Finite Density Condensation and Scattering Data: A Study in ϕ^4 Lattice Field Theory

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We study the quantum field theory of a charged ϕ^4 field in lattice regularization at finite density and low temperature in 2 and 4 dimensions with the goal of analyzing the connection of condensation phenomena to scattering data in a nonperturbative way. The sign problem of the theory at nonzero chemical potential μ is overcome by using a worldline representation for the Monte Carlo simulation. At low temperature we study the particle number as a function of μ and observe the steps for 1-, 2-, and 3-particle condensation. We determine the corresponding critical values μ_n^{crit} , $n = 1, 2, 3$ and analyze their dependence on the spatial extent L of the lattice. Linear combinations of the μ_n^{crit} give the interaction energies in the 2- and 3-particle sectors and their dependence on L is related to scattering data by Lüscher's formula and its generalizations to three particles. For two dimensions we determine the scattering phase shift and for four dimensions the scattering length. We cross-check our results with a determination of the mass and the 2- and 3-particle energies from conventional 2-, 4-, and 6-point correlators at zero chemical potential. The letter demonstrates that the physics of condensation at finite density and low temperature is closely related to scattering data of a quantum field theory.

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Introduction.—It is well known that phenomena in low energy physics can be described in terms of a few low energy parameters, which in the context of this Letter was, e.g., discussed in the seminal paper [1]. As a particular instance of this relation the condensation of particles at low temperature and nonzero chemical potential can be related to scattering data of the corresponding quantum field theory. More specifically one may show [2] that the critical values of the chemical potential where one observes condensation steps at low temperature and small volume are related to the finite volume many particle energies, which in turn are related to the scattering length [1].

For studying low energy properties, nonperturbative methods need to be applied, e.g., lattice simulations. However, for many finite density lattice field theories the action is complex. The Boltzmann factor has a complex phase and cannot be used as a probability in a lattice Monte Carlo study. This “sign problem” has recently been overcome for several theories by exactly mapping them to a worldline representation with only real and positive weights (see Refs. [3–7] for the model considered here).

In this Letter we study the complex ϕ^4 field at finite chemical potential using a worldline representation. We compute the particle number as a function of the chemical

potential at low temperature and determine the condensation steps for the 1-, 2-, and 3-particle sectors. Analyzing their volume dependence we show nonperturbatively that the condensation steps are indeed related to the scattering data of the theory.

Worldline representation.—The dynamical degrees of freedom of the charged ϕ^4 field are the complex valued fields ϕ_x assigned to the sites x of a d -dimensional lattice with periodic boundary conditions. Here we consider $d = 2$ and $d = 4$; i.e., we work on lattices with volumes $V = N_s \times N_t$ and $V = N_s^3 \times N_t$, where N_s is the spatial extent in lattice units. N_t is the extent in the Euclidean time direction (the d direction), which also equals the inverse temperature β in lattice units. The grand canonical partition sum is given by the path integral $Z = \int D[\phi] e^{-S[\phi]}$ with the product measure $\int D[\phi] = \prod_x \int_{\mathbb{C}} d\phi_x / 2\pi$. The lattice action is given by

$$S[\phi] = \sum_{x \in \Lambda} \left(\eta |\phi_x|^2 + \lambda |\phi_x|^4 - \sum_{\nu=1}^d [e^{\mu \delta_{\nu,d}} \phi_x^* \phi_{x+\hat{\nu}} + e^{-\mu \delta_{\nu,d}} \phi_{x+\hat{\nu}}^* \phi_x] \right). \quad (1)$$

The bare mass m_b enters via the parameter $\eta \equiv 2d + m_b^2$, λ denotes the coupling of the quartic self-interaction and μ is the chemical potential.

For nonzero μ the action (1) is complex and the model has a sign problem in the conventional formulation. The sign problem can be solved by exactly mapping the theory

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to a worldline representation where also at finite μ all weights are real and positive, such that a simulation is possible directly in terms of the worldlines [3–7]. In the worldline form the partition sum is given by

$$Z = \sum_{\{k\}} \left[\prod_x \delta(\vec{\nabla} \cdot \vec{k}_x) \right] e^{\mu \beta \omega[k]} B[k]. \quad (2)$$

The sum is over all configurations of the worldline variables $k_{x,\nu} \in \mathbb{Z}$ assigned to the links of the lattice. The worldline variables $k_{x,\nu}$ obey a zero divergence constraint, which we write as a product over all lattice sites and at each site x a Kronecker delta $\delta(j) \equiv \delta_{j,0}$ enforces vanishing divergence $\vec{\nabla} \cdot \vec{k}_x \equiv \sum_{\nu} (k_{x,\nu} - k_{x-\hat{\nu},\nu}) = 0$. Consequently, the worldline variables $k_{x,\nu}$ must form closed loops of conserved flux.

The chemical potential μ couples to the temporal winding number $\omega[k]$ of the conserved flux: By comparing the μ -dependent term in Eq. (2) to the standard form $e^{\mu \beta N}$ for the μ dependence of the grand canonical partition sum, we conclude that the net-particle number N is given by the temporal net winding number $\omega[k]$ of the worldlines. Finally each configuration comes with a weight factor

$$B[k] \equiv \sum_{\{a\}} \prod_{x,\nu} \frac{1}{(a_{x,\nu} + |k_{x,\nu}|)! a_{x,\nu}!} \prod_x I(s_x),$$

with $I(s_x) = \int_0^\infty dr r^{s_x+1} e^{-\eta r^2 - \lambda r^4}.$ (3)

The weight factor is itself a sum over configurations $\sum_{\{a\}}$ of auxiliary link variables $a_{x,\nu} \in \mathbb{N}_0$. The integrals $I(s_x)$ come from integrating out the radial degrees of freedom of the original field variables at site x . The argument s_x is a non-negative integer combination of the auxiliary variables and the moduli of all k fluxes that run through x , defined as $s_x = \sum_{\nu} [|k_{x,\nu}| + |k_{x-\hat{\nu},\nu}| + 2(a_{x,\nu} + a_{x-\hat{\nu},\nu})]$. For the numerical simulation the integrals $I(s_x)$ are precalculated and stored for sufficiently many values of the arguments $s_x \in \mathbb{N}_0$. In a Monte Carlo simulation of the worldline form the variables $k_{x,\nu}$ and the auxiliary variables $a_{x,\nu}$ need to be updated, such that the $k_{x,\nu}$ obey all constraints. We apply a strategy based on the worm algorithm [8] with the details discussed in Ref. [9].

For the 4D simulations we use lattices with $N_t = 320$ and 640, and N_s between 3 and 10 at coupling values of $\eta = 7.44$ and $\lambda = 1.0$. The statistics is 10^5 to 2×10^5 configurations. For two dimensions we use $N_t = 400$ and N_s between 2 and 16 with $\eta = 2.6$, $\lambda = 1.0$ and a statistics of 4×10^5 .

We conclude this section with an estimate of discretization effects for the 4D case. As we will see below, at the couplings we use the infinite volume mass m_∞ of the lowest excitation is $m_\infty \sim 0.168/a$, where a is the lattice constant.

For the momentum cutoff $p_c = \pi/a$ we thus find $p_{\text{cut}}/m_\infty = \pi/0.168 \sim 18.9$. The largest energy we use in our study is the 3-particle energy W_3 for $N_s = 4$, which at $W_3(4) \sim 0.93/a$ is less than 6 times m_∞ . We expect that with $p_c/W_3(4) = \pi/0.93 \sim 3.4$ cutoff effects are small. A similarly good ratio holds for our 2D study.

Condensation thresholds and multiparticle energies.— Using the worldline representation summarized in the previous section we now analyze the particle number N as a function of the chemical potential μ . We have already discussed that in the worldline representation the particle number N is represented by the temporal winding number $\omega[k]$ of the worldlines, and thus we study the expectation value $\langle N \rangle \equiv \langle \omega[k] \rangle$, where the vacuum expectation value on the right-hand side of this equation is evaluated in the worldline representation.

In Fig. 1 we show the expectation value of the particle number $\langle N \rangle$ as a function of the chemical potential μ for the 4D case with $N_s = 6$. We split the figure into 3 plots, choosing the ranges of μ such that we see the condensation thresholds for 1-, 2-, and 3-particle condensation, i.e., the values μ_n^{crit} , $n = 1, 2, 3$, where $\langle N \rangle$ quickly climbs from $\langle N \rangle = n - 1$ to $\langle N \rangle = n$. One observes that $\langle N \rangle$ has

FIG. 1. The expectation value of the particle number $\langle N \rangle$ as a function of μ for the 4D case with $N_s = 6$. We show the regions of 1- (top plot), 2- (middle), and 3-particle condensation (bottom). The Monte Carlo data (symbols) are fit with the logistic function (full curve).

shoulders at the integers 0,1,2,3 and shows a rapid increase in between. In the zero temperature limit, i.e., for $N_t \rightarrow \infty$ this turns into steps, which here at finite N_t are rounded due to temperature effects.

Near the transition from $\langle N \rangle = n - 1$ to $\langle N \rangle = n$ we fit the data with a logistic function shifted by a constant, $\langle N \rangle = [1 + \exp(-a_n[\mu - \mu_n^{\text{crit}}])]^{-1} + n - 1$. The plots show that this two-parameter (a_n and μ_n^{crit}) fit function describes the data very well and allows us to determine the critical values μ_n^{crit} , $n = 1, 2, 3$ of the chemical potential. As a cross-check we determined the critical values μ_n^{crit} also from the peaks of the particle number susceptibility and found excellent agreement of the two determinations.

In Ref. [2] it was pointed out, that the critical values μ_n^{crit} , $n = 1, 2, 3$ at low temperature are related to the 1-, 2-, and 3-particle energies at finite volume, i.e.,

$$\begin{aligned}\mu_1^{\text{crit}} &= m, \\ \mu_1^{\text{crit}} + \mu_2^{\text{crit}} &= W_2, \\ \mu_1^{\text{crit}} + \mu_2^{\text{crit}} + \mu_3^{\text{crit}} &= W_3,\end{aligned}\quad (4)$$

where m is the renormalized physical mass, W_2 the 2-particle energy, and W_3 the 3-particle energy.

When changing the spatial extent N_s of the lattice one observes a shift of the condensation steps μ_n^{crit} and thus of m , W_2 and W_3 . In Fig. 2 we show the N_s dependence of

FIG. 2. The physical mass m and the 2- and 3-particle energies W_2 and W_3 for the 4D case as a function of the spatial extent N_s . We compare the results from the n -particle energy thresholds (squares) to the results from a direct determination with correlators (diamonds). The fits to m and W_2 are shown as a solid red curve, and the prediction for W_3 based on these fits is shown as a dashed purple curve.

these three quantities (squares), which in the next section we will use to determine scattering data.

Before we come to the analysis of the finite volume effects and their connection to scattering data we present an important cross-check of our worldline results. The mass m , as well as W_2 and W_3 can also be computed from the exponential decay of Euclidean $2n$ -point functions in the conventional representation. More specifically, we consider the spatially Fourier transformed fields at zero momentum, $\tilde{\phi}_t = (N_s)^{-3} \sum_{\vec{x}} \phi_{\vec{x},t}$, and compute the connected $2n$ -point functions for $n = 1, 2, 3$:

$$\langle (\tilde{\phi}_t)^n (\tilde{\phi}_0^*)^n \rangle_c \propto A e^{-tE_n}, \quad (5)$$

where $E_1 = m$ and $E_n = W_n$ for $n = 2, 3$. From a fit to the correlators we determined the values for m , W_2 and W_3 , which in Fig. 2 are shown as diamonds. As a cross-check we determined m , W_2 and W_3 also using a full correlation matrix and got values agreeing very well with those from the $2n$ -point functions (5), which indicates that contributions of excited states are negligible.

Figure 2 shows that the values for m , W_2 and W_3 as determined from the condensation steps agree very well with the values from the $2n$ -point functions. This establishes that the condensation steps observed for the particle number are indeed determined by the corresponding n -particle energies via the relations (4). The same comparison was done also for the 2D case and again we found excellent agreement of the energies determined from the critical μ_n^{crit} and those from the $2n$ -point functions.

Volume dependence and scattering.—Having shown that the low temperature condensation steps are indeed governed by the n -particle energies we can now apply known finite volume relations to connect the condensation steps with scattering data.

We begin this analysis with the 2-d case following [10]. There the 2-particle energy W_2 is related to the relative momentum k of the particles via $W_2 = 2\sqrt{m^2 + k^2}$, and we can invert this equation to determine the momentum k for each value of W_2 . On our finite lattice with spatial extent N_s the momentum k is subject to the quantization condition $e^{2i\delta(k)} = e^{-ikN_s}$, where $\delta(k)$ is the phase shift for that momentum. Combining this relation with the relation between W_2 and k , we can extract the scattering phase shift $\delta(k)$ from W_2 . Varying N_s gives rise to different values of the relative momentum k such that $\delta(k)$ can be determined for a whole range of momenta.

In Fig. 3 we plot the results for $\delta(k)$ as a function of k and again compare the data determined from the n -particle energy thresholds ($m = \mu_1^{\text{crit}}$, $W_2 = \mu_1^{\text{crit}} + \mu_2^{\text{crit}}$) to the results obtained by determining m from 2-point functions and W_2 from 4-point functions. We find very good agreement of the two data sets and thus establish the relation of the condensation steps to the scattering phase shift for the 2D case.

FIG. 3. Scattering phase shift $\delta(k)$ for two dimensions as a function of the momentum k . We compare the results from the worldline calculation to the data from the conventional approach.

For the 4D case we use the finite volume relations for m [11], the result [1,12] for the 2-particle energy W_2 (using the notation of [13]) and the results [13–17] for the 3-particle energy W_3 :

$$m = m_\infty + \frac{A}{L^{\frac{3}{2}}} e^{-Lm_\infty}, \quad (6)$$

$$W_2 = 2m + \frac{4\pi a}{mL^3} \left[1 - \frac{a\mathcal{I}}{L\pi} + \left(\frac{a}{L}\right)^2 \frac{\mathcal{I}^2 - \mathcal{J}}{\pi^2} + \mathcal{O}\left(\frac{a}{L}\right)^3 \right], \quad (7)$$

$$W_3 = 3m + \frac{12\pi a}{mL^3} \left[1 - \frac{a\mathcal{I}}{L\pi} + \left(\frac{a}{L}\right)^2 \frac{\mathcal{I}^2 + \mathcal{J}}{\pi^2} + \mathcal{O}\left(\frac{a}{L}\right)^3 \right]. \quad (8)$$

Fit parameters are the infinite volume mass m_∞ , the amplitude A , and the scattering length a . The numerical constants $\mathcal{I}$ and $\mathcal{J}$ are given by $\mathcal{I} = -8.914$, $\mathcal{J} = 16.532$.

We identify $L \equiv N_s$ and fit the data for $m(N_s)$ as determined from μ_1^{crit} in the range between $N_s = 4$ and $N_s = 10$ with the functional form (6). This fit gives the amplitude parameter A and the infinite volume mass m_∞ in lattice units. Subsequently, we fit $W_2(N_s)$ determined from $\mu_1^{\text{crit}} + \mu_2^{\text{crit}}$ with the functional form (7), again in the range between $N_s = 4$ and $N_s = 10$. We use $m(N_s)$ from the previous step, such that this second fit is a one-parameter fit that gives the scattering length a in lattice units. From Fig. 2 it is obvious that the fits for $m(N_s)$ and $W_2(N_s)$ describe the data very well and indeed the reduced χ^2 is close to 1 for both fits.

For $W_3(N_s)$ no additional free parameter is needed such that we simply can compare our data to the curve for W_3 that we obtain from Eq. (8) using the fit parameters of the previous fits as input. In Fig. 2 we observe good agreement of this “predicted” W_3 with the data from the condensation

steps. Only for the smallest $L (\equiv N_s)$ we observe a deviation which shows that here higher order corrections in a/L start to play a role. However, it has to be remarked that cleanly determining the higher order power law corrections in W_2 and W_3 or exponential terms of the form $e^{-L/R}$, where R is the range for an interaction with an exponential tail, is a nontrivial numerical challenge. Such terms contribute significantly only for very small extent L and for a serious determination one should resolve small L with several data points, which in turn implies working with very fine lattices and very high statistics.

For completeness we quote our results for the two physical parameters, i.e., the mass m_∞ and the scattering length a . In lattice units we obtain $m_\infty = 0.168(1)$ and $a = -0.078(7)$ and a value of $am_\infty = -0.013(1)$ for their dimensionless product.

Discussion and concluding remarks.—In this Letter we determined the n -particle energy thresholds μ_n^{crit} , $n = 1, 2, 3$ in a worldline simulation of the charged ϕ^4 field at finite density. These thresholds correspond to the first three unit steps of the particle number expectation value $\langle N \rangle$ and emerge for small volumes and low temperatures. From the μ_n^{crit} we determined the mass m , as well as the 2- and 3-particle energies W_2 and W_3 using Eq. (4). We studied their dependence on the spatial extent N_s and cross-checked the condensation results with those from $2n$ -point functions. We found very good agreement of the data for all values of N_s we analyzed, thus demonstrating that the condensation thresholds are indeed governed by the lowest n -particle energies, which correspond to the mass and 2- and 3-particle scattering states. This is the first time that this agreement is shown nonperturbatively in four dimensions, since the necessary worldline techniques for finite density lattice simulations became available only recently.

Subsequently, we analyzed the volume dependence of W_2 and W_3 in order to make contact to scattering data. For the 2D case such an analysis allows for a complete determination of the scattering phase $\delta(k)$ from W_2 . In four dimensions we fit the L dependence of m and W_2 to determine the infinite volume mass m_∞ and the scattering length a . Inserting these parameters in the functional form for W_3 determines the 3-particle energy up to $1/L^6$ corrections. We compared this “prediction” with our results for W_3 from the condensation data and found very convincing agreement. This demonstrates that the finite density condensation steps at low temperature are indeed governed by the scattering data of the theory.

We stress at this point that the scenario for the condensation which was exploited in our analysis requires a repulsive interaction. In the case of an attractive interaction one expects condensation thresholds at the masses of the bound states, and a nice example of this scenario is documented in Ref. [18] for the model of QCD with the exceptional gauge group G_2 , which is free of sign problems.

It is well known that in four dimensions ϕ^4 theory is trivial. The renormalized coupling vanishes when approaching the continuum limit and one may expect that also the scattering length vanishes. Consequently, our study in ϕ^4 theory deals with an effective theory which, however, has a large scaling region where it essentially behaves like a continuum theory at low energies, as has been demonstrated in Ref. [19]. In two dimensions, on the other hand, one could try to run towards the Ising fixed point to construct a nontrivial continuum limit, where one expects a constant phase shift of $\delta(k) = -\pi/2$ [20].

Having established the interesting connection between scattering data and thermodynamical properties at low temperature in a simple scalar theory it is of course interesting to ask if this can also be seen in more rich theories. The key issue is to be able to simulate the theory at finite density, which often is spoiled by the sign problem. However, two interesting cases can be addressed immediately, namely, QCD with only two colors and QCD with an isospin chemical potential. In both cases the sign problem is absent, but the former case clearly is of more academic interest. However, using an isospin chemical potential one can condense pions in full QCD and study the relation of the second and third condensation thresholds to scattering data. This is a highly interesting connection that could be studied along the lines presented in this Letter.

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