TALENT/INT Course on Nuclear Forces
Exercises and Discussion Questions M3

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Monday 3: Many-body problem and basis considerations; MBPT

There are quite a few problems and questions in this exercise set. Be sure to jump around so that you try all of the topics in the available time.

1. Two-minute and discussion questions:

   (a) Which of the many-body methods discussed could use the Entem-Machleidt N^3LO 500 MeV interaction as input and which could not?

   (b) What is a *reference state* and how is it used in MBPT?

   (c) Does the diagonalization in a major harmonic-oscillator shell lead to positive and negative parity states?

   (d) Why are only even $N_{\max}$ results shown in the typical convergence plots with $N_{\max}$ in the NCSM?

   (e) IM-SRG and Coupled Cluster.

      i. In what way are these methods very similar conceptually? (Hint: what do you decouple in each case?)

      ii. What is the role of the reference state in these approaches?

      iii. Two possibilities for reference states for closed-shell nuclei are a Hartree-Fock Slater determinant from the input potential or a Slater determinant with harmonic oscillator single-particle wave functions. Which do you think will be more effective (and why)?

   (f) At present, the only known way to remove cutoff dependence order-by-order in the EFT expansion with Weinberg counting is to include the Hamiltonian beyond leading order perturbatively.

      i. Which of the many-body methods we've discussed can do that?

      ii. How would the fitting procedure to phase shifts have to be changed?

   (g) What is the difference between Feynman diagrams and Goldstone diagrams? Which can you use to calculate ground-state energies?

2. Effects of a harmonic-oscillator basis truncation.

   (a) How are the UV and IR cutoffs from using a finite harmonic-oscillator basis analogous to those for a lattice with finite size and finite spacing?

   (b) What sets the scale for the UV and IR cutoffs?

3. Contractions between creation and annihilation operators are defined by the expectation values

$$\overbracket{\mathrm{a}_i^\dagger \mathrm{a}_j} \equiv \left\langle \Phi \right| \mathrm{a}_i^\dagger \mathrm{a}_j \left| \Phi \right\rangle , \quad \overbracket{\mathrm{a}_i \mathrm{a}_j^\dagger} \equiv \left\langle \Phi \right| \mathrm{a}_i \mathrm{a}_j^\dagger \left| \Phi \right\rangle , \ldots \tag{1}$$

where $\left|\Phi\right\rangle$ denotes the (arbitrary) reference state.

What are the values of the contractions $\overbracket{\mathrm{a}_i^\dagger \mathrm{a}_j}$ and $\overbracket{\mathrm{a}_i \mathrm{a}_j^\dagger}$ if $\left|\Phi\right\rangle$ is (i) the particle vacuum $\left|0\right\rangle$, (ii) a general Slater determinant, or (iii) a Hartree-Fock Slater determinant? Are there other non-vanishing contractions in each of the three cases?

4. Derive or justify the normal-ordering factors discussed in the lecture. That is, start from the second-quantized Hamiltonian with two- and three-body interactions,

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

and normal-order all operators with respect to a finite-density Fermi vacuum $|\Phi\rangle$ (for example, the Hartree-Fock ground state or the non-interacting Fermi sea in nuclear matter), as opposed to the zero-particle vacuum. Show that H can be *exactly* written as

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

where the zero-, one-, and two-body normal-ordered terms are given by

$$E_0 = \langle \Phi|H|\Phi\rangle = \sum_1 T_{11} n_1 + \frac{1}{2} \sum_{12} \langle 12|V|12\rangle n_1 n_2 + \frac{1}{3!} \sum_{123} \langle 123|V^{(3)}|123\rangle n_1 n_2 n_3 \,,$$

$$f_{12} = T_{12} + \sum_i \langle 1i|V|2i\rangle n_i + \frac{1}{2} \sum_{ij} \langle 1ij|W|2ij\rangle n_i n_j \,,$$

$$\langle 12|\Gamma|34\rangle = \langle 12|V|34\rangle + \sum_i \langle 12i|V^{(3)}|34i\rangle n_i \,,$$

where n_i denote the sharp occupation numbers (0 or 1) in the reference state.

5. Wick's theorem for commutators and products of normal-ordered operators. Wick's theorem allows us to expand a product of two normal-ordered operators purely in terms of *external* contractions, i.e., each contraction must involve at least one $\mathrm{a}^\dagger$ or a from either of the two operators. For example,

$$:\mathrm{a}_a^\dagger \mathrm{a}_b::\mathrm{a}_k^\dagger \mathrm{a}_l: = - :\mathrm{a}_a^\dagger \mathrm{a}_k^\dagger \mathrm{a}_b \mathrm{a}_l: - \overbracket{\mathrm{a}_a^\dagger \mathrm{a}_l} :\mathrm{a}_k^\dagger \mathrm{a}_b: + \overbracket{\mathrm{a}_b \mathrm{a}_k^\dagger} :\mathrm{a}_a^\dagger \mathrm{a}_l: + \overbracket{\mathrm{a}_a^\dagger \mathrm{a}_l} \overbracket{\mathrm{a}_b \mathrm{a}_k^\dagger} \,. \tag{4}$$

   (a) Briefly discuss why only external contractions appear in the expansion.

   (b) When can 0-body operators appear in the Wick expansion of a product of normal-ordered K- and N-body operators? Which A-body components are possible in general?

(c) Show that the commutator between normal-ordered $K-$ and N-body operators,

$$\left[:\mathrm{a}^\dagger_{k_1}\dots\mathrm{a}^\dagger_{k_K}\mathrm{a}_{k'_1}\dots\mathrm{a}_{k'_K}:, :\mathrm{a}^\dagger_{n_1}\dots\mathrm{a}^\dagger_{n_N}\mathrm{a}_{n'_1}\dots\mathrm{a}_{n'_N}:\right]$$

has no $(N+K)$-body component.

6. In-Medium SRG flow equation. In previous lectures, we encountered the SRG flow equation in operator form,

$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right]. \tag{5}$$

In the In-Medium SRG, the medium is introduced by choosing a reference state $\left|\Phi\right\rangle$, and normal ordering the operators. Let us assume that $\left|\Phi\right\rangle$ is a Hartree-Fock Slater determinant in the following. This allows us to construct a basis of the many-body Hilbert space which consists of $\left|\Phi\right\rangle$ and all possible particle-hole excitations, $\left|\Phi^p_h\right\rangle =:\mathrm{a}^\dagger_p\mathrm{a}_h: \left|\Phi\right\rangle$, $\left|\Phi^{pp'}_{hh'}\right\rangle =:\mathrm{a}^\dagger_p\mathrm{a}^\dagger_{p'}\mathrm{a}_{h'}\mathrm{a}_h: \left|\Phi\right\rangle$, etc.

To determine the system's ground-state energy, we integrate the flow equation in order to decouple $\left|\Phi\right\rangle$ from excitations as $s\to\infty$. This defines a unitary transformation between $H(0)$ and $H(\infty)$, or conversely $\left|\Phi\right\rangle$ and the true ground state. A generator which achieves the desired decoupling is $\eta = \left[H^d, H^{od}\right]$, where the off-diagonal Hamiltonian that is driven to zero is defined as

$$H^{od} \equiv \sum_{ph} f_{ph}\ :\mathrm{a}^\dagger_p\mathrm{a}_h: + \sum_{pp'hh'}\Gamma_{pp'hh'}\ :\mathrm{a}^\dagger_p\mathrm{a}^\dagger_{p'}\mathrm{a}_{h'}\mathrm{a}_h: + \mathrm{H.c.} \tag{6}$$

(the s-dependence is suppressed for brevity).

(a) In current applications, we treat η and H as normal-ordered operators containing up to two-body components. Why is this an approximation?

(b) A two-body Hamiltonian can couple $\left|\Phi\right\rangle$ to up to $2p$-$2h$ excitations. Evaluate the matrix elements $\left\langle 0\right| H\left|\Phi^p_h\right\rangle$ and $\left\langle 0\right| H\left|\Phi^{pp'}_{hh'}\right\rangle$ with Wick's theorem in order to show that these are precisely the matrix elements which define H^{od}.

(c) Use the elementary commutator expressions from the exercise on Wick's theorem to derive the IM-SRG flow equation for the ground-state energy ($\bar{n}_i = 1 - n_i$),

$$\frac{d}{ds}E = \sum_{ab}\left(n_a - n_b\right)\ \eta_{ab}f_{ba} + \frac{1}{2}\sum_{abcd} n_a n_b \bar{n}_c \bar{n}_d\ \eta_{abcd}\Gamma_{cdab} \tag{7}$$

(d) Show that $\frac{d}{ds}E = 0$ if H^{od} vanishes. (Hint: what are the occupation numbers n_i for particle and hole states?)

7. Lattice effective field theory. Here are some results by Epelbaum et al. from lattice EFT calculations for the ground-state energies of light nuclei:

nucleus	^{4}He	^{8}Be	^{12}C	^{16}O
LO $[Q^0]$	$-28.0(3)$	$-57(2)$	$-96(2)$	$-144(4)$
NLO $[Q^2]$	$-24.9(5)$	$-47(2)$	$-77(3)$	$-116(6)$
NNLO $[Q^3]$	$-28.3(6)$	$-55(2)$	$-92(3)$	$-135(6)$
experiment	-28.30	-56.5	-92.2	-127.6

(a) Why might you expect the structure of these nuclei to be heavily influenced by "alpha clusters"? Why is lattice EFT well suited to efficiently include the effects of alpha clusters? Which other methods can do this efficiently?

(b) The numbers in parenthesis are the statistical errors for each calculation. Why don't they get smaller as you go to higher order in the EFT expansion? How would you make them smaller?

(c) If the lattice spacing for these calculations was $a = 2\,\mathrm{fm}$ and the typical momentum in these nuclei was about m_π, what would you expect the expansion parameter to be? How does that compare to the pattern of convergence in the table? Can you explain the differences from naive expectations?

(d) Why will it be useful to have additional calculations with different cutoffs (i.e., different lattice spacings)?

8. Consider the power counting formula for k_{F}^{β} for a uniform, dilute, natural Fermi system (rules on slide 17, formula on slide 18, diagrams on slide 19 in M3b slides).

   (a) Verify for the diagrams that the claimed power of k_{F} is reproduced from the formula.

   (b) Why does the formula for β ensure that: i) only a finite number of diagrams contributes at each order in k_{F}/Λ; ii) β is at least 6; iii) increasing the number of derivatives at a vetex or increases the number of lines increases β? Argue that this means we will have a controlled perturbative expansion. (Must it converge?)

   (c) Why is this not a good model for infinite nuclear systems (neutron or nuclear matter) at low densities? What about densities comparable to the interior of heavy nuclei?

9. Brueckner-Bethe-Goldstone (BBG) power counting and MBPT.

   (a) Why is it necessary to do G-matrix summations of ladder diagrams for traditional nucleon-nucleon potentials (such as the local phenomenological potentials)?

   (b) How can you use Weinberg eigenvalues to test if this is necessary for softened potentials (either from chiral EFT with a lower cutoff or RG-softened interactions)?

   (c) Why is the MBPT expansion still non-perturbative in terms of G-matrices (rather than "bare" interactions) for traditional potentials? Why is this not true for softer potentials?

   (d) What is the expansion parameter for the hole-line expansion?