Progress Report

Quantum Monte Carlo Calculations of Nucleon Systems and Cold Atom Gases

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Abstract

We present our progress on the projects we have been developing. In our study of strongly interacting Fermi gases, we investigated core structure properties of two-dimensional Fermi gas vortices in the BEC-BCS crossover region. The manuscript with our findings is currently under review by Physical Review A journal. Also, we have been developing light nuclei wave functions which include explicit pion contributions. In our study of improved trial wave functions for nucleon systems, we have results for ^{4}He, ^{16}O, and symmetric nuclear matter.

1 Scientific discoveries

1.1 Strongly paired fermionic systems of cold atoms

Our findings regarding cold gases systems were summarized in the article "Core structure of two-dimensional Fermi gas vortices in the BEC-BCS crossover region" [1], which has been submitted to the Physical Review A journal.

We reported $T = 0$ diffusion Monte Carlo results for the ground-state and vortex excitation of unpolarized spin-1/2 fermions in a two-dimensional disk. We investigated how vortex core structure properties behave over the BEC-BCS crossover. We calculated the vortex excitation energy, density profiles, and vortex core properties related to the current. We found a density suppression at the vortex core on the BCS side of the crossover, and a depleted core on the BEC limit. Size-effect dependencies in the disk geometry were carefully studied.

1.2 QMC simulations with explicit contributions from the pion field

We begun our study of explicit contributions of the pion field to QMC simulations by studying one nucleon in a box. As a starting point, we can try to determine the self energy (effective mass) of a nucleon of bare mass m_b, which should be equal to its physical mass. Since we consider dynamical pions, we are effectively including processes like the ones in Fig. 1.

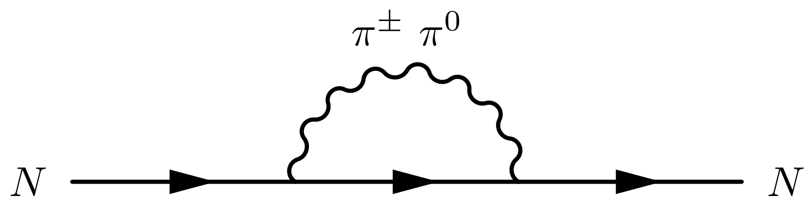

Figure 1

The corresponding Hamiltonian can be written as

$$\hat{H} = \sum_{k=0}^{k_c} \left\{ -\frac{1}{2}\nabla^2_{\pi^c_{k_\beta}} - \frac{1}{2}\nabla^2_{\pi^s_{k_\beta}} + \frac{1}{2}(k^2 + m_\pi^2)(\pi^{c2}_{k_\beta} + \pi^{s2}_{k_\beta}) \right\}$$
$$+ \frac{g_a}{2f_\pi}\frac{1}{\sqrt{2\pi}} \sum_{\alpha,\beta} \sum_{k=0}^{k_c} \sigma_\alpha \tau_\beta (k_\alpha \pi^s_{k\beta} \cos(\mathbf{k}\cdot\mathbf{x}) - k_\alpha \pi^c_{k\beta} \sin(\mathbf{k}\cdot\mathbf{x})) + \frac{p_i^2}{2m_b} + m_b', \tag{1}$$

where $\mathbf{k}$ are wave vectors compatible with the simulation box, k_c is a cutoff, $\pi_{\mathbf{k}}$ are pionic degrees of freedom, m_π is the pion mass, g_a and f_π are coupling constants, $\mathbf{x}$ are the spatial coordinates of the nucleon, $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ are the usual Pauli matrices which act on spin and isospin, respectively, and $\mathbf{p}$ is the momentum of the nucleon.

The trial wave function which we developed is

$$\psi_T(\boldsymbol{\pi}^c_{\mathbf{k}}, \boldsymbol{\pi}^s_{\mathbf{k}}, \mathbf{x}) = \prod_{k=0}^{k_c} \exp\left[-\sqrt{k^2 + m_\pi^2} \left\{ \boldsymbol{\pi}^{c2}_{k_\beta} + \boldsymbol{\pi}^{s2}_{k_\beta} + \tilde{G}_k \mathbf{k}\cdot\boldsymbol{\sigma} \left[-\sin(\mathbf{k}\cdot\mathbf{x})\boldsymbol{\pi}^c_{\mathbf{k}}\cdot\boldsymbol{\tau} \right.\right.\right.$$
$$\left.\left.\left. + \cos(\mathbf{k}\cdot\mathbf{x})\boldsymbol{\pi}^s_{k_\beta}\cdot\boldsymbol{\tau} \right] + \tilde{G}_k^2 (\boldsymbol{\sigma}\cdot\mathbf{k})^2 \boldsymbol{\tau}^2 \right\} \right] \phi \tag{2}$$

where the $\tilde{G}_k$ are variational parameters and

$$\phi = \begin{pmatrix} \phi^{p\uparrow} \\ \phi^{p\downarrow} \\ \phi^{n\uparrow} \\ \phi^{n\downarrow} \end{pmatrix}$$

is a 4-spinor.

1.3 Improved trial wave functions for nuclei and nuclear matter

Auxiliary Field Diffusion Monte Carlo (AFDMC) calculations depend heavily on having a good estimate to the ground-state wave function of the system. This estimate is called the trial wave function. The ideal set of spin-isospin dependent correlations are an exponential of spin-isospin operators. In the past this exponential was expanded and truncated at linear correlations [2]. We have expanded the trial wave function to include quadratic correlations. The addition of these correlations has lowered the energies for each system that we have calculated compared to the same calculation with linear correlations. We have currently done correlations for the nuclei ^{4}He and ^{16}O, and for symmetric nuclear matter. Our preliminary results are summarized in Tab. 1. We have also calculated the energy per nucleon of symmetric nuclear matter (SNM) with density $\rho = 0.16\text{fm}^{-3}$ of 28 particles with periodic boundary conditions. The energy per nucleon was -13.92(6) MeV for linear correlations, -14.80(7) MeV for independent pair correlations, and -14.70(11) MeV with the full set of quadratic correlations.

Table 1: Energy in MeV for ^{4}He and ^{16}O as calculated with all three types of correlations compared to experimental energies.

	Linear	Independent Pair	Quadratic	Experimental
^{4}He	-27.17(4)	-26.33(3)	-25.35(3)	-28.295
^{16}O	-115.7(9)	-121.5(1.5)	-120.0(1.4)	-127.619

It would be beneficial to include the full exponential correlations in the trial wave function if possible. To propagate the positions and spins of the configurations of particles we use a Green's function or propagator. The propagator involves the exponential of the Hamiltonian, which contains the same spin-isospin dependent operators as the wave function correlations. Currently the spin-isospin dependent propagator is calculated with the aid of the Hubbard-Stratanovich transformation as described in [3]. We plan to use the Hubbard-Stratanovich transformation to calculate the full exponential correlation operator. This should improve the trial wave function even further than the quadratic correlations.

With this improved trial wave function we will investigate the clustering of two neutrons and two protons into alpha particles in mostly neutron matter. Alpha particle clustering has been investigated and has shown a dependence on density in mostly nuclear matter [4]. We plan to show that AFDMC is a viable tool to investigate this clustering.

2 Scientific production

Our findings regarding cold gases systems were summarized in the article "Core structure of two-dimensional Fermi gas vortices in the BEC-BCS crossover region" [1], which is under review by the Physical Review A journal.

References

[1] Lucas Madeira, Stefano Gandolfi, and Kevin E. Schmidt. Core structure of two-dimensional Fermi gas vortices in the BEC-BCS crossover region. *arXiv pre-print*, 2017. arXiv:1703.01998 [cond-mat.quant-gas].

[2] S. Gandolfi, A. Lovato, J. Carlson, and Kevin E. Schmidt. From the lightest nuclei to the equation of state of asymmetric nuclear matter with realistic nuclear interactions. *Phys. Rev. C*, 90:061306, Dec 2014.

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[4] P Schuck, Y Funaki, H Horiuchi, G Röpke, A Tohsaki, and T Yamada. Alpha-Particle Condensation in Nuclear Systems. *Journal of Physics: Conference Series*, 413(1):012009, 2013.