Monte Carlo Calculation of Phase Shift in Four Dimensional $O(4) \phi^4$ Theory

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Abstract

The phase shift of the $O(4)$ symmetric $\phi^4$ theory in the symmetric phase is calculated numerically using the relation between phase shift and energy levels of two-particle states recently derived by Lüscher. The results agree with the prediction of perturbation theory. A practical difficulty of the method for a reliable extraction of the phase shift for large momenta due to the necessity of a precise determination of excited two-particle energy levels is pointed out.

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Monte Carlo simulation techniques enable us to study various non-perturbative phenomena of field theories defined on a space-time lattice. Because of the Euclidean formalism of lattice field theories, however, the method does not allow a direct evaluation of physical quantities characterizing scattering processes such as phase shift.

It has been known for some time\[1, 2, 3\] that finite-size effects in energy levels are closely related to scattering amplitudes. Indeed, asymptotic behavior of energy levels of two-particle states for large volume can be written in terms of scattering length \[4\] (see Refs. \[4, 5, 6, 7\] for its applications). Recently this asymptotic formula has been generalized to an exact relation between energy levels of two-particle states in a finite box and phase shift \[5\]. Since two-particle energy levels are calculable through standard Monte Carlo techniques, this relation opened a possibility of extracting phase shift through numerical simulations. Of particular interest is that the relation may allow a determination of resonance parameters in QCD\[9\].

The corresponding relation in two dimension has been used to numerically extract the phase shift of the O(3) non-linear σ model\[10\] and a coupled Ising system\[11\] and a good agreement has been found between the numerical results and analytic predictions. These results encourage us to examine the practical applicability of the method for realistic field theories in four dimensions. In this article we report on our attempt to extract the phase shift of the four-dimensional O(4) symmetric \(\phi^4\) theory in the symmetric phase. This model provides a good testing ground of the method since the triviality of the theory, which is confirmed in many ways\[12\] though no exact proof exists, enables us to check the results against perturbative calculations.

Consider a system of two identical particles in a cubic box of a size \(L^3\), whose states are classified by the irreducible representations of the cubic group SO(3,\(\mathbb{Z}\)). Let \(W_j\) (\(j = 0, 1, 2, \ldots\); \(W_0 < W_1 < \cdots\)) be the energy levels of the two-particle states in an irreducible representation of SO(3,\(\mathbb{Z}\)). Let \(m\) be the mass of the particle and define the momentum \(k_j\) corresponding to \(W_j\) by

\[
W_j = 2\sqrt{m^2 + k_j^2}.
\]

(1)

Lüscher’s formula\[8\] relates \(k_j\) to the set of phase shifts \(\delta_l(k_j)\) having the angular momentum \(l\) not excluded by the symmetry of the two-particle state. For the states in the \(A_1^+\) representation the relevant phase shifts are \(\delta_0, \delta_4,\)
At low energies the s-wave phase shift $\delta_0$ dominates. Neglecting the phase shifts $\delta_l$ with $l \geq 4$ the formula takes the form

$$- \delta_0(k_j) = \phi \left( \frac{k_j L}{2\pi} \right) - j\pi,$$

(2)

where $\phi(q)$ is given by

$$e^{-2i\phi(q)} = \frac{Z_{00}(1; q^2) + i\pi^{3/2}q}{Z_{00}(1; q^2) - i\pi^{3/2}q}, \quad \phi(0) = 0,$$

(3)

with $Z_{00}(1; q^2)$ defined by an analytic continuation of

$$Z_{00}(s; q^2) = \frac{1}{\sqrt{4\pi}} \sum_{n \in \mathbb{Z}^3} \frac{1}{(n^2 - q^2)^s}.$$

(4)

In a numerical simulation of a given size $L$, the formula (2) determines the phase shift only at a discrete set of momenta $k_0, k_1, \cdots$ corresponding to the energy levels $W_0, W_1, \cdots$. The momenta, however, can be shifted by using a different lattice size. Combining the results for various lattice sizes one can obtain the full momentum dependence of the phase shift.

We apply the method above to the $\phi^4$ theory in four dimensions with O(4) symmetry, employing the standard lattice action given by

$$S = -2\kappa \sum_{\alpha} \sum_{\mu=1}^{4} \phi_\mu^\alpha \phi_\mu^{\alpha*}, \quad \sum_{\alpha} \phi_\mu^\alpha \phi_\mu^{\alpha*} = 1.$$

(5)

The system undergoes a second-order phase transition at $\kappa = \kappa_c \equiv 0.30411(6)$, above which the O(4) symmetry is spontaneously broken. The simulations are made at $\kappa = 0.297$ in the symmetric phase on an $L^3 \times 16$ lattice with $L = 8$ and 12. We carried out $4 \times 10^6$ sweeps of the heat bath algorithm for each lattice size, measuring observables at every 10 sweeps.

We extract single-particle energies from the exponential decay of the propagator

$$\sum_{\alpha} \langle \phi_\mu^\alpha(t) \phi_\mu^{\alpha*}(0) \rangle \longrightarrow \text{const.} e^{-E(p)t}$$

(6)

with $\phi_\mu^\alpha(t)$ the projection of $\phi_n^\alpha$ to the spatial momentum $p$ at a time slice $t$. The exponential fits are made over the range $t = 3 - 6$ for the spatial size $L = 8$ and $t = 4 - 6$ for $L = 12$. The results for the momenta $p =$
\((0, 0, 0), (1, 0, 0), (1, 1, 0)\) and \((1, 1, 1)\) (in units of \(2\pi/L\)) are given in Table 1. The errors are estimated by the jackknife method with the bin size of \(10^6\) sweeps. Our values for the mass \(m = E(0)\) are consistent with those of Ref. [5] for the same choice of \(\kappa\) and \(L\).

The \(O(4)\)-scalar two-particle operator for a center-of-mass momentum \(\mathbf{p}\) is given by

\[
\mathcal{O}_p(t) = \sum_{\alpha} \sum_{R} \phi^\alpha_{R\mathbf{p}}(t) \phi^\alpha_{-R\mathbf{p}}(t)
\]

where the summation over cubic rotation \(R\) ensures the projection onto the \(A_1^+\)-sector. The corresponding two-point function is defined by

\[
G_{pp'}(t) = \langle \mathcal{O}_p(t) \mathcal{O}_{p'}(0) \rangle - \langle \mathcal{O}_p(t) \rangle \langle \mathcal{O}_{p'}(0) \rangle
\]

Inserting the complete set of states, one can rewrite the two-point function as

\[
G_{pp'}(t) = \sum_j v_j^p v_j^{p'} e^{-W_j t},
\]

with \(v_j^p\) the coupling of the state \(j\) to the two-particle operator \(\mathcal{O}_p\). The two-particle energy levels \(W_j\)'s can be extracted by diagonalizing \(G_{pp'}(t)\) as a matrix in \(p, p'\) at each time slice \(t\), and fitting the eigenvalues \(\lambda_j(t)\) to a single exponential\[10\]

\[
\lambda_j(t) \xrightarrow{t \to \infty} C_j e^{-W_j t}.
\]

In our calculation we truncate the momenta to the subset \(p = (0, 0, 0), (1, 0, 0), (1, 1, 0), (1, 1, 1)\). For the lowest state a \(\chi^2\) fit is made to the exponential form \([10]\) for \(t = 2 - 7\), while for higher states we used the range \(t = 2 - 4\) as errors in the eigenvalues become quite significant for larger values of \(t\). The results for the two-particle energies are given in Table 2 where we also list the values of the momentum \(k = \sqrt{(W/2)^2 - m^2}\) with \(m = E(0)\) taken from Table 1. The errors are estimated by the jackknife method with the bin size of \(10^6\) sweeps.

We have made a one-loop perturbative calculation of the phase shift to compare with numerical results. For the \(O(N)\)-symmetric \(\phi^4\) theory in the continuum defined by the Lagrangian

\[
\mathcal{L} = \frac{1}{2} \sum_{\alpha=1}^{N} \partial_{\mu} \phi^\alpha \partial^{\mu} \phi^\alpha - \frac{1}{2} m_R^2 \sum_{\alpha=1}^{N} \phi^\alpha \phi^\alpha - \frac{1}{4!} g_R \left( \sum_{\alpha=1}^{N} \phi^\alpha \phi^\alpha \right)^2 + (\text{counterterms}),
\]

\(\mathcal{L}\) is the action for the \(O(N)\)-symmetric \(\phi^4\) theory in the continuum defined by the Lagrangian
the two-particle scattering amplitude up to one-loop level, renormalized by
the momentum subtraction at $p = 0$, is given by

$$
T(k, k') = \frac{4\pi^2}{\omega_k^2} A \left[ \alpha_R + \frac{1}{2} \alpha_R^2 \left\{ A \varphi(s) + B(\varphi(t) + \varphi(u)) + O(\alpha_R^3) \right\} \right],
$$

where $s, t, u$ are the Mandelstam variables constructed from the initial and
final momentum $k$ and $k'$ in the center-of-mass frame, $k \equiv |k| = |k'|$, $\alpha_R = g_R/16\pi^2$, and $\omega_k \equiv \sqrt{k^2 + m_R^2}$. The coefficients take the values $A = (N+2)/3$ and $B = 1$ for the scalar channel ($A = 2/3$ and $B = (N + 6)/6$ for the tensor
channel), and the function $\varphi$ is defined by

$$
\varphi(z) = \int_0^1 dx \ln \left( 1 - \frac{z}{m_R^2} x(1-x) \right).
$$

The phase shifts $\delta_l(k)$ are defined through the partial-wave expansion of
$T(k, k')$

$$
T(k, k') = -\frac{8\pi}{\omega_k} \sum_{l=0}^{\infty} (2l + 1) P_l(\cos \theta) \frac{e^{2i\delta_l(k)}}{2ik},
$$

with $\theta$ the angle between $k$ and $k'$. The s-wave phase shift $\delta_0(k)$ is therefore
obtained as

$$
\delta_0(k) = -\frac{\pi}{2} \frac{k}{\omega_k} A \left[ \alpha_R + \alpha_R^2 \left\{ Af(k) + Bg(k) \right\} + O(\alpha_R^3) \right],
$$

where the functions $f(k)$ and $g(k)$ are given by

$$
f(k) = \frac{k}{\omega_k} \ln \left( \frac{\omega_k + k}{m_R} \right) - 1,
$$

$$
g(k) = \frac{1}{2} \int_0^\pi d\theta \sin \theta \left( \frac{\omega_k \sin \frac{\theta}{2}}{k \sin \frac{\theta}{2}} \ln \left( \frac{\omega_k \sin \frac{\theta}{2} + k \sin \frac{\theta}{2}}{m_R} \right) - 1 \right) + \frac{1}{2} \int_0^\pi d\theta \sin \theta \left( \frac{\omega_k \cos \frac{\theta}{2}}{k \cos \frac{\theta}{2}} \ln \left( \frac{\omega_k \cos \frac{\theta}{2} + k \cos \frac{\theta}{2}}{m_R} \right) - 1 \right).
$$

Lüscher’s formula (2) is derived in the continuum space-time and the
dispersion relation of the one-particle energy $E(p) = \sqrt{p^2 + m^2}$ enters into
the proof in an essential way. The simulation results for the one-particle
energy are compared with the continuum dispersion relation in fig.1. We
find a good agreement \( E(p)/\sqrt{p^2 + m^2} = 0.994(6) \) for the lowest momentum \( p = 2\pi/L \sim 0.5 \) for the lattice size \( L = 12 \). An increasing deviation for larger momenta indicates that finite lattice spacing effects become non-negligible for higher momenta.

In fig.2 we show by filled circles our results for the s-wave phase shift \( \delta_0(k) \) in the scalar channel extracted from the lowest two-particle state (see Table 2 for numerical values). The dotted lines show the function \( \phi(kL/2\pi) \) and the solid line represents the one-loop perturbative result \([15]\) calculated with the infinite volume estimates for the renormalized parameters \( m_R = 0.3044 \) and \( \alpha_R = 0.142 \) for \( \kappa = 0.297 \)[5]. We have also used the data of ref.[5] for the lowest two-particle energy to calculate the phase shift. The results are plotted by open circles in fig.2 and are consistent with our values. We observe a reasonable agreement between the results of simulations and that of one-loop perturbation theory. A trend may be present, however, that the numerical results become smaller than the perturbative prediction as the lattice size decreases. This may represent a systematic bias due to an increase of vacuum polarization effects for small lattice sizes, which are not taken into account in \([2]\).

As is seen from the figure, the phase shift is almost linear in the region of momenta which can be explored by the lowest two-particle states. These states therefore do not give information on the phase shift beyond the scattering length, which has already been calculated \([1\ 3]\) using the leading term of Lüscher’s formula in \( 1/L \) expansion derived earlier\[3\]. In order to extract the phase shift for large momenta we must therefore examine excited two-particle states. The rightmost point in fig.3 shows the phase shift extracted from the first excited state for \( \kappa = 0.297 \) and \( L = 12 \). The agreement with the perturbative prediction, albeit with a sizable error, is quite encouraging.

We note that fig.3 reveals an important point in practical applications of Lüscher’s formula. The function \( \phi(kL/2\pi) \) increases very rapidly for momenta corresponding to excited states (this is specific to four dimensions; in two dimensions \( \phi(kL/2\pi) = kL/2 \) and the slope is constant\[10\]). As a consequence, a reliable extraction of the phase shift for large momenta requires quite a precise determination of the momentum \( k = \sqrt{(W/2)^2 - m^2} \), and hence that of the two-particle energy \( W \). For example, reducing the error of the phase shift for the first excited state in fig.3 to a 10% level ne-
cessitates a calculation of the momentum within 0.5\% accuracy compared to the 2\% error of the present data. Achieving such an accuracy requires an order of magnitude more computer time (our run for the size $L = 12$ took 20 hours for $4 \times 10^6$ sweeps on HITAC S820/80 with the peak speed of 3 Gflops). The requirement becomes rapidly more demanding as we go to higher excited states. For instance, with the present statistics we only obtained $-\delta_0(k) = 0.4(9)$ for the second excited state.

To conclude, the method works well for momenta which can be explored by the lowest two-particle state. We find, however, that extraction of phase shifts for large momenta requires quite a high statistics determination of excited two-particle state energies due to the steep increase of the function $\phi(kL/2\pi)$. We feel that this presents an obstacle in practical applications of the method, with which one can in principle extract scattering data beyond scattering lengths in four dimensions.

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Table 1: Single-particle energy $E(p)$ in lattice unit for $\kappa = 0.297$ for $L = 8$ and 12.

| $p$  | $0$        | $1$        | $2$        | $3$        |
|------|------------|------------|------------|------------|
| $L = 8$ | 0.321(2)  | 0.819(7)   | 1.11(2)    | 1.24(4)    |
| $L = 12$ | 0.305(2)  | 0.602(3)   | 0.783(6)   | 0.91(1)    |

Table 2: Two-particle energy $W_j$, the corresponding momentum $k_j$ in lattice unit and the s-wave phase shift $-\delta_0(k_j)$ calculated through (2) for $\kappa = 0.297$ for the size $L = 8$ and 12. Values for the cases when errors are too large are omitted.

| $L$ | $j$     | 0        | 1        | 2        | 3        |
|-----|---------|----------|----------|----------|----------|
| 8   | $W_j$  | 0.73(2)  | 1.6(2)   | $-$      | $-$      |
|     | $k_j$  | 0.17(2)  | 0.74(11) | $-$      | $-$      |
|     | $-\delta_0(k_j)$ | 0.14(4) | $-$      | $-$      | $-$      |
| 12  | $W_j$  | 0.646(9) | 1.26(3)  | 1.66(9)  | 1.72(15) |
|     | $k_j$  | 0.106(6) | 0.552(11)| 0.77(7)  | 0.80(10) |
|     | $-\delta_0(k_j)$ | 0.12(2) | 0.40(15) | 0.4(9)   | $-$      |
Figure captions

Fig. 1 $E(p)/\sqrt{p^2 + m^2}$ as a function of $p = |p|$ for $L = 8$ (squares) and $L = 12$ (circles) at $\kappa = 0.297$ with $m = 0.321(2)$ for $L = 8$ and $m = 0.305(2)$ for $L = 12$ as input.

Fig. 2 S-wave phase shift calculated from the lowest two-particle state energy for $\kappa = 0.297$ with various lattice sizes $L$. Momentum $k$ is in lattice unit. Dashed lines represent the right hand side of (2) for each $L$. Solid line represents the one-loop result(15).

Fig. 3 S-wave phase shift calculated from the first excited two-particle state energy for $\kappa = 0.297$ and $L = 12$. Those from the lowest ones are also plotted.