Ab initio nuclear thermodynamics

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In this letter we present the first ab initio calculations of nuclear thermodynamics using lattice effective field theory. The simulations use a new approach called the pinhole trace algorithm to calculate thermodynamic observables for a fixed number of protons and neutrons enclosed in a finite box. In this framework, we calculate the equation of state, liquid-vapor coexistence line and critical point of neutral symmetric nuclear matter with high precision. The calculated critical temperature, density and pressure are \( T_c = 15.80(3) \text{ MeV}, \rho_c = 0.089(1) \text{ fm}^{-3}, \) and \( P_c = 0.260(3) \text{ MeV/fm}^3, \) respectively. Since the algorithm uses a canonical ensemble with a fixed number of particles, it provides a sizable computational advantage over grand canonical ensemble simulations that can be a factor of several thousands to as much as several millions for large volume simulations.

**Introduction**— The equation of state of strongly interacting matter is one of the central topics in contemporary nuclear physics, as it plays an important role in the early universe, heavy-ion reactions and the generation of gravitational waves in violent neutron star mergers. In Fig. 1 we show the phase diagram of symmetric nuclear matter with equal numbers of protons and neutrons (or equal numbers of up and down quarks). The horizontal axis is the nucleon density \( \rho \) as a fraction of the saturation density \( \rho_0 \), and the vertical axis is temperature in units of MeV. The nuclear equation of state for both symmetric and asymmetric matter is of great relevance to the evolution and dynamics of core-collapse supernovae [1], neutron star cooling [2], and neutron star mergers [3]. There are also important connections between the nuclear equation of state and heavy-ion collisions. It is well established that highly-excited nuclear states can be treated en masse as part of an equilibrium thermal distribution. The large density of states at high energies allows a treatment in terms of thermodynamic concepts, such as temperature, entropy, and free energy. Simple statistical models have been used to address processes such as compound nucleus reactions [4], nuclear multifragmentation [5], nuclear liquid-gas phase transitions [6], and stellar nucleosynthesis [7]. Hot nuclei can, for example, be modeled by a simple Fermi gas model (FGM), where many-body correlations and shell effects are neglected.

Although it can explain some basic properties, the FGM does not reflect many details of nuclear structure and fails in explaining phenomena associated with strong correlations such as clustering [8]. At relatively low temperatures, these problems have been solved by many-body methods such as the shell model Monte Carlo (SMMC) approach [9], which includes many-body correlations within a major shell using stochastic methods. When applied to medium mass nuclei, the SMMC method improves the FGM level densities for excitation energies of a few MeV, which is important for both slow and rapid neutron capture processes in astrophysics [10–12]. At higher temperatures, however, continuum states comprised of nucleons and nuclear fragments play important roles in nuclear breakup, and these are not well described in the shell model valence space. In such cases, the available methods are transport models [13, 14], cluster models [15, 16], and molecular dynamics [17], where clustering correlations are either disregarded or included explicitly. Recent efforts to introduce important correlations into transport models can be found in Ref. [18]. As each of the above methods employs effective interactions selected to reproduce a few chosen observables,
the uncertainties can be significant, especially at high temperatures or densities where less empirical data is available.

In recent years much progress has been made in ab initio or fully microscopic calculations of the nuclear Hamiltonian starting from underlying nuclear forces. When combined with a systematic framework for the nuclear forces such as effective field theory [25], these first-principles calculations can reduce systematic errors order by order and generate important many-body correlations such as those responsible for clustering. Unfortunately, most ab initio methods rely on computational strategies which are not designed for calculations at nonzero temperature. One exception is the method of lattice effective field theory. There have been some early efforts to describe nuclear thermodynamics using lattice simulations [26, 27], however there has been little progress to report since then. The difficulties stem from the amount of computational effort needed to perform grand-canonical simulations of nucleons in large spatial volumes.

In this letter we report a new paradigm for calculating ab initio nuclear thermodynamics with lattice simulations. We demonstrate an efficient method, called the pinhole trace algorithm, for computing nuclear observables at nonzero temperature using a canonical ensemble with fixed numbers of protons and neutrons. We show that the approach can provide reliable results from absolute zero to temperatures high enough to completely dissociate nuclei.

Method——Our ab initio calculations are based on nuclear lattice effective field theory (NLEFT) using a leading-order pionless EFT interaction as defined in [28]. Despite the simplicity of the interaction, the ground-state energies and charge radii of the light and medium-mass nuclei are well reproduced, as well as the zero-temperature equation of state of pure neutron matter [28]. When applied to zero-temperature neutral symmetric nuclear matter as explained in Methods, we obtain $\rho_0 = 0.205$ fm$^{-3}$ and $E/A = -16.9$ MeV at the saturation point. The lattice simulations are performed using auxiliary-field Monte Carlo as described in the review [29] and the book [30].

For a canonical ensemble with fixed nucleon number $A$, volume $V$ and temperature $T$, the expectation value of any observable $O$ can be measured as

$$\langle O \rangle_\beta = \frac{Z_\beta}{Z(\beta)} = \frac{\text{Tr}_A(e^{-\beta H}O)}{\text{Tr}_A(e^{-\beta H})},$$

where $Z(\beta)$ is the canonical partition function, $\beta = T^{-1}$ is the inverse temperature, $H$ is the Hamiltonian, and $\text{Tr}_A$ is the trace over the $A$-body Hilbert space. Throughout, we work in canonical units with $\hbar = c = k_B = 1$. In this letter we use a novel algorithm called pinhole trace algorithm (PTA) to efficiently compute $Z(\beta)$ and $Z_\beta(\beta)$ on the lattice. The pinhole trace algorithm is an extension of the pinhole algorithm introduced in Ref. [19] to sample the spatial positions and spin/isospin indices of the nucleons. The new feature is that we also perform a quantum mechanical trace over all possible states, see Methods.

Naively, one might expect the pinhole trace algorithm to suffer from severe Monte Carlo sign oscillations. By sign oscillations we mean the cancellation of positive and negative matrix determinants in our auxiliary-field Monte Carlo simulations [20, 21]. In auxiliary-field simulations with attractive pairing interactions, the sign problem is held in check by pairing symmetries. The pairing symmetries produce matrices with eigenvalues that come in complex conjugate pairs so that the corresponding matrix determinants remain positive. Since the pinholes’ positions and indices are allowed to explore unpaired configurations, they could spoil the protection from sign oscillations provided by pairing symmetries. Indeed, this worry is one reason why the method had not been considered earlier, and why grand-canonical ensemble simulations have instead been used for simulations of the thermodynamics of nuclear systems as well as ultracold atoms [22, 23]. Fortunately, we find that this is not the case. Although there are some sign oscillations, the pinholes are dynamically driven by the underlying particle interactions to form pairs, thereby quenching the problem of sign oscillations.

In this work we perform simulations on a $6 \times 6 \times 6$ cubic lattice with a spatial lattice spacing $a = 1/150$ MeV$^{-1}$ $\approx 1.32$ fm, such that the corresponding momentum cutoff is $\Lambda = \pi/a \approx 471$ MeV. The temporal lattice spacing is $a_t = 1/2000$ MeV$^{-1}$. We impose twisted boundary conditions along the $x$-, $y$- and $z$-directions [12]. The twist angles are averaged over all possible values by Monte Carlo sampling to remove the fictitious finite-volume shell effect (see Methods).

As the first application of the PTA, we study the nuclear liquid-vapor phase transition by examining the finite-temperature equation of state. Throughout, we only consider symmetric nuclear matter with equal numbers of protons and neutrons and the Coulomb interaction is neglected. Note that in realistic systems the Coulomb interaction is also important. In Fig. 2 we present the calculated chemical potential and pressure isotherms. Each point represents a separate simulation. The temperature $T$ covers the range of $10.0$ MeV $\leq T \leq 20.0$ MeV and the nucleon number $A$ varies from 4 to 100, which corresponds to densities from $0.008$ fm$^{-3}$ to $0.2$ fm$^{-3}$. These settings allow us to explore the whole region relevant to the nuclear matter liquid-vapor phase transition. In this paper we use a quantum Widom insertion method (QWIM) to extract the chemical potential $\mu$, in which we randomly insert or remove nucleons in the system and measure the corresponding free-energy differences, see Methods. We found that QWIM gives highly precise measurements of $\mu$ for a large range of densities from a dilute nucleon gas to supersaturation density $2\rho_0$ over the entire temperature regime considered in this paper. All the Monte Carlo errors for $\mu$ are smaller than $0.02$ MeV and not shown explicitly in Fig. 2. Based on the lattice results, we map the whole $\mu$-$\rho$-$T$ equation of state in this area using interpolation. The critical point is then deduced from solving the equations $d\mu/d\rho = d^2\mu/d\rho^2 = 0$. The uncertainties in the critical values are estimated by propagating the simulation and interpolation errors. We found
The calculated critical pressure is \( p = 0 \). In the middle panel of Fig. 3 we show the free energy curve across the liquid-vapor coexistence line. We subtract \( \mu_{\text{coex}} \) and \( p_{\text{coex}} \) can have different values. A well-known example is that the pressure of the vapor in equilibrium with small liquid drops can be larger than its thermodynamic-limit value, with the difference compensated by the contribution of the surface tension. Bearing the importance of the surface contributions in mind, we can easily interpret the \textit{ab initio} calculations presented in Fig. 2.

The most prominent feature of the isotherms in Fig. 2 is the backbending in the coexistence regime below \( T_c \). Note that the origin of this backbending is completely different from that of similar structures found in the van der Waals model or other mean-field calculations. The mean-field models always describe homogeneous systems and the backbending of the \( p-\rho \) isotherms result in a negative compressibility, and in this regard the assumption of homogeneity conflicts with the condition of mechanical equilibrium. Conversely, in \textit{ab initio} calculations we do not rely on the assumption of homogeneity; the results always describe realistic systems. In particular, phase separation occurs spontaneously whenever it is favored by the free-energy criterion. In the coexistence regime, the most probable configurations consist of high-density liquid regions and low-density vapor regions, the surface spatially separating these regions gives rise to a positive contribution to the total free energy, which prohibits the formation of small liquid drop in vapor or small bubbles in liquid. The distortions of the isotherms reflect the efforts of the system to overcome such a surface-energy barrier.

In Fig. 3 we show schematic plots illustrating the underlying mechanism. Given a fixed volume \( V \) and a temperature \( T \) below the critical value \( T_c \), the free energy \( F \) is a function of the nucleon number \( A \). In the middle panel of Fig. 3 we show the free energy curve across the liquid-vapor coexistence region. We subtract \( \mu_{\text{coex}}A \) from \( F \) to remove most of the \( A \)-dependence, with \( \mu_{\text{coex}} \) assuming the value at the thermodynamic limit. For a finite system the surface free energy \( F_{\text{surf}} \) is approximately proportional to the area of the surface. In the upper panel of Fig. 3 we show the most probable configurations for different densities. At low densities we have a
nucleus surrounded by small clusters, while at high densities we see bubbles in a nuclear liquid. At intermediate densities the system contains bulk nuclear matter with appreciable surface areas. The surface area first increases after the formation of a nucleus then decreases when most of the volume is occupied by the liquid phase. Correspondingly $F_{\text{surf}}$ has a unique maximum and creates a bump in the free energy curve. In the lower panel of Fig. 3 we show the corresponding chemical potential $\mu = \partial F / \partial A$. Apparently the backbending is a natural result of the surface free energy contributions.

**Summary and perspective**—— In this letter we have presented a novel method called the pinhole trace algorithm for simulating a nucleus at fixed temperature $T$, volume $V$, and particle number $A$. We trace over the $A$-body Hilbert space using auxiliary-field Monte Carlo method and find that the Monte Carlo sign oscillations are under control. Because we are working with the canonical ensemble, it suffices to propagate in imaginary time only $A$ single-nucleon states, in contrast with the grand canonical ensemble where the full $4L^3$ space of single-nucleon states must be propagated. This provides an enormous computational advantage over grand canonical ensemble simulations that can be a factor of several thousands to as much as several millions for large volume simulations.

Compared with shell-model based methods, the *ab initio lattice* formalism enables us to explore a much larger configuration space, which is essential for studying phenomena involving high excitation energies and strong many-body correlations. This work is only a first exploration into *ab initio* nuclear thermodynamics with realistic interaction; there is plenty of more work to be done. When combined with high-accuracy lattice chiral interactions that are improved systematically order by order [34], we can perhaps finally realize the goal of *ab initio* calculations with controlled systematic errors that explore all aspects of the nuclear equation of state as a function of density, temperature, and proton fraction.

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[1] H. Togashi, K. Nakazato, Y. Takehara, S. Yamamuro, H. Suzuki, M. Takanobe, Nucl. Phys. A 961, 78 (2017).
[2] D. Page, J. M. Lattimer, M. Prakash, A. W. Steiner, Astrophys. J. Suppl. 155, 623 (2004).
[3] E. R. Most, L. J. Papenfort, V. Dexheimer, M. Hanauske, S. Schramm, H. Stöcker, L. Rezzolla, Phys. Rev. Lett. 122, 061101 (2019).
[4] W. Hauser and H. Feshbach, Phys. Rev. 87, 366 (1952).
[5] N. Bohr, Nature 137, 351 (1936).
[6] P. J. Siemens, Nature 305, 410 (1983).
[7] P. Seeger, W. Fowler, and D. Clayton, The Astrophysical Journal (1965).
[8] M. Freer, H. Horiiuchi, Y. Kanada-En’yo, D. Lee, and U.-G. Meißner, Rev. Mod. Phys. 90, 035004 (2018).
[9] S. E. Koonin, D. J. Dean, and K. Langanke, Phys. Rep. 278, 1 (1997).
[10] D. J. Dean, S. E. Koonin, K. Langanke, P. B. Radha, and Y. Alhassid, Phys. Rev. Lett. 74, 2909 (1995).
[11] H. Nakada and Y. Alhassid, Phys. Rev. Lett. 79, 2939 (1997).
[12] Y. Alhassid, G. F. Bertsch, S. Liu, and H. Nakada, Phys. Rev. Lett. 84, 4 (2000).
[13] J. Aichelin, Phys. Rep. 202, 233 (1991).
[14] A. Ono, H. Horiiuchi, T. Maruyama, A. Ohnishi, Phys. Rev. Lett. 68, 2898 (1992).
[15] M.E. Fisher, Physics-New York 3, 255 (1967).
[16] M.E. Fisher, Rep. Prog. Phys. 30, 615 (1967).
[17] T. Furuta and A. Ono, Phys. Rev. C 74, 014612 (2006)
[18] A. Ono, Prog. Part. Nucl. Phys. 105, 139 (2019).
[19] S. Elhatisari, E. Epelbaum, H. Krebs, T. A. Lähde, D. Lee, N. Li, B. Lu, U.-G. Meißner, and G. Rupak, Phys. Rev. Lett. 119, 222505 (2017).
[20] M. Troyer and U.-J. Wiese, Phys. Rev. Lett. 94, 170201 (2005).
[21] C. E. Berger, L. Rammelmüller, A. C. Loheac, F. Ehmann, J. Braun, J. E. Drut, arXiv:1907.10183
[22] A. Bulgac, J.E. Drut, P. Magierski, Phys. Rev. Lett. 96, 090404 (2006).
[23] A. Bulgac, J.E. Drut, P. Magierski, Phys. Rev. A 78, 023625 (2008).
[24] C. Lin, F.-H. Zong, D. M. Ceperley, Phys. Rev. E 64, 016702 (2001).
[25] E. Epelbaum, H.-W. Hammer, and U.-G. Meißner, Rev. Mod. Phys. 81, 1773 (2009).
[26] H. M. Müller, S. E. Koonin, R. Seki, U. van Kolck, Phys. Rev. C 61, 044320 (2000).
[27] D. Lee, B. Borasoy, T. Schäfer, Phys. Rev. C 70, 014007 (2004).
[28] B.-N. Lu, N. Li, S. Elhatisari, D. Lee, E. Epelbaum, U.-G. Meißner, arXiv:1812.10928[nucl-th].
[29] D. Lee, Prog. Part. Nucl. Phys. 63, 117 (2009).
[30] T. A. Lähde, U.-G. Meißner, “Nuclear Lattice Effective Field Theory: An Introduction”, Lecture Notes in Physics, Volume 957, Springer, (2019).
[31] J. B. Elliott, P. T. Lake, L. G. Moretto, L. Phair, Phys. Rev. C 87, 054622 (2013).
[32] Y. Alhassid, S. Liu, and H. Nakada, Phys. Rev. Lett. 99, (2007).
[33] K. Hagel, D. Fabris, P. Gonthier, H. Ho, Y. Lou, Z. Majka, G. Mouchaty, M. N. Namboodiri, J. B. Natowitz, G. Nebbia, R. P. Schmitt, G. Viesti, R. Wada, and B. Wilkins, Nucl. Phys. A 486, 429 (1988).
[34] N. Li, S. Elhatisari, E. Epelbaum, D. Lee, B.-N. Lu, and U.-G. Meißner, Phys. Rev. C 98, 044002 (2018).
METHODS

Pinhole trace algorithm

In this section we give the details of the pinhole trace algorithm (PTA). We also discuss its performance, including acceptance rate, auto-correlation, sign problem and time complexity.

The canonical partition function of $A$ fermions can be written in the single particle basis as

$$
\Omega(\beta, A) = \sum_{c_1, c_2, ..., c_A} \langle c_1, c_2, ..., c_A | \exp(-\beta H) | c_1, c_2, ..., c_A \rangle,
$$

where $c_i = (n_i, \sigma_i, \tau_i)$ are the quantum numbers of the $i$-th particle, with $n_i$ an integer triplet specifying the lattice coordinate, $\sigma = \pm 1/2$ the spin along the $z$-axis and $\tau = \pm 1/2$ the isospin. On the lattice the components of $n_1$ take integer values from 0 to $L - 1$, with $L$ the box size in units of the lattice spacing. $\beta$ is the inverse temperature $\beta = 1/T$ and $H$ the Hamiltonian. For nuclear systems the neutron number $N$ and proton number $Z$ are conserved separately, the summation in Eq. (2) is limited to the subspace with specific $N$ and $Z$.

In lattice effective field theory [29], $\beta$ can be recognized as the imaginary time and discretized into $L_t$ slices with equal width $a_t$, $\beta = L_t a_t$. For each time slice the two- and three-body interactions can be decomposed using the auxiliary field transformation. Taking a two-body contact interaction and Hubbard-Stratonovich transformation as example, we have

$$
\exp \left( - \frac{C}{2} \rho^2 \right) = \frac{1}{2\pi} \int ds \exp \left( - \frac{s^2}{2} + \sqrt{-Cs^2} \right),
$$

where $C$ is the coupling constant, $\rho$ is the density operator. The two- and three-body interactions are then substituted by the interaction of the particles with external auxiliary fields. The fluctuations of the auxiliary fields should be integrated out to restore the original partition function. Putting these pieces together, we end up with a path integral expression,

$$
\Omega(\beta, A) = \sum_{c_1, c_2, ..., c_A} \int Ds_{L_t} Ds_{L_t-1} ... Ds_1 \times \langle c_1, c_2, ..., c_A | M(s_{L_t}) M(s_{L_t-1}) \times \cdots \times M(s_1) | c_1, c_2, ..., c_A \rangle,
$$

where $M(s_{n_t}) = \exp(-a_t H(s_{n_t}))$ is the transfer matrix for the $n_t$-th imaginary time interval $[n_t a_t, (n_t + 1)a_t]$, $s_{n_t}$ is the corresponding auxiliary field(s). For brevity, in following sections we use the abbreviation $\bar{c} = \{c_1, c_2, ..., c_A\}$, $\bar{s} = \{s_{L_t}, s_{L_t-1}, ..., s_1\}$, $\bar{c_i} = \{c_1, ..., c_i-1, c_{i+1}, ..., c_A\}$, $\bar{s_{n_t}} = \{s_{n_t}, ..., s_{n_t+1}, s_{n_t+1}, ..., s_1\}$.

In the pinhole trace algorithm we evaluate Eq. (4) using Monte Carlo method with importance sampling. We generate an ensemble $\Omega$ of $\{\bar{s}, \bar{c}\}$ configurations with probability distribution

$$
P(\bar{s}, \bar{c}) = \left\langle \left| \bar{c} \right| \prod_{n_t=1}^{L_t} M(s_{n_t}) \left| \bar{c} \right\rangle, \right.
$$

then the expectation value of operator $\hat{O}$ can be expressed as

$$
\langle \hat{O} \rangle = \langle \mathcal{M}_0(\bar{s}, \bar{c}) \rangle / \langle \mathcal{M}_1(\bar{s}, \bar{c}) \rangle,
$$

where $\langle \cdot \rangle_\Omega$ denotes the average in ensemble $\Omega$, the amplitudes $\mathcal{M}_{0,1}$ are defined as

$$
\mathcal{M}_{1,0}(\bar{s}, \bar{c}) = \left\langle \bar{c} \prod_{n_t=1}^{L_t} M(s_{n_t}) \right\rangle / P(\bar{s}, \bar{c}).
$$

In the PTA the central problem is to generate the configurations according to the probability Eq. (5). Here we use the Metropolis algorithm to update $\bar{s}$ and $\bar{c}$ alternately. We first fix the nucleon configuration $\bar{c}$ and update the auxiliary fields $\bar{s}$. Starting from the rightmost time slice $s_1$, we update $s_1$, $s_2$, ..., $s_L$, successively. For updating $s_n$, we generate a new configuration $s'_n$, with probability distribution

$$
P_0(s'_n) = C \exp \left( - \frac{s_n^2}{2} + s_n \frac{\partial \ln P}{\partial s_n} |_{s_n=0} \right),
$$

$C$ is the normalization constant. We accept the new configuration if

$$
\frac{P((\bar{s}-s_n, s'_n), \bar{c})/P_0(s'_n)}{P(\bar{s}, \bar{c})/P_0(s_n)} > r,
$$

where $r$ is a random number uniformly distributed in $[0, 1]$. Whether the new configuration is accepted or not, we progress to $s_{n+1}$ and repeat this procedure. Note that the partial derivative in Eq. (8) can be evaluated exactly using Jacobi’s formula. For $a_t = 1/2000$ MeV$^{-1}$ used in this paper, this algorithm gives an acceptance rate as high as 70% to 90% in most calculations.

When all $L_t$ time slices are updated, we fix the auxiliary field(s) $\bar{s}$ and turn to the updates of the nucleon configuration $\bar{c}$. We randomly choose a nucleon $i$, move it to one of its neighbouring vacancies or flip its spin with equal probability,

$$
c_i = \{n_i, \sigma_i, \tau_i\} \rightarrow c'_i = \{n'_i, \sigma_i, \tau_i\},
$$

with $0 \leq r < 1$ a random number. As in each update we only change the quantum number of a single nucleon, the calculation of the new probability in the denominator of Eq. (11) is
fast, thus we need not to use weighted sampling in $\vec{c}$ updates. The acceptance rate in most calculations is about 30%.

Because in $\vec{c}$ update only a fraction of the nucleons are moved/hipped, the successive configurations are correlated. Only when all nucleons have been updated we can obtain statistically independent configurations. In order to reduce the autocorrelation, we need to use multiple $\vec{c}$ updates. In this work we make 16 $\vec{c}$ updates every 1 $\vec{s}$ update. In Fig. 4 we show the auto-correlation coefficient

$$\rho(n) = \frac{\text{Cov}[E(n_0), E(n_0 + n)]}{\sqrt{\text{D}[E(n_0)] \text{D}[E(n_0 + n)]}},$$

where $E(n_0)$ and $E(n_0 + n)$ are the energies calculated after $n_0$ and $n_0 + n$ update cycles, respectively. Cov and D are covariance and variance, respectively. It is clearly seen that the auto-correlation length increases with the nucleon number, which means that for larger systems more $\vec{c}$ updates will be needed to accelerate the convergence to the equilibrium or reduce the uncertainties. Nevertheless, in all calculations presented in this paper, 16 $\vec{c}$ updates every cycle is sufficient for getting reliable results.

At low temperatures the Monte Carlo simulations for the Fermion system face the notorious sign problem, which means large cancellation between positive and negative amplitudes and we end up with extremely noisy results. The average phase

$$\langle e^{i\theta} \rangle = \langle M_1(\vec{s}, \vec{c}) \rangle_\Omega$$

signifies the severity of the sign problem. For its value close to 1 most of the amplitudes are positive and we can expect a small uncertainty, whereas for $\langle e^{i\theta} \rangle < 0.1$ the results are usually not acceptable. In Fig. 5 we show the average phase of PTA for temperatures from 1 MeV to 15 MeV in the $^{16}$O nucleus. Here the average phase is a monotonically increasing function of the temperature and converges to 1 at high temperatures. Note that the sign problem is due to the antisymmetrized nature of the Fermion wave functions, at high temperatures the system behaves more classically and the sign problem disappears. For temperatures as low as 1 MeV, the average phase decreases to 0.3-0.4, which requires more measurements to achieve a prescribed precision. Nevertheless, for all temperatures above 1 MeV, we found that the sign problem is rather mild.

In Fig. 6 we show the real calculation time for generating a single configuration. By single configuration we mean go through one $\vec{s}$ updates and 16 $\vec{c}$ updates. $A$ is the nucleon number and $L$ is the box size. $L_i$ is fixed to 100. The grey line shows the fitted linear function, which clearly shows that for large $A$ or $L$ the time scales exactly as $A^2 L^3$. From these results one can estimate how many CPU hours are needed to perform a specific calculation using PTA. For example, if we set $\alpha_t = 1/2000$ MeV$^{-1}$, the simulation for 100 nucleons in a $L = 6$ box at temperature $T = 20$ MeV will cost

$$\Delta t = 2.25 \times 10^{-6} s \times 100^2 \times 6^3 = 4.86 s$$

(14)
to generate every configuration. Note that these CPU times are estimated on a supercomputer equiped with Intel Xeon 24-core Skylake CPUs and may vary depending on the hardware.

Widom insertion method

In the pinhole trace algorithm the volume $V$ and particle number $A$ are both fixed, the corresponding intensive variables pressure $p$ and chemical potential $\mu$ must be measured or calculated. In this section we apply a quantum version of the Widom insertion method (QWIM) to solve this problem.

In classical thermodynamics simulations the Widom insertion method (WIM) [1] is conventionally used to determine the statistical mechanical properties [2, 3]. In WIM we freeze the motion of the molecules and insert a test particle to the system and measure the insertion parameter,

$$B = \langle \exp(-\Psi/T) \rangle_\Omega,$$

(15)

where $\langle \rangle_\Omega$ denotes the ensemble average and $\Psi$ is the interaction energy of the test particle with the other particles in the
method to the PTA to extract the intensive variables. This similarity allows us to apply the Widom insertion in a molecular dynamics simulation, with the only difference. The particle basis serves as a counterpart of the classical particles at low temperatures. On the other hand, in PTA the single particle basis induces large uncertainties due to sign problem at very small volumes or different volumes. Despite of this fact the volume can only be inferred with an integration from the absolute zero, the limit of the lattice structure, the absolute free energy can be calculated exactly. However, this involves multiple calculations with different particle numbers or different volumes. Despite of the fact that the volume can not change continuously due to the finite volume together with the specific boundary condition induce fictitious shell structures for fermions. Especially, the finite volume together with the specific bound-ary condition induce fictitious shell structures for fermions. As only one particle is inserted/removed in each measurement, we found that the QWIM is very efficient and precise in calculating the chemical potential. In Fig. 7 we benchmark the QWIM using free nucleon gas, in which we turn off the interaction and the chemical potential can be calculated exactly. In grand-canonical ensemble the chemical potential µ can be determined by solving the equation

\[ \int_0^\Lambda \frac{\rho(\epsilon)}{1 + e^{-\beta(\epsilon - \mu)}} d\epsilon = A, \]  

where

\[ \rho(\epsilon) = \frac{2}{\pi} mV \sqrt{2m\epsilon} \]  

is the level density for free Fermion gas with two species, \( m \) is the nucleon mass, \( \Lambda = (\pi/a)^2/(2m) \) with \( a \) the lattice spacing is the energy cutoff imposed by the lattice. In Fig. 7 the solid line shows the exact solutions and the circles show lattice results calculated using the QWIM. The temperature is \( T = 10 \text{ MeV} \) and box size is \( L = 5 \). We found that the lattice results fit well to the exact solutions for \( A \leq 100 \). The deviation for small \( A \) is due to the difference between canonical (with a fixed \( A \)) and grand-canonical ensemble (with a fixed \( \mu \)).

### Finite volume effects

In nuclear matter and neutron matter calculations the results are usually contaminated by the finite volume effects. Especially, the finite volume together with the specific boundary condition induce fictitious shell structures for fermions. New lattice magic numbers for protons or neutrons emerges at which the calculated observables exhibit unphysical kinks. It was claimed that 66 particles for one-species Fermion give results close to the thermodynamic limit. This number was extensively used in most of the nuclear matter, neutron matter or cold atom simulations [4, 5]. However, in lattice effective field theory the lattice spacing is fixed and we are not allowed to change the volume continuously, leaving large gaps in scanning state variables like the densities. An alternative is to fix the volume and explore different densities by varying

\[
F(A \pm 1) - F(A) = -T \ln \left[ \frac{\langle B_{A+1} \rangle}{\langle A \pm 1 \rangle} \right].
\]

Finally, with symmetric difference formalism we have

\[
\mu = [F(A+1) - F(A-1)]/2 = -\frac{T}{2} \ln \left[ A(A+1) \frac{\langle B_{-1} \rangle}{\langle B_{1} \rangle} \right].
\]

In PTA the summations in Eq. (16) can be calculated using random sampling. For \( B_1 \) we insert a nucleon with random spin to random lattice site and propagate it through all time slices, while for \( B_{-1} \) we simply remove one of the existing nucleon. As only one particle is inserted/removed in each measurement, we found that the QWIM is very efficient and precise in calculating the chemical potential. In Fig. 7 we benchmark the QWIM using free nucleon gas, in which we turn off the interaction and the chemical potential can be calculated exactly. In grand-canonical ensemble the chemical potential \( \mu \) can be determined by solving the equation

\[
\int_0^\Lambda \frac{\rho(\epsilon)}{1 + e^{-\beta(\epsilon - \mu)}} d\epsilon = A,
\]

where

\[
\rho(\epsilon) = \frac{2}{\pi} mV \sqrt{2m\epsilon}
\]

is the level density for free Fermion gas with two species, \( m \) is the nucleon mass, \( \Lambda = (\pi/a)^2/(2m) \) with \( a \) the lattice spacing is the energy cutoff imposed by the lattice. In Fig. 7 the solid line shows the exact solutions and the circles show lattice results calculated using the QWIM. The temperature is \( T = 10 \text{ MeV} \) and box size is \( L = 5 \). We found that the lattice results fit well to the exact solutions for \( A \leq 100 \). The deviation for small \( A \) is due to the difference between canonical (with a fixed \( A \) and grand-canonical ensemble (with a fixed \( \mu \)).
the nucleon numbers. With this regard we must eliminate the fictitious shells explicitly.

The origin of the finite volume shell effects is the constraint imposed by the boundary conditions on the particle momenta. For a cubic box with periodic boundary conditions (PBC), particles are only allowed to have integer momenta \( p = \frac{2\pi}{L} n \), which results in a series of magic numbers 2, 14, 38, ... for one species Fermion. One solution is to apply the twisted boundary conditions (TBC) [6] which attach extra phases to wave functions when the particle cross the borders. TBC allows the particle to explore different momenta combinations other than the integer points prescribed by the PBC. In particular, averaging over all possible twist angles provides an efficient way of approaching the infinite volume limit [7, 8].

The TBC method was first proposed for exactly solvable models [7–11] and then found applications in quantum Monte Carlo methods [12]. Last few years have witnessed a boom in applying TBC to lattice QCD calculations to find infinite volume results otherwise not accessible with present computational power [13–16]. Meanwhile, application of TBC to lattice effective field theory is shown to be successful but still limited to few-body and exactly solvable systems [17]. In this section we discuss the application of the TBC to the lattice Monte Carlo calculations and show how it help us remove the annoying finite volume shell effects in thermodynamics calculations.

We apply the twisted boundary conditions to the single particle wave functions,

\[
\begin{align*}
\psi(x + L, y, z, \sigma, \tau) &= \exp(i2\sigma\theta_x)\psi(x, y, z, \sigma, \tau), \\
\psi(x, y + L, z, \sigma, \tau) &= \exp(i2\sigma\theta_y)\psi(x, y, z, \sigma, \tau), \\
\psi(x, y, z + L, \sigma, \tau) &= \exp(i2\sigma\theta_z)\psi(x, y, z, \sigma, \tau),
\end{align*}
\]

with \(-\pi \leq \theta_x, \theta_y, \theta_z \leq \pi\) the independent twist angles in three directions. Note that for spin \( \sigma = \pm 1/2 \) we use the opposite twist angles, which is necessary for avoiding the sign problem. In this paper we utilize the TBC by averaging over all possible \((\theta_x, \theta_y, \theta_z)\) (average twisted boundary conditions, ATBC). This can be easily implemented in Monte Carlo calculations by allocating every thread a random phase triplet with elements uniformly distributed in \([-\pi, \pi]\).

In Fig. 8 we compare the binding energies at \( T = 0 \), \( T = 16 \text{ MeV} \) and the chemical potential at \( T = 16 \text{ MeV} \) calculated with different boundary conditions. For the same density, different box sizes correspond to different nucleon...
numbers. The open symbols denote the results calculated with periodic boundary conditions, the full symbols show the results for the average twisted boundary conditions. Here we see clear shell effects for PBC calculations. For each box size the energy and chemical potential oscillates with respect to the nucleon number and exhibit extrema at lattice magic numbers $A = 4, 28, 76, \ldots$. The amplitudes of the oscillation are smaller for larger boxes, but for $L = 6$ the fictitious shell effects are still apparent. For example, for $T = 0$ MeV the energy minimum occurs at $\rho \approx 0.153$ fm$^{-3}$, which is just a shell effect corresponds to $A = 76$. These results can be misleading if we do not take into account the finite volume corrections.

With ATBC all kinks found above disappear and the results collapse into single curves. We found that even a small box $L = 4$ with ATBC is sufficient for giving converging results. In particular, the chemical potential or the Fermi level, which is very sensitive to the shell structure, can be precisely calculated. Based on these results, in the nuclear matter equation of state calculations presented in the main text, we use $L = 6$ together with the ATBC, which gives results sufficiently close to the infinite volume limit.

Some remarks must be added for the finite volume effects. Here we distinguish between finite volume effects and finite size effects. The former comes into play together with the boundary conditions and can be removed by using twisted boundary conditions. However, the latter is due to the finite particle number and manifests itself mainly through the surface effects. That is, the finite size effects are maximized for inhomogeneous systems, in particular, the system comprising of two or more phases. The contact surfaces of the different phases give positive contributions to the free energy, which will vanish at the thermodynamic limit. For example, for symmetric nuclear matter with sub-saturation density, the surface effects will eventually disappear.

The finite size effects scale with the surface-volume ratio, which in turn scales as $O(A^{-1/3})$ with respect to the nucleon number. Thus these effects decay very slowly and can not be removed with present computational settings. One example of the surface effects are the upbending of the $T = 0$ energy curves at low densities in Fig. 8. For infinite nuclear matter, at the sub-saturation densities the density and the binding energy per nucleon will be exactly the value at the saturation point. However, for finite systems the extra surface energy causes the upbending of the energy curve and makes it converging to the binding energy per nucleon of small nucleus in the vacuum, $E/A \approx -8$ MeV.

In Fig. 9 we show the energy per nucleon at $T = 0$ calculated with different box sizes. In order to show the finite size effects we have removed the finite volume effects by imposing the average twisted boundary conditions. The calculated energies at sub-saturation energy tend to increase with respect to the box size. However, the convergence is extremely slow. To reduce the finite size effects by one order of magnitude, we have to use $10^3$ times more nucleons and $10^3$ times larger volume, which is not affordable at present.

We must stress that the existence of the surface effects at phase coexistence is not a deficiency of our method. Instead of studying the infinite homogeneous matter, our method focuses on the real finite systems, which can also be prepared in the laboratory. The advantage of the ab initio calculation is that we can prepare the system under various constraints, including temperature, volume, pressure, etc., most of which are not directly accessible in the experiments. The phenomena involving strong correlations, like clustering and phase transition, can now be completely simulated starting from the scratch. Consequently, we believe that our formalism, together with the advanced nuclear interactions, will pave the way of fully understanding the nuclear thermodynamic processes.

### Interpolation and error analysis

In extracting the equation of state and critical point, we make an interpolation for the lattice results using the 5-th order virial expansion,

$$
\mu(\rho, T) = a_0 + a_1 \ln \rho + \sum_{i=1}^{4} a_{i+1} \rho^i,
$$

(22)

where $a_i$ are functions of $T$ and should be fitted for each isotherm separately. Note that this expression is only meant to parametrize the isotherms and the resulting parameters can not be compared directly with the real virial coefficients. For non-integer temperatures the chemical potential is obtained by cubic spline interpolation. The differentiation, integration, etc. are performed based on the interpolated equation of state.

The error in the critical values are estimated by the bootstrap method, by which we resample every lattice results with variance given by the Monte Carlo simulation several times,
and estimate the variance of the critical values by the resulting distribution.

[1] B. Widom, J. Chem. Phys. 39, 2808 (1963).
[2] K. Binder, Rep. Prog. Phys. 60, 487 (1997).
[3] R.P.A. Dullens, Mol. Phys. 103, 3195 (2005).
[4] M. Forbes, S. Gandolfi, and A. Gezerlis, Phys. Rev. Lett. 106, 235303 (2011).
[5] J. Carlson, Sefano Gandolfi, Kevin E. Schmidt, Shiwei Zhang, Phys. Rev. A 84, 061602R (2011).
[6] N. Byers and C. N. Yang, Phys. Rev. Letts. 7, 46 (1961).
[7] E. Y. Loh, Jr. and D. K. Campbell, Synthetic Metals 27, A499 (1988).
[8] R. Valenti, C. Gros, P. J. Hirschfeld and W. Stephan, Phys. Rev. B 44, 13203 (1991).
[9] C. Gros, Z. Phys. B 86, 359 (1992).
[10] J. Tinka Gammel, D. K. Campbell, and E. Y. Loh, Jr., Synthetic Metals 55, 4437 (1993).
[11] C. Gros, Phys. Rev. B 53, 6865 (1996).
[12] C. Lin, F.-H. Zong, D. M. Ceperley, Phys. Rev. E 64, 016702 (2001).
[13] Paulo F. Bedaque, Phys. Lett. B 593, 82 (2004).
[14] G. M. Divitiis, R. Petronzio, N. Tantalo, Phys. Lett. B 595, 408 (2004).
[15] Paulo F. Bedaque, Jiunn-Wei Chen, Phys. Lett. B 616, 208 (2005).
[16] C. T. Sachrajda, G. Villadoro, Phys. Lett. B 609, 73 (2005).
[17] C. Körber, T. Luu, Phys. Rev. C 93, 054002 (2016).