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Spectroscopy from canonical partition functions

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A spectroscopical method for staggered fermions based on thermodynamical considerations is proposed. The canonical partition functions corresponding to the different quark number sectors are expressed in the low temperature limit as polynomials of the eigenvalues of the reduced fermion matrix. Taking the zero temperature limit yields the masses of the lowest states. The method is successfully applied to the Goldstone pion and both dynamical and quenched results are presented showing good agreement with that of standard spectroscopy. Though in principle the method can be used to obtain the baryon and dibaryon masses, due to their high computational costs such calculations are practically unreachable.

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1. Introduction

One of the most critical steps in hadron spectroscopy is the choice of the wave function for the searched particle. Without finding the proper interpolating operator contamination from other particle states can often occur. Therefore, a spectroscopical method where the knowledge of the wave function is not required would be desirable. The question was first addressed by P. E. Gibbs. He found a formula that gives the Goldstone pion mass configuration by configuration using the eigenvalues of the fermion propagator matrix [1].

There has been many advances lately in the canonical approach to finite density QCD [2, 3, 4]. Using the canonical partition functions we give a method which, in principle, can be used to obtain the masses of different particles.

2. Canonical partition functions on the lattice

Let $\hat{H}$ be the Hamiltonian of a QCD-like system with n_s different flavors. Let $\hat{N}_i$ and μ_i denote the quark number operator and the quark number chemical potential corresponding to the ith quark field, respectively. Then the grand canonical partition function at a given set of chemical potential values $(\mu_1, \mu_2, \ldots, \mu_{n_s})$ and temperature T is given by

$$Z(\mu_1, \mu_2, \ldots, \mu_{n_s}, T) = \mathrm{Tr}\left[e^{-(\hat{H}-\mu_1\hat{N}_1-\mu_2\hat{N}_2-\ldots-\mu_{n_s}\hat{N}_{n_s})/T}\right]. \tag{2.1}$$

The canonical partition function corresponding to a given set of quark number values $N_1, \ldots, N_{n_s}$ can be obtained by taking the trace only over the subspace $\hat{N}_1 = N_1, \ldots, \hat{N}_{n_s} = N_{n_s}$.

$$Z_{N_1,\ldots,N_{n_s}}(T) = \mathrm{Tr}\left[e^{-\hat{H}/T} \cdot \delta_{\hat{N}_1,N_1} \ldots \delta_{\hat{N}_{n_s},N_{n_s}}\right] \tag{2.2}$$

When one introduces imaginary chemical potentials [5], the different canonical partition functions become the coefficients in the Fourier expansion of the grand canonical partition function.

$$Z_{N_1,\ldots,N_{n_s}}(T) = \frac{1}{(2\pi T)^{n_s}} \int_0^{2\pi T} \mathrm{d}\mu_1 \ldots \int_0^{2\pi T} \mathrm{d}\mu_{n_s}\, e^{-i\mu_1 N_1/T} \cdots e^{-i\mu_{n_s} N_{n_s}/T}\, Z(i\mu_1, \ldots, i\mu_{n_s}, T) \tag{2.3}$$

$$Z(i\mu_1, \ldots, i\mu_{n_s}, T) = \sum_{N_1=-\infty}^{\infty} \cdots \sum_{N_{n_s}=-\infty}^{\infty} Z_{N_1,\ldots,N_{n_s}}(T)\, e^{i\mu_1 N_1/T} \ldots e^{i\mu_{n_s} N_{n_s}/T} \tag{2.4}$$

The canonical partition function can be written as

$$Z_{N_1,\ldots,N_{n_s}}(T) = \sum_{k=0}^{\infty} n_k^{(N_1,\ldots,N_{n_s})}\, e^{-E_k^{(N_1,\ldots,N_{n_s})}/T}, \tag{2.5}$$

where $E_k^{(N_1,\ldots,N_{n_s})}$ and $n_k^{(N_1,\ldots,N_{n_s})}$ are the energy and the multiplicity of the kth state in sector $(N_1, \ldots, N_{n_s})$, respectively. In sector $(0, \ldots, 0)$ the lowest state is the vacuum, which is assumed to be non-degenerate.

The mass of the lowest state in sector $(N_1, \ldots, N_{n_s})$ is the difference of the energy of the ground state in this sector and the energy of the vacuum state,

$$m_0^{(N_1,\ldots,N_{n_s})} = E_0^{(N_1,\ldots,N_{n_s})} - E_0^{(0,\ldots,0)}. \tag{2.6}$$

In order to obtain this mass one needs to consider the free energy of the given channel.

$$F_{N_1,\ldots,N_{n_s}}(T) = -T\ln Z_{N_1,\ldots,N_{n_s}}(T) \tag{2.7}$$

If the temperature is sufficiently low then the difference of the free energies of the channel we are looking for and the channel of the vacuum as a function of the temperature follows a linear behaviour,

$$F_{N_1,\ldots,N_{n_s}}(T) - F_{0,\ldots,0}(T) \approx m_0^{(N_1,\ldots,N_{n_s})} - T\ln n_0^{(N_1,\ldots,N_{n_s})}, \tag{2.8}$$

where the slope of the linear depends only on the multiplicity of the ground state. Therefore, the mass of the lightest particle carrying quantum numbers $(N_1,\ldots,N_{n_s})$ and its multiplicity can be obtained by a linear extrapolation to the $T = 0$ limit.

$$m_0^{(N_1,\ldots,N_{n_s})} = \lim_{T\to 0}\left[F_{N_1,\ldots,N_{n_s}}(T) - F_{0,\ldots,0}(T)\right] \tag{2.9}$$

The temperature on the lattice is given by $T = 1/aL_t$, where L_t is the number of sites in the temporal direction and a is the lattice spacing. Let $\hat{\mu}_i = \mu_i a$ denote the chemical potentials in lattice units. Then the grand canonical partition function using staggered lattice fermions can be written as the path integral over all lattice configrations

$$Z(i\hat{\mu}_1,\ldots,i\hat{\mu}_{n_s}) = \int [\mathrm{d}U]\, e^{-S_g[U]} \prod_{i=1}^{n_s} \det M(m_i, i\hat{\mu}_i, U)^{n_i/4}, \tag{2.10}$$

where m_i denotes the bare mass and n_i denotes the number of tastes of the ith staggered quark field. The ratios of the determinants can be treated as observables while the functional integral can be taken using the measure at $\hat{\mu}_i = 0$. Then the partition function becomes the expectation value of the determinant ratios taken over the ensemble generated at zero chemical potentials,

$$Z(i\hat{\mu}_1,\ldots,i\hat{\mu}_{n_s}) = Z\cdot\left\langle \prod_{i=1}^{n_s}\left(\frac{\det M(m_i, i\hat{\mu}_i, U)}{\det M(m_i, 0, U)}\right)^{n_i/4}\right\rangle_{\mu_i=0}, \tag{2.11}$$

where Z denotes the zero chemical potential value of the partition function [6]. Therefore, the canonical partition functions are obtained by taking the expectation values of the Fourier components of the determinant ratios.

$$Z_{N_1,\ldots,N_{n_s}} = Z\cdot\left\langle \prod_{i=1}^{n_s}\frac{L_t}{2\pi}\int_0^{\frac{2\pi}{L_t}} \mathrm{d}\hat{\mu}_i\, e^{-i\hat{\mu}_i N_i L_t}\left(\frac{\det M(m_i, i\hat{\mu}_i, U)}{\det M(m_i, 0, U)}\right)^{n_i/4}\right\rangle_{\mu_i=0} \tag{2.12}$$

In order to perform the assigned Fourier transformations, we need the analytic $\hat{\mu}$–dependence of $\det M(i\hat{\mu})$. In temporal gauge, the fermion matrix can be written as

$$M(i\hat{\mu}) = \begin{pmatrix} B_0 & e^{i\hat{\mu}} & 0 & \ldots & 0 & Ue^{-i\hat{\mu}} \\ -e^{-i\hat{\mu}} & B_1 & e^{i\hat{\mu}} & \ldots & 0 & 0 \\ 0 & -e^{-i\hat{\mu}} & B_2 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & B_{L_t-2} & e^{i\hat{\mu}} \\ -U^\dagger e^{i\hat{\mu}} & 0 & 0 & \ldots & -e^{-i\hat{\mu}} & B_{L_t-1} \end{pmatrix}, \tag{2.13}$$

where U denotes the remaining time direction links on the last timeslice (including the correct staggered phases) and B_k is the spacelike staggered fermion matrix on timeslice k. In matrix (2.13) each block is a $3V \times 3V$ matrix, where $V = L_s^3$ and L_s is the spatial size of the lattice. After performing $L_t - 2$ steps of Gaussian elimination [7], the determinant of (2.13) can be written as

$$\det M(i\hat{\mu}) = e^{3VL_t i\hat{\mu}} \prod_{k=1}^{6V} \left(\lambda_k - e^{-i\hat{\mu}L_t}\right), \tag{2.14}$$

where λ_k denote the eigenvalues of the $6V \times 6V$ sized reduced fermion matrix

$$S = \begin{pmatrix} 0 & 1 \\ 1 & B_{L_t-1} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & B_{L_t-2} \end{pmatrix} \cdots \begin{pmatrix} 0 & 1 \\ 1 & B_0 \end{pmatrix} \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}. \tag{2.15}$$

The eigenvalues of matrix S have a symmetry, according to which whenever λ is an eigenvalue of S then $1/\lambda^*$ is also an eigenvalue of S [7]. Therefore, each eigenvalue whose absolute value is greater than 1 has a pair with an absolute value smaller than 1, and vice versa. Then the ratio of the determinants appearing in eq. (2.12) can be written as

$$\frac{\det M(i\hat{\mu})}{\det M(0)} = e^{3VL_t i\hat{\mu}} \prod_{k=1}^{3V} \frac{\lambda_k - e^{-i\hat{\mu}L_t}}{\lambda_k - 1} \, \frac{\frac{1}{\lambda_k^*} - e^{-i\hat{\mu}L_t}}{\frac{1}{\lambda_k^*} - 1} = \prod_{k=1}^{3V} \left| \frac{1 - \lambda_k e^{i\hat{\mu}L_t}}{1 - \lambda_k} \right|^2, \tag{2.16}$$

where the product is taken over only the eigenvalues lying inside the unit circle. From now on when the limits of a sum or product taken over the eigenvalues of S are from 1 to $3V$, then the sum or product is meant to be taken over only the "small" eigenvalues, that is, the eigenvalues with absolute value smaller than 1.

When the temperature is low ($T \ll T_c$) a gap appears between these "small" and the "large" eigenvalues of S. This makes a Taylor expansion of (2.16) in the small eigenvalues possible. As the temperature decreases the small eigenvalues become exponentially smaller, increasing the validity of the series expansion. After performing the Taylor expansion the canonical partition functions $Z_{N_1,\ldots,N_{n_s}}$ can be explicitly written as polynomials of a given order of the eigenvalues λ_k.

In the simplest case, when all the staggered fields have four tastes ($n_i = 4$), that is, there is no root taking, the leading order term for sector $(N_1, \ldots, N_{n_s})$ can be written as

$$Z_{N_1,\ldots,N_{n_s}} \overset{\text{LO}}{=} Z \cdot \left\langle \prod_{i=1}^{n_s} \left[(-1)^{|N_i|} \sum_{1 \le k_1^{(i)} < \cdots < k_{|N_i|}^{(i)} \le 3V} \left(\lambda_{k_1^{(i)}}^{(i)} \cdots \lambda_{k_{|N_i|}^{(i)}}^{(i)} \right)^{*(\operatorname{sgn} N_i)} \right] \right\rangle, \tag{2.17}$$

where $*(\operatorname{sgn} N_i)$ in the exponent means that there is a complex conjugation if N_i is negative and there is not if N_i is positive, and $\lambda_k^{(i)}$ stands for the kth eigenvalue of the reduced matrix $S^{(i)}$ obtained from the fermion matrix of the ith quark field. The more complicated but similar leading order term in case of arbitrary number of tastes n_i can be obtained in the same manner.

3. Application to baryons

If one would like to use this method to measure the mass of a baryon, for example the proton, then two staggered fields are needed. One for the u quark with n_u tastes and one for the d quark with n_d tastes. The proton is believed to be the lowest state in the $N_u = 2, N_d = 1$ channel, therefore, its mass is obtained as the zero temperature limit

$$am_p = \lim_{T\to 0} F_{N_u=2,N_d=1}(T) - F_{N_u=0,N_d=0}(T) = \lim_{T\to 0} -T \ln\left(\frac{Z_{2,1}(T)}{Z_{0,0}(T)}\right). \tag{3.1}$$

After performing the series expansion one arrives at the task of evaluating the expectation value

$$am_p = \lim_{L_t\to\infty} -\frac{1}{L_t}\ln\left\langle \frac{n_u n_d}{32}\left(\sum_{k=1}^{3V}\lambda_k^{(u)2}\right)\left(\sum_{k=1}^{3V}\lambda_k^{(d)}\right) - \frac{n_u^2 n_d}{128}\left(\sum_{k=1}^{3V}\lambda_k^{(u)}\right)^2\left(\sum_{k=1}^{3V}\lambda_k^{(d)}\right)\right\rangle. \tag{3.2}$$

The formulas for the masses of the 2-baryon, 3-baryon, etc. channels can be similarly obtained. These can in principle be used to measure the bonding energy of several-baryon states.

Unfortunately the expression inside the expectation value in equation (3.2) can be any complex number. Its real part can be both positive and negative, and on a typical gauge configuration it is many orders of magnitude larger than the expectation value itself. The problem becomes even more severe when one decreases the temperature in order to get closer to the $T \to 0$ limit. Therefore, in case of baryons the evaluation of these expectation values is beyond the reach of present day calculation capabilities.

4. Application to mesons

If $n_d = n_u = n_t/2$, $m_d = m_u$ and we are looking at one of the $N_d = -N_u$ sectors this sign problem does not arise. These sectors can be parametrized by one quantum number, the third component of the isospin $I_3 = (N_u - N_d)/2$. Since $\lambda_k^{(u)} = \lambda_k^{(d)}$ for all k, we will write λ_k only.

The lowest state in the $I_3 = 1$ sector is expected to be the Goldstone pion. Its partition function can be written as the expectation value

$$Z_{I_3=1} \overset{\text{LO}}{=} Z_{N_u=1,N_d=-1} \overset{\text{LO}}{=} Z \cdot \left\langle \frac{n_t^2}{64}\left|\sum_{k=1}^{3V}\lambda_k\right|^2\right\rangle, \tag{4.1}$$

which is a manifestly positive polynomial of the eigenvalues. Therefore, it can be easily evaluated, and by taking the zero temperature limit

$$am_{I_3=1,\pi} = \lim_{L_t\to\infty} -\frac{1}{L_t}\ln\left\langle \frac{n_t^2}{64}\left|\sum_{k=1}^{3V}\lambda_k\right|^2\right\rangle \tag{4.2}$$

one directly obtains the mass of the lowest state in the $I_3 = 1$ channel.

The Goldstone pion mass $am_{I_3=1,\pi}$ obtained by (4.2) using purely thermodynamic considerations can be compared to the mass $m_{\pi,\text{sp}}$ obtained on the same configurations using conventional spectroscopical methods.

Equation (4.2) can be rewritten as

$$am_{I_3=1,\pi} = \lim_{L_t\to\infty}\left[-\frac{1}{L_t}\ln\left(\frac{n_t^2}{64}\right) - \frac{1}{L_t}\ln\left\langle\left|\sum_{k=1}^{3V}\lambda_k\right|^2\right\rangle\right] = \lim_{L_t\to\infty} -\frac{1}{L_t}\ln\left\langle\left|\sum_{k=1}^{3V}\lambda_k\right|^2\right\rangle. \tag{4.3}$$

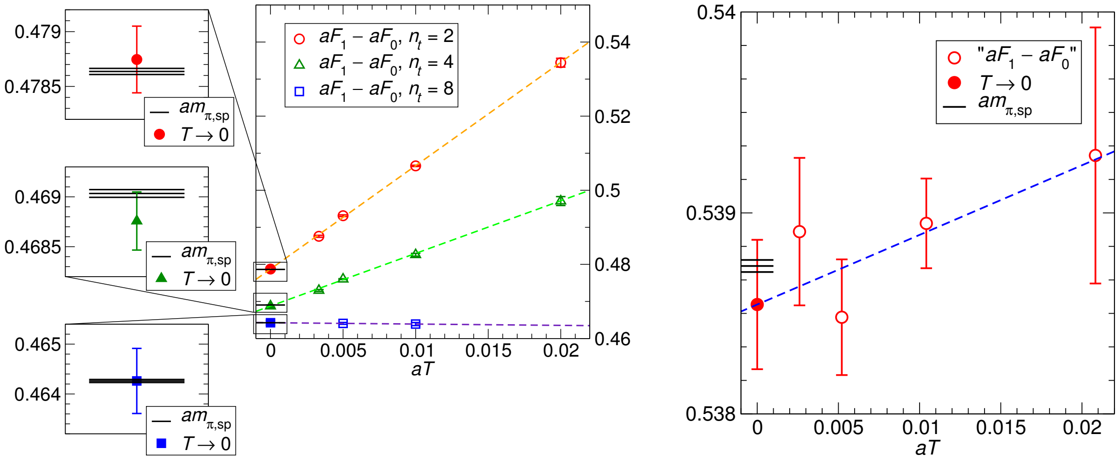

Figure 1: The differences of the free energies of the isospin one and isospin zero sectors as a function of the temperature on dynamical staggered (left panel) and quenched (right panel) configurations with a spatial volume of 6^3 and bare quark mass $am_q = 0.04$. The dashed lines show the linear fits to the data points. The $T \to 0$ extrapolated values are compared to the spectroscopical pion masses $m_{\pi,\mathrm{sp}}$.

One can see that the number of staggered tastes appears explicitly only as an additional term, which modifies only the slope of the linear, but not the $T \to 0$ limit. Therefore, the quantity

$$\text{“}aF_{I_3=1} - aF_{I_3=0}\text{”} = -\frac{1}{L_t} \ln \left\langle \left| \sum_{k=1}^{3V} \lambda_k \right|^2 \right\rangle , \tag{4.4}$$

whose zero temperature limit also yields the pion mass, can be evaluated on quenched configurations as well. The such obtained pion mass then can be compared to the pion mass obtained using quenched spectroscopy.

5. Results

We performed several calculations using dynamical staggered as well as quenched configurations to measure the Goldstone pion mass. For the dynamical simulations we used the Wilson plaquette action for the gauge fields and unimproved staggered fermion action. Calculations were done using rooted staggered fermions with $n_t = 2$ ($n_u = n_d = 1$) and $n_t = 4$ ($n_u = n_d = 2$) as well as unrooted fermions with $n_t = 8$ ($n_u = n_d = 4$). For the $n_t = 2$ runs the gauge coupling was $\beta = 4.8$. The lattice spacing was $a = 0.41$ fm, measured from the string tension σ using the value of $\sqrt{\sigma} = 465$ MeV [8]. For the $n_t = 4$ case $\beta = 4.3$ and $a = 0.42$ fm and for the $n_t = 8$ case $\beta = 3.8$ and $a = 0.44$ fm. In all three cases the bare quark mass was $am_q = 0.04$ and the spatial extension of the lattice was $L_s = 6$. In the two rooted case we used temporal lattice extensions of $L_t = 50, 100, 200, 300$ while in the unrooted case only $L_t = 100, 200$ was used.

The quenched calculations were performed using the Wilson plaquette gauge action. The spatial extension of the lattice was $L_s = 6$, the gauge coupling was $\beta = 5.6$ and the corresponding lattice spacing was $a = 0.21$ fm [8]. The time extension of the used lattices were $L_t = 48, 96, 192, 384$ and for the measurements we used a bare quark mass of $am_q = 0.04$.

The difference of the free energies $aF_{I_3=1} - aF_{I_3=0}$ was measured on each set of configurations. According to equation (2.8) the mass of the ground state in the $I_3 = 1$ channel can be obtained using a linear extrapolation to $T = 0$. For comparison we measured the pion mass in all cases using the ordinary spectroscopical method. The measured free energy values, the fitted linear and the comparision to the spectroscopical pion mass can be seen in Figure 1. The comparision shows that the mass of the ground state is in agreement with the spectroscopical pion mass.

6. Conclusion

We proposed a spectroscopical method based on completely thermodynamical considerations. In principle, using the method one can obtain the mass of the lightest particle in a given quark number sector without the knowledge of its wave function. The case of baryons is computationally very demanding, but we successfully applied our method to the Goldstone pion. Our results were in good agreement with the results obtained using conventional spectroscopy in both the dynamcal and staggered cases.

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