Simulation of Scalar Field Theories with Complex Actions

Leandro Medina and Michael C. Ogilvie
Dept. of Physics, Washington University, St. Louis, MO 63130 USA

We develop a method for the simulation of scalar field theories with complex actions which is local, simple to implement and can be used in any number of space-time dimensions. For model systems satisfying the $P\bar{T}$ symmetry condition $L^*(\phi) = L(-\phi)$, the complex weight problem is reduced to a sign problem. The sign problem is eliminated completely for a large subclass of these models; this class includes models within the $i\phi^3$ universality class, and also models with nonzero chemical potential. Simulations of models from this subclass show a rich set of behaviors. Propagators may exhibit damped oscillations, indicating a clear violation of spectral positivity. Modulated phases occur in some models, exhibiting striping and other pattern-forming behaviors. These field theory models are connected to complex systems where pattern formation occurs because of competition between interactions at two different length scales.

The sign problem is a significant obstacle in theoretical physics. Computational methods for averaging over positive weights have been highly developed in lattice field theory and statistical physics, but averaging with real or complex weights has proven difficult. Two examples of sign problems in lattice field theory are associated with QCD with nonzero chemical potential.

where the sum is over all lattice sites $x$ and $\partial_\mu \chi = \chi(x+\hat{\mu}) - \chi(x)$. We take the potential $V$ to satisfy $V(-\chi) = V(\chi)^*$. Because of this condition, the Fourier transform $\tilde{w}(\tilde{\chi})$ of $w(\chi) \equiv \exp[-V(\chi)]$ with respect to $\chi$ is real. If $\tilde{w}(\tilde{\chi})$ is everywhere positive, we say that the dual positivity condition is satisfied and define a real function $\tilde{V}(\tilde{\chi}) = -\log(\tilde{w}(\tilde{\chi}))$. The partition function is

$$Z[h] = \int \prod_x d\chi(x) \exp \left[ -S(\chi(x)) + \sum_x i\hbar(x)\chi(x) \right]$$

where $h(x)$ is an arbitrary source. We rewrite $Z$ as

$$Z = \int \prod_x d\pi_\mu(x)d\bar{\chi}(x)d\chi(x) \exp \left\{ -\sum_x \left[ \frac{1}{2}\pi^2_\mu(x) + i\pi_\mu(x)\partial_\mu \chi(x) + \bar{V}(\bar{\chi}(x)) + i\chi(\bar{\chi}(x) + h(x)) \right]\right\}.$$
After a lattice integration by parts, the integral over $\phi$ yields

$$Z = \prod_x d\pi(x) \exp \left\{ -\sum_x \left[ \frac{1}{2} \pi^2(x) + \tilde{V}(\partial \cdot \pi(x) - h(x)) \right] \right\}. \quad (4)$$

This represents a dual form of the partition function for fields defined on the real line, similar to dual forms for models with fields defined on compact manifolds. In the more general case where the dual positivity condition does not hold, the same procedure reduces the problem of simulating a complex action to the simulation of a system with a true sign problem. The strategy for simulation of the model is now clear: one simulates the new action

$$\tilde{S}[\pi] = \sum_x \left[ \frac{1}{2} \pi^2(x) + \tilde{V}(\partial \cdot \pi(x)) \right]. \quad (5)$$

There is a clear extension to the case of more than one $\mathcal{PT}$-symmetric scalar field. Correlation functions of the original field $\chi$ may be obtained in the usual way by differentiation with respect to $h(x)$. In particular, non-coincident correlation functions of $\chi$ are obtained in the new representation using the field $i\tilde{V}^\prime(\partial \cdot \pi(x))$. Note that the expectation value of $\chi$ is either zero or purely imaginary.

The allowed forms of $V$ are constrained by Bochner’s theorem, which states that a function $\tilde{w}(k)$ on a locally compact Abelian group is positive if and only if $w(x)$ is positive-definite, that is, the matrix $w(x_j - x_k)$ has positive eigenvalues for any choice of the set $\{x_j\}$. This theorem is easily understood from the formula

$$\int dx \psi^*(x)w(x)\psi(x) = \int dk dq \tilde{\psi}^*(k)\tilde{w}(k-q)\tilde{\psi}(q). \quad (6)$$

The simplest of the constraints imposed by Bochner’s theorem is $V(x) + V(-x) > 2V(0)$. This constraint excludes the double-well potential and other potentials that lead to conventional spontaneous symmetry breaking at tree level. This is consistent with $\mathcal{PT}$ symmetry which requires $\langle \chi \rangle^* = -\langle \chi \rangle$, i.e., that $\langle \phi \rangle$ be purely imaginary. We do not view this limitation as fundamental, because this constraint does not appear in other duality-based treatments of complex actions [13].

It is simplest to take the form of the dual potential $\tilde{V}$ as given, and determine the parameters of $V$ from it. If one parametrizes $V$ as a polynomial in $\phi$, $V = \sum_n g_n \phi^n/n!$, then the coefficients $g_n$ are naturally obtained from the generating functional of the zero-dimensional dual theory defined by

$$g_n = \left. \frac{\partial^n V}{\partial \chi^n} \right|_{\chi = 0} = -(i)^n \langle \tilde{\chi}^n \rangle_c, \quad (7)$$
the cumulant of the dual variable $\tilde{\chi}$ averaged with weight $\tilde{w}(\tilde{\chi})$. The mass parameter of $V$ is given by $g_2 = \langle \chi^2 \rangle_c = \langle \tilde{\chi}^2 \rangle - \langle \tilde{\chi} \rangle^2$ and is therefore always positive. It follows that in the dual theory the case $g_2 = 0$ can only be obtained by a limiting process, and the region with $g_2 < 0$ is not directly accessible. Note that $g_2$ is the bare parameter, defined at the scale of a lattice spacing. For a generic dual potential $\tilde{V}$, the coupling $g_3$ is nonzero and imaginary, so critical behavior is naturally in the $i\phi^3$ universality class.

It is very interesting to consider the coupling of $\mathcal{PT}$-symmetric scalar fields to normal fields [14]. We write the action as

$$S(\phi) = \sum_x \left[ \frac{1}{2} (\partial_\mu \phi(x))^2 + \frac{1}{2} (\partial_\mu \chi(x))^2 + V(\phi(x), \chi(x)) \right]$$

where the potential obeys the condition $V(\phi(x), \chi(x))^\ast = V(\phi(x), -\chi(x))$. Following similar steps applied to $\chi$ as those given above, we arrive at a dual action of the form

$$\tilde{S} = \sum_x \left[ \frac{1}{2} (\partial_\mu \phi(x))^2 + \frac{1}{2} \pi_\mu^2(x) + \tilde{V}(\phi(x), \partial \cdot \pi(x) - h(x)) \right].$$

As in the case of a single field, expectation values involving $\chi$ can be obtained from $i\partial \tilde{V}'(\phi, \partial \cdot \pi) / \partial (\partial \cdot \pi)$. The case of a complex field with a nonzero chemical potential $\mu$ is similar, but the complex contribution to action arises in the kinetic term rather than in $V$, and requires a separate treatment.

In this class of models $\phi$ and $\chi$ play roles similar to the real and imaginary parts of the Polyakov loop, $P_R$ and $P_I$, in QCD at finite temperature $T$ and chemical potential $\mu$. The Polyakov loop $P = P_R + i P_I$ is associated with the free energy required to insert a very heavy quark into the system via $\langle P \rangle = \text{exp}(-F_Q/T)$; $\langle P^\ast \rangle$ is related to the free energy $F_Q$ for insertion of a heavy antiquark. When $\mu = 0$, $P_R$ develops a real expected value and $\langle P_I \rangle = 0$ such that $F_Q = F_{\tilde{Q}}$. When $\mu \neq 0$, QCD has a sign problem, and a variety of techniques show that $P_I$ acquires an imaginary expectation value [15][19]. This implies that $\langle P \rangle \neq \langle P^\ast \rangle$ and $F_Q \neq F_{\tilde{Q}}$. Both phenomenological models [17][18] as well as simplified lattice models of QCD at nonzero density [19] show that correlation functions may exhibit damped oscillatory behavior for some range of parameters.

As a demonstration of the technique and the variety of results which may be obtained, we consider three different models. In all three models, $S$ is quadratic in $\chi$ so that both $V$ and $\bar{V}$ are known analytically. Our first model is exactly solvable but displays nontrivial behavior. This imaginary-coupled quadratic (ICQ) model has a potential $V$ of the form $V(\phi, \chi) = m_\phi^2 \phi^2/2 + m_\chi^2 \chi^2/2 - ig_2 \phi \chi$. The eigenvalues of the mass matrix are given by $(m_\phi^2 + m_\chi^2 \pm \sqrt{(m_\phi^2 - m_\chi^2)^2 - 4g_2^2})/2$, so there are either two real masses or a complex conjugate pair, as required by the $\mathcal{PT}$ symmetry of the model. A quantum mechanical model of this form was considered in [14][20]. The dual potential takes the form $\tilde{V}(\phi, \partial \cdot \pi) = m_\phi^2 \phi^2/2 + (\partial \cdot \pi - g_2 \phi)^2/2m_\chi^2$. In figure 1, we show results for one-dimensional simulations of the ICQ model in the two different regions on a lattice of size $N = 256$: the difference in behavior
We show in figure 3, configuration snapshots of $\phi$ in the $d=2$ ICDW model on a $64^2$ lattice for several values of $g$. From left to right, top to bottom: $g = 0.9, 1.0, 1.1, 1.2, 1.3$ and $1.5$. The other parameters are $m_\chi^2 = 0.5, \lambda = 0.1$ and $v = 3$.

is striking between the upper curve where there are two real masses, and the lower curve where there is a complex conjugate mass pair. Similar results were obtained in two-dimensional simulations. The lines represent the analytical form of the continuum result for the propagators, and the error bars on the points are smaller than the points themselves. The nonmonotonicity of the lower curve makes the violation of spectral positivity obvious; in fact the lower curve is a damped sinusoid. The analytical result for the upper curve shows that it is the difference of two decaying exponentials, and therefore also violates spectral positivity. It is interesting to note that with the definition $\psi = (\partial \cdot \pi - g \phi)/m_\chi^2$, the equations of motion obtained from $S$ can be reduced to a set of real linear equations for $\phi$ and $\psi$. These equations may be derived from a Lagrangian of the form
\begin{equation}
\frac{1}{2} (\partial \phi)^2 + \frac{1}{2} m_\phi^2 \phi^2 - \frac{1}{2} (\partial \psi)^2 - \frac{1}{2} m_\psi^2 \psi^2 - g \phi \psi
\end{equation}
but this Lagrangian is not suitable for lattice simulation due to the negative quadratic terms.

A second interesting model is the imaginary coupling Yukawa (ICY) model, where the potential has the form $V(\phi, \chi) = m_\phi^2 \phi^2/2 + m_\chi^2 \chi^2/2 - ig \chi \phi^2$. This in turn leads to a dual potential $\tilde{V}(\phi, \partial \cdot \pi) = m_\phi^2 \phi^2/2 + (\partial \cdot \pi - g \phi^2)^2/2m_\chi^2$. We show in figure 4 the typical behavior of the propagator $\langle \phi(x)\phi(y) \rangle$ as a function of $|x - y|$ for the $d=2$ ICY model. An extensive search indicated no signs for a region of parameter space with complex conjugate mass pairs, but we were not able to rule out violations of spectral positivity of the type seen in the ICQ model when both masses are real. It seems possible that this is a model where masses are always real. This is consistent with the large-$m_\chi$ limit: After the rescaling $\pi \mu \to m_\chi \pi \mu$ and the definition $\lambda = g^2/m_\chi^2$ we can take the limit $m_\chi \to \infty$ to obtain a potential $\lambda \phi^4/2$. This is a bosonic form of a familiar argument for fermions: the $ig \chi \phi^2$ interaction is repulsive and in the large $m_\chi$ limit becomes a repulsive four-boson interaction [21].

Our third example also generalizes the first: we take $V(\phi, \chi) = U(\phi) + m_\phi^2 \chi^2/2 - ig \chi \phi$, leading to $\tilde{V}(\phi, \partial \cdot \pi) = U(\phi) + (\partial \cdot \pi - g \phi^2)^2/2m_\chi^2$. The potential $U$ can be chosen to give a first-order or second-order transition as a function of its parameters when $g = 0$. We will consider here the specific case of the imaginary-coupled double well (ICDW) model, where the potential has the form $U(\phi) = \lambda (\phi^2 - v^2)^2$. Because the field $\chi$ enters quadratically, it may be integrated out, yielding an effective action of the form
\begin{equation}
S = \sum_x \left[ \frac{1}{2} (\partial \chi \phi(x))^2 + U(\phi) \right] + \frac{g^2}{2} \sum_{x,y} \phi(x)\Delta(x - y)\phi(x)
\end{equation}
where $\Delta(x)$ is a free Euclidean propagator with mass $m_\chi$, i.e., a Yukawa potential. This additional term in the action acts to suppress spontaneous symmetry breaking. Models of this type have been used to model a wide variety of physical systems and are known to produce spatially modulated phases [22, 23]. In this class of models the complex form of the action intermediates between a real local form and a real quasi-local form.
Constant solutions which extremize $S$ can be found by minimizing $U(\phi) + g^2\phi^2/2m_\chi^2$. Linearizing the equation of motion around such a solution $\phi_0$, the inverse propagator is found to be
\[ p^2 + U''(\phi_0) + \frac{g^2}{p^2 + m_\chi^2} \]
which has a minimum away from zero when $g > m_\chi^2$, given by $p_{\min}^2 = g - m_\chi^2$. For this value of $p^2$, the inverse propagator has the value $2g - m_\chi^2 + U''(\phi_0)$. As long as this quantity is positive, the constant solution is stable to fluctuations at $p^2 = p_{\min}^2$. On the other hand, if the two conditions
\[ U''(\phi_0) + \frac{g^2}{m_\chi^2} > 0 \]
\[ 2g - m_\chi^2 + U''(\phi_0) < 0 \]
are simultaneously satisfied, then $\phi_0$ will be unstable to modulated behavior with wavenumber $p_{\min}$. For $U(\phi)$ a double well, this instability leads to a region where spatially modulated behavior occurs in lattice simulations of the dual form of the theory, as shown in the configuration snapshots for $d = 2$ in figure[3]. Light and dark portions represent positive and negative values of $\phi$, respectively. The length scale of the modulations decreases as $g$ increases and the system moves toward restoration of the broken symmetry. Similar behavior is seen for $d = 1$ and $d = 3$.

For scalar field theories with sign problems satisfying the dual positivity condition, the methods developed here enable straightforward simulation with a real local action. Relatively simple models show complicated behaviors that do not occur in conventional field theories, such as complex conjugate mass eigenstates and spatially modulated phases. These models and our simulation method provide a benchmark against which other simulation methods and analytical techniques can be tested. This method allows for simulation of models in the $i\phi^3$ universality class as well as field theories with a nonzero chemical potential; we plan to return to both these topics in subsequent publications.

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