Analysis of unstable particle with the maximum entropy method in $O(4)\ \phi^4$ theory on the lattice

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Abstract

We explore applications of the maximum entropy method (MEM) to determine properties of unstable particles using the four-dimensional $O(4)\ \phi^4$ theory as a laboratory. The spectral function of the correlation function of the unstable $\sigma$ particle is calculated with MEM, and shown to yield reliable results for both the mass of $\sigma$ and the energy of the two-pion state. Calculations are also made for the case in which $\sigma$ is stable. Distinctive differences in the volume dependence of the $\sigma$ mass and two-pion energy for the stable and unstable cases are analyzed in terms of perturbation theory.

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In contrast to many successes in understanding of stable hadron states by numerical simulations, unstable hadrons and hadronic decay processes are not understood well on the lattice. An important example in QCD is $\rho \rightarrow \pi\pi$ decay. There are a number of difficulties in dealing with such decay processes. One of the difficulties is computer power. In full QCD lattice simulations accessible today, the pion is so heavy that the $\rho$ meson cannot decay. A more crucial problem is the difficulty first pointed out by Maiani and Testa [1]. Because the $\rho$ meson and the $\pi\pi$ state in the isospin $I = 1$ channel have the same quantum numbers, the correlation function of the $\rho$ meson behaves as a multi-exponential function corresponding to $\pi\pi$ states with various relative momenta as well as the $\rho$ meson. In general, it is very difficult to decompose the states and extract the energy of each state from such a correlation function.

In this article we explore application of the maximum entropy method (MEM) to extract the mass of unstable particle and the energies of states to which the unstable particle can decay. MEM has already been applied to extract the ground and first excited states of the stable mesons in QCD [2,3]. The masses of the two states were simultaneously extracted from the peak positions of the spectral function of the meson. This experience leads us to expect MEM to be useful for the multi-exponential correlation function of unstable particles such as the $\rho$ meson.

We employ the four-dimensional $O(4)$ $\phi^4$ theory for the present exploratory study. It is an effective theory of QCD, containing the pion and $\sigma$ particle. The $\sigma$ can be made either stable or unstable by choice of parameters. In the non-linear formulation with the constraint $\phi^\alpha(x)\phi^\alpha(x) = 1$, the action is given by

$$S = \sum_x \left\{ -\kappa \cdot \phi^\alpha(x) D\phi^\alpha(x) - J\phi^4(x) \right\},$$

where $\phi^\alpha(x) = (\pi^i(x), \sigma(x))$ for $i = 1, 2, 3$, and $D\phi(x) = \sum_\mu \phi(x + \hat{\mu}) + \phi(x - \hat{\mu})$. For $m_\sigma > 2m_\pi$, the $\sigma$ particle is unstable and can decay to the $I = 0$ two-pion state, similarly to the $\rho$ meson in QCD. We examine the efficiency of MEM for extracting the energies of $\sigma$ and $\pi\pi$ states for both the unstable $m_\sigma > 2m_\pi$ and stable $m_\sigma < 2m_\pi$ cases. Very recently a similar study for the three-dimensional four-fermion model has been carried out by Allton et al. [4].

Numerical simulations are carried out at $(\kappa, J) = (0.308, 0.0012)$ and $(0.30415, 0.003)$, corresponding to $m_\sigma/m_\pi \approx 3.7$ and $m_\sigma/m_\pi \approx 1.8$, for several spatial lattice sizes in the range $10^3 - 28^3$ to investigate the volume dependence of the spectral functions and energies. The temporal lattice size is fixed to $T = 64$. Configurations are generated by the multi-cluster algorithm [5]. The periodic boundary condition is imposed in all directions. We perform $0.6 \times 10^6 - 1.2 \times 10^6$ iterations per simulation point $(\kappa, J)$ and volume.

We calculate the correlation function matrix [5,6] given by $C_{ij}(\tau) = \langle (O_i(\tau) - O_i(\tau + 1))O_j(0) \rangle$ for $i, j = \sigma$ and $\pi\pi$, where $O_i$ is the interpolating operator either for the $\sigma$ or the $I = 0$ two-pion state with zero momentum, and the subtraction $O_i(\tau) - O_i(\tau + 1)$ is made for eliminating the vacuum contribution. We apply MEM to the diagonal parts of the correlation function matrix $C_{ii}(\tau)$.

In Fig. 1 we illustrate the correlation functions in the $\sigma$ and $\pi\pi$ channels for two volumes in the unstable case. The errors are estimated by the jackknife method with the bin size of 8000 to 16000 iterations. For the smaller volume the $\pi\pi$ correlation function exhibits a
change of slope at \( t \approx 10 \), from a larger slope corresponding to \( \sigma \) to a smaller one of the \( \pi \pi \) state. The \( \sigma \) correlator decays parallel to the latter, indicating dominance of the \( \pi \pi \) state for small volumes. For the larger volume, the trend is opposite, the \( \pi \pi \) correlation function showing a change of slope from the \( \sigma \) particle to \( \pi \pi \) state at \( t \approx 20 \), while the \( \pi \pi \) correlator is dominated by the \( \pi \pi \) state. The decrease of “off-diagonal” contributions with increasing volume in the correlation functions can be understood from a perturbative analysis: the overlaps \(|\langle 0|\sigma|\pi\pi\rangle|^2\) and \(|\langle 0|\pi\pi|\sigma\rangle|^2\) are proportional to \( 1/[L^3(m_\sigma - E_{\pi\pi})^2] \) where \( E_{\pi\pi} \) is the two-pion energy.

The spectral function \( f(\omega) \) in the \( \sigma \) and \( \pi \pi \) channels is defined in terms of the correlation function \( C_{ii}(\tau) \) \((i = \sigma, \pi\pi)\) through

\[
L^3 C_{ii}(\tau) = \int d\omega f_i(\omega) K(\omega, \tau),
\]

where \( K(\omega, \tau) = e^{-\tau \omega}(1 - e^{-\omega}) + e^{-(\tau - T)\omega}(1 - e^{-\omega}) \). In our MEM analysis the model function \( m(\omega) \) is chosen as \( m(\omega) = A(\omega_0) \cdot \omega^4 \), where \( \omega_0 \) is a reference point and \( A(\omega_0) \) is the perturbative \( \sigma \) spectral function at a reference point \( \omega_0 \), which is given by

\[
A(\omega_0) = \frac{M_I(\omega_0)}{\pi[(\omega_0^2 - \tilde{m}_\sigma^2 + M_R(\omega_0))^2 + M_I^2(\omega_0)]}/Z_\sigma.
\]

The functions \( M_R(\omega_0) \) and \( M_I(\omega_0) \) are defined by

\[
M_R(\omega_0) = C[\gamma_\sigma(\omega_0) - \gamma_\sigma(\tilde{m}_\sigma) + 3\gamma_\sigma(\omega_0)],
\]

\[
M_I(\omega_0) = C[\beta_\pi(\omega_0) + 3\beta_\sigma(\omega_0)],
\]

where \( \gamma_\alpha(\omega_0) = \beta_\alpha(\omega_0) \ln[(1 + \beta_\alpha(\omega_0))/(1 - \beta_\alpha(\omega_0))] \) and \( \beta_\alpha(\omega_0) = \sqrt{1 - (4\tilde{m}_\alpha^2/\omega_0^2) \theta(\omega_0 - 2\tilde{m}_\alpha)} \) for \( \alpha = \sigma \) and \( \pi \). The constant \( C \) in Eqs. (4) and (5) is given by \( C = 3Z_\sigma(\tilde{m}_\pi^2 - \tilde{m}_\sigma^2)^2/32\pi^2v^2 \), where \( v = (\sigma) \), and \( Z_\alpha \) \((\alpha = \sigma, \pi)\) is the wave function renormalization factor for \( \sigma \) and \( \pi \), respectively. We apply the same model function to the \( \sigma \) and \( \pi \pi \) correlation functions.

We choose \( \omega_0 = 2 \), and \( \tilde{m}_\alpha \) and \( Z_\alpha \) in Eq.(3) are fixed to the values estimated from inverse correlation functions in momentum space. The input parameters for the model function are compiled in Table I. The reconstruction is carried out in the region \( 0 \leq \omega \leq 3 \). We choose \( \Delta \omega = 5 \times 10^{-4} \) around the peaks corresponding to the \( \sigma \) and \( \pi \pi \) states to determine the energies accurately, and \( \Delta \omega = 10^{-2} \) in other regions. The number of data is taken as large as possible \( 0 \leq \tau \leq T/2 \). We also check that the final results for the spectral functions do not depend much on the model function.

In Fig. 2 we show the spectral functions for the \( \sigma \) and \( \pi \pi \) correlation functions, \( f_\sigma(\omega) \) and \( f_{\pi\pi}(\omega) \), in the unstable case. Since energy eigenvalues are discrete on a finite volume, the spectral function is a sum of \( \delta \) functions. We indeed observe sharp peaks for both spectral functions, which can be identified as the \( \pi \pi \) state with zero momentum at the first peak and the \( \sigma \) state at the second peak. The decrease of the peak height for the \( \pi \pi \) state in \( f_\sigma(\omega) \) and for the \( \sigma \) state in \( f_{\pi\pi}(\omega) \) agrees with the volume dependence of the correlation functions discussed above. In the figure for \( f_\sigma(\omega) \) the position of peak expected for the \( \pi \pi \) state with momentum \( p = 2\pi/L \) is indicated by a downward arrow. The absence of peak in our data implies that the overlap of \( \sigma \) with this state is very small.
Fig. 3 shows the spectral functions in the stable case. For $f_{\pi\pi}(\omega)$ the $\sigma$ contribution decreases with volume similar to the unstable case. We observe only a single peak in $f_\sigma(\omega)$, indicating that $|\langle 0|\sigma|\pi\pi\rangle|^2$ is very small in this case.

The $\sigma$ mass $m_\sigma$ and the $\pi\pi$ state energy $E_{\pi\pi}$ obtained from the peak positions of the spectral functions as functions of spatial lattice size $L$ are shown in Fig. 4 (unstable case) and 5 (stable case) by circles. For larger volumes $m_\sigma$ from $f_{\pi\pi}(\omega)$ and $E_{\pi\pi}$ from $f_\sigma(\omega)$ suffer from large errors or are not available. This is because the overlaps $|\langle 0|\sigma|\pi\pi\rangle|^2$ and $|\langle 0|\pi|\sigma\rangle|^2$ decrease as the volume increases.

We have seen in Figs. 2 and 3 that the $\sigma$ and $\pi\pi$ correlation functions are dominated by the $\sigma$ and $\pi\pi$ states with zero momentum, and other states are negligible. In this case we can apply the diagonalization method [6] to the $2 \times 2$ correlation function matrix $C(\tau)$ for extraction of the energy eigenvalues of these states. We diagonalize the matrix $D(\tau, \tau_0) = C^{-1/2}(\tau_0) C(\tau) C^{-1/2}(\tau_0)$ at each $\tau$, where $\tau_0$ is some reference time chosen to be $\tau_0 = 0$ in this work. The eigenvalue of $D(\tau, \tau_0)$ is given by $\lambda_\nu(\tau, \tau_0) = K(W_\nu, \tau)/K(W_\nu, \tau_0)$ with $K(W_\nu, \tau) = e^{-iW_\nu(1 - e^{-W_\nu}) + e^{W_\nu(\tau - T)}(1 - e^{W_\nu})}$, where $W_\nu$ is the energy of the states $\nu = \sigma, \pi\pi$.

The energies obtained by the diagonalization method are plotted by cross symbols in Figs. 4 and 5. The errors are estimated by the jackknife method with 8000 to 16000 eliminations. The results for $m_\sigma$ and $E_{\pi\pi}$ are consistent with those with MEM, but the statistical error with the diagonalization method is much smaller. This is because the diagonalization makes full use of the $2 \times 2$ correlation function matrix while MEM utilizes on the diagonal element.

For the application of the diagonalization method, it is essential that the dominant states in the correlation functions are known. Otherwise we need to consider the correlation function matrix of all possible states with the same quantum numbers, which is a difficult task. MEM is useful for identifying the dominant states, as exemplified with our example.

Comparing Fig. 4 with Fig. 5 we find an essential difference in the volume dependence of the $\sigma$ mass and $\pi\pi$ energy between the unstable and stable cases. In the unstable case, the $\pi\pi$ energy increases and the $\sigma$ mass decreases as the volume increasing, while an opposite trend is seen in the stable case.

The volume dependence of the $\sigma$ mass expected from perturbation theory is given by

$$m_\sigma(L, m_\sigma, g_R) = m_\sigma + g_R(\Delta m_\sigma(L) - \Delta m_\sigma(\infty)).$$

Here $m_\sigma$ is the $\sigma$ mass for infinite volume, $g_R$ is the renormalized coupling constant, and

$$\Delta m_\sigma(L) = \frac{1}{4m_\sigma L^3} \sum_\vec{p} \sum_{\alpha = \pi, \sigma} \left[ \frac{D}{W_\alpha(p)} + A_\alpha C_\alpha(p) \right],$$

with $A_\alpha = 2, 6$ for $\alpha = \pi, \sigma$, $D = 1 - 3(m_\sigma^2 - m_\pi^2)/m_\pi^2$, and

$$C_\alpha(p) = \frac{m_\sigma^2 - m_\pi^2}{W_\alpha(p)(m_\sigma^2 - W_\alpha^2(p))},$$

where $W_\alpha(p) = 2\sqrt{m_\alpha^2 + 4\sum_{i=1}^{3} \sin^2(p_i/2)}$ with $p_i$ being the spatial momenta.

We fit our results for the $\sigma$ mass obtained by the diagonalization method to Eq.(6), taking $m_\sigma$ and $g_R$ as fit parameters and setting $m_\pi$ to the value obtained from the pion
correlation function at \( L = 28 \). The fit curves are plotted in Fig. 4 and Fig. 5 for each case, where the data at \( L = 10 \) are excluded from the fitting. The fit parameters and \( \chi^2 \) are compiled in Table II. The fits agrees quite well with the simulation results. We then realize that the different volume dependence between the unstable and stable cases originates from an opposite sign of \( C_\pi(p) \) in Eq.(7) in the two cases.

In order to understand the volume dependence of the \( \pi\pi \) energy, we consider the scattering length \( a_0 \). It is related to the energy shift of the two-pion state through L"uscher's formula [7] given by

\[
E_{\pi\pi} - 2m_\pi = -\frac{4\pi a_0}{m_\pi L^3} \left( 1 + c_1 \frac{a_0}{L} + c_2 \frac{a_0^2}{L^2} \right),
\]

where \( c_1 = -2.837297, \ c_2 = 6.375183 \). The results for \( a_0 \) obtained from \( E_{\pi\pi} \) calculated with the diagonalization method are tabulated in Table III in the column entitled “Simu. diago.”. Here \( m_\pi \) is fixed to the value at \( L = 28 \). The sign of \( a_0 \) differ in the two cases, which reflects the difference in the volume dependence of \( E_{\pi\pi} \).

We can estimate the scattering length in perturbation theory. From results for the perturbative phase shift [5] we obtain

\[
a_0 = \frac{g_R m_\pi}{96\pi m_\sigma^2} \left( 7R^2 + 8 \right) \frac{1}{R^2 - 4},
\]

where \( R = m_\sigma/m_\pi \). To evaluate the right handside, we use the fit result for \( m_\sigma \) given in Table II. The coupling constant \( g_R \) is obtained in two ways, either from the perturbative definition [5,8] denoted as \( g_R(\text{def.}) = 3Z_\pi (m_\pi^2 - m_\sigma^2)/v^2 \) or from the fit of the volume dependence of the \( \sigma \) mass given in Table II denoted as \( g_R(\text{fit}) \). For \( m_\pi, Z_\pi \) and \( v \) we use the results at \( L = 28 \) as before.

In Table III the simulation results for \( a_0 \) are compared with the two estimates using the perturbative formula Eq. (10). While we cannot claim a precise agreement, we observe consistency in the value and sign obtained with simulation and perturbation theory for both the unstable and stable cases. Thus it is the factor of \( R^2 - 4 \) in the perturbative formula which leads to the the opposite volume dependence of the \( \pi\pi \) energy in the two cases found by the simulation.

In this paper, we have investigated the efficiency of the maximum entropy method for study of unstable particle systems using the four-dimensional \( O(4) \phi^4 \) theory. We have demonstrated that the \( \sigma \) mass and \( \pi\pi \) energy can be obtained from the \( \sigma \) correlation function alone. We have also explained that the difference in the volume dependences of the \( \sigma \) mass and \( \pi\pi \) energy between the unstable and stable cases can be understood by perturbation theory. It is an advantage of MEM that only the single particle correlation function of the unstable particle is needed to analyze both the particle itself and the multi-particle decaying states. Furthermore it works even when the dominant states in the correlation functions are not known. We expect the MEM analysis to play a useful role in future studies of unstable particles and decays in lattice QCD.

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TABLES

|   | unstable case |stable case |
|---|---|---|
|L  | $\tilde{m}_\pi$  | $Z_\pi$| $\tilde{m}_\sigma$ | $Z_\sigma$ | $v$ |
|10 | 0.1138(2)     | 0.961(1) | 0.309(2) | 0.956(1) | 0.112921(7) |
|12 | 0.1084(2)     | 0.9657(8)| 0.337(2) | 0.949(1) | 0.127042(4) |
|14 | 0.1053(2)     | 0.9667(6)| 0.351(1) | 0.944(1) | 0.13351169(4) |
|16 | 0.1041(3)     | 0.9674(6)| 0.359(1) | 0.938(1) | 0.136818(1) |
|18 | 0.1036(2)     | 0.9676(6)| 0.362(1) | 0.935(1) | 0.138598(1) |
|24 | 0.1024(2)     | 0.9678(8)| 0.365(1) | 0.928(1) | 0.140646(2) |
|28 | 0.1024(2)     | 0.9685(7)| 0.365(1) | 0.925(2) | 0.1410983(6) |
|24 | 0.1024(2)     | 0.9685(7)| 0.365(1) | 0.925(2) | 0.1410983(6) |
|28 | 0.1024(2)     | 0.9685(7)| 0.365(1) | 0.925(2) | 0.1410983(6) |

TABLE I. The input parameters for the model function of the MEM in the unstable and stable cases.

|   | unstable | stable |
|---|---|---|
| $m_\sigma$ | 0.3765(2) | 0.3285(1) |
| $g_R$ | 14(1) | 9(1) |
| $\chi^2$/d.o.f. | 0.23 | 2.5 |

TABLE II. Fit parameters and $\chi^2$/d.o.f. (degrees of freedom) of the volume dependence of the $\sigma$ mass.

|   | unstable | stable |
|---|---|---|
| $a_0$ | 0.289(9) | $-2.49(19)$ |
| Pert. $g_R$(def.) | 0.494(1) | 19.1(2) | $-3.62(11)$ | 17.8(1) |
| Pert. $g_R$(fit) | 0.361(3) | 14(1) | $-1.98(23)$ | 9(1) |

TABLE III. Scattering lengths for the the simulation (Simu.) and perturbative (Pert.) results.
FIG. 1. Correlation functions for the $\sigma$ and $\pi\pi$ in the unstable case.

FIG. 2. Spectral functions reconstructed from $\sigma$ (left line) and $\pi\pi$ (right line) correlation functions in the unstable case.
FIG. 3. Spectral functions reconstructed from $\sigma$ (left line) and $\pi\pi$ (right line) correlation functions in the stable case.

FIG. 4. Energies for $\sigma$ and $\pi\pi$ with the MEM and diagonalization in the unstable case.

FIG. 5. Energies for $\sigma$ and $\pi\pi$ with the MEM and diagonalization in the stable case.