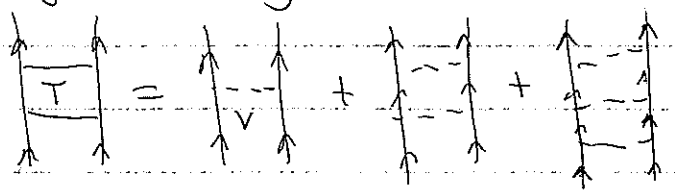
MBPT2-I

12/5/14 MBPT Revisited

- Reminder: softened potentials at finite density
  - Weinberg eigenvalue analysis applied to the T-matrix Lippmann-Schwinger equation
    $\hat{T}(E) = V + V\frac{1}{E-H_0}V + V\frac{1}{E-H_0}V\frac{1}{E-H_0}V + \ldots$
    showed increased convergence (smaller eigenvalue) when SRG λ or $V_{low\,k}$ Λ is reduced.
  - At finite density, the intermediate states are Pauli blocked ⇒ changes the convergence even more ⇒ perturbation theory in particle-particle ladders works.

- Diagrammatically, the Lippmann-Schwinger equation is



"particle-particle ladder diagrams"

- That's all there is in free space. At finite density many more diagrams are possible. (Why?)
- The question of MBPT is how to power count these diagrams:
  - What is an organizational principle that allows for systematic calculations?
  - How does the power counting depend on resolution of the interaction?

- go to finite density by closing lines

2/15/14

(MBPT2-1)

Traditional BBG power counting: G-matrix and hole-line expansion

Plan: Highlight the important features that depend on the interaction and how it changes with low-resolution interactions.

- For (much) more details, see the review by B. Day (RMP, 1978) on the original BBG theory and references therein and the many-body book by Negele and Orland.

- BBG → Brueckner-Bethe-Goldstone
  - Developed to deal with potentials with strongly repulsive cores
- Basics:
  - Write the Hamiltonian as $\hat{H} = \hat{H}_0 + \hat{H}_1$

    where

    $$\hat{H}_0 = \hat{T} + \hat{U} \quad \text{and} \quad \hat{H}_1 = \hat{V} - \hat{U}$$

    with $\hat{U}$ a single-particle potential to be specified
  - Great freedom to choose $\hat{U}$ (eg. could be $\hat{U}_{HF}$ → Hartree-Fock)
  - $\hat{H}_0 |\Phi_0\rangle = E_0 |\Phi_0\rangle$ is the reference state (in a finite system where $\rho(\vec{x})$)
    - In DFT, need freedom to make the density of $|\Phi_0\rangle$ the same as the full, exact density, order-by-order in an expansion. (Kohn-Sham reference system has same density as exact system)
    - In conventional BBG, freedom is needed to enhance convergence, so not available for DFT

- Restatement of time-independent perturbation theory for ground-state energy E:

$$E = E_0 + \langle \Phi_0 | \hat{H}_1 \sum_{n=0}^{\infty} \left(\frac{1}{E_0 - \hat{H}_0} \hat{H}_1 \right)^n | \Phi_0 \rangle_{\text{connected}}$$

($E_0 = \langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle$)

looks like perturbation theory!

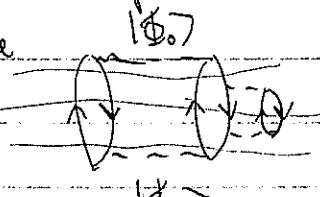
cf. Feynman diagrams
⇒ Feynman perturbation theory has time (or frequency) integrals. Do these and we get time-ordered Goldstone diagrams

(MBPT 2-B)

12/5/18

• Diagrammatic expansion called Goldstone diagrams

• Example



with ⇒ $V^{(2)}$ ← 2-body

index convention: single-particle

• start with $|\Phi_0\rangle$ and apply $|\hat{H}_1\rangle$, which creates particles and holes (all possible)

• For $V^{(2)}$, this is two particles and 2 holes

• $\frac{1}{E_0 - \hat{H}_0}$ propagates the state ↑ particle lines up ↑ $\varepsilon > \varepsilon_F$
⇒ involves single-particle energies (sum of particle − sum of hole energies) . hole lines down ↓ $\varepsilon < \varepsilon_F$

schematic, see refs for details

• "Connected" means $|\Phi_0\rangle$ is not an intermediate state
• put in $\hat{P} = 1 - |\Phi_0\rangle\langle\Phi_0|$ projector

$$\Rightarrow E - E_0 = \sum_{\text{connected diagrams}} \frac{(-1)^{n_h+n_p}}{2^{n_\ell}} \prod \frac{1}{\left(\sum_a \varepsilon_a - \sum_h \varepsilon_h\right)} \prod \{ij|\hat{V}_{NN}|kl\}$$

(product) ; anti-symmetrized

n_e = # energy denom.
n_ℓ = # of closed loops
n_h = # of hole lines

single particle energies according to $\hat{H}_0$

hole energies ↑ particle energies ↑ ⇐ sum of particle energies − hole energies

• The details are not so important to us as the basic organization and the consequences for a diagrammatic expansion.

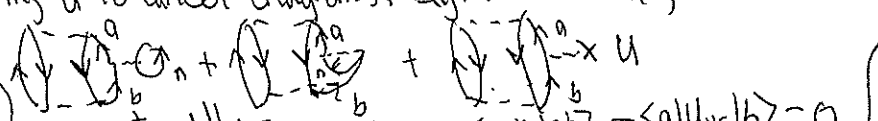
For denials with pulsive ones

• What happens if you try to apply this in an expansion in the number of times $\hat{H}_1$ acts? Two infinite-order resummations needed:

① Successive particle-particle ladders within a series of diagrams are all the same size ⇒ sum into G matrices

② Expansion in # of G matrices is still not perturbative: only adding an independent hole line to a diagram makes it smaller
⇒ sum all diagrams with a given number of hole lines (infinite!)

Choosing $\hat{U}$ to cancel diagrams. E.g. if $U = U_{HF}$, the Hartree-Fock potential, then

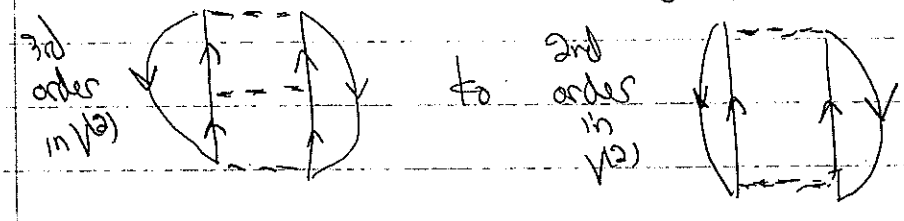


same except middle: $\sum_{n \le \epsilon_F} \langle an|V|bn\rangle - \langle an|V|nb\rangle - \langle a|U_{HF}|b\rangle = 0$

MBPT 2-4

12/5 HH

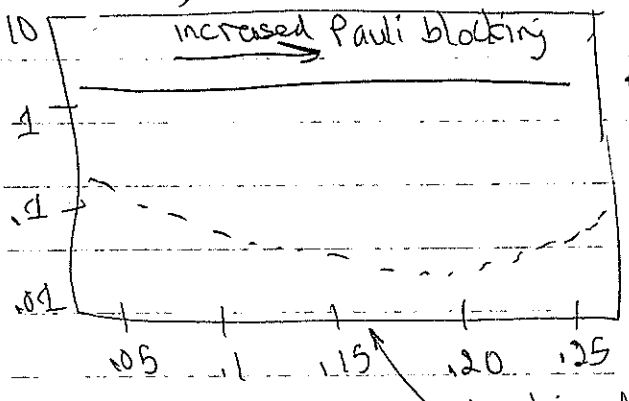
Lets start with numerical study of the ratio of



Is it bigger or smaller, (And 4th to 3rd, 5th to 4th, etc.)

(see slides as well)

[log plot]



3rd order / 2nd order

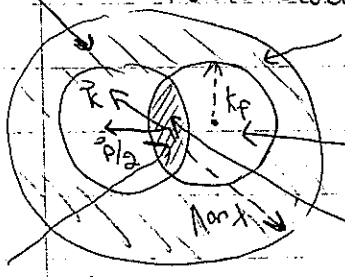
← AV18 (ratio 1.7 independent of density)

← evolved by $V_{low\,k}$ RG to $\Lambda = 2.1$ fm

- Uses Hartree-Fock (HF) continuous single-particle spectrum
  - : contributions from higher-orders for AV18 have similar ratio

- N^{3}LO picture is much more favorable (less than unity) but still a dramatic reduction when evolved to $V_{low\,k}$ $\Lambda = 2$ fm^{-1} or SRG $\lambda = 2$ fm

- Why does decoupling high and low momentum lead to smaller contributions?
  - : Pauli blocking and weaker interaction in relevant phase space for S-waves



- For large Λ and strong repulsive $V^{(2)}$, contribution is from large region and part excluded by Pauli blocking is small ⇒ density independent.
- For low Λ, there is a smaller and smaller region as density increases, and matrix elements are weaker there

sum and relative momenta of pair

$|\frac{P}{2} \pm k| > k_F$ and $|k| < \Lambda$

$|\frac{P}{2} \pm k| < k_F$

12/5/19

- So SRG or $V_{low\,k}$ at $\lambda, \Lambda \lesssim 2\,fm^{-1}$ is perturbative, each ladder rung added makes the diagram smaller
  - exactly consistent with Weinberg eigenvalues.

- For hard potentials, must add up the rungs, as we did in free space to form the T-matrix ← Pauli-blocking operator

$$\frac{1}{E-H_0}\ (\text{free space}) \Longrightarrow \frac{Q_F}{E-H_0}\ (\text{in-medium})$$

- It has been said in the literature that $V_{low\,k}$ interaction is just like a G-matrix.
  - But only true at low momentum (under certain assumptions for the treatment of the single-particle energies)
  - but there is still a lot of off-diagonal strength in the G-matrix and this makes the energy still non-perturbative in the G-matrix while perturbative in the $V_{low\,k}$ or V_{SRG} low-momentum potential

(see pictures)

- Hole-line expansion: power counting for the G-matrix
  - an analysis shows that the size of a diagram with conventional potentials doesn't relate to how many particle lines there are, but how many (independent hole lines)
  - see slides for examples of 4th order to third-order diagram, where one 4th order has another particle line while the other adds a hole line ← extra hole line

12/5/14

The estimate for the ratio of 4th to 3rd order when a particle line is added goes like the defect wave function at the origin (in coordinate space) [see B. Day, RMP (1967)]

- This is the two-particle relative wf compared to non-interacting relative plane waves.
- This defect is almost complete for highly repulsive cores but largely gone for low-momentum $^1S_0$ and greatly reduced for $^3S_1$ (see graphs ⇒)

⇒ adding an interaction doesn't reduce the diagram in the hard case (so resum all) but does in the soft case.

- When a hole line is added, the relevant expansion parameter is the excluded volume at short-range to the average volume occupied by a particle (proportional to $1/\rho$).
  - This is the so-called "wound-integral" κ
  - It is less than one ⇒ expansion for even hard potentials.
  - Still better for soft potentials (and no resummation)

- Bottom line: for soft potentials, adding another potential line reduces the size of the diagram (caveat: in all cases considered so far)

⇒ real perturbation theory may work. ∈ tested for neutron matter so far ✓ with QMC comparison

* • Regular hole-line expansion also needed to choose $\hat{U}$ to cancel diagrams to enhance convergence.
  - With low-momentum potentials we are free to choose it to make Kohn-Sham DFT work.