1}{2} \sum_{\nu\nu'} \langle \nu\nu' | V \Psi_2 | \nu\nu' \rangle_A$$

$$S^{(1,2)} = s(p) a_p^+ a_0^+ a_0^2 + s(p, q) a_p^+ a_q^+ a_0^2$$

with  $s(p) \rightarrow \mathcal{S}(n_p)$  and  $s(p, q) \rightarrow \mathcal{S}(n_p + n_q + l_p)$



To obtain the TICC2 equation for the amplitudes  $S(n)$  we have to project onto the appropriate admixture of 1p-1h and 2p-2h, characterized by the quantum number  $N_x$  (excitation energy  $2N_x\hbar\omega$ )

The TI excited state:

$$\langle \Phi | [c(p)a_p a_0 (a_0^+)^2 + c(p,q)a_p a_q (a_0^+)^2] | \Phi \rangle$$

$$c(p) = \delta(l_p, 0)\delta(m_p, 0)2\langle n_p 0, 00, 0 | n_p 0, 00, 0 \rangle$$

$$c(p,q) = C(l_p, l_q, 0; m_p, m_q, 0)\langle n_p + n_q + l_p 0, 00, 0 | n_p l_p, n_q l_q, 0 \rangle$$

The resulting equation:

$$\begin{aligned} & \langle \Phi | [c(p)a_p a_0 (a_0^+)^2 + c(p,q)a_p a_q (a_0^+)^2] | H : e^{S^{(1,2)}} : | \Phi \rangle \\ & = E \langle \Phi | [c(p)a_p a_0 (a_0^+)^2 + c(p,q)a_p a_q (a_0^+)^2] : e^{S^{(1,2)}} : | \Phi \rangle \end{aligned}$$

Simplified notation:

$$\sum_{i_1, i_2, i_3, i_4=0}^{N_{\max}} F(N_x, i_1, i_2, i_3, i_4) S(i_1) S(i_2) S(i_3) S(i_4) = 0$$

with the convention  $S(0) = 1$

Example: Contribution of the potential energy

$$\langle \Phi | \left[ c(m)(a_0^+)^2 a_0 a_m + c(m,n)(a_0^+)^2 a_m a_n \right] V : e^{S^{(1,2)}} : | \Phi \rangle$$

to the equation

$$\sum_{i_1, i_2, i_3, i_4=0}^{N_{\max}} F(N_x, i_1, i_2, i_3, i_4) \mathcal{S}(i_1) \mathcal{S}(i_2) \mathcal{S}(i_3) \mathcal{S}(i_4) = 0$$

$$F(N_x, 0, 0, 0, 0) = \\ \text{np2} * ( 2 * (n-1) * c(m) * v(m, 0, 0, 0) \\ + 2 * c(m, n) * v(m, n, 0, 0) )$$

$$F(N_x, i_1, 0, 0, 0) = \\ \text{np2} * ( (n-1) ** 2 * (n-2) * c(m) * v(0, 0, 0, 0) * s(m) \\ + 2 * (n-2) * (n-3) * c(m, n) * v(0, 0, 0, 0) * s(m, n) \\ + 4 * (n-1) * (n-2) * c(m, n) * v(m, 0, 0, 0) * s(n) \\ + 4 * (n-1) * (n-2) * c(m) * v(0, 0, p, 0) * s(m, p) \\ + 4 * (n-1) ** 2 * c(m) * v(m, 0, p, 0) * s(p) \\ + 16 * (n-2) * c(m, n) * v(n, 0, p, 0) * s(m, p) \\ + 4 * (n-1) * c(m) * v(m, 0, p, q) * s(p, q) \\ + 4 * (n-1) * c(m, n) * v(m, n, p, 0) * s(p) \\ + 4 * c(m, n) * v(m, n, p, q) * s(p, q) )$$

$$\text{np2} = N(N-1)$$

$$\begin{aligned}
F(N_x, i_1, i_2, 0, 0) = & \\
np4 * ( & (n-2) * (n-3) * c(m, n) * v(0, 0, 0, 0) * s(m) * s(n) \\
& + 4 * (n-3) * c(m, n) * v(0, 0, p, 0) * s(m, n) * s(p) \\
& + 8 * (n-3) * c(m, n) * v(0, 0, p, 0) * s(m, p) * s(n) \\
& + 2 * (n-1) * (n-2) * c(m) * v(0, 0, p, 0) * s(m) * s(p) \\
& + 4 * c(m, n) * v(0, 0, p, q) * s(m, n) * s(p, q) \\
& + 8 * c(m, n) * v(0, 0, p, q) * s(m, p) * s(n, q) \\
& + 8 * (n-2) * c(m, n) * v(n, 0, p, 0) * s(m) * s(q) \\
& + 4 * (n-1) * c(m) * v(0, 0, p, q) * s(m, q) * s(p) \\
& + 2 * (n-1) * c(m) * v(0, 0, p, q) * s(m) * s(p, q) \\
& + 2 * (n-1) * c(m) * v(m, 0, p, q) * s(p) * s(q) \\
& + 16 * c(m, n) * v(n, 0, p, q) * s(m, q) * s(p) \\
& + 8 * c(m, n) * v(n, 0, p, q) * s(m) * s(p, q) \\
& + 2 * c(m, n) * v(m, n, p, 0) * s(p) * s(q) )
\end{aligned}$$

$$\begin{aligned}
F(N_x, i_1, i_2, i_3, 0) = & \\
np6 * ( & 2 * (n-3) * c(m, n) * v(0, 0, p, 0) * s(m) * s(n) * s(p) \\
& + (n-2) * c(m) * v(0, 0, p, q) * s(m) * s(p) * s(q) \\
& + 8 * c(m, n) * v(0, 0, p, q) * s(m, p) * s(n) * s(q) \\
& + 2 * c(m, n) * v(0, 0, p, q) * s(m, n) * s(p) * s(q) \\
& + 2 * c(m, n) * v(0, 0, p, q) * s(m) * s(n) * s(p, q) \\
& + 4 * c(m, n) * v(n, 0, p, q) * s(m) * s(p) * s(q) )
\end{aligned}$$

$$\begin{aligned}
F(N_x, i_1, i_2, i_3, i_4) = & \\
np8 * ( & c(m, n) * v(0, 0, p, q) * s(m) * s(n) * s(p) * s(q) )
\end{aligned}$$

$$np4 = N(N-1)(N-2)(N-3)$$

$$np6 = np4 (N-4)(N-5)$$

$$np8 = np6 (N-6)(N-7)$$

$$\sum_{i_1, i_2, i_3, i_4=0}^{N_{\max}} F(N_x, i_1, i_2, i_3, i_4) S(i_1) S(i_2) S(i_3) S(i_4) = 0$$

with  $S(0) = 1$

- The function  $F(N_x, i_1, i_2, i_3, i_4)$  contains combinations of excitation coefficients  $c(n)$ , and matrix elements of kinetic and potential energy
- TICC2 involves the solution of a coupled set of non-linear multinomial equations in the truncated set of coefficients  $\{S(n); n = 1, \dots, N_{\max}\}$
- This is a nonlinear problem: there is no *a priori* way to know whether all solutions have been determined in this way neither if the so obtained solutions are or not physically relevant
- TICI2  $|\Psi\rangle = (1 + :S^{(1,2)}:)|\Phi\rangle$  (linear approximation)

Solve

$$\sum_{i_1=0}^{N_{\max}} F(N_x, i_1, 0, 0, 0) S(i_1) + q \sum_{i_1=0, (i_2, i_3, i_4) \neq 0}^{N_{\max}} F(N_x, i_1, i_2, i_3, i_4) S(i_1) S(i_2) S(i_3) S(i_4) = 0$$

$q$  quenching factor slowly growing from 0 (TICI2) to 1 (TICC2)

- The use of a HO reference state introduces a free parameter  $\alpha$ , and a supplementary minimization of the ground state energy could also be envisaged

TIC12  
 S I  
 $N_{max}$   
 $\sum_{i=0}^{N_{max}} F(N_i, i, 0, 0, 0)$   
 $S(i, \alpha) = 0$   
 $S(0) = 1$

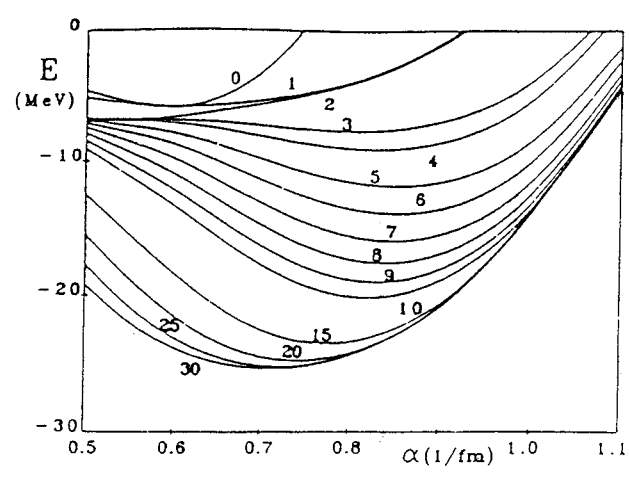


FIG. 2. The ground-state energy of the  ${}^4\text{He}$  nucleus calculated with the S3 potential and at various levels of basis truncation in the CI2 approximation, as a function of the oscillator parameter  $\alpha$  which characterizes the single-particle basis. The different curves are labeled by the respective order ( $n_{max}$ ) of the truncation.

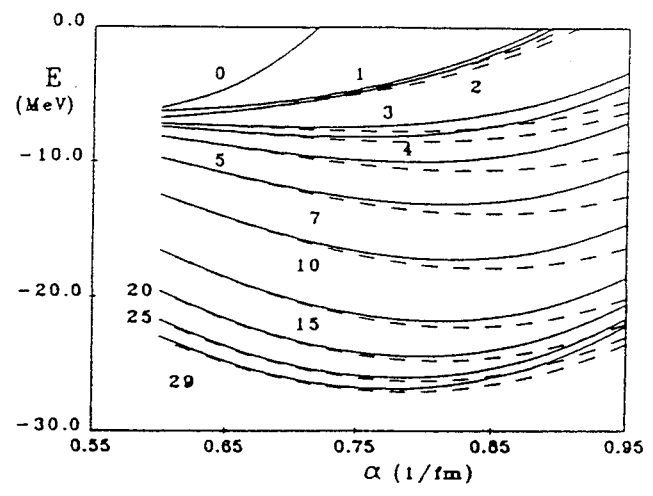


FIG. 3. The ground-state energy of the  ${}^4\text{He}$  nucleus calculated with the MT-V potential and at various levels of basis truncation in the CI2 approximation (solid lines) and the CC2 approximation (dashed lines), as a function of the oscillator parameter  $\alpha$  which characterizes the single-particle basis. The different curves are labeled by the order ( $n_{max}$ ) of the truncation.

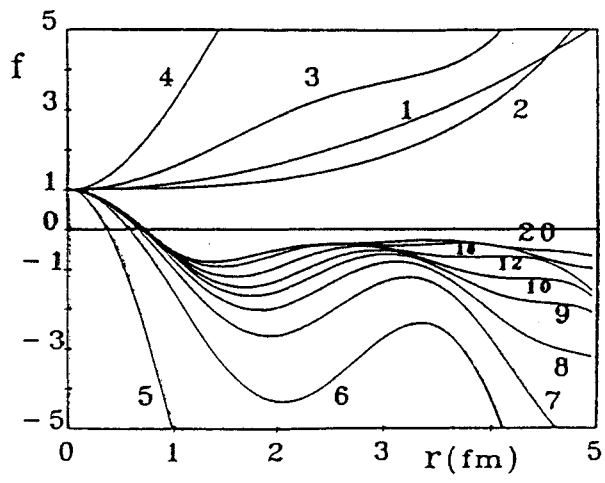


FIG. 4. The correlation factor  $f(r)$  that characterizes the CI2 approximation to the  ${}^4\text{He}$  ground-state wave function via the parametrization of Eq. (35). The calculation employs the S3 potential and a value  $\alpha = 0.7 \text{ fm}^{-1}$  for the oscillator parameter of the single-particle basis. The different curves are labeled by the respective order ( $n_{max}$ ) of the truncation.

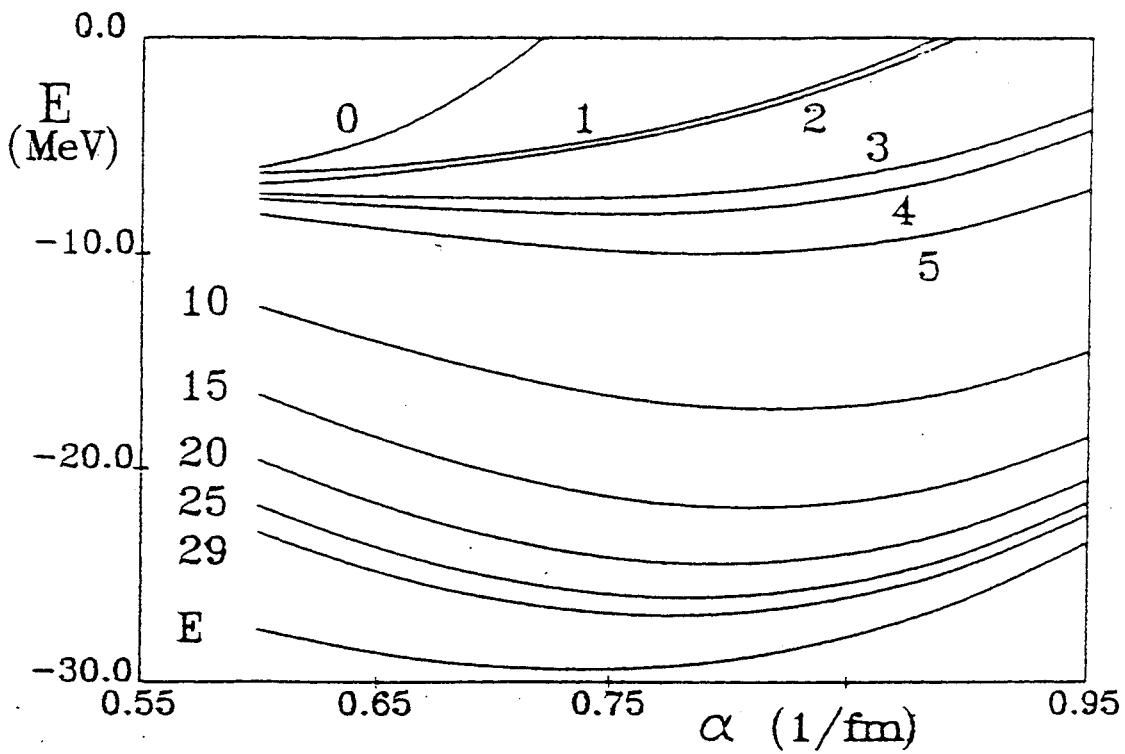
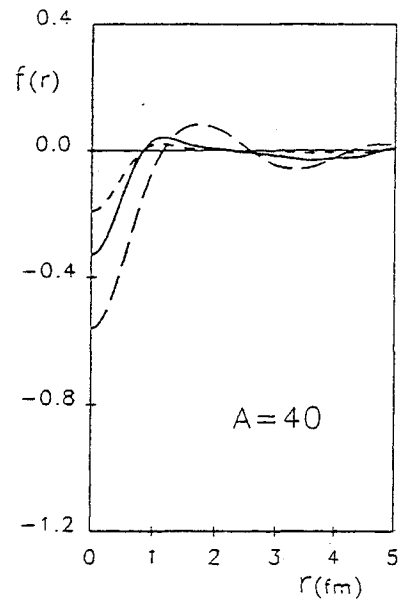
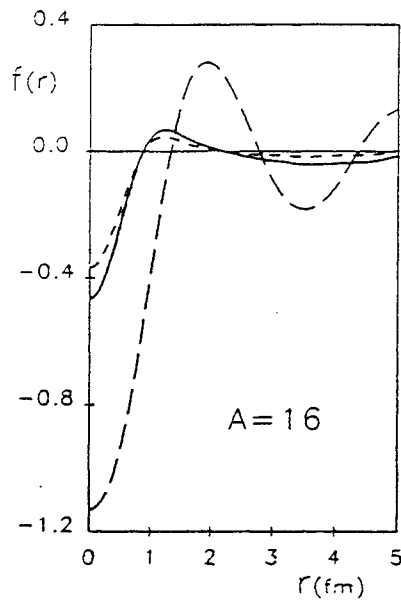
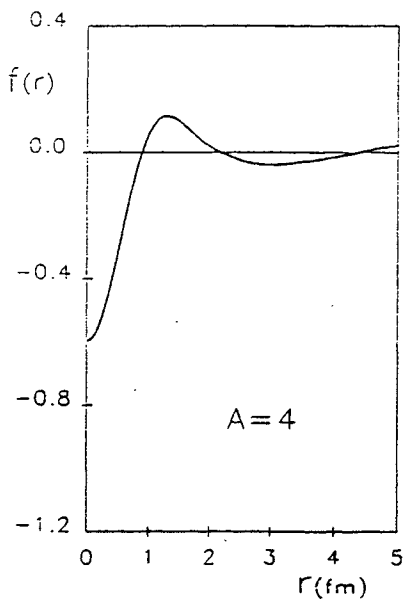
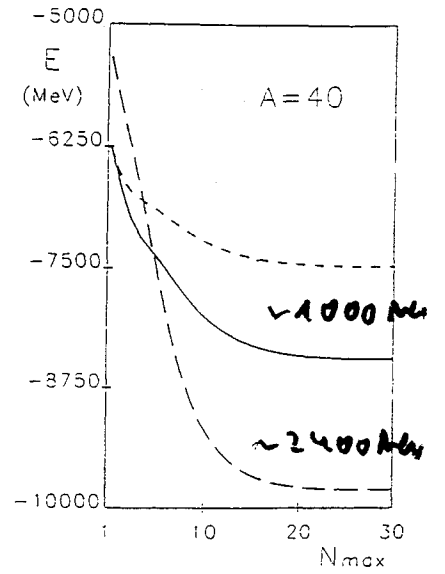
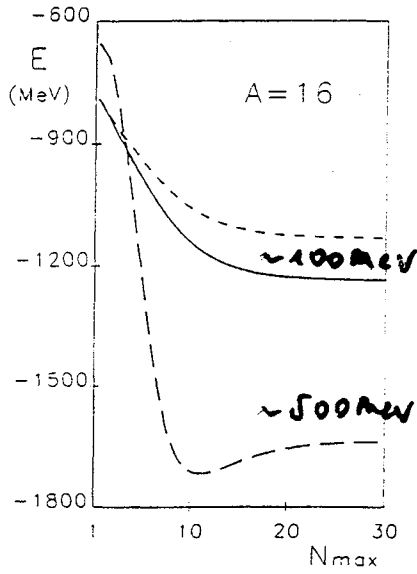
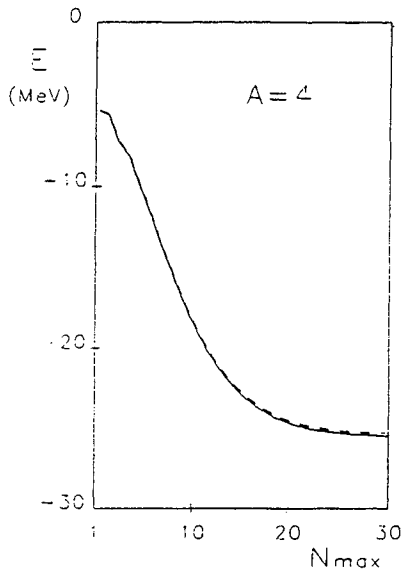


Figure 3. The GS energy in MeV of  ${}^4\text{He}$  corresponding to the MTV interaction versus the harmonic oscillator parameter  $\alpha$ . The lines labelled with an integer number  $n_{\text{max}}$  represent the shell-model calculation with  $2p$ - $2h$  excitations up to  $2n_{\text{max}}\hbar\omega$  in energy. The curve labelled E is the present Euler-Lagrange evaluation of this energy.

A BOSONS  
S<sub>2</sub> INTERACTION



$$\sum_{i < j} f(r_{ij}) |\phi\rangle$$

→ S7, S8, S9

Several comments regarding these three solutions

- All of them tend to stability with increasing values of  $N_{\max}$ , and at  $N_{\max} = 30$  they have already converged.
- There is a connection between the continuous line and the CI2 line in the quenching scheme and in both directions. This means that starting at CI2 solution ( $q = 0$ ) one arrives to the point in the continuous line (CC2 solution) when  $q = 1$  and conversely, starting at the CC2 solution ( $q=1$ ) from the continuous line one arrives to the CI2 solution by slowly decreasing  $q$  down to  $q = 0$ .
- There is not a connection path which starts at the long-dashed CC2 solution. When  $q$  is slowly decreased the solution disappears.



## 4.2 TICC2 in coordinate representation

Coordinate representation of operator  $S^{(1,2)}$

$$\langle \mathbf{r}_1 \dots \mathbf{r}_N | S^{(1,2)} | \Phi \rangle = 2 \sum_{n=1}^{\infty} S(n) \left[ \frac{2^n n!}{(2n+1)!!} \right]^{1/2} \sum_{i < j} L_n^{1/2} \left( \frac{1}{2} \alpha^2 r_{ij}^2 \right) \langle \mathbf{r}_1 \dots \mathbf{r}_N | \Phi \rangle$$

Completeness of the Laguerre polynomials:

$$f(r) = 2 \sum_{n=1}^{\infty} S(n) \left[ \frac{2^n n!}{(2n+1)!!} \right]^{1/2} L_n^{1/2} \left( \frac{1}{2} \alpha^2 r^2 \right)$$

$$\langle \mathbf{r}_1 \dots \mathbf{r}_N | S^{(1,2)} | \Phi \rangle = \sum_{i < j} f(r_{ij}) \langle \mathbf{r}_1 \dots \mathbf{r}_N | \Phi \rangle$$

The quadratic term:

$$\langle \mathbf{r}_1 \dots \mathbf{r}_A | : S^{(1,2)} S^{(1,2)} : | \Phi \rangle = \sum_{i < j} f(r_{ij}) \sum'_{k < l} f(r_{kl}) \langle \mathbf{r}_1 \dots \mathbf{r}_A | \Phi \rangle$$

Primed sum means that neither particle in pair  $kl$  in the second summation coincides with either particle in pair  $ij$  in the first one

TICC2 ground-state wave function in coordinate representation

$$\begin{aligned} \Psi(\mathbf{r}_1 \dots \mathbf{r}_A) &= \langle \mathbf{r}_1 \dots \mathbf{r}_A | : \exp S^{(1,2)} : | \Phi \rangle \\ &= \left( 1 + \sum_{i < j} f(r_{ij}) + \frac{1}{2!} \sum_{i < j} f(r_{ij}) \sum'_{k < l} f(r_{kl}) \right. \\ &\quad \left. + \frac{1}{3!} \sum_{i < j} f(r_{ij}) \sum'_{k < l} f(r_{kl}) \sum''_{m < n} f(r_{mn}) + \dots \right) \Phi(\mathbf{r}_1 \dots \mathbf{r}_A) \end{aligned}$$

convention: repeated indices in the products of primed sums are excluded

**In general: CC<sub>n</sub> deals only with independent *n*-body correlation operators**

Compare with a Jastrow correlation factor

$$\begin{aligned} &\exp \left( \sum_{i < j} h(ij) \right) \Phi(\mathbf{r}_1 \dots \mathbf{r}_A) \\ &= \left( 1 + \sum_{i < j} h(ij) + \frac{1}{2!} \sum_{i < j} \sum_{k < l} h(ij) \right. \\ &\quad \left. + \frac{1}{3!} \sum_{i < j} \sum_{k < l} \sum_{m < n} h(ij) h(kl) h(mn) + \dots \right) \Phi(\mathbf{r}_1 \dots \mathbf{r}_A) \end{aligned}$$

Repeated indices imply non trivial technical problems if functions *h* contain not commuting operators

## Properties of the correlation function $f(r)$

The intermediate normalization condition  $\langle \Phi | \Psi \rangle = 1$  implies

$$\langle \Phi | \left( \sum_{i < j} f(r_{ij}) + \frac{1}{2!} \sum_{i < j} f(r_{ij}) \sum'_{k < l} f(r_{kl}) + \dots \right) | \Phi \rangle = 0$$

In the case of a bosonic system this condition is always satisfied because

$$\langle \phi_{000}(\mathbf{r}_1) \phi_{000}(\mathbf{r}_2) | f(r_{12}) | \phi_{000}(\mathbf{r}_1) \phi_{000}(\mathbf{r}_2) \rangle = 0$$

HO single-particle wave functions

$$\phi_{000}(\mathbf{r}_i) = \left( \frac{\alpha}{\sqrt{\pi}} \right)^{3/2} \exp\left(-\frac{1}{2}\alpha^2 r_i^2\right)$$

Change of coordinates  $\{\mathbf{r}_1, \mathbf{r}_2\} \rightarrow \{\mathbf{r}, \mathbf{R}\}$

$$\begin{aligned} & \langle \phi_{000}(\mathbf{r}_1) \phi_{000}(\mathbf{r}_2) | f(r_{12}) | \phi_{000}(\mathbf{r}_1) \phi_{000}(\mathbf{r}_2) \rangle \\ &= \langle \phi_{000}(\mathbf{R}) \phi_{000}(\mathbf{r}) | f(r) | \phi_{000}(\mathbf{R}) \phi_{000}(\mathbf{r}) \rangle \\ &= \langle \phi_{000}(\mathbf{r}) | f(r) | \phi_{000}(\mathbf{r}) \rangle \\ &= 2 \sum_{n=1}^{\infty} S(n) \left( \frac{2^n n!}{(2n+1)!!} \right)^{1/2} \\ & \quad \langle \phi_{000}(\mathbf{r}) | L_n^{1/2} \left( \frac{1}{2} \alpha^2 r^2 \right) | \phi_{000}(\mathbf{r}) \rangle \end{aligned}$$

The red factor is identically zero due to the orthogonality properties of the Laguerre polynomials

The physical meaning is clear: the pair correlation function  $f(r_{12})$  projects the product  $\phi_{000}(\mathbf{r}_1) \phi_{000}(\mathbf{r}_2)$  of occupied functions onto the unoccupied subspace

## Projecting onto $T(1p-1h + 2p-2h)$ states

In coordinate representation the wave function is given by

$$\Psi = \left( 1 + \sum f(ij) + \frac{1}{2!} \sum \sum' f(ij)f(kl) + \dots \right) \Phi$$

Ground-state energy

$$\begin{aligned} E &= \langle \Phi | H | \Psi \rangle \\ &= \langle \Phi | H \left( 1 + \sum f(ij) + \frac{1}{2!} \sum \sum' f(ij)f(kl) + \dots \right) | \Phi \rangle \end{aligned}$$

A generic  $T(1p-1h + 2p-2h)$  excitation may be represented by an arbitrary function  $g(r_{ij})$  with the same characteristics as  $f$ , namely



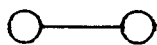

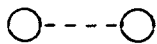
$$\langle \phi_{000}(\mathbf{r}_1)\phi_{000}(\mathbf{r}_2) | g(r_{12}) | \phi_{000}(\mathbf{r}_1)\phi_{000}(\mathbf{r}_2) \rangle = 0$$

Equation for  $f$

$$\langle \Phi | g H | \Psi \rangle = E \langle \Phi | g | \Psi \rangle,$$

The equation is most succinctly presented in a diagrammatic form.

Notation:

|               |  |
|---------------|--|
| Particle      |   |
| function $g$  |  |
| function $f$  |  |
| Action of $T$ |   |
| Action of $V$ |  |

## CC2 Equation in diagrammatic form

$$\begin{aligned}
 & 2 \text{---} + 2 \text{---} + 2C_1^2 \left\{ \text{---} + \text{---} + \text{---} \right\} \\
 & + 2C_2^2 \left\{ \text{---} + \text{---} \right\} \\
 & + \text{---} + \text{---} + 2C_1^2 \text{---} \\
 & + 2C_1^2 \left\{ \text{---} + \text{---} + \text{---} + \text{---} \right\} \\
 & + 2C_2^2 \left\{ \text{---} + \text{---} + \text{---} + \text{---} \right\} \\
 & + C_2^2 \left\{ \text{---} + \text{---} + 2 \text{---} + 2 \text{---} + 2 \text{---} \right\} \\
 & + 2C_3^2 \left\{ \text{---} + \text{---} + \text{---} + \text{---} + \text{---} \right\} \\
 & + 2C_4^2 \left\{ \text{---} + \text{---} \right\} \\
 & + E_2 \text{---} + E_3 2C_1^2 \text{---} + E_4 C_2^2 \text{---} \\
 & = E_0 \left\{ \text{---} + 2C_1^2 \text{---} + C_2^2 \text{---} \right\}
 \end{aligned}$$

Statistical factors  $C_k^n \equiv (N-n)(N-n-1)\dots(N-n-k+1)$

The quantities  $E_n$  are related to unlinked diagrams

$$\begin{aligned}
 E_n = & C_1^n \text{---} + C_2^n \text{---} + \frac{1}{2} C_2^n \text{---} + \frac{1}{2} C_2^n \text{---} \\
 & + C_3^n \text{---} + \frac{1}{2} C_4^n \text{---}
 \end{aligned}$$

$E_0$  corresponds to the ground-state energy

To clarify the diagrammatic notation:

$$\text{Diagram} \equiv \int \Phi^* g^*(r_{12}) V(r_{34}) f(r_{13}) f(r_{24}) \Phi \, d\mathbf{r}_1 \dots d\mathbf{r}_A$$

General form of the TICC2 equation

$$\int g^*(r_{12}) F[f] \, d\mathbf{r}_1 \dots d\mathbf{r}_A = 0.$$

$g(r)$  is not a fully arbitrary function, because of the required orthogonality of the excited states with respect to the reference state

Replace

$$g \longrightarrow G - \langle \Phi | G | \Phi \rangle$$

where  $G(r_{ij})$  is a completely arbitrary function

→ **EXERCISE 4**

Practical way to solve the integro-differential equation:  
Expand  $f$  using a suitable basis

- Gaussian basis  $f(r) = \sum_p C_p \exp(-\beta_p r^2)$   
(largely employed in atomic and molecular problems)  
Use negative and positive values for  $\{\beta_p\}$

Laguerre polynomial basis → TICC2 in configuration representation

## Example

Binding energies (in MeV) for various bosonic nuclei with the Wigner part of the S3 interaction and for the different orders of truncation of the equations in powers of  $f$

|         | $A = 4$ | $A = 8$ | $A = 16$ | $A = 40$ |
|---------|---------|---------|----------|----------|
| Order 1 | 25.42   | 225.46  | 1131.2   | 7495.3   |
| Order 2 | 25.60   | 235.12  | 1235.7   | 8457.1   |
| Order 3 |         | 235.12  | 1235.1   | 8458.5   |
| Order 4 |         | 235.12  | 1235.1   | 8458.7   |
| Conf.   | 25.49   | 235.03  | 1234.9   | 8456.6   |

Order 1 corresponds to the TIC12 case, and Order 4 is the full TICC2 result. The last row shows the full TICC2 configuration-space results

- The coordinate-space numbers are fully converged, with the use of between 10 and 14 gaussians  
By contrast, in HO configuration space up to 30 amplitudes were used (corresponding to single-particle excitation energies up to  $60\hbar\omega$ ), not reaching full convergence in some cases
- Working in coordinate-space results in a much faster computation of the required expansion coefficients
- The third- and fourth-order terms give an almost negligible contribution  $\rightarrow$  one may safely simplify the integro-differential equation by keeping only up to quadratic terms in  $f(r)$ .

## 4.3 The nuclei ${}^4\text{He}$ and ${}^{16}\text{O}$ in the TICI2 approximation

TICI2 in coordinate space

$$\Psi = \left( 1 + \sum_{i < j} f(r_{ij}) \right) \Phi \equiv \sum_{i < j} h(r_{ij}) \Phi$$

This ansatz is not exclusive of the bosonic nature of the particles we have assumed to obtain it

- The bosonic or fermionic character of the particles is contained in the reference state
- TICI2: the simplest way to consider TI pair correlations is to determine a correlation function  $h(r_{ij})$

In fermionic systems  $h(r_{ij})$  may be generalized to deal with discrete degrees of freedom

Suppose a V4 nucleon-nucleon interaction

$$V_{ij} = \sum_p V^{(p)}(r_{ij}) \Theta^{(p)}(ij),$$

$$\Theta^{(1)} = 1, \Theta^{(2)} = P_{ij}^\sigma, \Theta^{(3)} = P_{ij}^\tau, \Theta^{(4)} = P_{ij}^\sigma P_{ij}^\tau$$

It seems natural to consider an operatorial structure for the pair correlation operator also of the V4 form

$$h_{ij} = \sum_p h^{(p)}(r_{ij}) \Theta^{(p)}(ij)$$



## Practical calculation

$$h^{(p)}(r) = \sum_i c_i^{(p)} \exp(-\beta_i r^2),$$

$\{c_i^{(p)}\}$  = unknown coefficients to be determined

$\{\beta_i\}$  = set of pre-determined exponents (include negative as well as positive values)

- Note that this is completely different from the expansion in Laguerre polynomials  $\equiv$  TICI2 in configuration space
- The gaussian form is particularly adequate for the HO  $\Phi$ : the required space integrals are the product of an exponential of a positive-definite quadratic form with a polynomial
- The expectation value of the energy:

$$E(\{c_i^{(p)}\}) = \frac{\sum_{(ip),(jq)} c_i^{(p)*} \mathcal{H}_{ij}^{(pq)} c_j^{(q)}}{\sum_{(ip),(jq)} c_i^{(p)*} \mathcal{N}_{ij}^{(pq)} c_j^{(q)}}$$

(the different components in this decomposition are not orthogonal)

Optimize with respect to  $c_i^{(p)}$   $\rightarrow$  a generalized eigenvalue problem

$$\sum_{(jq)} \mathcal{H}_{ij}^{(pq)} c_j^{(q)} = \lambda \sum_{(jq)} \mathcal{N}_{ij}^{(pq)} c_j^{(q)}$$

The lowest eigenvalue  $\lambda$  gives an upper bound to the ground state energy (TICI2 is variational!)

Results for  $^4\text{He}$  and  $^{16}\text{O}$  with V4-interactions

V4-interactions: B1, S3, MS3, MT I/III and MT V

- This choice allows for the best comparison with existing results in the literature
- Some of these interactions are semi-realistic in the sense that they fit some of the two-nucleon properties

Two types of calculations, according to the two-body correlation operator

- state-independent (SI): restricted to the first term in 
$$h_{ij} = \sum_p h^{(p)}(r_{ij}) \Theta^{(p)}(ij)$$
- fully state-dependent (SD): four correlation functions are to be determined
- The value of the HO parameter  $\alpha$  has been optimized for the SI case, and this value is kept fixed for the ensuing SD calculations

The interactions

$$V_{B1}(r) = [595.5455e^{-(r/0.7)^2} - 72.2116e^{-(r/1.4)^2}] + [206.0455e^{-(r/0.7)^2} + 68.38784e^{-(r/1.4)^2}]P^\sigma P^\tau$$

$$V_{S3}(r) = [500.e^{-3r^2} - 81.675e^{-1.05r^2} - 10.75e^{-0.6r^2} - 41.5e^{-0.8r^2} - 5.75e^{-0.4r^2}] + [-81.675e^{-1.05r^2} - 10.75e^{-0.6r^2} + 41.5e^{-0.8r^2} + 5.75e^{-0.4r^2}]P^\sigma + [81.675e^{-1.05r^2} + 10.75e^{-0.6r^2} - 41.5e^{-0.8r^2} - 5.75e^{-0.4r^2}]P^\tau + [-500.e^{-3r^2} + 81.675e^{-1.05r^2} + 10.75e^{-0.6r^2} + 41.5e^{-0.8r^2} + 5.75e^{-0.4r^2}]P^\sigma P^\tau$$

$$V_{MS3}(r) = 500.e^{-3r^2} + V_{S3}(r)$$

$$V_{MTV}(r) = [1458.2687 \frac{e^{-3.11r}}{r} - 578.1769 \frac{e^{-1.55r}}{r}]$$

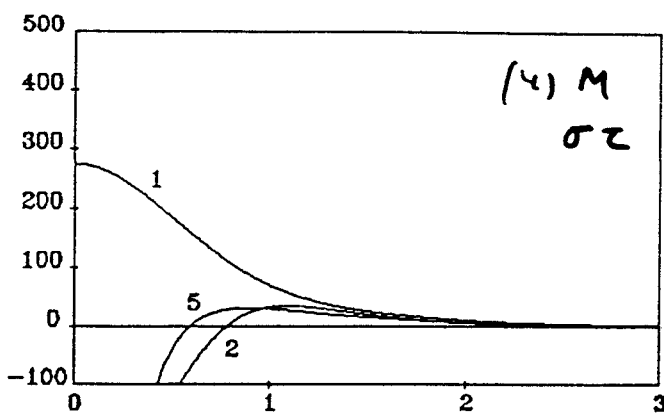
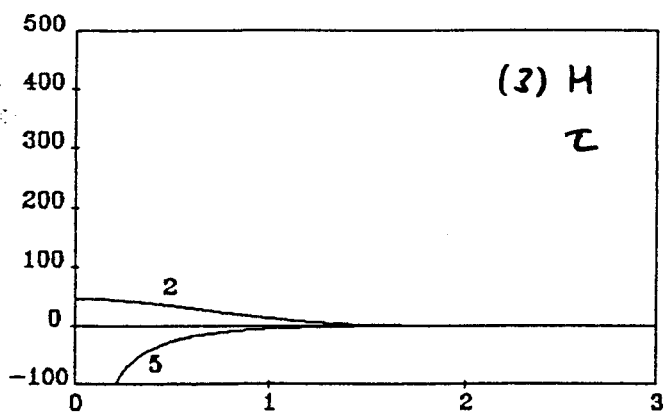
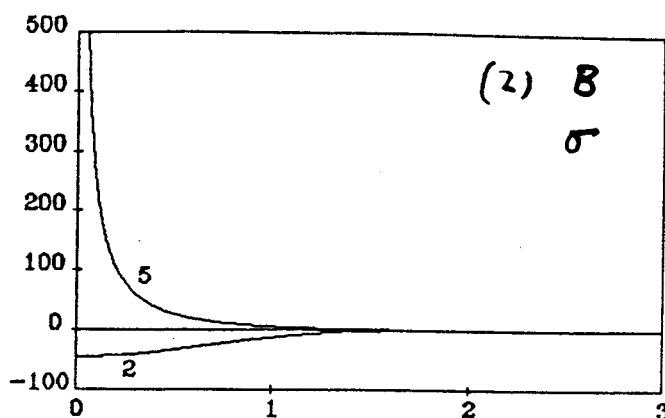
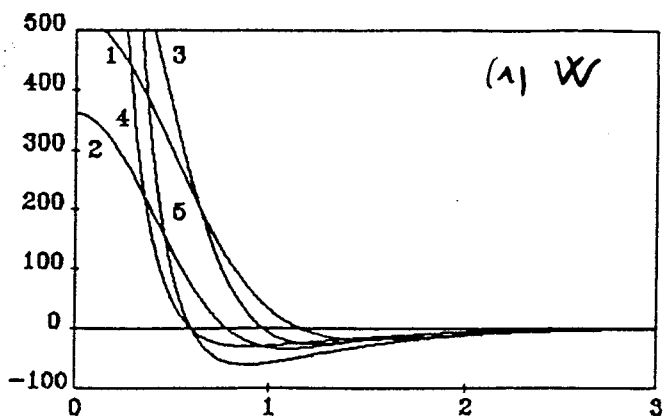
$$V_{MTI/III}(r) = [729.13435 \frac{e^{-3.11r}}{r} - 289.08845 \frac{e^{-1.55r}}{r}]$$

$$+ [28.61285 \frac{e^{-1.55r}}{r}]P^\sigma$$

$$+ [-28.61285 \frac{e^{-1.55r}}{r}]P^\tau$$

$$+ [-729.13435 \frac{e^{-3.11r}}{r} + 289.08845 \frac{e^{-1.55r}}{r}]P^\sigma P^\tau$$

→ S10



- 1: B1 (1), (4)
- 2: S3 (1), (2), (3), (4)
- 3: MS3 (1),  $\frac{1}{2}$  (2), (3), (4)  $\equiv$  S3
- 4: MT-V (1)
- 5: MT-I/III (1), (2), (3), (4)

$^4\text{He}$  and  $^{16}\text{O}$  nuclei

TICI2 ground-state energies (in MeV)

Nuc. Phys. **A609** (1996) 218

| Interaction | Nucleus         | $\alpha$ (fm $^{-1}$ ) | SI      | SD      |
|-------------|-----------------|------------------------|---------|---------|
| B1          | $^4\text{He}$   | 0.729                  | -37.86  | -37.86  |
|             | $^{16}\text{O}$ | 0.602                  | -145.94 | -167.30 |
| S3          | $^4\text{He}$   | 0.717                  | -25.41  | -28.19  |
|             | $^{16}\text{O}$ | 0.707                  | -141.64 | -164.88 |
| MS3         | $^4\text{He}$   | 0.713                  | -25.41  | -27.99  |
|             | $^{16}\text{O}$ | 0.596                  | -85.56  | -105.64 |
| MT I/III    | $^4\text{He}$   | 0.741                  | -29.45  | -30.81  |
|             | $^{16}\text{O}$ | 0.744                  | -194.10 | -207.52 |
| MT V        | $^4\text{He}$   | 0.741                  | -29.45  | -29.45  |
|             | $^{16}\text{O}$ | 1.078                  | -966.65 | -973.67 |

- SD variational space larger than the SI one: it should produce a lower value for the ground state energy  
 → (0 - 4) MeV for  $^4\text{He}$ , (10 - 20) MeV for  $^{16}\text{O}$
- Interactions B1 and MTV contain only Wigner and Majorana terms: do not couple to the spin-dependent piece of the correlation operator in  $^4\text{He}$   
 → No difference in the SD and SI energies for these interactions in  $^4\text{He}$   
 However, even for those potentials, spin-dependent correlations do play a role for  $^{16}\text{O}$  (← the uncorrelated state is not fully space symmetric)

Comparing with other techniques

Interaction: MTV

MTV does not saturate nuclear matter  $\rightarrow$  it produces high-density systems. Ideal case to test the importance of three- and more-body correlations

|          | ${}^4\text{He}$ (MTV) | ${}^{16}\text{O}$ (MTV) |
|----------|-----------------------|-------------------------|
| TICI2-SI | 29.45                 | 966.65                  |
| TICI2-SD | 29.45                 | 973.67                  |
| GFMC [a] | $31.3 \pm 0.2$        | $1194 \pm 20$           |
| DMC      | $31.32 \pm 0.02$ [b]  | $1189 \pm 1$ [c]        |
| VMC      |                       | $1138.5 \pm 0.2$ [c]    |
| FHNC/0   |                       | 987/1152 [d]            |
|          |                       | 1059/1055 [e]           |
| IDEA [f] | 30.7-31.2             | 1021-1027               |

${}^4\text{He}$ : TICI2  $\simeq$  94% GFMC, DMC energy

${}^{16}\text{O}$ : TICI2  $\simeq$  80% GFMC, DMC energy

the effects due to the non-linear terms neglected in TICI2, and the correlations neglected in TICCC2 are comparatively more important for heavier systems

[a] J.G. Zabolitzky et al: NP A356 ('81) 114; PR C25 ('82) 1111; NP A442 ('85) 109

[b] R.F. Bishop et al: JP G18 ('92) L21

[c] S.A Chin, E. Krotscheck: NP A560 ('93) 151

[d] G. Co', A. Fabrocini, S. Fantoni: NP A568 ('94) 73

[e] E. Krotscheck: NP A465 ('87) 461

[f] R. Brizzi et al: NP A596 ('96) 199

$\rightarrow$  S11

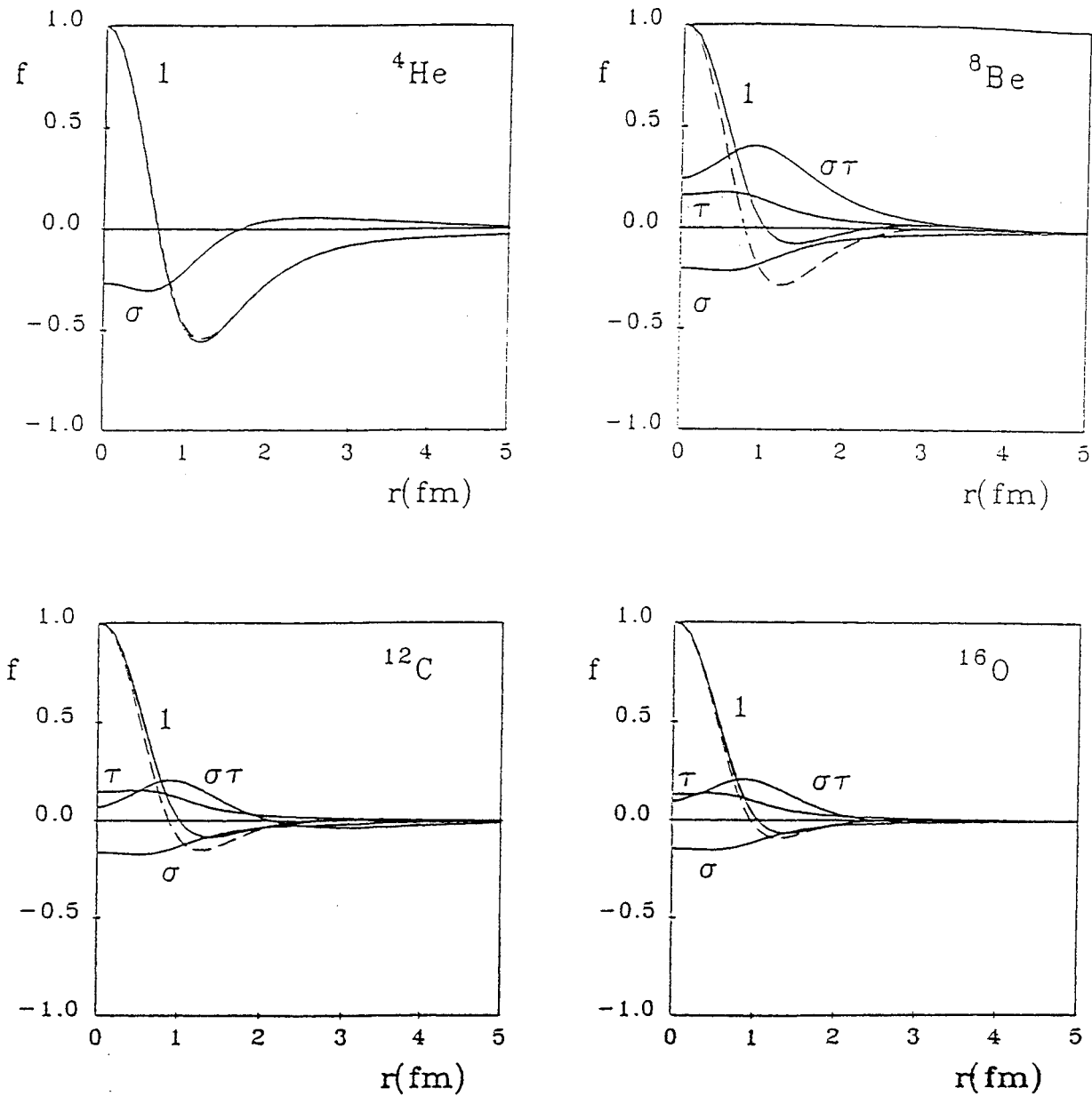


Fig. 1. The calculated correlation functions in the case of the MS3 potential. Dashed lines correspond to purely central scalar SI correlations and solid lines to SD correlations of V4 type. In the latter case the labels 1,  $\sigma$ ,  $\tau$  and  $\sigma\tau$  correspond to the terms  $k = 1, 2, 3$  and 4 in the parametrisation of eqs. (8) and (9). As discussed in the text, for helium only two such functions should be used.

SI - - -

SD ———

## V6-Interactions

$$V_{ij} = \sum_p V^{(p)}(r_{ij}) \Theta^{(p)}(ij),$$

Add two more terms containing the tensor operator

$$\begin{aligned}\Theta^{(5)}(ij) &= S_T(ij) \\ \Theta^{(6)}(ij) &= S_T(ij) P_{ij}^{(\tau)}\end{aligned}$$

We use the following interactions:

|         |   |
|---------|---|
| GPDT    | D. Gogny et al: PLB32('70)591             |
| SSC     | R. de Tournell, D. Sprung: NPA201('73)193 |
| AV14    | R.B. Wiringa et al: PRC29('84)1207        |
| AV18    | R.B. Wiringa et al: PRC51('95)38          |
| Reid-V6 | J. Carlson: PRC38('88)1879                |

They contain more terms (spin-orbit,  $L^2$ , ...), which will be ignored. Only the 4-central plus the 2-tensor terms are considered

Exception: Reid-V6, which is a V6 adaptation of Reid SC (R.V. Reid: AP 50 ('68) 411)

All these interactions are realistic: they include at least the one pion exchange part of the NN interaction plus a short-range phenomenological part, adjusted so as to reproduce experimental phase-shifts



The introduction of tensor correlations increases dramatically the computer time needed in the calculations

V4:

Potential matrix element of a generic diagram

$$\langle \phi | h^+(ij) V(kl) h(mn) | \Phi \rangle =$$

$$W_d \sum_{pqr} \sum_{i_1^* \dots i_N^* = 1}^{A/4} \sum_P \epsilon_P \text{Tr}(\Theta_{ij}^p \Theta_{ij}^p \Theta_{ij}^r P_{P i_1^* \dots P i_N^*}^\sigma P_{P i_1^* \dots P i_N^*}^r)$$

$$\langle \phi_{i_1^*}(1) \dots \phi_{i_N^*}(N) | h^{p*}(r_{ij}) V^q(r_{kl}) h^r(r_{mn}) | \phi_{P i_1^*}(1) \dots \phi_{P i_N^*}(N) \rangle$$

$W_d$ : statistical weight of the diagram

$\phi$ 's: spatial part of sp wave functions

$P_{P i_1^* \dots P i_N^*}^\sigma$ : representation of the spin part of the permutation

V6:

The tensor operator contributes both to the traces and to the spatial terms

→ The number of traces is much higher

→ More types of spatial integrals

→ **S12**

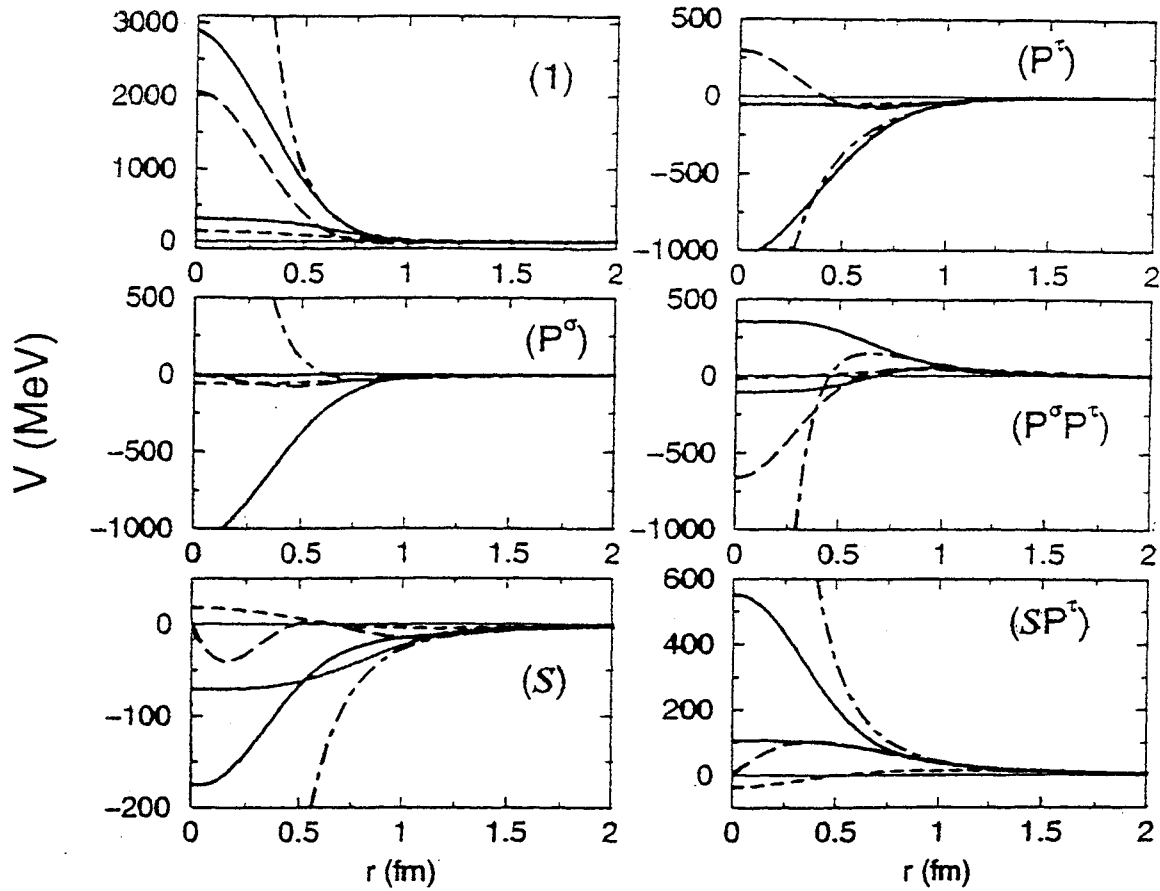


Fig. 2. A comparison between the V6 potentials used in this paper. The horizontal axis in each panel shows  $r$  (in fm), the vertical axis the potential strength (in MeV). Each panel represents one operatorial channel, for each of the operators used to expand the correlation functions, as indicated in the figure. The solid line is AV14, the long-dashed line is AV18. The dotted line is the SSC, and the medium dashed line is the Gogny. The short-long dashed line is the Reid-V6 potential.

$^4\text{He}$  and  $^{16}\text{O}$  nuclei  
 TICI2 ground-state energies (in MeV)  
 Nuc. Phys. **A643** (1998) 243

| Interaction | Nucleus         | -E      | $\alpha$ ( $\text{fm}^{-1}$ ) |
|-------------|-----------------|---------|-------------------------------|
| GPDT        | $^4\text{He}$   | -27.36  | 0.70                          |
|             | $^{16}\text{O}$ | -128.68 | 0.64                          |
| SSC         | $^4\text{He}$   | -24.12  | 0.68                          |
|             | $^{16}\text{O}$ | -63.55  | 0.55                          |
| AV14        | $^4\text{He}$   | -14.77  | 0.59                          |
|             | $^{16}\text{O}$ | -14.97  | 0.40                          |
| AV18        | $^4\text{He}$   | -15.40  | 0.61                          |
|             | $^{16}\text{O}$ | -23.76  | 0.46                          |
| Reid-V6     | $^4\text{He}$   | -5.67   |                               |

There is a competition between central and tensor forces:  
 Most binding is obtained from the off-diagonal tensor interaction (matrix element between the central and the tensor-correlated channel)

This matrix element competes with a strong repulsion in the central channel

The origin of the problem is to be related to the size of the repulsive core of the potential

Solution: Include more correlations

## 4.4 Beyond the TICI2 approximation

### 4.4.1 TICC[2]

Lessons from TICC2 for bosons

Binding energies (in MeV) for various bosonic nuclei with the Wigner part of the S3 interaction and for the different orders of truncation of the equations in powers of  $f$

|         | $A = 4$ | $A = 8$ | $A = 16$ | $A = 40$ |
|---------|---------|---------|----------|----------|
| Order 1 | 25.42   | 225.46  | 1131.2   | 7495.3   |
| Order 2 | 25.60   | 235.12  | 1235.7   | 8457.1   |
| Order 3 |         | 235.12  | 1235.1   | 8458.5   |
| Order 4 |         | 235.12  | 1235.1   | 8458.7   |

Order 1 corresponds to the TICI2 case, and Order 4 is the full TICC2 result

The third- and fourth-order terms give an almost negligible contribution  $\rightarrow$  one may safely simplify the integro-differential equation by keeping only up to quadratic terms in  $f(r)$

### TICC[2] Approximation

$$\Psi(\mathbf{r}_1 \dots \mathbf{r}_A) = \Phi(\mathbf{r}_1 \dots \mathbf{r}_A) \left( 1 + \sum_{i < j} f(r_{ij}) + \frac{1}{2!} \sum_{i < j} f(r_{ij}) \sum_{k < l} f(r_{kl}) \right)$$

A significant difference between the bosonic and fermionic cases arises

Consider the following diagram

$$\begin{array}{c}
 \circ \text{---} \circ \\
 \equiv \langle \Phi | g(12) W(12) f(34) | \Phi \rangle \\
 \circ \text{~~~~} \circ
 \end{array}$$

( $W$  is the Wigner part of the interaction)

In the bosonic case the unlinked diagrams factorise because in the reference state all the particles are in the lowest HO state

$$\begin{aligned}
 \longrightarrow & \langle \phi_0(1) \phi_0(2) | g(12) W(12) | \phi_0(1) \phi_0(2) \rangle \\
 & \times \langle \phi_0(3) \phi_0(4) | f(34) | \phi_0(3) \phi_0(4) \rangle
 \end{aligned}$$

The second factor vanishes. All the diagrams containing a disconnected  $f$  give a null contribution

This is not the case with fermions because the permutations in the reference state involve different HO states

→ The number of diagrams to consider is much greater than in the bosonic case

It turns out that the contribution of disconnected diagrams is almost negligible, at least to compute the ground state energies of light nuclei

TICI2 and TICC[2] binding energies (in MeV)  
 No unlinked diagrams are considered in TICC[2]

|            | ${}^4\text{He}$ | ${}^{16}\text{O}$ |
|------------|-----------------|-------------------|
| B1         |                 |                   |
| TICI2-SI   | -37.86          | -145.94           |
| TICC[2]-SI | -37.92          | -149.36           |
| MS3        |                 |                   |
| TICI2-SI   | -25.41          | -85.56            |
| TICC[2]-SI | -25.59          | -94.71            |
| TICI2-SD   | -27.99          | -105.64           |
| TICC[2]-SD | -28.21          | -123.79           |

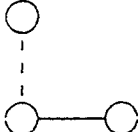
The improvement is quite remarkable, specially for the MS3 interaction which has a stronger short-range repulsion than the B1 potential

Calculations for realistic calculations have not yet been performed

## 4.4.2 J-TICI2

The problem with strong-repulsive potentials

  $\rightarrow$  screened by correlation

  $\rightarrow$  not screened

Recall:  $CC_n$  deals only with independent  $n$ -body correlation operators

Hybrid Method:

TICI2 additive state-dependent correlations

Jastrow multiplicative state-independent correlations

$$\Psi(1\dots A) = \left( \prod_{i < j} g(ij) \right) \left( \sum_{k < l} \sum_p h^{(p)}(kl) \Theta^{(p)}(kl) \right) \Phi(1\dots A)$$

(similar to the CBF of Feenberg, Clark, ..., in which are combined Jastrow correlations and non-orthogonal perturbation theory)

For simplicity:  $g(r) = 1 + ae^{-br^2}$

Variational problem: Minimize the ground state energy with respect to parameters  $\alpha, a, b$  and functions  $h^{(p)}$

## Results for $^4\text{He}$

|          | TICI2 |          | J-TICI2 |          |       |     |
|----------|-------|----------|---------|----------|-------|-----|
|          | -E    | $\alpha$ | -E      | $\alpha$ | $a$   | $b$ |
| B1       | 37.86 | 0.73     | 38.28   | 0.77     | -0.41 | 1.8 |
| S3       | 28.19 | 0.72     | 30.16   | 0.78     | -0.70 | 2.1 |
| MS3      | 27.99 | 0.71     | 29.97   | 0.74     | -0.70 | 2.1 |
| MT I/III | 30.81 | 0.74     | 32.70   | 0.75     | -0.88 | 5.0 |
| MT V     | 29.45 | 0.74     | 31.21   | 0.75     | -0.87 | 5.6 |
| GPDT     | 27.36 | 0.70     | 27.58   | 0.72     | -0.29 | 1.9 |
| SSC      | 24.12 | 0.68     | 26.74   | 0.75     | -0.66 | 2.1 |
| AV14     | 14.77 | 0.59     | 20.37   | 0.71     | -0.93 | 2.7 |
| AV18     | 15.40 | 0.61     | 21.08   | 0.74     | -0.92 | 3.2 |
| Reid-V6  | 5.67  | 0.43     | 22.70   | 0.72     | -1.05 | 2.4 |

For comparison

|         |                  |      |
|---------|------------------|------|
| B1      | $38.32 \pm 0.01$ | DMC  |
| MTV     | $31.32 \pm 0.02$ | DMC  |
| AV14    | $24.79 \pm 0.20$ | GFMC |
| Reid-V6 | $28.30 \pm 0.12$ | GFMC |

V4 interactions: Energies very close to DMC ones

V6 interactions: Impressive effects for strongly repulsive interactions (Reid-V6)

### **J-TICI2: Division of roles**

**Jastrow: short-range correlations**

**TICI2: medium and long-range  
correlations**

→ S13



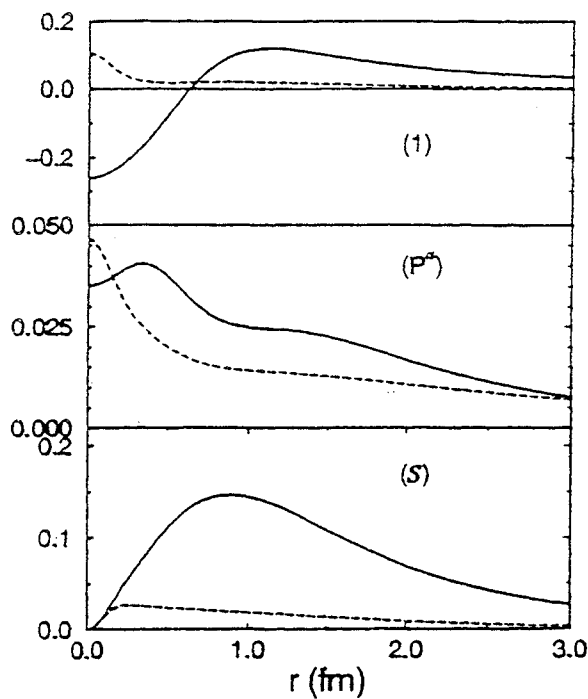


Fig. 3. A comparison between the TIC12 (solid line) and J-TIC12 (dashed line) correlation functions  $f^P$ , multiplied with  $\exp(-\alpha^2 r^2/8)$ , for  ${}^4\text{He}$  obtained from a solution to the generalised eigenvalue problem (7). We have chosen the V6 part of the AV14 potential as an example, and only plot the range for  $r$  from 0 to 3 fm. The normalisation of each of the correlation functions is as in the normalised ground-state eigenfunction, but we present separate results for each of the three operatorial channels.

# 5.1 The Approximation

## J-TICI3

$$\Psi(\mathbf{R}) = \Phi_{TICI3}(\mathbf{R}) \Phi_J(\mathbf{R})$$

*Correlated reference state*

$$\Phi_J(\mathbf{R}) = \prod_{i < j} g(r_{ij}) \Phi(\mathbf{R})$$

- Jastrow factor

$$g(r) = \exp \left[ -\frac{1}{2} \left( \frac{b}{r} \right)^\nu \right]$$

with fixed values  $\nu = 5.2$ ,  $b = 2.95 \text{ \AA}$  ( $^4\text{He}$ ),  $2.85 \text{ \AA}$  ( $^3\text{He}$ )

→ **EXERCISE 5**

- Reference state

$$^4\text{He}: \quad \Phi(\mathbf{R}) = \prod_{i < j} \exp \left( -\frac{\alpha^2}{2N} r_{ij}^2 \right)$$

Boson HO condensate

$$^3\text{He}: \quad \Phi(\mathbf{R}) = \Phi_\uparrow(\mathbf{R}) \Phi_\downarrow(\mathbf{R})$$

Product of HO Slater determinants  
referred to  $\uparrow, \downarrow$  spin particles

Backflow correlations are also included:

$$\mathbf{r}_i \longrightarrow \mathbf{r}_i + \sum_{i \neq j} \frac{\lambda}{r_{ij}^3} (\mathbf{r}_i - \mathbf{r}_j)$$

with fixed value  $\lambda = 5 \text{ \AA}^3$

Correlated reference state

$$\Phi_{TICI3}(\mathbf{R}) = 1 + \sum_{i<j} f_2(r_{ij}) + \sum_{i<j<k} f_3(r_{ij}, r_{ik}, r_{jk})$$

In practice, expansion on a Gaussian basis

$$\Phi_{TICI3}(\mathbf{R}) = \sum_{p<q<r}^{N_g} C_{\{\mu\}} G_{\{\mu\}}(\mathbf{R})$$

$$G_{\{\mu\}}(\mathbf{R}) = \mathcal{S} \left( \sum_{i<j<k} e^{-\beta_p r_{ij}^2} e^{-\beta_q r_{ik}^2} e^{-\beta_r r_{jk}^2} \right)$$

with  $\{\mu\} \equiv \{p, q, r\}$

Our choice: five Gaussians with widths

$$\begin{aligned} (\beta_p/\alpha^2) &= (0, -0.05, 0.5, 1, 4) && (^4\text{He}) \\ &= (0, 0.5, 1, 2, 4) && (^3\text{He}) \end{aligned}$$

Interest of using  $\beta_1 = 0$

- Three labels  $p, q, r = 1 \rightarrow \Phi_{TICI3} \equiv 1$
- Two labels  $= 1 \rightarrow \Phi_{TICI3} \equiv TICI2$

## Generalized eigenvalue problem

$$\sum_{\mu_2} (\mathcal{K}_{\mu_1, \mu_2} + \mathcal{V}_{\mu_1, \mu_2}) C_{\mu_2} = E \sum_{\mu_2} \mathcal{N}_{\mu_1, \mu_2} C_{\mu_2}$$

$$\mathcal{N}_{\mu_1, \mu_2} = \int d\mathbf{R} |\Phi_J(\mathbf{R})|^2 G_{\mu_1}^*(\mathbf{R}) G_{\mu_2}(\mathbf{R})$$

$$\mathcal{V}_{\mu_1, \mu_2} = \int d\mathbf{R} |\Phi_J(\mathbf{R})|^2 G_{\mu_1}^*(\mathbf{R}) \sum_{m < n} V(r_{mn}) G_{\mu_2}(\mathbf{R})$$

We choose

$$\mathcal{K}_{\mu_1, \mu_2} = \int d\mathbf{R} |\Phi_J(\mathbf{R})|^2 G_{\mu_1}^*(\mathbf{R}) \frac{1}{\Phi_J(\mathbf{R})} \left( -\frac{\hbar^2}{2m} \sum_n \Delta_n \right) G_{\mu_2}(\mathbf{R}) \Phi_J(\mathbf{R})$$

Multidimensional integrals calculated by means of the MC method, using the positive definite function  $|\Phi_J(\mathbf{R})|^2$  as the guide of a Metropolis random walk

- No subtraction of the CMM is necessary, as we are using a TI wave function
- The number of unknown amplitudes  $C_\mu$  is

$$\binom{N_\beta + 2}{3}$$

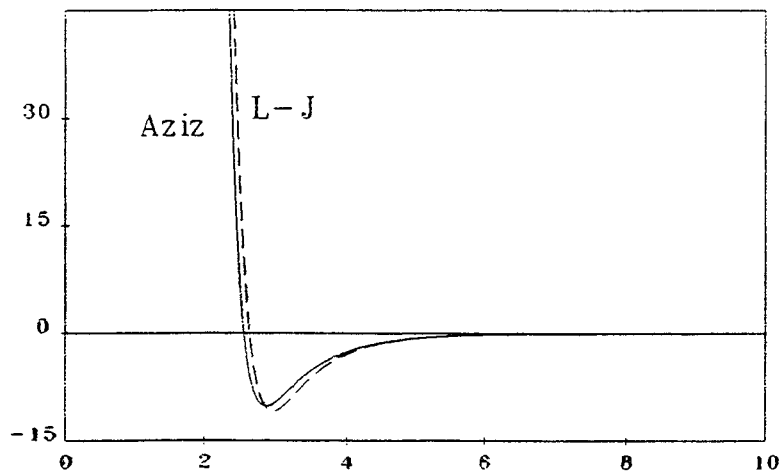
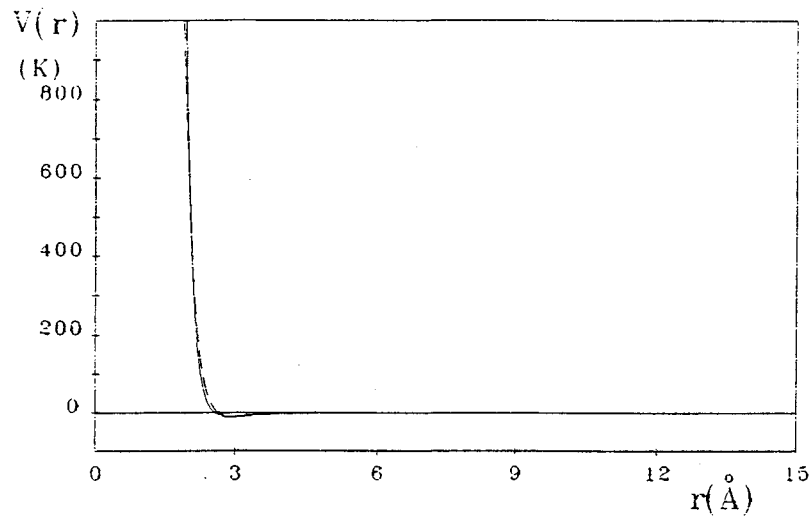
In our case,  $N_\beta = 5 \rightarrow 35$

# He-He interaction: Aziz HFD-B(HE)

$$V(r) = \epsilon \left[ Ae^{-\alpha x + \beta x^2} - F(x) \left( \frac{C_6}{x^6} + \frac{C_8}{x^8} + \frac{C_{10}}{x^{10}} \right) \right]$$

$$F(x) = \begin{cases} e^{-(D/x-1)^2} & x < D \\ 1 & \text{elsewhere} \end{cases}$$

$$x = r/r_m$$

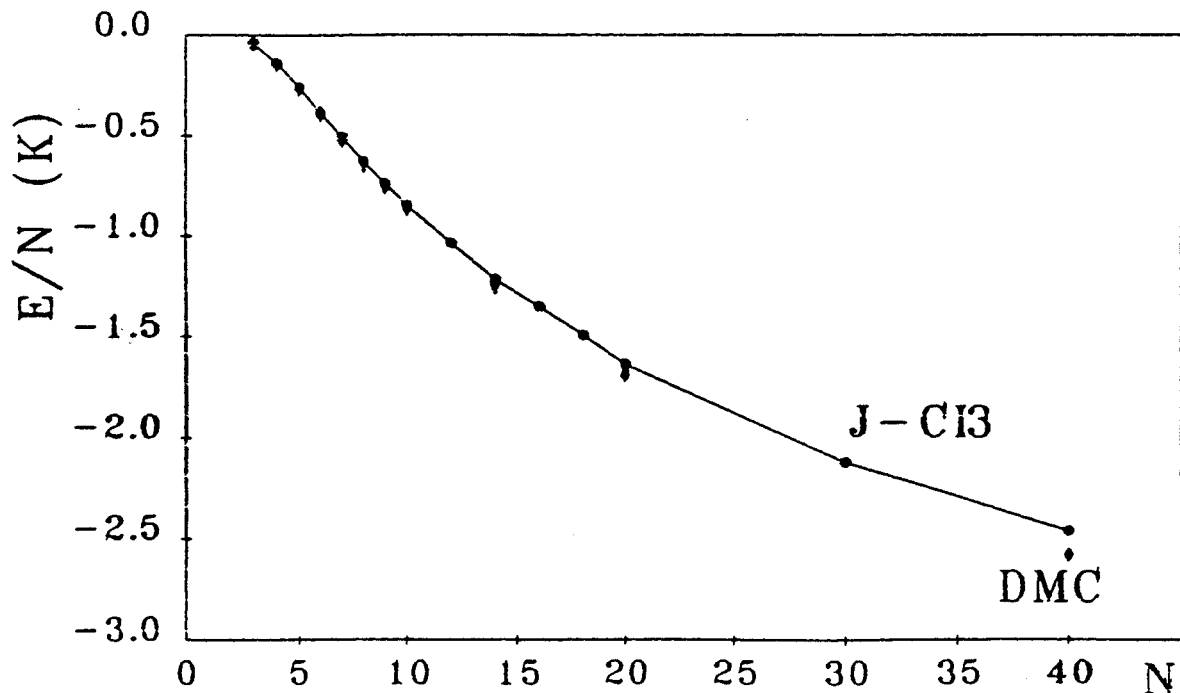


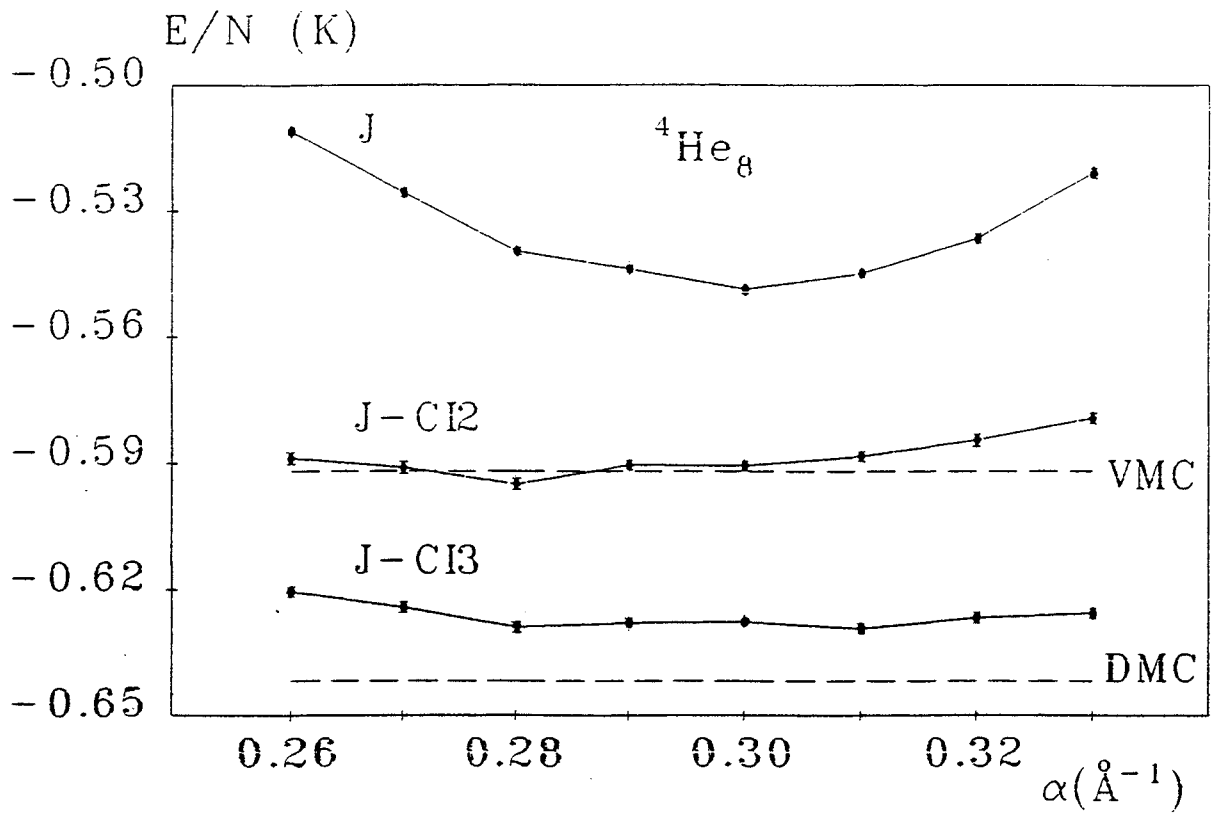
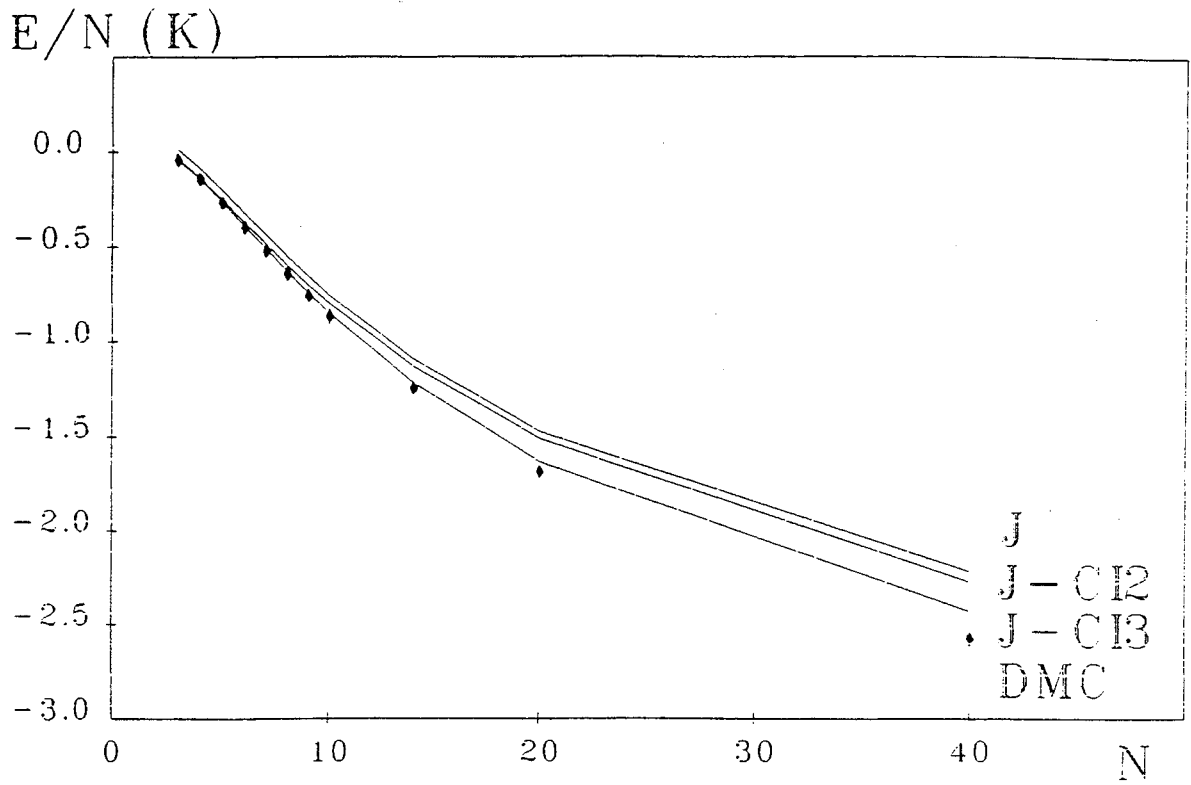
## 5.2 Drops of $^4\text{He}$ atoms

Ground state results

PR B60 (99') 6288

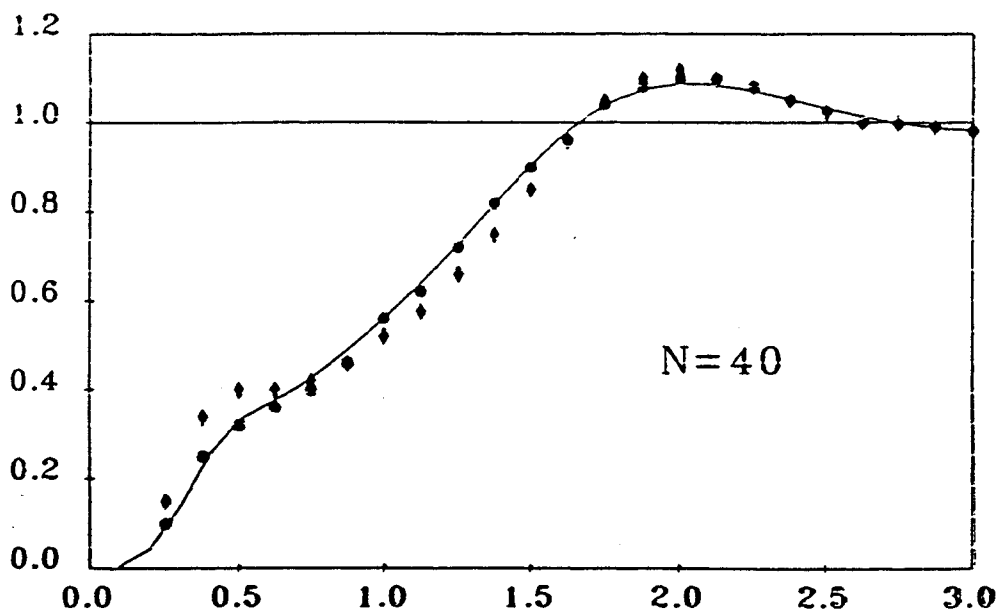
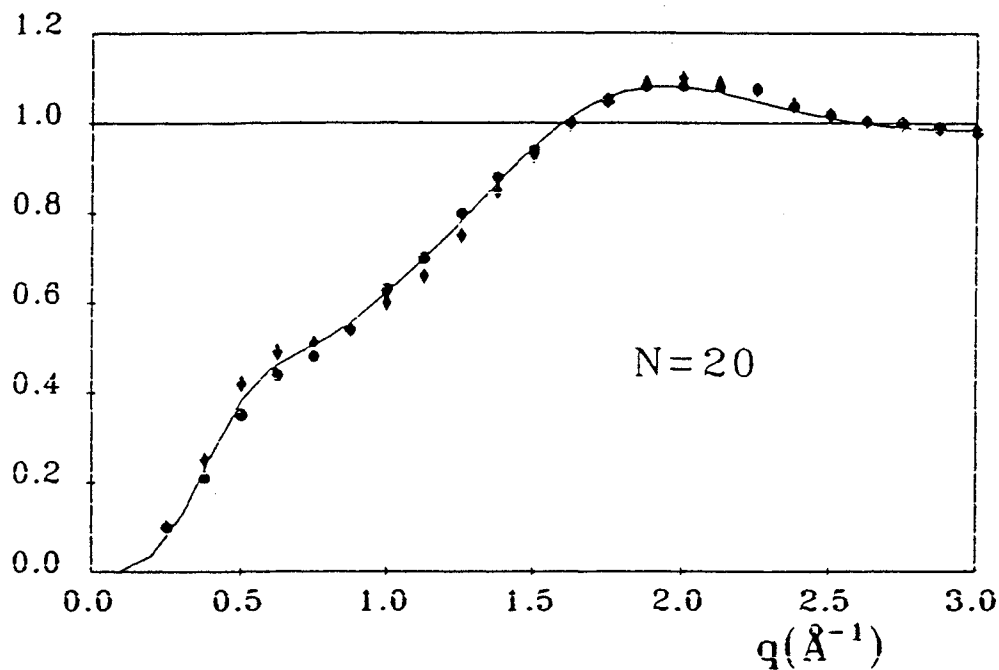
| N  | E/N (K)     |             | $r_0(\text{\AA})$ |      |
|----|-------------|-------------|-------------------|------|
|    | J-CI3       | DMC         | J-CI3             | DMC  |
| 3  | -.0430(10)  | -.0436(2)   | 5.4(2)            | 5.59 |
| 4  | -.1398(15)  | -.1443(2)   | 4.11(11)          | 4.13 |
| 5  | -.2616(13)  | -.2670(3)   | 3.66(7)           | 3.65 |
| 6  | -.3868(11)  | -.3950(2)   | 3.42(6)           |      |
| 7  | -.5081(12)  | -.5206(4)   | 3.31(5)           | 3.22 |
| 8  | -.6289(13)  | -.6417(4)   | 3.18(4)           |      |
| 9  | -.7392(12)  | -.7563(6)   | 3.11(3)           |      |
| 10 | -.8484(19)  | -.8654(7)   | 3.01(3)           |      |
| 14 | -1.215(2)   | -1.2478(12) | 2.91(2)           | 2.83 |
| 20 | -1.6336(15) | -1.688(2)   | 2.727(14)         | 2.69 |
| 40 | -2.4563(14) | -2.575(3)   | 2.578(8)          |      |





## Static structure factor

$$S(q) = 1 + \frac{2}{N} \langle \sum_{i < j} e^{i\vec{q} \cdot \vec{r}_{ij}} \rangle - \frac{1}{N} \left| \langle \sum_i e^{i\vec{q} \cdot (\vec{r}_i - \vec{R})} \rangle \right|^2$$



J-TICI3 (solid), VMC-triplets (circles), DMC (diamonds)



Excited states (angular momentum  $L$ )

Generalize the reference state

$$\Phi_J^{(L)} = \prod_{i < j} e^{-\frac{1}{2} \left(\frac{b}{r_{ij}}\right)^\nu} \prod_{i < j} e^{-\frac{\alpha^2}{2N} r_{ij}^2} \sum_{i < j} r_{ij}^L Y_{L0}(\hat{r}_{ij})$$

$$\Psi^{(L)}(\mathbf{R}) = \Phi_{CI3}^{(L)}(\mathbf{R}) \Phi_J^{(L)}(\mathbf{R})$$

$$\Phi_{CI3}^{(L)} = 1 + \sum_{i < j} f_2(r_{ij}) + \sum_{i < j < k} f_3(r_{ij}, r_{ik}, r_{jk})$$

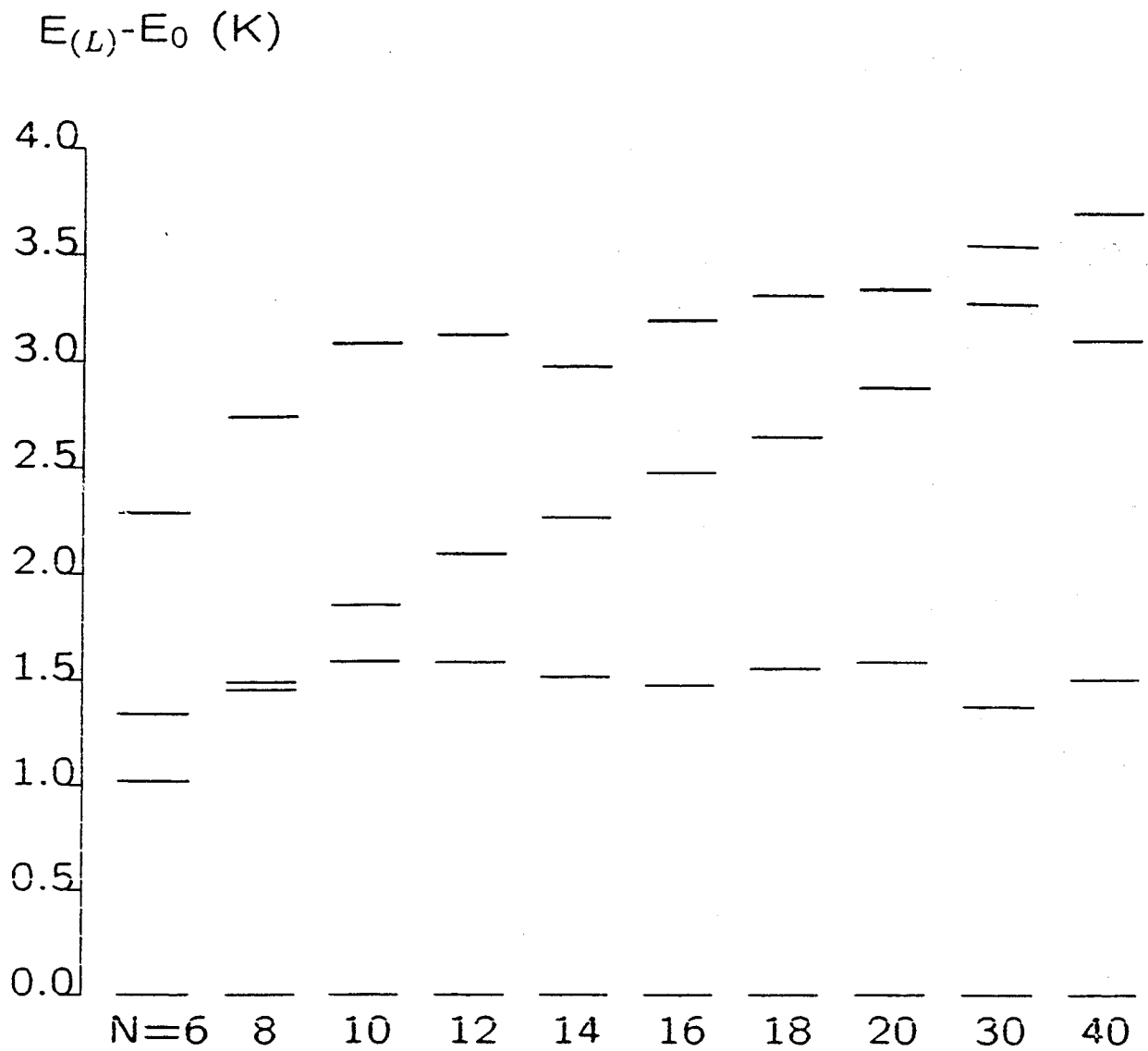
Note that ( $f_2$  and  $f_3$  depend implicitly on  $L$ )

Variational problem: minimize

$$E_L = \langle \Psi^{(L)} | H | \Psi^{(L)} \rangle / \langle \Psi^{(L)} | \Psi^{(L)} \rangle$$

with respect to  $f_2$  and  $f_3$

Random walk guided by  $|\Phi_J^{(L)}(\mathbf{R})|^2$



**L=2, L=4** excitation energies

Chemical potential  $|\mu(N)| = |E(N) - E(N - 1)|$

Discrete excitations:

**L=2** for  $N \geq 10$ ,  $\simeq 1.5$  K

**L=4** for  $N \geq 30$ ,  $\simeq 3.1$  K

## Other calculations: $\Psi_{\text{exc}} = F(\mathbf{R})\Psi_{\text{gs}}$

- Use exact  $\Psi_{\text{gs}}$  and solve the variational problem for  $F$  (Chin-Krotscheck DMC)

Define

$$M_1 = \frac{1}{2} \langle \Psi_{\text{gs}} | [F, [H, F]] | \Psi_{\text{gs}} \rangle$$

$$M_0 = \langle \Psi_{\text{gs}} | F^2 | \Psi_{\text{gs}} \rangle - (\langle \Psi_{\text{gs}} | F | \Psi_{\text{gs}} \rangle)^2$$

Excitation energy  $\hbar\omega = M_1/M_0$

⇒ Upper bound for excitation energy

- Use trial  $\Psi_{\text{gs}}$  (VMC) and minimize the centroid energy  $\hbar\omega$  (Krishna-Whaley, Chin-Krotscheck VMC)

- Our trial wave function for  $L \neq 0$

$$\Psi_{JCI3}^{(L)} = \frac{\Phi_{CI3}^{(L)}(\mathbf{R})}{\underbrace{\Phi_{CI3}^{(L=0)}(\mathbf{R})}_{\sum_{i < j} r_{ij}^L Y_{10}(\hat{r}_{ij})}} \Psi_{JCI3}^{(0)}$$

≠ one-body excitation operator  $F(\mathbf{R})$

|           | N=20 |      |      | N=40 |      |      |
|-----------|------|------|------|------|------|------|
|           | L=0  | L=2  | -μ   | L=0  | L=2  | -μ   |
| KW        | 2.67 |      |      |      |      |      |
| VMC       | 2.79 | 2.03 |      | 3.44 | 1.77 |      |
| DMC       | 2.80 | 2.26 |      | 3.68 | 2.04 |      |
|           | 2.72 | 1.75 | 2.91 | 3.60 | 1.37 | 3.67 |
|           | 2.80 | 1.71 |      | 3.68 | 1.22 |      |
| Ours      |      | 1.58 | 2.87 |      | 1.45 | 3.72 |
| $M_1/M_0$ | 3.57 | 1.78 |      | 3.93 | 1.79 |      |

## 5.3 Drops of $^3\text{He}$ atoms

Differences with respect to  $^4\text{He}$  drops

- $m_3 < m_4 \rightarrow$  Large zero point motion
- Fermions  $\rightarrow$  Pauli repulsion

Mass and statistics act in the same direction

$N=8$

J-CI3 results

|          | Aziz HDF-B(HE) interaction |                  |
|----------|----------------------------|------------------|
|          | $m_4$                      | $m_3$            |
| Bosons   | $-4.78 \pm 0.04$           | $-0.53 \pm 0.07$ |
| Fermions | $-0.78 \pm 0.05$           | $+2.57 \pm 0.07$ |

Existence of a minimum number of atoms below which  $^3\text{He}$  drops are unbound

Determination of  $N_{\min}$

- NLDF + shell model  
HO magic numbers  
 $N_{\min} \simeq 30$
- J-CI3  
(approximating mixing of subshells)

## A comparison with previous calculations

Binding energies (K) with HFDHE-2 interaction

| $N$ | VMC              | J-CI3            |
|-----|------------------|------------------|
| 20  | $4.12 \pm 0.14$  | $3.44 \pm 0.05$  |
| 40  | $-1.44 \pm 0.08$ | $-2.55 \pm 0.07$ |

VMC: Trial WF includes pair plus triplet Jastrow and backflow correlations (Pandharipande et al, PRB34 ('86) 4571)

$$\longrightarrow 20 < N_{\min} < 40 \text{ (1f2p shell)}$$

Use cartesian coordinates (L not well defined)

Occupation numbers for configurations in the 1f2p active shell in cartesian coordinates giving rise to wave functions invariant under  $90^\circ$  rotations, as a function of the number of atoms of a given  $\sigma_z$

| orbitals | $n=10$ | 9 | 7 | 6 | 4 | 3 | 1 |
|----------|--------|---|---|---|---|---|---|
| $x^3$    | 1      | 1 | 0 | 0 | 1 | 1 | 0 |
| $y^3$    | 1      | 1 | 0 | 0 | 1 | 1 | 0 |
| $z^3$    | 1      | 1 | 0 | 0 | 1 | 1 | 0 |
| $x^2y$   | 1      | 1 | 1 | 1 | 0 | 0 | 0 |
| $x^2z$   | 1      | 1 | 1 | 1 | 0 | 0 | 0 |
| $y^2x$   | 1      | 1 | 1 | 1 | 0 | 0 | 0 |
| $y^2z$   | 1      | 1 | 1 | 1 | 0 | 0 | 0 |
| $z^2x$   | 1      | 1 | 1 | 1 | 0 | 0 | 0 |
| $z^2y$   | 1      | 1 | 1 | 1 | 0 | 0 | 0 |
| $xyz$    | 1      | 0 | 1 | 0 | 1 | 0 | 1 |

Binding energy (in K) determined at the J-CI3 approximation for several  ${}^3\text{He}_N$  drops as a function of the number of spin up ( $N_\uparrow$ ) and spin down ( $N_\downarrow$ ) atoms. Results are given for the Aziz potential HFD-B(HE)

PRL 84 (00') 1144

| $N$ | $N_\uparrow$ | $N_\downarrow$ | $S_z$ | HFD-B(HE)        |
|-----|--------------|----------------|-------|------------------|
| 40  | 20           | 20             | 0     | $-3.90 \pm 0.07$ |
| 39  | 20           | 19             | 1/2   | $-3.17 \pm 0.10$ |
| 38  | 19           | 19             | 0     | $-2.29 \pm 0.11$ |
| 37  | 20           | 17             | 3/2   | $-1.62 \pm 0.09$ |
| 36  | 20           | 16             | 2     | $-1.09 \pm 0.09$ |
| 36  | 19           | 17             | 1     | $-0.86 \pm 0.10$ |
| 35  | 19           | 16             | 3/2   | $-0.33 \pm 0.09$ |
| 34  | 20           | 14             | 3     | $0.09 \pm 0.06$  |
| 34  | 17           | 17             | 0     | $0.67 \pm 0.06$  |
| 33  | 20           | 13             | 7/2   | $0.56 \pm 0.09$  |
| 33  | 19           | 14             | 5/2   | $0.66 \pm 0.09$  |
| 33  | 17           | 16             | 1/2   | $1.15 \pm 0.10$  |
| 32  | 19           | 13             | 3     | $1.04 \pm 0.09$  |
| 32  | 16           | 16             | 0     | $1.81 \pm 0.08$  |
| 31  | 20           | 11             | 9/2   | $1.42 \pm 0.07$  |
| 31  | 17           | 14             | 5/2   | $1.62 \pm 0.09$  |
| 30  | 20           | 10             | 5     | $1.35 \pm 0.09$  |
| 30  | 19           | 11             | 4     | $1.73 \pm 0.07$  |
| 30  | 17           | 13             | 2     | $2.02 \pm 0.06$  |
| 30  | 16           | 14             | 1     | $2.09 \pm 0.07$  |
| 20  | 10           | 10             | 0     | $3.01 \pm 0.05$  |

$$N_{\min} \simeq 34$$

GS with maximum spin

Fill either  $1f^n 2p^6$  or  $1f^{14} 2p^n$  subshells  
(L well defined)

Binding energy (in K) (PRB 62 (01') 3415)

| N  | Conf.        | L            | S   | E (K)            |
|----|--------------|--------------|-----|------------------|
| 34 | $p^6 f^8$    | 3            | 3   | $-0.03 \pm 0.05$ |
|    |              | 7            | 2   | $0.17 \pm 0.08$  |
|    |              | 8            | 2   | $0.35 \pm 0.12$  |
|    |              | 10           | 1   | $0.41 \pm 0.06$  |
|    |              | 11           | 1   | $0.46 \pm 0.10$  |
|    |              | 12           | 0   | $0.55 \pm 0.09$  |
| 35 | $p^6 f^9$    | 1            | 5/2 | $-0.52 \pm 0.09$ |
|    |              | 3            | 5/2 | $-0.59 \pm 0.09$ |
|    |              | 5            | 5/2 | $-0.39 \pm 0.06$ |
|    |              | 8            | 3/2 | $-0.16 \pm 0.08$ |
|    |              | 9            | 3/2 | $-0.23 \pm 0.08$ |
|    |              | 10           | 1/2 | $-0.15 \pm 0.10$ |
|    |              | 11           | 1/2 | $-0.03 \pm 0.06$ |
| 36 | $p^6 f^{10}$ | 0            | 2   | $-0.97 \pm 0.08$ |
|    |              | 2            | 2   | $-1.04 \pm 0.10$ |
|    |              | 3            | 2   | $-1.01 \pm 0.10$ |
|    |              | 4            | 2   | $-0.93 \pm 0.08$ |
|    |              | 6            | 2   | $-1.00 \pm 0.10$ |
|    |              | 8            | 1   | $-0.80 \pm 0.07$ |
|    |              | 9            | 1   | $-0.78 \pm 0.09$ |
|    |              | $p^2 f^{14}$ | 1   | 1                |
| 38 | $p^6 f^{12}$ | 1            | 1   | $-2.23 \pm 0.09$ |
|    |              | 3            | 1   | $-2.22 \pm 0.09$ |
|    |              | 5            | 1   | $-2.21 \pm 0.05$ |
|    | $p^4 f^{14}$ | 1            | 1   | $-2.31 \pm 0.07$ |

$$N_{\min} \simeq 34$$

GS with maximum spin

For a given S, degeneracy with L

## EXERCISE 1

The CCM equations have been written in two different ways:

$$\langle \Phi | C_I H e^S | \Phi \rangle = E \langle \Phi | C_I e^S | \Phi \rangle \quad I \neq 0$$

and

$$\langle \Phi | C_I e^{-S} H e^S | \Phi \rangle = 0 \quad I \neq 0$$

with  $E = \langle \Phi | H e^S | \Phi \rangle$ . Show that both sets of equations are identical.

Hint: Use the identities

$$1 = e^S e^{-S} = \sum_J e^S C_J^+ | \Phi \rangle \langle \Phi | e^{-S}$$

(index  $J$  includes 0)

## EXERCISE 2

Calculate the ground state energy, in successive CCn approximations, of the one-dimensional anharmonic oscillator described by the Hamiltonian

$$H = \frac{1}{2} (p^2 + x^2) + \lambda x^4$$

You have to choose a reference state, construct the CCn ansatz for the ground state wave function, derive the equations for amplitudes, solve them (you only need a pocket calculator), and finally calculate the ground state energy. It is convenient to use the set of equations

$$\langle \Phi | C_I e^{-S} H e^S | \Phi \rangle = 0 \quad I \neq 0$$

and express the operator  $e^{-S} H e^S$  in terms of nested commutators.

You should reproduce (or correct!) the results displayed in the following table for several values of the coupling



constant  $\lambda$ . The column "exact" corresponds to energies obtained integrating numerically the Schrödinger equation.

| $\lambda$ | exact | CC2   | CC4   | CC6   | CC8   |
|-----------|-------|-------|-------|-------|-------|
| 0.1       | 0.559 | 0.560 | 0.559 | 0.559 | 0.559 |
| 1         | 0.804 | 0.796 | 0.805 | 0.805 | 0.804 |
| 10        | 1.508 | 1.424 | 1.497 | 1.507 | 1.509 |
| 100       | 3.131 | 2.834 | 3.075 | 3.124 | 3.138 |
| 1000      | 6.694 | 5.895 | 6.513 | 6.651 | 6.695 |

### EXERCISE 3

Show that for an homogeneous system of bosons the HCSUB(2) equation in coordinate representation may be written as

$$-\Delta S_2(r) + V(r)(1 + S_2(r)) = 4\epsilon S_2(r)$$

where

$$\epsilon = \frac{1}{2}\rho \int dr V(r) (1 + S_2(r))$$

is the energy per particle, and  $\rho$  is the particle density. (Units:  $\hbar^2/m = 1$ )

Suppose the bosons interact through a hard sphere potential:  $V(r) = \infty$  if  $r < a$ ,  $= 0$  otherwise. In the low-density limit, the energy per particle is given by the series (see e.g. Fetter-Walecka)

$$\epsilon = 2\pi\rho a \left( 1 + \frac{128}{15} \left( \frac{\rho a^3}{\pi} \right)^{1/2} + \dots \right)$$

Calculate the HCSUB(2) energy  $\epsilon$  in the low-density limit.

## EXERCISE 4

A generic TI (1p-1h+2p-2h) excitation has been represented by a function  $g(ij)$  with the property  $\langle \Phi | g | \Phi \rangle = 0$ . Let us call TICC2[g] the corresponding TICC2 equation. To deal with a completely arbitrary function, the change  $g \rightarrow G \langle \Phi | G | \Phi \rangle$  has been made. Write the new TICC2[G] equation and compare with the TICC2[g]. Explain the result (at first sight surprising).

## EXERCISE 5

Consider two helium atoms, interacting through a Lenard-Jones potential

$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

with  $\epsilon = 10.22\text{K}$  and  $\sigma = 2.556\text{\AA}$ . Obtain the very short-range behaviour of the relative wave function, thus justifying the choice of the Jastrow factor in J-TICI3. To be quantitative, use the values  $\hbar^2/m = 12.1194\text{ K \AA}^2$  and  $16.084\text{ K \AA}^2$ , respectively for  $^4\text{He}$  and  $^3\text{He}$