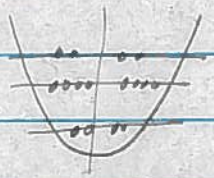
Lecture M3a Many-body problem and basis considerations

(1) Shell closures and reference states
(2) Many-body configurations ad expansions
(3) Normal ordering
(4) Residual 3-body forces
(5) Preview on exotic nuclei

(1) Shell closures and reference states

recall ^{16}O



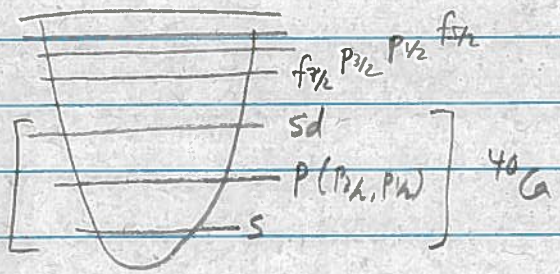
closed shell or sub-shell nuclei
can be used as (single) reference states

in shell model we take as reference states cores that are particularly good closed shell nuclei
→ minimizes core polarization effects ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{100}Sn, ^{88}Sr, ^{132}Sn, ...

shell closures can be seen in masses, rapid decrease in S_{2n} (S_{2p} for proton shell closures) after closed shell
$S_{2n}(N,Z) = B(N,Z) - B(N-2,Z)$
Q: Why not in S_n?
pairing leads to odd-even staggering in S_n

and by high excitation energy → Thursday lecture

Example: Calcium isotopes



Q: What are good closed shell/sub-shell reference states?

^{40}Ca → magic numbers N=Z=20 } stable
^{48}Ca → " " N=28 }
^{52}Ca → new magic number N=32
^{54}Ca → closed subshell maybe also magic
↳ particularly well-bound
^{60}Ca → has not been produced in laboratory, but good closed shell reference state

distinguish: reference state in calculation vs. experimental closed-shell nucleus

(2) Many-body configurations and expansions

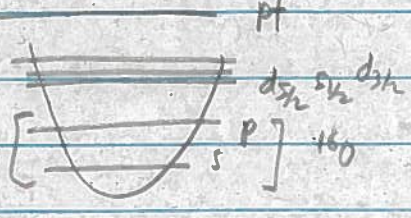
$\psi_i(\vec{r}) = \langle \vec{r} | a_i^\dagger | 0 \rangle$

Hartree-Fock reference state: optimal single-particle states determined so that single Slater determinant $a_1^\dagger \dots a_A^\dagger |0\rangle$ minimizes energy

Other reference state: closed shell/subshell with lowest s.p. harmonic oscillator states occupied
→ single reference
(or multi-reference for open-shell nuclei)

Strategies for many-body calculation

→ Q: What's the difference in this picture for HF or Other?



1) closed shell/subshell case: take ^{16}O as example

start from HF or Other reference state

a) include many-body configurations with increasing N_{max} or E_{max} to convergence

N_{max} = maximal $N_{max}\hbar\omega$ excitations

e.g. $N_{max} = 2$ → 2 particles can be excited by $1\hbar\omega$ each
1 particle " " " $2\hbar\omega$

E_{max} = maximal $E_{max}\hbar\omega$ for each particle $E_{max} = (1+1)\hbar\omega$
↑ ^{16}O core

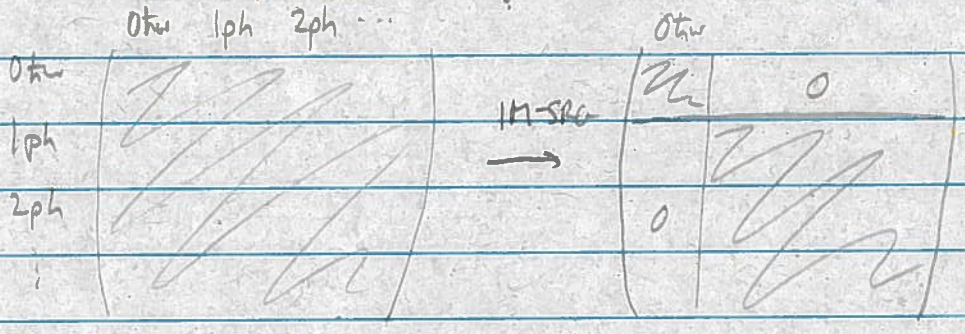
→ all 16 particles can be excited by $1\hbar\omega$ each

possible methods: No-core shell model (NCSM): diagonalize with increasing N_{max} (N_{max} cut-off guarantees that can separates)

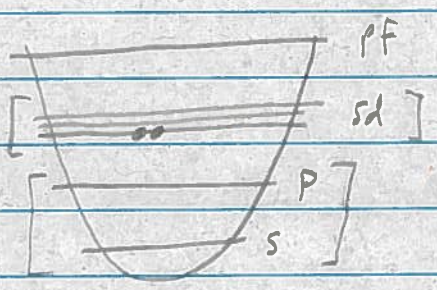
Many-body perturbation theory (MBPT) usually in E_{max}
→ need to check convergence in E_{max} and in order of MBPT (→ usually difficult)

In-Medium SRG decouple beyond 0ħω configurations

From 0ħω reference state by SRG



2) open shell case take ^{18}O as example



Q: How many 0ħω states?

$\binom{12}{2} = 66$ but can reduce this # using angular mom coupling

possible methods: NCSM diagonalization for finite N_{max} + check convergence with increasing N_{max} (same as in 1)

MBPT + often nonperturbative resummation to guarantee size extensivity with increasing $N_{valence}$

→ shell model define valence space of low-energy configurations

- e.g. sp core + sd shell = P-space

calculate perturbatively contribution from Q=1-P space

diagonalize in valence space

Q. Why do we need to introduce P-space?

various IM-SRG decoupling strategies

(3) Normal ordering

until now we have normal-ordered operators with respect to the vacuum $|0\rangle$

$$H = \sum_{12} T_{12}\, a_1^\dagger a_2 + \frac{1}{(2!)^2}\sum_{1234}\langle 12|V_{NN}|34\rangle\, a_1^\dagger a_2^\dagger a_4 a_3 + \frac{1}{(3!)^3}\sum_{123456}\langle 123|V_{3N}|456\rangle\, a_1^\dagger a_2^\dagger a_3^\dagger a_6 a_5 a_4$$

normal ordering: all operators that annihilate reference state (so far $|0\rangle$) to the right and all operators that create a new state to the left

for general reference state $|\phi\rangle$: define <u>normal-ordered operator</u> $:a_1^\dagger a_2^\dagger \cdots a a \cdots:$

by definition $\langle\phi|:a_1^\dagger a_2^\dagger \cdots a a \cdots:|\phi\rangle = 0$

Example: $|\phi\rangle$ = Fermi gas $= \prod_{k\le k_F} a_k^\dagger |0\rangle$

$$a_p^\dagger a_p |\phi\rangle = \begin{cases} 0, & p > k_F \\ |\phi\rangle, & p \le k_F \end{cases} \quad \text{but} \quad :a_p^\dagger a_p:|\phi\rangle = 0$$

define contractions between $a^\dagger$ and a by $\quad \overbrace{a_i^\dagger a_j} \equiv \langle\phi|a_i^\dagger a_j|\phi\rangle$

$$\overbrace{a_i a_j^\dagger} \equiv \langle\phi|a_i a_j^\dagger|\phi\rangle$$

Q: What is $\overbrace{a_i^\dagger a_j}$ for Fermi gas? $= \delta_{ij} n_i$ with occupation number $n_i = \begin{cases} 0 & p > k_F \\ 1 & p \le k_F \end{cases}$

<u>Wick's theorem</u> can write any string of $a^\dagger$ and a (generically A) as

$$A_1 A_2 \cdots A_n = :1 \cdots n: + \sum_{\text{one contraction}} :1 \cdots \overbrace{i \cdots j} \cdots n: + \sum_{\text{two contractions}} :1 \cdots \overbrace{i \cdots k \cdots j \cdots k} \cdots n: + \cdots$$

(proof by induction)

Using Wick's theorem one can exactly rewrite $\hat{H}$ with normal-ordered operators with respect to a reference state $|\phi\rangle$ with $a_i^\dagger a_j = \delta_{ij}\, n_i$ as

$$H = E_0 + \sum_{12} f_{12} :a_1^\dagger a_2: + \frac{1}{(2!)^2} \sum_{1234} \langle 12|\Gamma|34\rangle :a_1^\dagger a_2^\dagger a_4 a_3: + \frac{1}{(3!)^2} \sum_{123456} \langle 123|V_{3N}|456\rangle :a_1^\dagger a_2^\dagger a_3^\dagger a_6 a_5 a_4:$$

with 0-, 1-, 2-, 3-body normal ordered terms

$$E_0 = \langle\phi|H|\phi\rangle = \sum_1 T_{11} n_1 + \frac{1}{2}\sum_{12} \langle 12|V_{NN}|12\rangle n_1 n_2 + \frac{1}{3!}\sum_{123} \langle 123|V_{3N}|123\rangle n_1 n_2 n_3$$

Q: What is E_0?

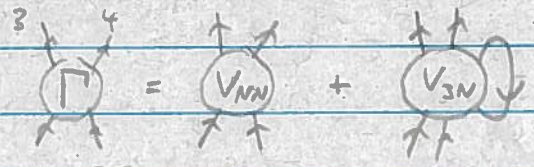
$$f_{12} = T_{12} + \sum_i \langle 1i|V_{NN}|2i\rangle n_i + \frac{1}{2}\sum_{ij} \langle 1ij|V_{3N}|2ij\rangle n_i n_j$$

e.g. for Hartree-Fock reference state E_0 = HF energy

$$\langle 12|\Gamma|34\rangle = \langle 12|V_{NN}|34\rangle + \sum_i \langle 12i|V_{3N}|34i\rangle n_i$$

also sometimes called residual 1-, 2-, 3-body interactions

diagrammatically



↳ for infinite matter: density-dependent two-body interaction

Remarks: (i) E_0, f_{12}, Γ_{1234} different for different reference states!

(ii) careful about normal ordering factors

→ V_{3N} enters in E_0, residual 1- and 2-body interactions with different factors

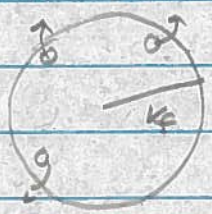
(iii) given "density-dependent" interactions with density of given reference state maybe the only way to justify "density dependent" Hamiltonian

otherwise: density functional not Hamiltonian → see Friday

(4) Residual 3-body forces

residual 3-body forces take 3 particles from reference state and excite them above Fermi level/energy → 3ph excitations

Can show for normal Fermi system
↳ with Fermi surface



that contribution from residual 3-body is suppressed by $\frac{\Delta}{E_F}$
with Δ typical scale of low-energy excitations and E_F Fermi energy
compared to the contribution from f and Γ.

physics behind this: phase space is limited by Pauli blocking
vs. f and Γ get enhanced by summing over occupied states in density or A_{core}

→ for same reason there are no 3-body Fermi liquid interactions

→ in shell model calculations with $N_{valence}$ and N_{core}
contributions from residual 3-body forces will be suppressed by $N_{valence}/N_{core}$
compared to f and Γ.