

# Grand Canonical Ensembles, Multiparticle Wave Functions, Scattering Data, and Lattice Field Theories

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We show that information about scattering data of a quantum field theory can be obtained from studying the system at finite density and low temperatures. In particular we consider models formulated on the lattice that can be exactly dualized to theories of conserved charge fluxes on lattice links. Apart from eliminating the complex action problem at nonzero chemical potential  $\mu$ , these dualizations allow for a particle world line interpretation of the dual fluxes from which one can extract data about the two-particle wave function. As an example we perform dual Monte Carlo simulations of the two-dimensional O(3) model at nonzero  $\mu$  and finite volume, whose nonperturbative spectrum consists of a massive triplet of particles. At nonzero  $\mu$  particles are induced in the system, which at sufficiently low temperature give rise to sectors of fixed particle number. We show that the scattering phase shifts can be obtained either from the critical chemical potential values separating the sectors or directly from the wave function in the two-particle sector. We find that both methods give excellent agreement with the exact result. We discuss the applicability and generality of the new approaches.

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In many quantum field theories the low energy excitations are very different from the field content of the elementary Hamiltonian or Lagrangian. Indeed, excitations, rather than fundamental degrees of freedom, are responsible for many important phenomena, ranging from superconductivity in condensed matter to confinement and dynamical mass generation in quantum chromodynamics (QCD). These excitations are often referred to as particles (or quasiparticles in condensed matter literature) with particular masses, charges, and interactions, although their internal structure may be rather complicated. For a satisfactory theoretical description nonperturbative methods are needed, often complemented with numerical simulations.

In the approach discussed here we consider lattice field theories with a chemical potential  $\mu$ . In recent years there was quite some progress with finding so-called dual representations (see Refs. [1,2] for reviews), which provide an exact mapping to new (dual) degrees of freedom, which are fluxes for matter and surfaces for gauge fields. Initially, dualization was motivated to overcome the complex action problem (at nonzero  $\mu$  the action  $S$  is complex and the Boltzmann factor  $e^{-S}$  cannot be used as a probability in a Monte Carlo simulation). Here, we show that very precise information about scattering phases and interactions can be obtained based on two simple observations. 1. At finite volume and zero temperature the one, two, three, etc.,

charge sectors are separated by finite energy steps, and hence these charges will appear in the system at certain chemical potential thresholds  $\mu_1, \mu_2, \mu_3, \dots$ , the difference of which contains information about the interaction energy of particles carrying charges. 2. The dual variables allow a particle world line interpretation from which the multiparticle ground state wave function can be obtained. The latter in principle contains all the information about the interactions. It is these two observations that are the cornerstone of the two methods we develop in this work: the *charge condensation method* and the *dual wave function method*, respectively.

We develop the ideas using the two-dimensional O(3) model, and discuss their generality in the end. In addition to being an important condensed matter system, the O(3) model is a widely used toy theory for QCD because of common features such as asymptotic freedom, a dynamically generated mass gap, and topological excitations. Moreover, there exist exact results [3] for the scattering phase shifts, i.e., the physical observables that we aim at in our new approach. Suitable dual representations at nonzero  $\mu$  are known [4,5] and the basics of the finite density behavior were discussed for the related case of the O(2) model in Ref. [6].

The Lagrangian of a quantum field theory typically shows some continuous symmetries resulting in

corresponding conserved Noether charges. These symmetries and charges play a twofold role in our approach: when transforming the theory to the dual representation the symmetries give rise to constraints of the dual variables making flux conservation explicit. The resulting “world lines of flux” transport the corresponding charge in space and time, and the particle number turns into a topological invariant: the winding number of the corresponding flux around the compact Euclidean time.

The second important aspect of the symmetries and the corresponding charges is that a chemical potential can be coupled to the associated charge, which then can be used to populate the corresponding charge sector. In the dual representation the chemical potentials introduce an additional weight for the winding number of the corresponding flux lines.

At sufficiently low temperature  $T$  and finite volume one can control the particle number with the chemical potential and systematically probe the system in the different charge sectors, which are separated by the aforementioned critical values  $\mu_i$ ,  $i = 1, 2, 3, \dots$  of the chemical potential. The critical values  $\mu_i$  are clearly marked by steps when plotting the expectation value of the charge  $Q$  at low  $T$  as a function of  $\mu$  (see Ref. [6] and Fig. 1 below). In the presence of a mass gap  $m$ , the (“Silver blaze”) range from  $\mu = 0$  to  $\mu = \mu_1$  corresponds to the charge-0 sector; no particle is present, and for sufficiently large spatial volume one has  $\mu_1 = m$ . The interval  $\mu \in (\mu_1, \mu_2)$  delimits the charge-1 sector, where  $\mu_2$  corresponds to the energy of the lowest charge-2 state, i.e., containing two particle masses plus their interaction energy [7]. At finite volume, it is exactly this two-particle energy that can be related to scattering data using the Lüscher formula [9–11], and analyzing the two-particle condensation threshold  $\mu_2$  as a function of the volume constitutes our first approach to extract scattering

data from nonzero density and finite volume. We refer to this approach as the “charge condensation method.”

Our second approach—which we refer to as the “dual wave function method”—is based on a direct analysis of the dual fluxes in the two-particle sector, i.e., the interval  $\mu \in (\mu_2, \mu_3)$ , where  $\mu_3$  marks the onset of the charge-3 sector. In this interval we analyze the two winding flux loops that characterize the charge-2 sector and determine the distribution of their spatial distance, which we relate to the two-particle wave function, from which we again compute scattering data.

Both methods are presented in detail for the 2D O(3) model. We begin with discussing the dual representation as derived in Ref. [4] where the details of the dualization and also the conventional form of the model are presented. We consider the O(3) model with a single chemical potential coupled to one of the conserved charges. The conventional degrees of freedom are O(3) rotors and the chemical potential is coupled to the 3-component of the corresponding angular momentum. In the dual form the partition sum  $Z$  is exactly rewritten into a sum over configurations  $\{m, l, k\}$  of three sets of dual variables  $m_{x,\nu} \in \mathbb{Z}$ ,  $l_{x,\nu}, k_{x,\nu} \in \mathbb{N}$  on the links  $(x, \nu)$  of a  $N_t \times N_s$  lattice (periodic boundary conditions, lattice constant  $a$ ):

$$Z(\mu) = \sum_{\{m,l,k\}} B_J[m, l, k] e^{-a\mu \sum_x m_{x,0}} \times \prod_x \delta\left(\sum_\nu [m_{x,\nu} - m_{x-\hat{\nu},\nu}]\right). \quad (1)$$

Each configuration of the variables  $m_{x,\nu}$ ,  $l_{x,\nu}$ ,  $k_{x,\nu}$  comes with a real non-negative weight  $B_J[m, l, k]$  that depends on the coupling  $J$ .  $B_J[m, l, k]$  is given explicitly in Ref. [4], but is irrelevant for the discussion here. A second weight factor  $e^{-a\mu \sum_x m_{x,0}}$  originates from the chemical potential  $\mu$  that couples to the temporal component of the current  $m_{x,\nu}$  (in our notation  $\nu = 0, 1$  and  $\nu = 0$  denotes Euclidean time). Obviously, all weights are real and positive such that the complex action problem is solved in the dual formulation for arbitrary  $\mu$ .

The dual variables  $m_{x,\nu}$ , which correspond to one of the O(2) subgroups of O(3), obey constraints at each site  $x$ . The product of Kronecker deltas  $\delta(\dots)$  enforces  $\nabla_{\vec{m}_x} \equiv \sum_\nu [m_{x,\nu} - m_{x-\hat{\nu},\nu}] = 0 \quad \forall x$ , which is a discrete version of a vanishing divergence condition. Thus, the flux  $m_{x,\nu}$  is conserved and the admissible configurations of  $m_\nu$ -flux are closed loops.

Since the  $m_\nu$ -flux must form loops, the term in Eq. (1) that multiplies  $\mu$  can be written as  $a \sum_x m_{x,0} = a N_t w[m_\nu]$ , where  $w[m_\nu]$  is the total winding number of  $m_\nu$ -flux around the compact time direction with extent  $a N_t \equiv 1/T$  (we use natural units with  $k_B = \hbar = c = 1$ ). Thus, we identify the winding number  $w[m_\nu]$  as the particle number in the dual formulation.

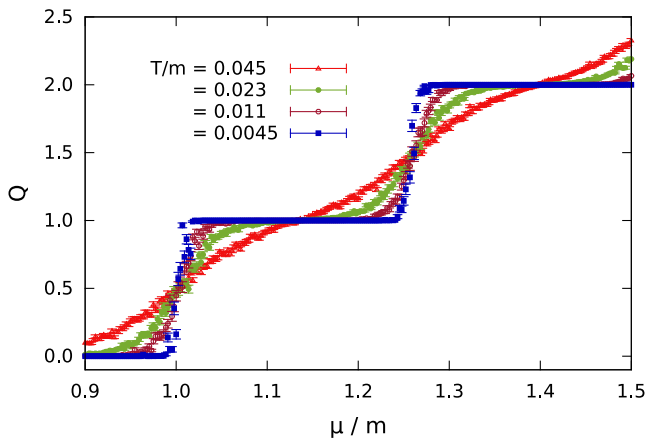


FIG. 1 (color online). The charge  $Q$  as a function of  $\mu$  (in units of the mass  $m$ ). We compare different temperatures  $T$  at fixed spatial extent  $Lm = 4.4$  ( $N_t = 100, 200, 400, 1000$  at  $N_s = 20$  using  $J = 1.3$ ).

The constrained  $m_\nu$ -fluxes can be updated with a generalization of the worm algorithm [12], while for the other fluxes local Monte Carlo updates are sufficient. Most of the Monte Carlo results presented in this Letter were computed at fixed coupling  $J = 1.3$  (with some scaling checks performed also at  $J = 1.4$  and  $J = 1.5$ , i.e., closer to the continuum). The temperature  $T = 1/aN_t$  was varied by changing the temporal extent  $N_t$  of the lattice, and the spatial size  $L = aN_s$  by changing  $N_s$ . Dimensionful quantities are expressed in units of the mass  $m$  of the lowest excitation, which was determined from propagators in the conventional representation, and, at, e.g.,  $J = 1.3$ , is  $am = 0.222$ .

To substantiate the above discussion of sectors with fixed  $Q$ , we show in Fig. 1 our  $J = 1.3$  results for  $Q = \langle w[m_\nu] \rangle$  as a function of  $\mu$  for several low temperatures, at fixed  $mL = 4.4$ . Decreasing the temperature we indeed find the expected formation of plateaus in Fig. 1, which correspond to the sectors of fixed charge, and we can read off the critical values  $\mu_i$ . In a practical calculation one actually determines the  $\mu_i$  from the peaks of the corresponding particle number susceptibility  $\chi = \langle (w[m_\nu] - Q)^2 \rangle / L$ . These susceptibilities are shown as a function of  $\mu$  in the top panel of Fig. 2, and we compare results for different spatial extents  $L$  in units of  $m$ . The susceptibilities show pronounced peaks, which we can use to determine the values  $\mu_i$ . We remark that the position  $\mu_1$  of the first peak is independent of  $L$ , while the second peak  $\mu_2$  shifts to smaller values when increasing  $L$  (see the discussion below).

We now make quantitative the above arguments connecting the critical chemical potentials  $\mu_1$  and  $\mu_2$  with the mass  $m$  of the lightest particle and the energy of the two-particle states. We write the grand-canonical partition sum  $Z(\mu)$  with a grand potential  $\Omega(\mu)$  in the form ( $\hat{H}$  and  $\hat{Q}$  denote the Hamiltonian and charge operator)

$$Z(\mu) = \text{tr} e^{-(\hat{H} - \mu \hat{Q})/T} \equiv e^{-\Omega(\mu)/T}. \quad (2)$$

The small- $T$  limit is governed by the minimal exponents, i.e., in each sector with charge  $Q$  the corresponding minimal energy  $E_{\min}^Q$  dominates and the grand potential in the different sectors is

$$\Omega(\mu) \xrightarrow{T \rightarrow 0} \begin{cases} E_{\min}^{(Q=0)} = 0 & \text{for } \mu \in [0, \mu_1), \\ E_{\min}^{(Q=1)} - \mu = m - \mu & \text{for } \mu \in (\mu_1, \mu_2), \\ E_{\min}^{(Q=2)} - 2\mu = W - 2\mu & \text{for } \mu \in (\mu_2, \mu_3), \\ \dots, \end{cases} \quad (3)$$

where we introduced the minimal two-particle energy  $W$ . Note that in the charge-1 sector we assumed  $\mu_1 = m$ ; i.e., we neglected possible finite volume corrections (see below for a cross-check).

The two-particle energy  $W$  can be calculated from  $\mu_1$  and  $\mu_2$ : the first two transitions between neighboring sectors

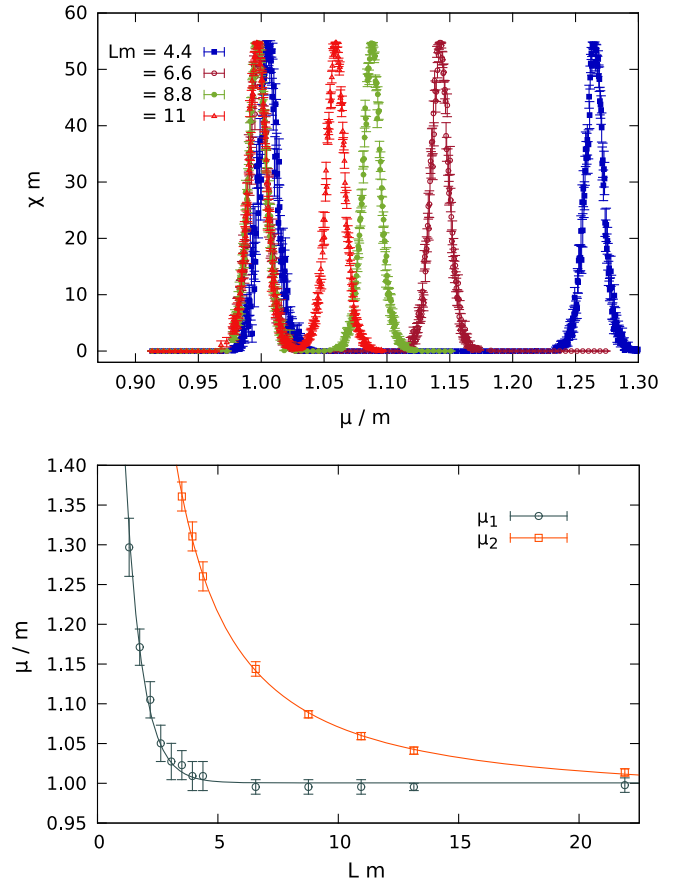


FIG. 2 (color online). Top: the susceptibility  $\chi$  at fixed temperature  $T/m = 0.0045$  as a function of chemical potential for different spatial extensions  $L$  ( $N_t = 1000$  with  $N_s = 20, 30, 40$ , and  $50$ ). For each  $L$  we show the first two peaks corresponding to the critical chemical potentials  $\mu_1$  and  $\mu_2$ . Bottom: the critical chemical potentials at the same temperature now as a function of  $L$ . The solid curves are results of fits (exponential for  $\mu_1$  and power law for  $\mu_2$ ).

occur when  $0 = m - \mu_1$  and  $m - \mu_2 = W - 2\mu_2$ , respectively, and thus we find

$$W = m + \mu_2 = \mu_1 + \mu_2. \quad (4)$$

So far we have not discussed the role of nonzero spatial momenta of the states, which for our two-dimensional model are given by  $2\pi n/L = 2\pi n/aN_s$ ,  $n = 0, 1, \dots, N_s - 1$ . We stress again that at very low  $T$  only states with vanishing total momentum contribute to the partition sum. Thus, in the charge-1 sector we have one particle at rest, in the charge-2 sector two particles with opposite spatial momentum, etc. We can combine this with the discreteness of the momenta to understand the  $L$  dependence of the  $\mu_i$ , which is documented in the bottom panel of Fig. 2, where we plot the values of  $\mu_1$  and  $\mu_2$  as a function of  $L$ .

For  $\mu_1$  we expect a dependence on  $L$  only when  $L$  becomes smaller than the Compton wavelength of the

lightest excitation [13] and self-interactions around periodic space alter the mass. This is indeed what we observe in the right panel of Fig. 2. For  $\mu_2$  a nonvanishing dependence on  $L$  is expected throughout, since the box size  $L$  controls the allowed relative momentum. Also, such a nontrivial dependence is obvious from Fig. 2.

For a short ranged potential one can write the two particle energy  $W$  as twice the energy of an asymptotically free particle

$$W = 2\sqrt{m^2 + k^2}, \quad (5)$$

where  $k$  denotes the relative momentum, which is shifted from the values  $2\pi n/L$  of the free case. In a finite volume, only certain quantized values of  $k$  can account for the scattering phase shift  $\delta(k)$  of the interaction and the periodicity, as expressed by the Lüscher formula [9]

$$e^{2i\delta(k)} = e^{-ikL}. \quad (6)$$

Varying  $L$  allows one to scan a whole range of momenta  $k$ . The temperature must be low enough for pronounced plateaus to form (see Fig. 1), which gives rise to the following two conditions:  $T \ll m$  and  $T/m \ll 1/(Lm)^2$ . Our numerical results for this extraction are given in Fig. 3. In the top panel we show our data for  $k$  as a function of  $L$  and compare to the exact result [3] for “isospin 2,” which is the relevant case for our choice of the chemical potential that excites the 3-component of the O(3) angular momentum. We also include results from the numerical spectroscopy calculation in the two-particle channel [11] and find excellent agreement of our results with the analytical and numerical reference data. In the bottom panel we give the results for the phase shift  $\delta(k)$  as a function of  $k$ , and again find excellent agreement with the reference data.

Our second approach for the determination of scattering data, the dual wave function method, is based on a direct analysis of the flux variables  $m_{x,\nu}$  that carry the charge: in the charge-2 sector we identify the two flux lines that wind around the compact time and interpret their temporal flux segments  $m_{x=(x_0,x_1),\nu=0} = 1$  as the spatial position  $x_1$  of the charge at time  $x_0$ . Thus, for a given time  $x_0$  we obtain two positions  $x_1^{(1)}, x_1^{(2)}$  and identify  $\Delta x = |(x_1^{(1)} - x_1^{(2)})|$  as the distance of the two charges at that time. Sampling over time and many configurations we obtain the probability distribution of the distance  $\Delta x$ , and the square root of this distribution can be identified as the relative wave function  $\psi(\Delta x)$  of the two charges.

In Fig. 4 we show  $\psi(\Delta x)$  for different spatial extents  $L$ . Except for very small  $\Delta x$  the wave functions are very well described by shifted cosines

$$\psi(\Delta x) \propto \cos(k(\Delta x - L/2)). \quad (7)$$

This finding confirms the applicability of Eq. (5): outside the interaction range the wave functions for the relative

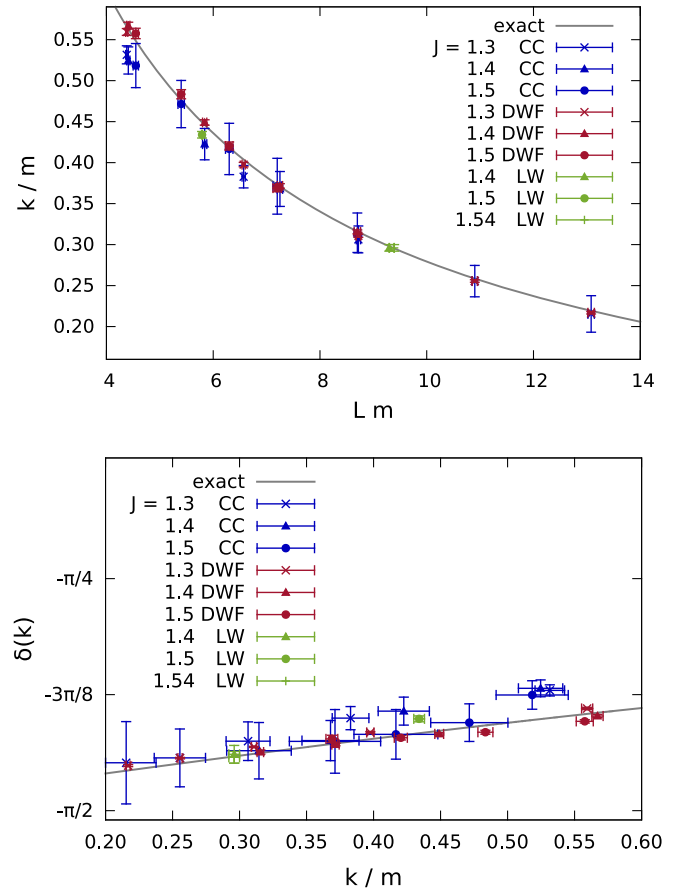


FIG. 3 (color online). Results from the charge condensation method (blue symbols, labeled CC) and the dual wave function method (red, DWF) using different  $J$  and  $N_s$ . We compare our results to the analytic solution [3] (full curves) and the analysis based on two-particle spectroscopy [11] (blue, LW). In the top panel we show the momenta  $k$  as a function of  $L$  and in the bottom panel the phase shift  $\delta(k)$  versus  $k$  ( $k$  and  $L$  in units of  $m$ ).

motion of the two particles are standing waves with momenta  $k$  that are related to the scattering phase shifts via Eq. (6). Thus, we can fit the data for  $\psi(\Delta x)$  with the cosines (7) and obtain the momenta  $k$  from that fit. The fit results are also shown in Fig. 4 and in the legend we give the corresponding momenta  $k$ . From these one again obtains the phase shift  $\delta(k)$  via Eq. (6). The results from the dual wave function method are included in Fig. 3 and agree very well with the charge condensation method and the reference data.

Let us summarize the two approaches for obtaining scattering data presented here and comment on their generality: both methods are based on simulations at nonzero chemical potential  $\mu$  at very low temperatures. The charge condensation method relates the critical chemical potentials  $\mu_1$  and  $\mu_2$  to the two-particle energy, which in turn can be related to the scattering phase shift via the Lüscher formula. Technically, this method assumes that nonzero chemical potential simulations are feasible, which,

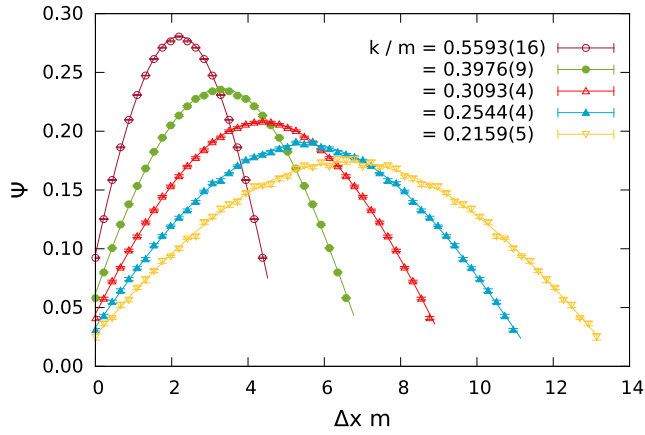


FIG. 4 (color online). The relative wave function  $\psi(\Delta x)$  as determined from analyzing the flux lines in the charge-2 sector. We show results for  $J = 1.3$  at  $T/m = 0.0045$  ( $N_t = 1000$ ) and different spatial extents,  $Lm = 4.4, 6.6, 8.8, 11, 13.2$  ( $N_s = 20, 30, 40, 50, 60$ ). The wave functions are fit according to Eq. (7) and in the legend we give the corresponding fit results for  $k$ .

for example, is the case for the isospin potential in QCD. The basic concept of the charge condensation method is generalizable also to higher dimensions, in particular, the relation of the condensation thresholds  $\mu_1, \mu_2$  to the two-particle energy. In higher dimensions a full partial wave analysis would be necessary for complete information about scattering, but at least the scattering length can be extracted from the two-particle energy [9,10]. For the second approach, the dual wave function method, the chemical potential is adjusted such that the system is in the charge-2 sector. This method is rather general in arbitrary dimensions. The relative two-particle wave function can be determined from the fluxes in the charge-2 sector and in principle this gives access to the complete scattering information.

We remark that both methods can be straightforwardly generalized to three and more particles. A second remark concerns the possibility to couple different chemical potentials to different conserved charges. Using such a setting one can also populate two-particle sectors with two different particle species and study their scattering properties. While the charge condensation method is independent of the representation of the system, we emphasize that the dual wave function method requires a suitable dualization and makes explicit use of the world line interpretation. The latter method opens the possibility to study particles and antiparticles, i.e., charges of opposite sign.

This exploratory Letter is a first step towards a full understanding of the relation between low temperature multiparticle sectors and scattering data. We believe that this is an interesting connection to explore, and understanding the physics involved clearly goes beyond the development of a new method for determining scattering data in lattice simulations.

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