F2a-1

7/12/13

Plan for Lecture F2a:

① Follow-ups from Th2a: ← supplemented by reference state normal ordering
- SRG 3-body evolution Th2a-II, Th2a-III
- Weinberg eigenvalues: the short version
- Computational aspects

② Many-body overview (mostly slides)
- after overview, come back to discuss classification & methods before resuming slide show

- Participant talks at 2pm.

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Th2a-10

How do we know that SRG evolution of operators (including the Hamiltonian) must generate many-body terms?

- In exercises: think about physics. Here: formal discussion.

- Consider 2nd quantization. This is defined with two ingredients
  1. a single-particle basis (eg. plane waves [in a box] or HO wfns)
  2. a reference state that serves as the "vacuum".

examples:
- could be the actual vacuum
- or a filled core (Fermi sea or a closed shell)

$\Big\} a_i|0\rangle = 0$

- Kinetic energy: $T = \sum_{ij} \frac{\hat{p}^2}{2m} a_i^\dagger a_j \to \sum_{ij} a_i^\dagger \langle i|T|j\rangle a_j$

The labels $i, j, \ldots$ could refer to (discretized) momenta, or to harmonic oscillators, or ...

- Two body potential: $\frac{1}{4}\sum V^{(2)}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$

- 3-body potential: $\frac{1}{36}\sum V^{(3)}_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l$

or $\hat{A} = \sum_{ij} a_i^\dagger \langle i|T|j\rangle a_j + \frac{1}{4}\sum_{ijkl} a_i^\dagger a_j^\dagger \langle ij|V^{(2)}|kl\rangle a_l a_k + \frac{1}{36}\sum_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger \langle ijk|V^{(3)}|klm\rangle$

(m, n: anti-symmetrized matrix element $\Rightarrow \frac{1}{4}, \frac{1}{36}$)

- These operators have anti-commutation relations:

$\{a_i, a_j^\dagger\} = a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij}$, $\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0$

Claim: $\frac{dV_s}{ds} = \Big[\Big[\underbrace{\sum a^\dagger a}_{G_s = T}, \underbrace{\sum a^\dagger a^\dagger a a}_{2\text{-body}}\Big], \underbrace{\sum a^\dagger a^\dagger a a}_{2\text{-body}}\Big] = \ldots + \underbrace{\sum a^\dagger a^\dagger a^\dagger a a a}_{3\text{-body!}}$

show this in the exercises

- And this is just one time step!
- $\Rightarrow$ A-body operators generated
- Is this a problem?
  - depends: we need to be able to truncate $\Rightarrow$ need hierarchy
  - also need to be able to calculate with minimal (usually 2-body)

In-medium SRG $\Rightarrow$ Alternative: Pick a different reference state $\Rightarrow$ reshuffles what is many-body!

F2a-1a

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To be concrete, consider N neutrons in a volume Ω that we take to ∞ at the end, with a short-range interaction $V(\vec{x}) = C_0 \delta^3(\vec{x})$. (to avoid confusing with potential)

- basis is discretized plane waves: $\psi_{\vec{k}\alpha}(\vec{x}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{x}} \eta_\alpha$ (normalized; also isospin)

$\Rightarrow \eta_\uparrow = \begin{pmatrix}1\\0\end{pmatrix}$, $\eta_\downarrow = \begin{pmatrix}0\\1\end{pmatrix}$ and $\eta_\alpha^\dagger \eta_\beta = \delta_{\alpha\beta}$ ($\alpha=0,1$; $\beta=0,1$)

(spin function for spin-1/2 along $\hat{z}$ axis)

- periodic boundary conditions $k_i = 2\pi n_i / L$, $n_i = 0, \pm 1, \pm 2, \ldots$

- ~~1st~~ quantized $H = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} C_0 \sum_{i \neq j}^{N} \delta^3(\vec{x}_i - \vec{x}_j)$

(one body; two body)

- 2nd quantized

$$\hat{H} = \sum_{k\alpha} \frac{k^2}{2m} a^\dagger_{k\alpha} a_{k\alpha} + \frac{1}{2} \frac{C_0}{\Omega} \sum\sum\sum\sum_{k_1\alpha_1, k_2\alpha_2, k_3\alpha_3, k_4\alpha_4} a^\dagger_{k_1\alpha_1} a^\dagger_{k_2\alpha_2} a_{k_3\alpha_3} a_{k_4\alpha_4} \times \delta_{\alpha_1\alpha_3} \delta_{\alpha_2\alpha_4} \delta_{\vec{k}_1+\vec{k}_2, \vec{k}_3+\vec{k}_4}$$

("normal-ordered with respect to vacuum" $\Rightarrow$ all $a^\dagger$'s to right of a's $\Rightarrow$ ready to apply Wick's theorem)

(add up the kinetic energy of each occupied mode, as checked by the number operator $a^\dagger_{k\alpha} a_{k\alpha}$)

This comes from

$$\langle k_1\alpha_1 | \frac{\hat{p}^2}{2m} | k_2\alpha_2 \rangle = \frac{1}{\Omega} \int d^3x\, e^{-i\vec{k}_1\cdot\vec{x}} \eta^\dagger_{\alpha_1} \left(-\frac{\nabla^2}{2m}\right) e^{i\vec{k}_2\cdot\vec{x}} \eta_{\alpha_2}$$

$$= \frac{k_2^2}{2m\Omega} \delta_{\alpha_1\alpha_2} \int d^3x\, e^{i(\vec{k}_2 - \vec{k}_1)\cdot\vec{x}} \quad \leftarrow \Omega \delta_{\vec{k}_1,\vec{k}_2}$$

$$= \frac{k_2^2}{2m} \delta_{\alpha_1\alpha_2} \delta_{\vec{k}_1\vec{k}_2}$$

Unsymmetrized potential energy (so $\frac{1}{2}\sum V_{unsym}$ vs. $\frac{1}{4}\sum V_{sym}$)

$$\langle k_1\alpha_1, k_2\alpha_2 | V | k_3\alpha_3, k_4\alpha_4 \rangle = \frac{1}{\Omega^2} \iint d^3x_1 d^3x_2\, e^{-i\vec{k}_1\cdot\vec{x}_1} \eta^\dagger_{\alpha_1}(1) e^{-i\vec{k}_2\cdot\vec{x}_2} \eta^\dagger_{\alpha_2}(2) \times C_0 \delta^{(3)}(\vec{x}_1 - \vec{x}_2) e^{i\vec{k}_3\cdot\vec{x}_1} \eta_{\alpha_3}(1) e^{i\vec{k}_4\cdot\vec{x}_2} \eta_{\alpha_4}(2)$$

(particle 1, particle 2; from WF's)

$$= \frac{C_0}{\Omega} \delta_{\alpha_1\alpha_3} \delta_{\alpha_2\alpha_4} \delta_{\vec{k}_1+\vec{k}_2, \vec{k}_3+\vec{k}_4}$$

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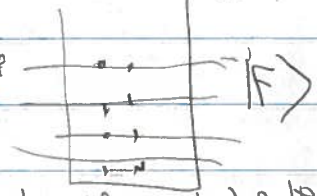
- Now suppose as a reference state we have the free Fermi gas $|F\rangle$
  - call the spin-isospin degeneracy ν (here $\nu=2$)
  - fill lowest momentum states up to k_F.
    - you can check that $N = \langle F | \sum_{k\alpha} a^\dagger_{k\alpha} a_{k\alpha} | F \rangle = \sum_{k\alpha} \theta(k_F - k)$ ($a_{k\alpha}|0\rangle = 0$ for all k,α; $a^\dagger_{k\alpha}$ = number operator; $|0\rangle$ = vacuum.)

$$N \to \frac{\nu k_F^3}{6\pi^2}$$



- As defined so far, $a_{k\alpha}|0\rangle = 0$ for all k,α
  - but $a_{k\alpha}|F\rangle \neq 0$ if $|k| < k_F$

with reference to $|F\rangle$ $\Rightarrow$ $a_{k\alpha}$ is destruction operator for $|k| > k_F$, but creation operator (of a hole) for $|k| < k_F$

- So with respect to reference state $|F\rangle$, we can redefine $a_{k\alpha}$

$$\Rightarrow a_{k\alpha} \to \theta(|k| - k_F)\, a_{k\alpha} + \theta(k_F - |k|)\, b^\dagger_{-k\alpha}$$

- But my Hamiltonian will not be normal-ordered wrt F now.
  For example, if $k_3 \to k_4$ are all in the Fermi sea $|k_i| \le k_F$, then the 2-body potential will have $b_1 b_2 b^\dagger_3 b^\dagger_4$ (where $1 \equiv k_1\alpha_1$)
  - we want to normal order wrt $|F\rangle$ as for Wick's theorem
    $\Rightarrow$ move b_1, b_2 to the right.
  - but $\{b_i, b^\dagger_j\} = \delta_{ij} \Rightarrow b_2 b^\dagger_3 = \delta_{23} - b^\dagger_3 b_2$

$$\Rightarrow b_1 b_2 b^\dagger_3 b^\dagger_4 = \delta_{23} b_1 b^\dagger_4 - b_1 b^\dagger_3 b_2 b^\dagger_4 \qquad (\delta_{13} - b^\dagger_3 b_1)$$

$$= \delta_{23}\delta_{14} - \delta_{23} b^\dagger_4 b_1 - \delta_{24} b_1 b^\dagger_3 + b_1 b^\dagger_3 b^\dagger_4 b_2$$

- $\delta_{23}\delta_{14}$: 0-body
- $\delta_{23} b^\dagger_4 b_1$: 1-body, normal ordered
- $\delta_{24} b_1 b^\dagger_3$: now bring b_1 through $\Rightarrow$ more 0-body, 1-body and finally 2-body $b^\dagger_3 b^\dagger_4 b_1 b_2$

or, apply Wick's theorem $\Rightarrow$ sum of all contractions

- So reference state changes where many-body contributions enter.
- For 3-body, reshuffles (most important) contributions to 0-body, 1-body, 2-body, with much smaller 3-body, so truncation of two-body force still captures much (most) of 3 body.

Th2a-11

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SRG technology is to evolve 3-body forces.

Three methods now exist:

slides by Angelo Calci

⇒ i) evolve in a discrete harmonic oscillator basis — Eric Jurgenson
⇒ applied to No-Core Shell Model (tomorrow) — many developments in Bogner+Furnstahl, P. Navratil

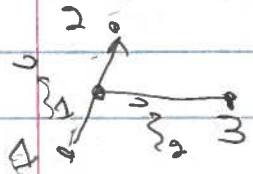
no disconnected pieces

(ii) evolve in a partial-wave momentum basis — Kai Hebeler (instructor next week!)
⇒ separate evolution of 2 and 3 body parts
⇒ applied to neutron matter (next week)

iii) evolve in a hyperspherical basis — Kyle Wendt (instructor last week)
⇒ good features, visualization

- more later on these comparisons
- Recent: 4-body evolution! (see Angelo Calci talk from Trento)

- Oscillator evolution is in a 3-body Jacobi basis



- generalization of center-of-mass and relative

$$\vec{\xi}_0 = \sqrt{\tfrac{1}{3}}\left[\vec{r}_1+\vec{r}_2+\vec{r}_3\right] \leftarrow \text{potential doesn't depend}$$

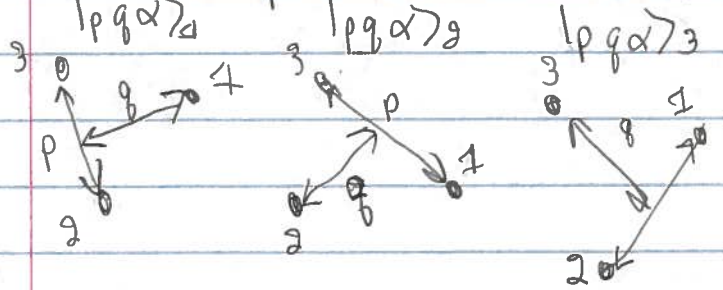
$$\vec{\xi}_1 = \sqrt{\tfrac{1}{2}}\left[\vec{r}_1-\vec{r}_2\right] \leftarrow \text{relative between 1 and 2.}$$

$$\vec{\xi}_2 = \sqrt{\tfrac{2}{3}}\left[\tfrac{1}{2}(\vec{r}_1+\vec{r}_2)-\vec{r}_3\right] \leftarrow \text{relative btwn 3 and com of 1 and 2}$$

(com of 1,2)

hard part: must antisymmetrize HO basis: $|\alpha\rangle = |[(N_1 L_1 S_1)J_1 (N_2 L_2 S_2)J_2]J m_J, (T_1 T_2)T m_T\rangle$

- momentum space evolution $|pq\alpha\rangle_i \equiv |p_i q_i; [(LS)J(l s_i)j]J\, J_z (T t_i)T\, T_z\rangle$



F2a-2

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Weinberg Eigenvalues: The Short Version (see Wednesday exercise problem)

- I've made the claim several times that softening nuclear interactions makes them more perturbative.
  - How can we make this statement more concrete?
    - ⇒ Weinberg eigenvalues
  - This will be a very abbreviated version to what your appetite.

- Start with the T-matrix in operator form:

$$\hat{T}(E) = \hat{V} + \hat{V}\frac{1}{E-\hat{H}_0}\hat{V} + \hat{V}\frac{1}{E-\hat{H}_0}\hat{V}\frac{1}{E-\hat{H}_0}\hat{V} + \ldots$$

- How do we judge convergence?
  - Look at the eigenvalues and eigenvectors of $\frac{1}{E-H_0}V$
  - Do this for every E ← not the eigenvalue of this operator.
  - In practice, take matrix elements in a basis and diagonalize ⇒ η_ν and $|\Gamma_\nu\rangle$ such that

$$\frac{1}{E-H_0}\hat{V}|\Gamma_\nu\rangle = \eta_\nu|\Gamma_\nu\rangle$$

  - η_ν is in general complex (it is real for $E<0$).

- Then $\hat{T}(E)|\Gamma_\nu\rangle = \hat{V}|\Gamma_\nu\rangle + \hat{V}(\eta_\nu)|\Gamma_\nu\rangle + \hat{V}\eta_\nu^2|\Gamma_\nu\rangle + \ldots$

$$= \hat{V}|\Gamma_\nu\rangle(1 + \eta_\nu + \eta_\nu^2 + \ldots)$$

⇒ T diverges if <u>any</u> $|\eta_\nu(E)| \geq 1$

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- Look for the largest eigenvalues, one positive and one negative
  - These are clearly distinguished for $E<0$, then follow their trajectory as E increases.

- General trends:
  - Repulsive cores lead to very large negative eigenvalues
    $\Rightarrow$ very nonperturbative
  - relatively little different with positive eigenvalues, which as associated with bound states in the S-waves, and are close to 1.
  - Lowering a cutoff Λ for $V_{low\,k}$ or evolving in λ will steadily reduce the negative eigenvalues
    - also to zero for ${}^1S_0$
    - from non-converging to converging in ${}^3S_1 - {}^3D_1$,
      - N^3LO (500 fm) is like $\Lambda \cong 3\,fm^{-1}$.
    - below $\Lambda = 2.5\,fm^{-1}$, all potentials are similar
  - If we now do it at finite density $\Rightarrow$ include "Pauli blocking" (can't use intermediate states already filled)
    both positive and negative eigenvalues decrease rapidly with density.
    - for the positive one, the deuteron "dissolves" in the ${}^3S_1 - {}^3D_1$ channel. [not all intermediate states are available for binding contribution]

$\Rightarrow$ Pauli blocking makes soft interactions even more perturbative.

$\Rightarrow$ good sign for successful many body calculations, $\Rightarrow$ MBPT on Monday.

** $\Rightarrow$ other slides

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Computational aspects at NN level.

- Momentum-space flow equations have integrals like:

$$I(p,q) \equiv \int_0^\infty dk\, k^2\, V(p,k)\, V(k,q)$$

these have some built in cutoff so integrals go to k_{max} instead of ∞

- Introduce Gaussian nodes and weights $\{k_n, w_n\}$ $(n=1,N)$

$$\Rightarrow \int_0^{k_{max}} dk\, f(k) \doteq \sum_n w_n f(k_n)$$

- Then $I(p,q) \to I_{ij}$ where $p=k_i$ and $q=k_j$

$$\Rightarrow I_{ij} = \sum_n k_n^2 w_n V_{in} V_{nj}$$

- we can make this look just like matrix multiplication by rescaling the V's to absorb the $k_n^2 w_n$ factor

$$\Rightarrow \tilde{V}_{ij} = \sqrt{w_i}\, k_i\, V_{ij}\, k_j \sqrt{w_j} \Rightarrow \tilde{I}_{ij} = \sum_n \tilde{V}_{in} \tilde{V}_{nj}$$

where $\tilde{I}_{ij} = \sqrt{w_i} k_i\, I_{ij}\, k_j \sqrt{w_j}$

$\Rightarrow$ SRG and Lippmann-Schwinger and simple diagonalization of H_s become basic matrix operations.

look at a few slides first

F2c-5

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Classification of many-body methods

"ab initio" → starting from microscopic 2+3-body forces

"configuration interaction" → traditional shell model → diagonalize a semi-empirical Hamiltonian within a restricted space

"density functional theory" (DFT) → Skyrme, Gogny, relativistic mean field energy density functionals (EDF)

These lectures: How developments in nuclear forces impact calculations in each of these categories.

- ab initio now part of all three categories
- put EDF's in more general context

Laundry list of ab initio methods:

① continuum Monte Carlo
- GFMC; A=1-12, many observables, needs local potential (AV18+3NF)
- AFDMC (Alex G's lectures); established for neutron matter, nuclear matter and larger nuclei? (sample spin-and spin/isospin), new N²LO local potential

② configuration interaction: matrix diagonalization in a basis (often HO) (separable center-of-mass)
- NCSM: no core shell model → all nucleons active
- NCFC: no core full configuration → see Maris, Vary for definitions
- needs soft interaction for adequate convergence
  - chiral EFT → Lee Suzuki unitary transformation or SRG/Vlowk
  - JISP potentials (some of separable terms — use off-shell freedom to reduce 3NF contributions)

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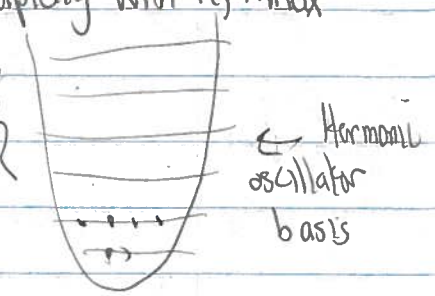
- limited by matrix size ⇒ grows very rapidly with A, N_{max}

^{4}He $N_{max}=4 \Rightarrow 10^3$ dimension $(10^3 \times 10^3)$
$N_{max}=8 \Rightarrow 4\times10^4$
$N_{max}=14 \Rightarrow \sim 3\times10^6$

^{12}C $N_{max}=4 \Rightarrow 10^6$
$N_{max}=8 \Rightarrow 7\times10^8$



- Feasible to do several billion size matrix (i.e. $10^9 \times 10^9$)
- How is this possible at all? Sparse matrices ⇒ mostly 0's.
  - Use Lanczos method:
    If $H|\psi_k\rangle = E_k|\psi_k\rangle$, then $H^m|\psi\rangle = \sum_k C_k E_k^m |\psi_k\rangle$ ← arbitrary
    ⇒ largest eigenvalue $|E_k|$ in magnitude dominates
  - Use $(H-\sigma I)^m$ with $\sigma>0$ large so $|E_0-\sigma|$ is largest
    ⇒ project out lowest eigenvalues and vectors. Maybe 20 at a billions!
    (Iterate in m orthogonalizing as you go)
- How can we push higher?
  - Importance Truncated NCSM ⇒ don't use all the basis states
    - determine relevant basis states before diagonalizing using first-order perturbation theory.
    - reference state $|\psi_{ref}\rangle$ (from small N_{max} diagonalization), calculate
      $$\chi_\nu = \frac{-\langle \Phi_\nu | H_{int} | \psi_{ref}\rangle}{\varepsilon_\nu - \varepsilon_{ref}}$$ for all $|\Phi_\nu\rangle$ basis states
      ⇒ keep for $|\chi_\nu| \geq \chi_{min}$.
  - Perturbation theory must be reliable ⇒ enabled by soft interactions
  - R. Roth et al. using SRG evolved interactions

- CI applies to any nucleus, any observable (need operators!)

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③ Coupled Cluster – efficient resummation of many-body PT (infinite)

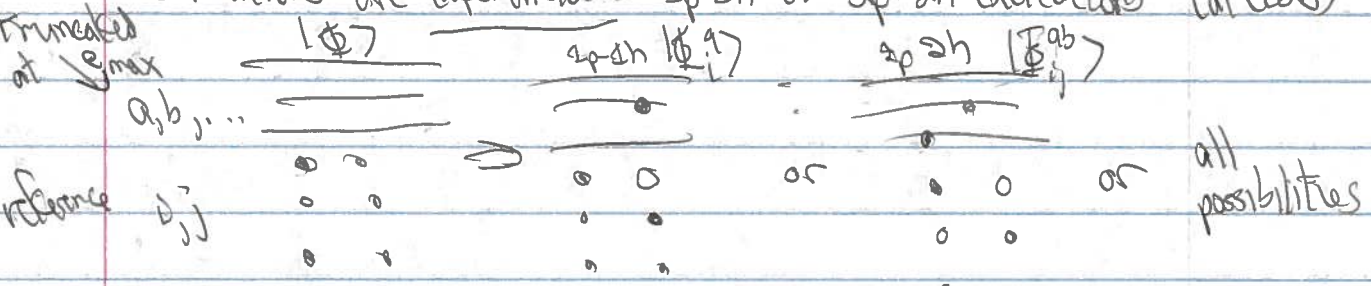
wf ansatz: $|\Psi\rangle = e^{T}|\Phi\rangle$ ← reference state

$T = T_1 + T_2 + \ldots$ ⇐ defines the truncation (eg. CCSD)

$T_1 = \sum_{ia} t_i^a a_a^\dagger a_i$, $T_2 = \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$, ...

Correlations are exponentiated 1p-1h and 2p-2h excitations (at CCSD)

truncated at e_{max}



- determine t_i^a, t_{ij}^{ab}, ... coefficients by requiring a similarity transformed Hamiltonian to decouple 1p-1h, 2p-2h

$\bar{H} = e^{T} H e^{T} \Rightarrow E = \langle\Phi|\bar{H}|\Phi\rangle$

$0 = \langle\Phi_i^a|\bar{H}|\Phi\rangle$ } CCSD

$0 = \langle\Phi_{ij}^{ab}|\bar{H}|\Phi\rangle$ }

- "triples" means $a^\dagger a^\dagger a^\dagger aaa$
- good scaling properties with A, size of space
- many on-going developments → ORNL/UT and Darmstadt groups
- uses chiral EFT forces as input (soft),
  - SRG would work well, but more development

④ Self-consistent Green's function
- Solve Dyson's equations non-perturbatively

{ recent developments using soft interactions → see INT program talks for March

See slide

⑤ In-medium SRG ⇒ SRG evolution with a reference state (cf. CC)

⑥ Lattice EFT

⑦ Other: MBPT (Manbuy), shell model EFT ← fit EFT interaction within shell model