Lattice QCD at non-zero isospin chemical potential

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Abstract. Systems of non-zero isospin chemical potential are studied from a canonical approach by computing correlation functions with the quantum numbers of $N \pi^+$'s ($C_{N\pi}$). In order to reduce the number of contractions required in calculating $C_{N\pi}$ for a large $N$ in the Wick's theorem, we constructed a few new algorithms. With these new algorithms, systems with isospin charge up to 72 are investigated on three anisotropic gauge ensembles with a pion mass of 390 MeV, and with lattice spatial extents $L \sim 2.0, 2.5, 3.0$ fm. The largest isospin density of $\rho_I \approx 9$ fm$^{-3}$ is achieved in the smallest volume, and the QCD phase diagram is investigated at a fixed low temperature at varying isospin chemical potentials, $m_\pi \leq \mu_I \leq 4.5$ $m_\pi$. By investigating the behaviour of the extracted energy density of the system at different isospin chemical potentials, we numerically identified the conjectured transition to a Bose-Einstein condensation state at $\mu_I \geq m_\pi$.

1. Introduction

An important goal of nuclear physics is to investigate interactions between hadrons; however studying many body systems are hampered by the factorially growing number of Wick contractions naively required in computing the corresponding correlation function. In order to study multi-meson systems, a few algorithms [1, 2] have been constructed to alleviate the cost of computing larger number of independent contractions. With these new algorithms, many-pion systems have been studied in Ref. [2, 3, 4], and many-kaon systems have been studied in Ref. [5], furthermore systems of mixed species have also been studied in Ref. [6]. In order to study more complicated multi-baryon systems, various methods have also been introduced. With methods constructed in [7], correlation functions of $^{28}$Si have been computed within a manageable amount of time.

Knowledge of systems at high density, with non-zero chemical potential, and non-zero temperature are vital to explore the QCD phase diagram. Systems with zero chemical potential have been investigated for a wide range of temperatures, and the transition from confined state at low temperature to the de-confined state at high temperature has been investigated substantially [8]. However, direct simulations of non-zero chemical potential systems are much harder due to the famous sign problem resulting from the non positive fermion determinants. But the sign problem does not exist for isospin chemical potential systems. Although QCD phase diagrams of these two systems are not the same, they do share some common properties, and it is also theoretical interesting to study non-zero isospin chemical potential systems.

In this proceeding, systems of non-zero isospin chemical potential are studied from a canonical approach by directly computing correlation functions of $n\pi^+$ systems. By applying algorithms constructed in [2], we studied systems containing up to 72 $\pi^+$'s on three anisotropic 2+1 flavor.
dynamical gauge ensembles, $16^3 \times 128$, $20^3 \times 256$ and $24^3 \times 128$, with $\xi = a_s/a_t = 3.5$, $a_s = 0.125$ fm, and with a pion mass of $m_\pi = 390$ MeV and a kaon mass of $m_K = 540$ MeV. The QCD phase diagram at a fixed low temperature, $T \sim 20$ MeV, for a range of isospin chemical potentials, $m_\pi \leq \mu_I < 4.5 \, m_\pi$, are investigated, and evidence for a phase transition from pion gasses to Bose-Einstein Condensate (BEC) state around $\mu_I = 1.3m_\pi$ is numerically identified.

The layout of this proceeding is as follows. In Sec.2, we briefly discuss the method applied to study $n$-$\pi$ systems. Main results from the simulation are presented in Sec.3, and we conclude in Sec.4.

2. Methodology
Non-zero isospin chemical systems can be investigated from the study of $n$-$\pi$ systems by directly computing their correlation functions. Because of the Pauli principle, the largest number of pions can be studied from a single source location is $N_s N_c = 12$. In order to study systems of more than 12 $\pi$'s, additional source locations are required. The correlation function for a system of total $\pi = \sum_{i=1}^{N} n_i \, \pi^+ \,$'s with $n_i \, \pi^+$'s from source locations $(y_i,0)$ is defined as:

$$
C_{n_1,...,n_N}(t) \equiv \left\langle \left( \sum_x \pi^+(x,t) \right)^{n_1} \left( \pi^-(y_1,0) \right)^{n_1} \cdots \left( \pi^-(y_N,0) \right)^{n_N} \right\rangle , \tag{1}
$$

where the interpolating operator $\pi^+(x,t) = \overline{d}(x,t)\gamma_5 u(x,t)$ and $\pi^-(x,t) = \overline{u}(x,t)\gamma_5 d(x,t)$.

Computing the above correlation function includes $O(\pi^n)$ contractions. For larger $\pi$ and $N$, number of ways to distribute pions over $N$ sources grows exponentially, which further increase the computational cost of all $C_{n_1,...,n_N}$'s. However, correlation functions of $\pi$ pions, $C_\pi$, without knowing details of the distributions of $n_i$ can be constructed, which significantly reduces the number of correlation functions to compute as energies extracted from $C_\pi$ is same as those extracted from $C_{n_1,...,n_N}$'s as long as $\pi = \sum_{i=1}^{N} n_i$. The explicit methods constructed in Ref.[2] are used to calculate $C_\pi$ in this proceeding. Detailed discussions of the method and evaluations of $n$-$\pi$ correlation functions in momentum space can be found in Ref.[2].

3. Lattice Results
Computations are performed on ensembles of $n_f = 2 + 1$ anisotropic gauge configurations with clover-improved fermions generated by the Hadron Spectrum Collaboration and the Nuclear physics with Lattice QCD collaboration. Pion correlations function, $C_{\pi\pi}(t)$, for $n = 1, 2, \ldots, 72$, are computed from three lattice ensembles of $L^3 \times T = 16^3 \times 128, 20^3 \times 256, 24^3 \times 128$. More details of these gauge ensembles can be found in Ref.[9].

The expected form of $C_{\pi\pi}(t)$ computed on a lattice with temporal extent $T$ is [6]

$$
C_{\pi\pi}(t) \equiv \sum_{m=0}^{\lfloor T/2 \rfloor} \binom{n}{m} A_m^n Z_m^n e^{-(E_{n-m}+E_m)T/2} \cosh((E_{n-m} - E_m)(t - T/2)) + \ldots , \tag{2}
$$

where $A_m^n = 1$ when $m = n/2$, otherwise $A_m^n = 2$. $E_m$ is the ground state energy of a $m$-$\pi$ system, the $Z_m^n$ are overlap factors of thermal states with $m \, \pi$'s propagating backward around the temporal boundary 1, and the ellipsis denotes contributions from excited states. For finite $T$, all thermal states vanish, and only the ground state survives, however the ground state is always contaminated by thermal states for finite $T$. Even for $C_{12\pi}$ computed on $T = 128$ ensembles, the ground state does not dominate in any region. Under the current precision, $C_{n\pi}$ computed from ensembles with a temporal extent $T = 256$ shows a clear plateau region even for $n = 72$. Thus, in order to reduce thermal contaminations, the anti-periodic plus periodic

1 When $m = 0$, $Z_0^n$ denotes the ground state contribution.
Figure 1. On the left plot, ground state energies of $n$-$\pi (E_{n\pi})$ systems extracted from ensembles $16^3 \times 128$ (red), $24^3 \times 128$ (blue) and $20^3 \times 256$ (green) are shown. The black line represents the free energy of $n$ non-interacting pions. Energy densities, $\epsilon(\rho_I)$, computed from three ensemble are compared on the right plot.

propagation ($A \pm P$) method [2] has been applied to effectively double the temporal extent of $T = 128$ ensembles.

3.1. Ground state energies
Ground state energies of $n$-$\pi$ systems are extracted by fitting a single exponential to $C_{n\pi}(t)$ within time slices where a clear plateau can be identified in the corresponding effective mass plot. Statistical uncertainties are evaluated from the bootstrap method, and systematic uncertainties are from averaging systematic uncertainties computed on each bootstrap sample by moving the fitting window forward and backward two time slices. Extracted ground state energies from three volumes are shown in the left plot of Fig. 1, and the corresponding energy densities, $\epsilon(\rho_I)$, are compared in the right. Because of the repulsive interactions between pions, $E_{n\pi}$ is larger in smaller volumes as pions are closer to each other, however energy densities computed from three volumes are approximately the same.

3.2. Isospin chemical potential
From the ground state energies of $n$-$\pi$ systems ($E_{n\pi}$), an effective isospin chemical potential $\mu_I(n) = \frac{dE}{dn}$ can be computed from a finite backward derivative, $\mu_I(n) = E_{n\pi} - E_{(n-1)\pi}$. In order to take into account the correlation between $E_{n\pi}$ and $E_{(n-1)\pi}$ extracted from the same bootstrap sample, $\mu_I(n)$ is also evaluated on each bootstrap sample. The extracted isospin chemical potential as a function of isospin density is plotted in Fig. 2.

At small isospin density, $\mu_I$ grows in an accelerating rate, agreeing with the prediction from $\chi$-PT [10], however it starts to deviate from the $\chi$-PT and begins to grow in a decelerating rate at large isospin densities, and at even larger isospin density it begins to flatten out.

3.3. QCD phase diagram
The change of the behavior of the isospin chemical potential at different isospin density signals a possible change of the physical state of the $n$-$\pi$ system. In order to investigate this change, we
Figure 2. The isospin chemical potential, $\mu_I$, is plotted as a function of the isospin density, $\rho_I$, from three lattice ensembles, $16^3 \times 128$ (red, $\rho_I = [0, 9]$), $20^3 \times 256$ (green, $\rho_I = [0, 4.7]$) and $24^3 \times 128$ (Blue, $\rho_I = [0, 2.8]$). The solid black line is from $\chi$-PT [10].

have studied the ratio of the energy density, $\epsilon$, to its zero temperature Stefan-Boltzmann limit,

$$\epsilon_{SB} = \frac{N_f N_c}{4\pi^2} \mu_I^4,$$

where $N_f = 3$ and $N_c = 3$ is used in this formula. The ratio is plotted in Fig. 3, where it grows at small $\mu_I$, reaches a peak around 1.3 $m_\pi$, starts to decrease after the peak, and begins to flatten out at large isospin chemical potential. With a linear extrapolation of the peak position for different volumes as a function of the inverse of volume, the peak position in the infinite volume limit is $\mu_I^{\text{peak}} = 1.30(7) \, m_\pi$.

At low temperature, as soon as $\mu_I$ reaches $m_\pi$, one pion is produced out of vacuum, and the system is an interacting pion gas. When $\mu_I$ reaches the peak at $\mu_I = 1.30(7) \, m_\pi$, pions start to condense and the $n$-$\pi$ system becomes Bose-Einstein Condenstate (BEC). Such a transition to BEC state at $\mu_I > m_\pi$ are also observed in two flavor QCD [11], and similar behavior occurs in two-color QCD [12].

4. Conclusion
In this proceeding, we studied $n$-$\pi$ systems from a canonical approach by explicitly computing correlation function of the $n$-$\pi$ system, $C_n(t)$. Ground state energies of the $n$-$\pi$ systems were extracted, and subsequently, the isospin chemical potential was computed as a function of the isospin density.
Figure 3. The $\epsilon/\epsilon_{SB}$ is plotted as a function of $\mu_I/m_\pi$.

By studying the ratio of the isospin energy density to its zero temperature Stefan-Bolzeman limit, the QCD phase diagram is investigated at a fixed low temperature, $T = 20$ MeV for a range of isospin chemical potentials, from $\mu_I = m_{\pi}$ to $\mu_I = 4.5 m_{\pi}$. An evidence of transition from a pion gas to BEC is identified at $\mu_I = 1.30(7) m_{\pi}$.

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