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Extended study for unitary fermions on a lattice using the cumulant expansion technique

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A recently developed lattice method for large numbers of strongly interacting nonrelativistic fermions exhibits a heavy tail in the distributions of correlators for large Euclidean time τ and large number of fermions N, which only allows the measurement of ground state energies for a limited number of fermions using standard techniques. In such cases, it is suggested that measuring the log of the correlator is more efficient, and a cumulant expansion of this quantity can be exactly related to the correlation function. The cumulant expansion technique allows us to determine the ground state energies of up to 66 unpolarized unitary fermions on lattices as large as 72×14^3, and up to 70 unpolarized unitary fermions trapped in a harmonic potential on lattices as large as 72×64^3. We have also improved our lattice action with a Galilean invariant form for the four-fermion interaction, which results in predictive volume scaling of the lowest energy of three fermions in a periodic box and in good agreement of our results for $N \leq 6$ trapped unitary fermions with those from other benchmark calculations.

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1. Introduction

One of the most challenging problems in physics is the quantitative understanding of a quantum system of many strongly interacting particles for which numerical simulations have played an important role. Among the variety of known systems, a dilute Fermi gas near unitarity has been noted for its pure form, which can be readily studied from theory, and for its realization by using ultra-cold atomic experiments (for a recent review, see [1, 2]). Besides the intrinsic physical interest, such as universal behavior, the unitary Fermi gas might also be considered as an ideal starting point to develop numerical techniques which can be applied to low energy nuclear physics, and to attack the noise problem which typically appears in numerical simulations of many particles.

In 2010 we presented a highly improved lattice method for non-relativistic fermions with four-fermion contact interactions [3] and its applications for trapped and untrapped unitary fermions [4, 5], where the largest numbers of fermions were restricted to $N = 20$ and 38, respectively, due to a statistical overlap problem. Since then, we have devised a tuning technique with a Galilean invariant form for the four-fermion interaction, which keeps the system at unitary up to Galilean boosts. We have also implemented an external harmonic potential in a more sophisticated way. Finally, we have developed a cumulant expansion technique to extract the ground state energies from data exhibiting a distribution overlap problem [6, 7]. As a result, we are able to extend our calculation of ground state energies of unpolarized fermions up to $N = 70$ and up to $N = 66$ unitary fermions with and without a harmonic trap, respectively. For the untrapped case, this extension leads us to the regime, $N \geq 38$, where the ground state energy E in units of that for non-interacting particles $E^{(0)}$ is constant; this implies that we are near the thermodynamic limit and can determine the universal dimensionless parameter $\xi = E/E^{(0)}$[1], called the Bertsch parameter. On the other hand, for the trapped case we find that $N = 70$ is insufficient to reach the thermodynamic limit.

2. Lattice construction for fermions at unitarity

We consider simulations of N non-relativistic two-component fermions $\psi = (\psi^{\uparrow}, \psi^{\downarrow})$ on a $T \times L^3$ Euclidean lattice, where periodic boundary conditions on the spatial directions and an open boundary condition on the temporal direction are imposed. The four-fermion contact interaction between different species of fermions is generated by Z_2 auxiliary fields ϕ which live on the time-like links of the lattice. A consequence of this set up is that the fermion-determinant does not depend on the ϕ field and thus the quenched simulation is exact [3].

The discretization errors for the energy of a single fermion are eliminated through the use of a perfect dispersion relation, while the unitarity limit may be achieved by tuning the interaction strength $C(\mathbf{q})$ to reproduce scattering data, $p \cot \delta_0 = 0$, using the Lüscher formula [3, 7]. Here the operator $\mathbf{q}$ for $|\mathbf{q}| < \Lambda$ corresponds to the momentum transfer between incoming and outgoing fermions, which makes the interaction Galilean invariant. The periodic function $C(\mathbf{q})$ is defined by

$$C(\mathbf{q}) = \frac{4\pi}{M} \sum_{n=0}^{N_O-1} C_{2n} O_{2n}(\mathbf{q}), \tag{2.1}$$

[1]The energies of non-interacting untrapped and trapped fermions are given by $E^{(0)}_{\text{untrapped}} = (3N)^{(5/3)}\pi^{4/3}/10ML^2$ and $E^{(0)}_{\text{trapped}} = (3N)^{4/3}\omega/4$, respectively. Here, ω is an oscillator frequency.

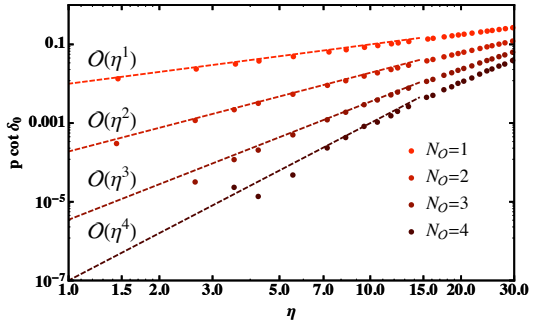

Figure 1: ln-ln plot of $p\cot\delta_0$ (dots) along with expected η scaling (dashed lines) for which $N_O = 1,2,3$ and 4 coefficients are tuned by exactly matching the first N_O energy eigenvalues for two particles in a box. Data is from an $L = 32$ and $M = 5$ lattice.

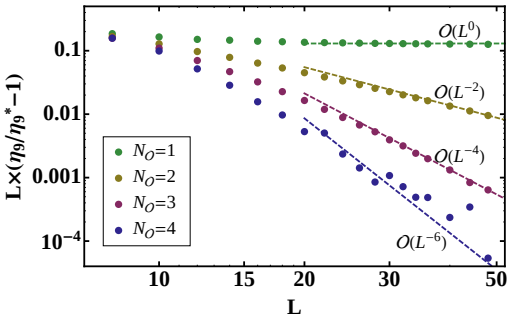

Figure 2: L dependence of the 9th energy eigenvalues for two particles in a box. The dashed lines are fit results of the data (dots) using Eq. 2.3.

where the basis functions are

$$O_{2n}(\mathbf{q}) = M_0^n \times \begin{cases} \left(1 - e^{-\mathbf{q}^2/M_0}\right)^n & |\mathbf{q}| \le \Lambda \\ \left(1 - e^{-\Lambda^2/M_0}\right)^n & |\mathbf{q}| > \Lambda \end{cases}, \tag{2.2}$$

for $\mathbf{q}$ within the first Brillouin zone and periodic from one Brillouin zone to the next. Although the parameter M_0 may in general be different from the fermion mass M, we use $M_0 = M$ in this work.

The coefficients C_{2n} are numerically determined by matching the lowest N_O energy eigenvalues of the two-body transfer matrix in our lattice theory with the lowest N_O Lüscher energy eigenvalues in the corresponding continuum theory. In Fig. 1 we plot the $p\cot\delta_0$ (dots), computed using the exact lattice energy eigenvalues and Lüscher's formula, which results from tuning the first N_O terms in the effective range expansion to zero. These results show an expected η scaling represented by the dashed lines in the figure. A systematic improvement is also seen for the energies of excited states above the lowest N_O tuned states, where the correction may be predicted by [7],

$$L\left(\frac{\eta_k}{\eta_k^*} - 1\right) \propto L^{2-2n}. \tag{2.3}$$

Here η_k are the kth eigenvalues of the two-body transfer matrix with N_O terms tuned, while η_k^* are the kth solutions of Lüscher's formula in the unitary limit, respectively. As an example, we plot $L(\eta_k/\eta_k^* - 1)$ with respect to L (dots) in Fig. 2 and find good agreement with Eq. 2.3.

In simulations of trapped unitary fermions, the external harmonic potential, $U = \frac{1}{2}\kappa\mathbf{x}^2$ with spring constant κ, has been implemented in the transfer matrix as

$$\begin{aligned} T_{trapped} &= e^{-b_\tau \mathbf{p}^2/4M} e^{-b_\tau U}(1 - b_\tau V) e^{-b_\tau U} e^{-b_\tau \mathbf{p}^2/4M} \\ &= e^{-b_\tau(\mathscr{H}+U)+O(b_\tau^3)}, \end{aligned} \tag{2.4}$$

where V represents the interaction and $\mathscr{H}+U$ is the target Hamiltonian for trapped unitary fermions. As seen in this formula, temporal discrerization errors appear at $O(b_\tau^2)$.[2]

[2]Throughout this paper, b_s and b_τ represent the spatial and temporal lattice spacings, respectively.

3. Measurement, overlap problem, and cumulant expansion method

The N-body correlators are constructed by taking determinants of the Slater matrix, where each element is obtained by evolving an initial state (source) at $\tau = 0$ with a single particle propagator and projecting onto a final state (sink) at $\tau = T$. The choice of sources and sinks for untrapped and trapped unitary fermions, which gives superior wave function overlap by imposing two-particle correlations at the sinks, has been described in [4] and [5], respectively.

One of the greatest difficulties in extending our study to large N was the apparent upward drift of the effective mass plot at large Euclidean time. By investigating the distribution of N-body correlators, we found that this difficulty arises from a heavily long-tailed distribution, requiring an exponentially large number of samples before the central limit theorem becomes applicable. In other words, the path-integral probability measure has small overlap with the dominant part of the operator being estimated. On the other hand, the distribution of the log of correlators is nearly Gaussian, implying that the standard estimation of the lower moments should succeed with moderately sized ensembles. A general relation between the expectation value of $\mathscr{C}$ and that of $\ln\mathscr{C}$ is given by [6]

$$\ln\langle\mathscr{C}(\tau)\rangle = \sum_{n=1}^{\infty} \frac{\kappa_n}{n!}, \tag{3.1}$$

where κ_k is the kth cumulant of $\ln\mathscr{C}$. The generalized effective mass and the ground state energy associated with each partial sum in Eq. 3.1 may be written as [7]

$$m_{\rm eff}^{N_k}(\tau) = -\frac{1}{\Delta\tau}\sum_{n=1}^{N_k}\frac{1}{n!}\left[\kappa_n(\tau+\Delta\tau)-\kappa_n(\tau)\right] \quad \text{and} \quad E_{N_k} = \lim_{\tau\to\infty} m_{\rm eff}^{N_k}(\tau). \tag{3.2}$$

Since the statistical uncertainties typically increase as N_k increases, one may determine the ideal value N_k^* for which the statistical uncertainties and truncation errors are comparable.

4. Ground state energy of unitary fermions

To extract the energies of the system, we perform standard bootstrap resamplings and correlated χ^2 fits to the plateau region of the generalized effective mass. Fitting systematic errors are obtained by varing the end points of the fitting interval. The quoted errors represent the combination of the statistical and fitting systematic errors added in quadrature.

4.1 Untrapped unitary fermions

As a nontrivial test of our lattice method, we have computed the lowest energy of three unitary fermions in a zero total momentum state with high precision. We performed the calculation for lattice sizes $L = 8, 10, 12, 14, 16$, tuning the coefficients of four O_{2n} operators for the $L = 8$ lattice, and five for the other lattices. Since the single particle and two particle s-wave sectors have been highly tuned, the leading L dependence will be L^{-3} due to the untuned two-derivative two-body p-wave operator. In Fig. 3 we plot the lowest energies versus L^{-3}. We perform two parameter fits of the $L \geq 10$ data to $c_1 + c_2/L^3$ and find an infinite volume energy of $0.3735^{+0.0014}_{-0.0007}$ in units of

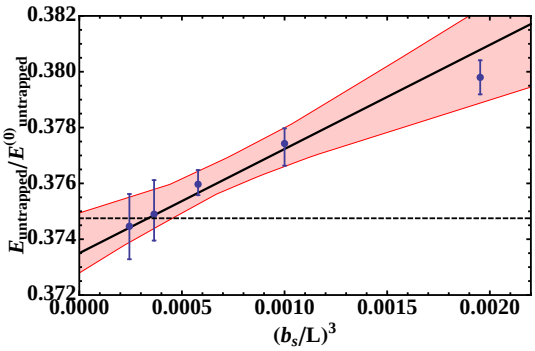

Figure 3: Energy of three untrapped unitary fermions in a zero total momentum eigenstate plotted versus $(b_s/L)^3$ for $L/b_s = 8, 10, 12, 14, 16$. The red band represents the uncertainty in two-parameter fits of the $L/b_s \geq 10$ data to the function $c_1 + c_2/L^3$. while the black line is the fit to the central values. The dashed line is the result from Ref. [8].

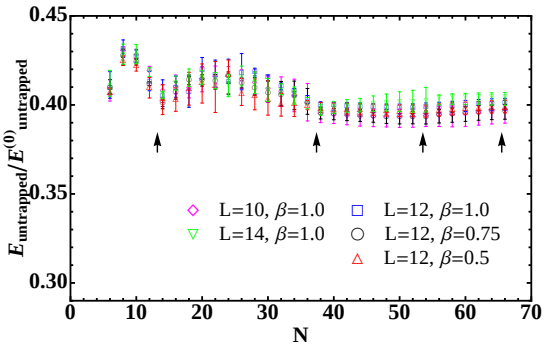

Figure 4: (Preliminary) Plot of ground state energies versus numbers of untrapped unitary fermions for $L = 10, 12$ and 14. For $L = 12$ we considered three different sinks, $\beta = 0.5, 0.75, 1.0$, to take into account any source dependence in our extraction of the energies. The arrows indicate the positions for which noninteracting fermions have fully occupied a given momentum shell.

the energy of three noninteracting fermions, which agrees with the high precision calculation by Pricoupenko and Castin [8] within our $\sim 0.3\%$ uncertainty.

The preliminary results for the ground state energies of up to 66 unpolarized unitary fermions in a periodic box are shown in Fig. 4. With the given statistics, we do not resolve any shell structure in the energy for $N \geq 38$ and believe that the system is close to the thermodynamic limit. By averaging the results obtained from a constant fit of $\xi(N)$ for $N \geq 38$ using five different ensembles, we find a preliminary result for the Bertsch parameter, $\xi = 0.399 \pm 0.002$. The unitary Fermi gas has been extensively studied using the Quantum Monte Carlo (QMC) technique and the most recent calculation reported is $\xi \leq 0.383(3)$ [9, 10]. Recent experimental results for this parameter are $\xi = 0.39(2)$ [11] and $0.41(1)$ [12].

4.2 Trapped unitary fermions

In numerical simulations of the trapped unitary Fermi gas, we have additional time scale $1/\omega$ and length scale $L_0 = (M\omega)^{-1/2}$ which should be chosen so that $b_s \ll L_0 \ll L$ and $b_\tau \ll 1/\omega$ in order to minimize the discretization and finite volume errors. To balance the need for small temporal discretization errors with the computational cost associated with the number of time steps required to reach the ground state, we have chosen $\omega b_\tau = 0.005$. An ideal L_0 has been determined by scanning the parameter space of L_0/b_s and L/L_0 and finding the region where both finite volume and spatial discretization errors are small. Fig. 5 presents our findings for the ground state energies of $N \leq 6$ fermions, with L_0/b_s ranging from 3 to 8 and fixed $L/b_s = 48$. For $L_0/b_s \leq 7$ we find that the systematic errors increase as L_0 decreases, which indicates that the discretization error is not negligible. For $L_0/b_s \geq 7$ we have also performed simulations with $L/b_s = 64$, which showed no volume dependence; and thus we conclude that both types of systematic errors are negligible. For $6 < N \leq 70$, based on the results of the L_0 scan for $N \leq 6$, we have chosen to perform the calculation for three volumes ($L = 48, 54, 64$) and at two values of the trap size ($L_0 = 7.5, 8$). We

Table 1: Results for $E_{\text{trapped}}/\omega$ for $N \leq 6$, including combined statistical and fitting systematic errors (first row). For comparison we give the exact $N = 3$ result [13] and results of Ref. [14] (second and third rows).

	3	4	5	6
this work	$4.243^{+0.037}_{-0.034}$	$5.071^{+0.032}_{-0.075}$	$7.511^{+0.051}_{-0.091}$	$8.339^{+0.080}_{-0.066}$
exact, Ref. [13]	4.2727	-	-	-
from Ref. [14]	4.273(2)	5.008(1)	7.458(10)	8.358(20)

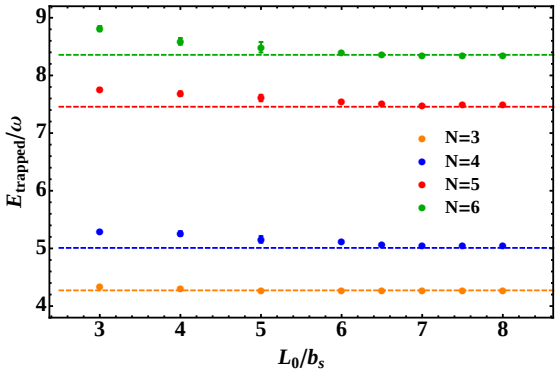

Figure 5: Ground-state energies (in units of ω) as a function of L_0/b_s at fixed $L/b_s = 48$ for various values of N. Dashed lines are results from Ref. [14].

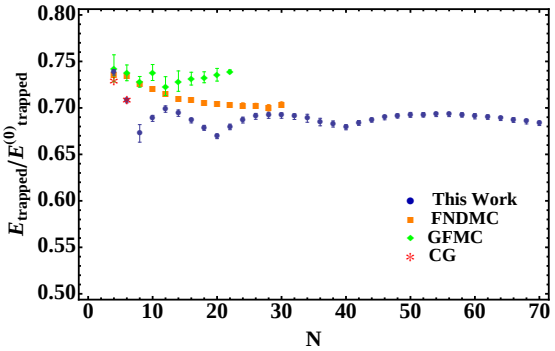

Figure 6: Ground-state energies of N-trapped unitary fermions.

find non-negligible volume dependence and perform an infinite volume extrapolation for each L_0. All of these considerations are included along with statistical, fitting systematic, and truncation of the cumulant expansion errors in the final quoted errors of ground state energies.

We first benchmark our method for up to $N = 6$ against high-precision solutions to the many-body Schrödinger equation [14], achieving agreement at 1% as shown in Tab. 1. In Fig. 6 we plot the results of the ground state energies for $N \leq 70$ along with the results from two fixed-node calculations for comparison: a Green's function Monte Carlo (GFMC) approach [15] and a diffusion Monte Carlo (FN-DMC) approach [16], which provide upper bounds on the ground state energies. We find that our energies are consistently lower than those obtained using both of these methods. However, our results show clear shell structure which indicates that $N \sim 70$ is insufficient to reach the thermodynamic limit.

5. Conclusion

A new statistical technique, called the cumulant expansion method, allows us to extend our studies up to $N \sim 70$ unitary fermions both with and without an external harmonic trap. We report a preliminary value of $\xi = 0.399 \pm 0.002$ from the calculation of the ground state energy for $N \geq 38$ untrapped unitary fermions. For $N \leq 70$ trapped fermions, we find that the shell structure is pronounced, which implies that we have not reached the thermodynamic limit, but our values of the ground state energies are consistently lower than those obtained from variational QMC calculations. In order to check the validity of our lattice method, we have performed high-precision

calculations for $N = 3$ untrapped fermions and $N \leq 6$ trapped fermions, and found good agreement with the results in [8] and [13, 14], respectively.

In the near future, we will present results for the pairing gap by calculating the ground state energies of the slightly unpolarized unitary Fermi gas ($N_\downarrow = N_\uparrow + 1$) and the integrated contact density by studying the dependence of the ground state energies on the s-wave scattering length near the unitary regime. Our lattice method combined with the new statistical technique is applicable for a wide range of nonrelativistic many-body systems.

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