## Lattice gas models derived from effective field theory

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We start from a low-energy effective field theory for interacting fermions on the lattice and expand in the hopping parameter to derive the nearest-neighbor interactions for a lattice gas model. In this model, the renormalization of couplings for different lattice spacings is inherited from the effective field theory, systematic errors can be estimated *a priori*, and the breakdown of the lattice gas model description at low temperatures can be understood quantitatively. We apply the lattice gas method to neutron matter and compare with results from a recent quantum simulation.

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# I. INTRODUCTION

Lattice gas models play an important role in many areas of physics from fluid mechanics [1-3] to quantum computing [4,5], alloy mixing [6,7], and nuclear physics. In nuclear physics, phenomenological lattice gas models have been used to model multifragmentation in heavy ion collisions and the thermodynamics of symmetric and asymmetric nuclear matter at nonzero temperature [8-16]. In this study, we attempt to broaden the scope of the lattice gas approach as applied to interacting fermions at nonzero temperature. We build a connection between lattice gas models and low-energy effective field theory on the lattice. While our main interest concerns interacting nucleons, our approach to lattice gas models should apply to systems such as trapped Fermi gases near a Feshbach resonance [17–22], where similar effective field theory descriptions are applicable.

For most applications of lattice gas models in nuclear physics, the coefficients of interactions are treated as adjustable parameters tuned to make the model realistic. Also, the lattice spacing is often chosen so that the completely filled lattice corresponds with normal nuclear matter density,  $\rho_N \approx 0.17 \text{ fm}^{-3}$ . While one cannot argue with the successes of this phenomenological approach, there remain some fundamental questions. How do we know which interactions are needed to describe the important low-energy physics? How can we determine the coefficients of the interactions directly from binding energies and/or few-body scattering data? How can we do simulations at different lattice spacings while keeping the low-energy physics the same?

In the full quantum theory, these questions are answered by effective field theory. In the low-energy limit, power counting schemes organize the interactions in order of importance [23–26]. Over the past few years, effective field theory methods have been used to study two- and three-nucleon systems at low energy [27–29]. There has also been recent progress in applying effective field theory to many-body nuclear lattice simulations [30–32]. In this approach, operator coefficients in the effective lattice Lagrangian are matched to few-body scattering data, and the renormalization group describes how the operator coefficients depend on the lattice spacing. The resulting lattice action can then be simulated using

standard lattice Monte Carlo methods to produce many-body results.

In this study, we attempt to bring lattice gas models into the framework of effective field theory. We make this connection by means of a spatial hopping parameter expansion. Starting from any effective field theory of interacting fermions, we show how to construct the rules for a corresponding lattice gas model. We discuss the convergence of the hopping parameter expansion as well as the uses and limits of the lattice gas approach. In particular, we clarify why it can describe a "classical" phase transition but not a truly "quantum" phase transition.

As an example, we consider low-energy neutron matter and compare it with recent quantum simulation results [32] for the energy per neutron as a function of density. In [32], it was shown that lattice effective field theory calculations for the equation of state for dilute neutron matter agree with the variational calculations of Friedman and Pandharipande [33] at temperatures of 4 and 8 MeV. Phenomenologically this is interesting since the equation of state for dilute neutron matter plays an important role in both the structure and evolution of neutron stars [34,35] and neutrino trapping in supernovae [36-38]. Furthermore, dilute neutron matter is also theoretically interesting for the reason that it lies very close to an important scaling limit. The neutron scattering length is  $a_{nn} \simeq -18$  fm, which implies that  $k_F |a_{nn}| \gg 1$  for densities  $\rho > 10^{-4}\rho_N$ . Here,  $k_F$  is the Fermi momentum. On the other hand, the effective range for neutron scattering is  $r_{nn} \simeq 2.8$  fm. So if the density is small,  $\rho < 0.1 \rho_N$ , then  $k_F |r_{nn}|$  is a small parameter, and neutron matter is close to the limit in which  $k_F|a_{nn}| \to \infty$  and  $k_F|r_{nn}| \to 0$ . In this limit, dimensional analysis implies that the energy per particle and the superfluid gap both have to be proportional to the free particle Fermi energy

$$\frac{E}{A} = \xi \frac{3}{5} \frac{k_F^2}{2m}, \quad \Delta = \zeta \frac{k_F^2}{2m}.$$
 (1)

The determination of these two dimensionless parameters  $\xi$  and  $\zeta$  is a nonperturbative problem that spans several branches of physics. Recently, it has been probed experimentally in cold, dilute gases of fermionic atoms tuned to be near a Feshbach resonance [17–20,39].

### **II. HOPPING EXPANSION**

Let us consider  $n_f$  species of fermions and any operator  $\hat{V}$  built up from the annihilation and creation operators. Let  $|\theta\rangle$  denote the eigenstates of  $\hat{V}$ ,

$$\hat{V}(\hat{a}^{\dagger},\hat{a})|\theta\rangle = V(\theta)|\theta\rangle.$$
<sup>(2)</sup>

Next we consider a tensor product space that represents the fermions at two different locations. For the moment, we single out one particular species *j* and define the Hamiltonian

$$\hat{H}_{j} = \hat{V}(\hat{a}^{\dagger}, \hat{a}) \otimes 1 + 1 \otimes \hat{V}(\hat{a}^{\dagger}, \hat{a}) - \varepsilon [\hat{a}_{j}^{\dagger} \otimes \hat{a}_{j} + \hat{a}_{j} \otimes \hat{a}_{j}^{\dagger}].$$
(3)

Let us define the matrix element

$$z_{j}^{\theta_{1},\theta_{2}}(\beta) = [\langle \theta_{1} | \otimes \langle \theta_{2} |] \exp[-\beta \hat{H}_{j}] [|\theta_{1}\rangle \otimes |\theta_{2}\rangle].$$
(4)

If we expand in  $\beta \varepsilon$ , we find

$$z_{j}^{\theta_{1},\theta_{2}}(\beta) = \exp\{-\beta[V(\theta_{1}) + V(\theta_{2})]\} \cdot \left[1 + \beta^{2} \varepsilon^{2} f_{j}^{\theta_{1},\theta_{2}}(\beta)\right] + O[(\beta \varepsilon)^{4}],$$
(5)

where

$$f_{j}^{\theta_{1},\theta_{2}}(\beta) = \sum_{\theta',\theta''} \begin{bmatrix} |\langle \theta'|\hat{a}_{j}|\theta_{1}\rangle|^{2} |\langle \theta''|\hat{a}_{j}^{\dagger}|\theta_{2}\rangle|^{2} \\ + |\langle \theta'|\hat{a}_{j}^{\dagger}|\theta_{1}\rangle|^{2} |\langle \theta''|\hat{a}_{j}|\theta_{2}\rangle|^{2} \end{bmatrix}$$
$$\times F\{\beta[V(\theta') + V(\theta'') - V(\theta_{1}) - V(\theta_{2})]\} \quad (6)$$

and

$$F(x) = \frac{e^{-x} - 1 + x}{x^2}, \qquad F(0) = \frac{1}{2}.$$
 (7)

We now generalize this result to a general three-dimensional periodic lattice Hamiltonian with nearest-neighbor hopping and single-site interactions,

$$\hat{H} = \sum_{\vec{n}} \hat{V}[\hat{a}^{\dagger}(\vec{n}), \hat{a}(\vec{n})] - \frac{1}{2m} \sum_{\vec{n}} \sum_{j=1, n_f} \sum_{l=1, 2, 3} \sum_{\vec{n} \in [\hat{a}_j^{\dagger}(\vec{n}) \hat{a}_j(\vec{n}+\hat{l}) + \hat{a}_j^{\dagger}(\vec{n}) \hat{a}_j(\vec{n}-\hat{l})].$$
(8)

In the following, we use dimensionless lattice parameters. If *a* is the lattice spacing, then the dimensionless mass parameter and inverse temperature are

$$m = m_{\rm phys}a,\tag{9}$$

$$\beta = \frac{1}{T_{\rm phys}a}.$$
 (10)

Let  $|\Theta\rangle$  be a configuration of fermion states at each lattice site,

$$|\Theta\rangle = \bigotimes_{\vec{n}} |\theta(\vec{n})\rangle. \tag{11}$$

Let us define

$$z(\beta,\Theta) = \langle \Theta | e^{-\beta \hat{H}} | \Theta \rangle.$$
 (12)

After applying the hopping corrections in (5) for each lattice site, fermion species, and dimension, we find

$$z(\beta, \Theta) = \exp\left\{-\beta \sum_{\vec{n}} V[\theta(\vec{n})]\right\} \prod_{\vec{n}} \prod_{j=1, n_f} \prod_{l=1, 2, 3} \times \left[1 + \left(\frac{\beta}{2m}\right)^2 f_j^{\theta(\vec{n}+\hat{l}), \theta(\vec{n})}(\beta)\right] + O\left[\left(\frac{\beta}{2m}\right)^4\right].$$
(13)

We have assumed that the lattice is longer than three sites in each dimension. If the lattice were three sites long in some dimension then there would be terms at  $O[(\frac{\beta}{2m})^3]$  which wind around the lattice.

We can introduce a chemical potential by adding  $-\mu \hat{N}$  to  $\hat{H}$ , where  $\hat{N}$  is the total fermion number operator. In order to compute

$$z(\beta, \mu, \Theta) = \langle \Theta | e^{-\beta(H - \mu N)} | \Theta \rangle, \qquad (14)$$

we can use the same expression in (13) if we redefine

$$\hat{V} \to \hat{V} - \mu \sum_{j} \hat{a}_{j}^{\dagger} \hat{a}_{j}.$$
(15)

By summing over all configurations  $\Theta$ , we now have an approximation to the grand canonical partition function,

$$Z_{G} = \operatorname{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] = \sum_{\Theta} z(\beta, \mu, \Theta)$$
$$\approx \sum_{\Theta} \exp\left\{-\beta \sum_{\vec{n}} V[\theta(\vec{n}), \mu]\right\} \prod_{\vec{n}} \prod_{j=1, n_{f}} \prod_{l=1, 2, 3} \left[1 + \left(\frac{\beta}{2m}\right)^{2} f_{j}^{\theta(\vec{n}+\hat{l}), \theta(\vec{n})}(\beta)\right].$$
(16)

We note the similarity to a  $2^{n_f}$ -state Ising model. The only differences are the nonexponential factors and the temperature dependence in the interactions. One could write everything in exponential form using

$$1 + \left(\frac{\beta}{2m}\right)^2 f_j^{\theta(\vec{n}+\hat{l}),\theta(\vec{n})}(\beta) \approx \exp\left[\left(\frac{\beta}{2m}\right)^2 f_j^{\theta(\vec{n}+\hat{l}),\theta(\vec{n})}(\beta)\right].$$
(17)

For weakly coupled systems, either form will do. However, we find that for very strongly coupled systems, the exponentiated form produces larger  $O[(\frac{\beta}{2m})^4]$  errors than the original expression.

#### **III. CONVERGENCE AND LONG-RANGE ORDER**

The spatial hopping parameter expansion can be extended to higher orders. At order  $O[(\frac{\beta}{2m})^n]$ , one must consider all *n*-step paths which are connected and form closed loops. On an  $L^3$  lattice where *L* is even, all closed paths must have an even number of steps. In that case, only even powers of  $\frac{\beta}{2m}$  are nonzero. When *L* is odd, there are winding paths that give nonzero contributions for odd powers greater than or equal to *L*. A similar expansion was used to derive the zone determinant expansion in [40], where the parameter  $\frac{\beta}{2m}$  was identified as a localization length in lattice units for a given fermion.

As the temperature increases, the hopping parameter expansion converges more quickly. However, if the temperature is too high, then the relevant physics may be at momenta too high for the chosen lattice spacing. The momentum cutoff scale on the lattice is  $\Lambda_a = \pi a^{-1}$ . The temperature must therefore lie well below the kinetic energy associated with this cutoff scale,

$$T_{\rm phys} \ll \frac{\Lambda_a^2}{2m_{\rm phys}}.$$
 (18)

In order to have a sensible effective theory, we need

$$\frac{1}{\pi^2} \ll \frac{\beta}{2m}.$$
(19)

If we combine this with the condition for convergence of the spatial hopping parameter expansion, we get

$$\frac{1}{\pi^2} \ll \frac{\beta}{2m} = \frac{1}{2m_{\text{phys}}T_{\text{phys}}a^2} \ll 1.$$
 (20)

Let us consider as an example  $T \approx 20$  MeV, roughly the temperature for the liquid-gas transition in symmetric nuclear matter. For a well defined lattice gas model based on a hopping parameter expansion, (20) tells us that the lattice spacing must lie in the range from about 1 to 3 fm. This is enough to probe a wide range of densities, including the saturation density  $\rho_N \approx 0.17$  fm<sup>-3</sup>. Therefore, it seems possible to describe the phase transition at several different lattice spacings.

While a lattice gas model may describe long-range particle density ordering in a liquid-gas transition, it cannot describe long-range order associated with "off-diagonal" operators. By off-diagonal operator, we mean operators which do not commute with the single-site operator  $\hat{V}$ . In our lattice gas model formalism, these operators are quite different from diagonal operators, such as the particle density operator, which commute with  $\hat{V}$ . We can compute the correlation functions of diagonal operators simply by computing the eigenvalues associated with each configuration state  $|\Theta\rangle$ . But in order to compute the correlation functions of off-diagonal operators, we need to consider entirely new hopping paths connecting one operator to another. It is clear that any long-range correlations would have to be built by hand from arbitrarily long paths in our hopping parameter expansion.

Therefore, we expect the lattice gas model approach to be ineffective for any truly "quantum" phase transition. Longrange order in a quantum phase transition becomes possible only when the quantum wave functions of individual particles

TABLE I.  $V(\theta, \mu)$ .

0	1	$\downarrow$	$\uparrow \downarrow$
0	$m-\mu+\frac{3}{m}$	$m-\mu+\frac{3}{m}$	$2(m-\mu+\frac{3}{m})+C$

TABLE II.  $f^{\theta_1,\theta_2}_{\uparrow}(\beta)$ .

	0	1	$\downarrow$	$\uparrow \downarrow$
0	0	$\frac{1}{2}$	0	$F(-\beta C)$
↑	$\frac{1}{2}$	Ō	$F(\beta C)$	0
$\downarrow$	0	$F(\beta C)$	0	$\frac{1}{2}$
↑↓	$F(-\beta C)$	0	$\frac{1}{2}$	0

overlap. Hence, the localization length  $\frac{\beta}{2m}$  must be greater than the interparticle spacing in lattice units, and so therefore  $\frac{\beta}{2m} \gtrsim 1$ .

## **IV. APPLICATION TO NEUTRON MATTER**

We now apply our hopping parameter expansion to an effective field theory for dilute neutron matter on the lattice. We focus on low energies and densities where the relevant momenta are smaller than the pion mass, and we use an effective field theory with only neutrons. We work with the lowest order effective Lagrangian which contains a neutron contact interaction that is adjusted to produce the physical  ${}^{1}S_{0}$  scattering length. Our lattice Hamiltonian with chemical potential included has the form

$$\begin{aligned} \hat{H} &-\mu \hat{N} \\ &= \left(m - \mu + \frac{3}{m}\right) \sum_{\vec{n}} \sum_{j=\uparrow,\downarrow} \hat{a}_j^{\dagger}(\vec{n}) \hat{a}_j(\vec{n}) \\ &+ C \sum_{\vec{n}} \hat{a}_{\uparrow}^{\dagger}(\vec{n}) \hat{a}_{\uparrow}(\vec{n}) \hat{a}_{\downarrow}^{\dagger}(\vec{n}) \hat{a}_{\downarrow}(\vec{n}) - \frac{1}{2m} \\ &\times \sum_{\vec{n}} \sum_{j=\uparrow,\downarrow} \sum_{l=1,2,3} [\hat{a}_j^{\dagger}(\vec{n}) \hat{a}_j(\vec{n}+\hat{l}) \\ &+ \hat{a}_j^{\dagger}(\vec{n}) \hat{a}_j(\vec{n}-\hat{l})]. \end{aligned}$$
(21)

We will use the labels  $\theta = 0, \uparrow, \uparrow, \uparrow\downarrow$  to represent the various zero-, one-, and two-neutron states on a single site. In Table I, we list  $V(\theta, \mu)$  for the various neutron states.

we list  $V(\theta, \mu)$  for the various neutron states. In Table II, we list  $f_{\uparrow}^{\theta_1,\theta_2}(\beta)$  for the various neutron states on nearest-neighbor sites, and in Table III, we list  $f_{\downarrow}^{\theta_1,\theta_2}(\beta)$ .

#### **V. RESULTS**

We have run lattice gas model simulations for both free and interacting neutron matter. The value for the interaction coefficient C is set by comparing with experimental data

TABLE III.  $f_{\perp}^{\theta_1,\theta_2}(\beta)$ .

	0	$\uparrow$	$\downarrow$	$\uparrow\downarrow$
0	0	0	$\frac{1}{2}$	$F(-\beta C)$
↑	0	0	$F(\hat{\beta}C)$	$\frac{1}{2}$
$\downarrow$	$\frac{1}{2}$	$F(\beta C)$	0	Ō
¢↓	$F(-\beta C)$	$\frac{1}{2}$	0	0

TABLE IV. Interaction coefficient C for different lattice spacings.

$a^{-1}$ (MeV)	$C ({ m MeV^{-2}})$
50	$-8.01 \times 10^{-5}$
60	$-6.73 \times 10^{-5}$
70	$-5.81 \times 10^{-5}$
80	$-5.10 \times 10^{-5}$

from nucleon-nucleon scattering. We sum all nucleon-nucleon scattering bubble diagrams on the lattice, locate the pole in the scattering amplitude, and compare with Lüscher's formula relating scattering lengths and energy levels in a finite periodic box [32,41,42]. The results are shown in Table IV.

We compute the energy per neutron E/A as a function of neutron density. The total number of neutrons A and average energy E are computed using

$$A = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z_G, \qquad (22)$$

$$E = -\frac{\partial}{\partial\beta} \ln Z_G - (m-\mu)A.$$
(23)

The results for T = 8 MeV are shown in Fig. 1. In Fig. 2, we show a similar plot from a full quantum lattice simulation [32]. The lattice volumes for our lattice gas models are chosen to be the same as those for the corresponding simulations in [32]. In both plots we use the abbreviation fc for free continuum results, f for free lattice results, and s for lattice simulation results. In Fig. 2, results for bubble chain diagrams calculations are also included and labeled with b. In addition to these abbreviations, we also use the shorthand labels shown in Table V for various combinations of spatial and temporal lattice spacing  $a_t$  is set to zero.

In Fig. 3, we show results at T = 4 MeV for the lattice gas model, and in Fig. 4 we show the full quantum simulation at T = 4 MeV.

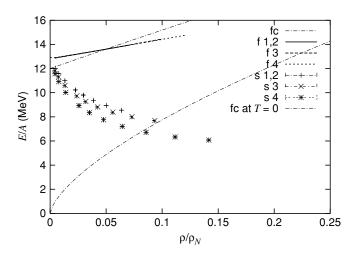


FIG. 1. Lattice gas model results for energy per neutron versus density at T = 8 MeV.

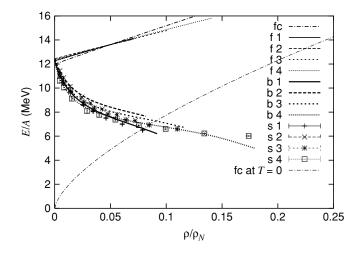


FIG. 2. Full quantum effective field theory results for energy per neutron versus density at T = 8 MeV.

TABLE V. Shorthand labels for various lattice spacings.

$a^{-1}$ (MeV)	$a_t^{-1}$ (MeV)	Label
50	24	0
60	32	1
60	48	2
70	64	3
80	72	4

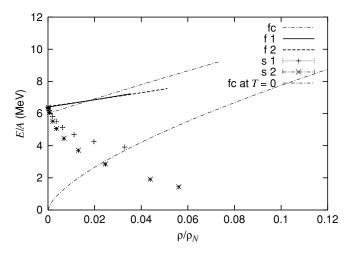


FIG. 3. Lattice gas model results for energy per neutron versus density at T = 4 MeV.

TABLE VI. Hopping parameters for various lattice spacings.

$a^{-1}$ (MeV)	50	60	70	80
$\frac{\beta}{2m}$ for $T = 8$ MeV	0.17	0.24	0.33	0.43
$\frac{\beta}{2m}$ for $T = 4$ MeV	0.33	0.48	0.65	0.85

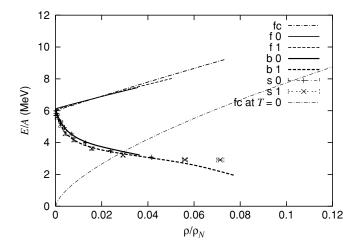


FIG. 4. Full quantum effective field theory results for energy per neutron versus density at T = 4 MeV.

For each of the temperatures and spatial lattice spacings, we show the corresponding spatial hopping parameter in Table VI.

As discussed in the previous section, the lattice gas model cannot describe the superfluid transition in neutron matter since this requires long-range ordering associated with neutron pairing. There may be some indication of this already in the T = 4 MeV data shown in Fig. 3. The points at higher density show considerable deviation from the full quantum simulation results in Fig. 4. Nevertheless, we see that the lattice gas results agree quite well with the quantum simulations when the spatial hopping parameter is less than about 0.4. This is a bit surprising considering that the computational cost for the lattice gas model simulation.

## VI. SUMMARY

Starting from a low-energy effective field theory for interacting fermions on the lattice, we derive the nearest-neighbor interactions for a lattice gas model by expanding in the spatial hopping parameter. Unlike most phenomenological approaches, we derive equivalent lattice gas models at different lattice spacings and determine coefficients directly from binding energies and/or few-body scattering data. We also give an estimate of the systematic errors and discuss the limits of the lattice model approach in describing long-range ordering. As a concrete example, we apply the effective field theory lattice gas approach to low-energy neutron matter and compare with results from a recent quantum simulation. Despite the very low computational cost, essentially the same as that for a  $2^{n_f}$ -state 3D Ising model, we find good agreement with full quantum simulation results when the hopping parameter is not too large.

In our approach, temperature-dependent interactions are naturally introduced into the lattice gas model. These are necessary to reproduce the physics of the full quantum theory at different temperatures. To our knowledge, neutron matter at this density and temperature has never been previously described using a lattice gas model. We hope that the broader application of lattice gas models as well as the connection with effective field theory will prove useful in the study of other many-body fermion systems at nonzero temperature.

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