Solution of the Bethe-Goldstone Equation Without Partial Wave Decomposition

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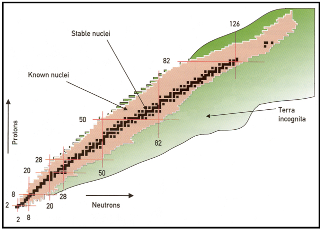
PhD Defense

Overview

- Motivation and methodology.
- Overview of the field
  1. The nucleon-nucleon (NN) potential.
  2. Use the NN potential in the kernel of Bethe-Goldstone scattering equation and calculate the effective interaction.
- Predictions
  1. Use the effective interaction as input to predict in-medium observables.

Motivation

- After more than 8 decades of nuclear physics, still a lot is unknown about the nuclear chart, particularly so for neutron rich nuclei (closely related to isospin asymmetric nuclear matter or IANM).



- The unknown region must be studied!
- These unknown nuclei could be beneficial to nuclear medicine, or aid in our understanding of neutron stars and matter at the beginning of the universe.
- Experimental programs such as FRIB will have widespread impact, filling some of the gaps in our incomplete knowledge of the nuclear chart.

Methodology

- The goal of microscopic nuclear physics is to derive the properties of nuclear systems from the basic nuclear interaction (ab initio).
- In the spirit of our ab initio methodology, we use a nuclear potential that has no free parameters (when we enter the medium).

Chiral and meson potentials

- Our present (incomplete) knowledge of the nuclear force is the result of decades of struggle.
- QCD (quantum chromodynamics) is the fundamental theory for the strong force. Unfortunately, this is often not a realistic option (it's non-perturbative).

Alternatives:

- QCD and its symmetries led to the development of chiral effective theories.
- Meson theory where the degrees of freedom are nucleons with mediating particles being mesons.

Which one?

- Chiral potentials are based on a low-momentum expansion and are of limited use for applications in dense matter.
- Thus, meson theory is a better choice.

Why we use meson potentials

- A high quality meson potential like the CD-Bonn does very well with nucleon-nucleon phase shits up to high energy.

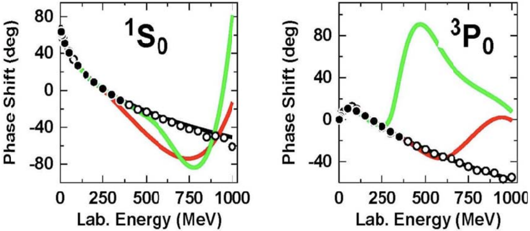


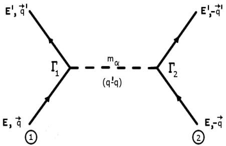
Figure: Some nucleon-nucleon phase shifts as predicted with meson and chiral potentials. Black dots correspond to the Meson potential (Bonn) and behind the open circles are experimental data points. The green and red curves are the chiral potentials.

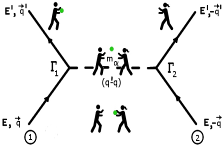
Bonn potentials

- To model the nuclear force, our group uses the Bonn potential.
- This potential will be used in the kernel of the scattering equation.
- The Bonn potential is constructed by exchanging six mesons

$$V_{Bonn} = V_\pi + V_\eta + V_\delta + V_\sigma + V_\rho + V_\omega \tag{1}$$

- The use of Feynman diagrams/rules aid in calculating the potential





IANM

- Hypothetical substance consisting of a huge number of protons and neutrons (with different concentrations) interacting only by the nuclear force (e.g. ignores the coulomb force).
- It's like a ball pit.

A closer look at the Bonn potential

Recall the Bonn potential

$$V_{Bonn} = V_\pi + V_\eta + V_\delta + V_\sigma + V_\rho + V_\omega \tag{2}$$

In literature V_δ is written as

$$\langle \boldsymbol{q}' \lambda_1' \lambda_2' | V_\delta | \boldsymbol{q} \lambda_1 \lambda_2 \rangle \propto \frac{W'W}{E'E} \left(1 - \frac{4\lambda_1 \lambda_1' \, |\boldsymbol{q}| \, |\boldsymbol{q}'|}{W'W} \right) \left(1 - \frac{4\lambda_2 \lambda_2' \, |\boldsymbol{q}| \, |\boldsymbol{q}'|}{W'W} \right) \langle \lambda_1' \lambda_2' | \lambda_1 \lambda_2 \rangle \tag{3}$$

where $E^2 = \boldsymbol{q}^2 + m^2$, $W = E + m$ and similar expressions for the primed value.

- Above m is the average of the proton and neutron mass. Since in free-space $m_{proton} \approx m_{neutron}$ this is fine.
- In IANM calculations (e.g. Bethe-Goldstone equation) $m_{proton} \not\approx m_{neutron}$, so it's more appropriate to keep the masses separate

$$\langle \boldsymbol{q}' \lambda_1' \lambda_2' | V_\delta | \boldsymbol{q} \lambda_1 \lambda_2 \rangle \propto \sqrt{\frac{W_1' W_2' W_1 W_2}{E_1' E_2' E_1 E_2}} \left(1 - \frac{4\lambda_1 \lambda_1' \, |\boldsymbol{q}| \, |\boldsymbol{q}'|}{W_1' W_1} \right) \left(1 - \frac{4\lambda_2 \lambda_2' \, |\boldsymbol{q}| \, |\boldsymbol{q}'|}{W_2' W_2} \right) \langle \lambda_1' \lambda_2' | \lambda_1 \lambda_2 \rangle \tag{4}$$

This generalization can be useful for calculations involving baryons with different masses and pseudovector coupling used for the exchange of pseudoscalar mesons.

A closer look at the Bonn potential conclusions

Notice the potential

$$\langle \boldsymbol{q}'\lambda_1'\lambda_2'|V_\delta|\boldsymbol{q}\lambda_1\lambda_2\rangle \propto \sqrt{\frac{W_1'W_2'W_1W_2}{E_1'E_2'E_1E_2}}\left(1-\frac{4\lambda_1\lambda_1'\,|\boldsymbol{q}|\,|\boldsymbol{q}'|}{W_1'W_1}\right)\left(1-\frac{4\lambda_2\lambda_2'\,|\boldsymbol{q}|\,|\boldsymbol{q}'|}{W_2'W_2}\right)\langle\lambda_1'\lambda_2'|\lambda_1\lambda_2\rangle \tag{5}$$

depends on

- Three momentum $\boldsymbol{q}, \boldsymbol{q}'$ with angles contained in the $\langle\lambda_1'\lambda_2'|\lambda_1\lambda_2\rangle$ term.
- Angular momentum via the helicities λ's, e.g. spin projection along the direction of the momentum.
- Isospin (not explicitly shown) has a formalism analogous to spin. For example, a nucleon with $I = +$ is a proton while one with $I = -$ is a neutron.

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Our traditional many-body framework

- Describing IANM requires a many-body theory (recall the ball pit).
- For this our group uses the Dirac-Brueckner-Hartree-Fock (DBHF) approach to symmetric and asymmetric nuclear matter.
- The Bonn potential in used as input to our many-body theory without free parameters when we enter the medium (ab initio methodology).
- Our group can then calculate things such as
    1. Equation of state (EoS) which is the energy per nucleon and is of fundamental importance (input for calculating nuclear binding energies, densities, neutron skins etc.).
    2. Effective interaction which is the solution to the Bethe-Goldstone equation.

Bethe-Goldstone equation

- Our goal is to solve the 3D angle dependent Bethe-Goldstone equation exactly for G i.e. without partial wave decomposition.

$$G(\boldsymbol{q}', \boldsymbol{q}) = V(\boldsymbol{q}', \boldsymbol{q}) + \lim_{\epsilon \to 0} \int \frac{V(\boldsymbol{q}', \boldsymbol{q}'')Q(\boldsymbol{q}'', \boldsymbol{P}, k_F)G(\boldsymbol{q}'', \boldsymbol{q})}{2(E^*_q - E^*_{q''} + i\epsilon)} \, \mathrm{d}^3 q'' \quad (6)$$

Medium effects come in through

- Effective masses, m^* which are included in the relativistic energy $E^*_p = \sqrt{p^2 + m^*}$ and also in the potential V (in accordance with the DBHF approach).
- The Pauli operator Q which prevents scattering into occupied states.

In free-space ($m^* = m, Q = 1$) you get the Thompson equation (integral version of the Schrodinger equation)

$$T(\boldsymbol{q}', \boldsymbol{q}) = V(\boldsymbol{q}', \boldsymbol{q}) + \lim_{\epsilon \to 0} \int \frac{V(\boldsymbol{q}', \boldsymbol{q}'')T(\boldsymbol{q}'', \boldsymbol{q})}{2(E_q - E_{q''} + i\epsilon)} \, \mathrm{d}^3 q'' \quad (7)$$

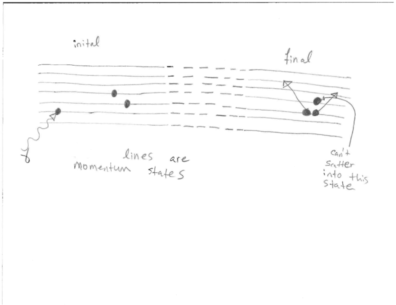
Motivation and purpose for Bethe-Goldstone equation

The G-matrix (effective interaction/solution to the Bethe-Goldstone equation) is very important.

Motivation

- Used in our EoS calculation.
- Used in nucleus-nucleus reaction calculations.

Purpose



Pauli Operator

- The Pauli operator in the Bethe-Goldstone equation is of central interest and is one of the most important medium effects in nuclear matter.
- The traditional solution of the Bethe-Goldstone equation uses partial wave decomposition along with the spherical approximation on the Pauli operator.
- On the other hand, in this project we solve the scattering equation in 3D space, that is, without the use of partial wave decomposition. This has the benefit of treating the Pauli operator exactly and allows us to investigate the validity of the spherical approximation.

Partial wave decomposition

You expand the free-space solution T [i.e. $T = V + \int VQT, Q = 1$] via the partial waves T^J

$$T(q', \theta', q) = \sum_J \frac{2J+1}{4\pi} d^J_{\lambda\lambda'}(\theta') T^J(q', q) \quad \text{where} \quad \lambda, \lambda' = \pm 1, 0 \tag{8}$$

with $d^J_{\lambda\lambda'}$ the reduced rotation matrix (Jacobi polynomials) and a similar expression for the potential V.
Then use this expression to re-write the Thompson equation

$$T^J(q', q) = V^J(q', q) + \int \frac{V^J(q', q'') T^J(q'', q)}{2(E_q - E_{q''} + i\epsilon)} q''^2 \, \mathrm{d}q'' \tag{9}$$

All you did is exchange the angle θ' with the partial waves J. Now you solve for $J = 0, 1, 2 \ldots N$ ($N = 15$ is usually high enough).

But what about the Bethe-Goldstone equation

- The partial wave expansion from the previous slide does not work on the Bethe-Goldstone equation because the Pauli operator has an angular dependence.
- The most naive thing to do is to take a functional average

$$\bar{Q}(q'') = \frac{\int Q(q'', \theta'', \phi'') \sin\theta'' \, \mathrm{d}\theta'' \, \mathrm{d}\phi''}{\int \sin\theta'' \, \mathrm{d}\theta'' \, \mathrm{d}\phi''} \tag{10}$$

This is known as the spherical or angle-average approximation. If this is used then partial wave decomposition can be preformed.

Numerical methods

- The Bethe-Goldstone equation is a set of six 3D coupled and complex Fredholm integral equations of the second kind (twelve if you include isospin).
- As a simple example consider the Fredholm integral equation of the second kind for the unknown function g

$$g(q) = v(q) + \int k(q, q') g(q') \, \mathrm{d}q' \tag{11}$$

- Approximate integral with Gauss-Legendre Quadrature

$$g(q) = v(q) + \sum_j w_j k(q, q_j) g(q_j) \tag{12}$$

- Now evaluate $q = q_i$ where q_i are the nodes q_j used in the Gauss-Legendre Quadrature rule.

$$g(q_i) = v(q_i) + \sum_j w_j k(q_i, q_j) g(q_j) \tag{13}$$

- Now define the vectors $g(q_i) = \boldsymbol{g}$, $v(q_i) = \boldsymbol{v}$, and the matrix $K = w_j k(q_i, q_j)$. In vector matrix form

$$\boldsymbol{g} = \boldsymbol{v} + K\boldsymbol{g} \implies \boldsymbol{g} = (1 - K)^{-1}\boldsymbol{v} \tag{14}$$

Numerical methods continued

- LU factorization from Lapack to solve the vector matrix equation.
- Had to use single precision complex numbers for the matrices otherwise we ran out of memory.
- OpenMP (parallel programming) to fill in the entries of the matrices.
- Needed a large number of Gauss-Legendre points to achieve stability [≈ 80 for $(0, \pi)$ and ≈ 100 for $(0, \infty)$] due to diagonal matrix entries creating long tailed functions.

Figure: “Dirac” nuclear theory group computer cluster.

Plot of Bonn potential

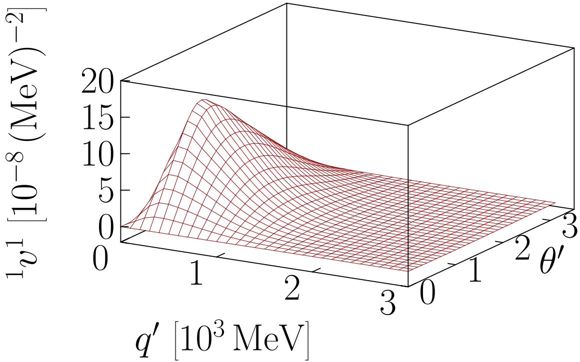


Figure: ϕ independent Bonn B potential evaluated at $\theta = \arccos(0.5)$ and $q = 306.42MeV$.

In-medium Observables

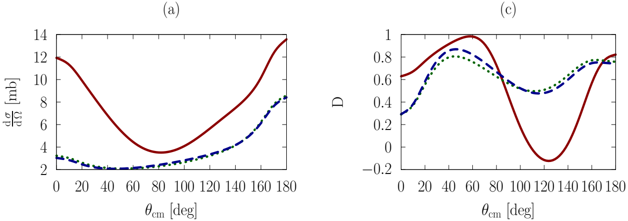
The solution of the Bethe-Goldstone equation can be used to calculate many in-medium observables. We selected two:

- The differential cross-section $\frac{d\sigma}{d\Omega}$.
- Depolarization D (i.e. a spin observable).

Particles incident in the area $d\sigma$ scatter into the solid area $d\Omega$.
The proportionality constant is $D(\theta) = \frac{d\sigma}{d\Omega}$ = Differential cross-section.

The spin polarization normal to the scattering plane is observed for the beam and scattered particle.

In-medium observable plots

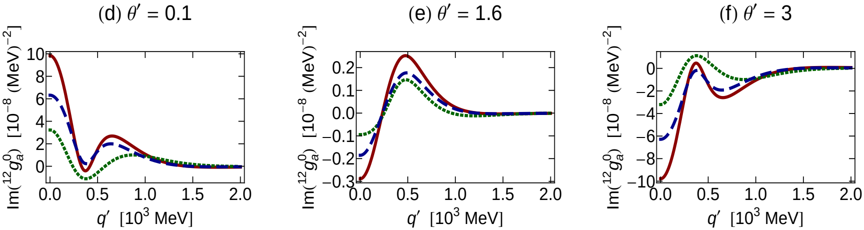


- Red: Free-space
- Blue: Exact solution
- Green: Spherical approximation

These plots use only the diagonal entries of the G-matrix.

In-medium observables continued

- These plots used all the entries of the G-matrix.
- Imaginary part of the physical G-matrix amplitudes.



- q $=$ 300 MeV and $\theta = \arccos(0.5)$.
- Red: Free-space
- Green: Exact solution
- Blue: Spherical approximation

Thus, there could be noticeable effects on processes which involve using all the entries of the G-matrix.

Conclusion

- Our standard DBHF many-body theory consists of a meson potential used as input. This allows us to calculate things such as the EoS or the G-matrix.
- In this work, we have specifically investigated the impact of removing the popular “spherical” approximation from the Pauli operator. For that purpose, we have solved the Bethe-Goldstone equation in 3D space, that is, without the use of partial wave decomposition.
- Although 3D solutions of the free-space scattering equation have been reported before, we are not aware of a similar calculation for the in-medium scattering equation.

Acknowledgments

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- Committee members:
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  3. Dr. You Qiang (Experimental Physics)
  4. Dr. Francesca Sammarruca (Theoretical Physics), Committee chair