

Covariant formulation of relativistic quantum molecular dynamics for a system of interacting wave packets

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We present a new formulation for the mean-field propagation part of relativistic quantum molecular dynamics, simulating an N -body system of interacting Gaussian wave packets via Lorentz scalar and vector potentials. Covariant equations of motion are derived based on the principle of least action with a weak form of mass-shell conditions and time-fixation constraints defined with respect to a chosen foliation. However, as is common with traditional relativistic quantum molecular dynamics, the dynamics exhibits a residual dependence on the chosen foliation, which is unavoidable because a finite number of interacting degrees of freedom is not strictly compatible with relativity. Nevertheless, we show that this dependence remains small for physically reasonable choices of the foliation in practical applications. By introducing a new approximation method to the spatial integral in the equations of motion, these covariant equations of motion can be solved with a computational cost comparable to that of conventional noncovariant quantum molecular dynamics. Furthermore, the new equations of motion accurately estimate the density-dependent potential, as demonstrated through comparison of the forces with the numerical integration. We apply them to N -body systems interacting via the Skyrme-type potentials or the relativistic mean field to simulate heavy-ion collisions. Our results show that the derived equations of motion provide a robust approximation to the dynamics of the full numerical integrations.

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I. INTRODUCTION

Microscopic transport models based on kinetic theories have been successful tools for investigating heavy-ion collisions across a wide range of collision energies. The evolution of the one-body phase-space distribution function is described by transport equations such as the Boltzmann-Uehling-Uhlenbeck (BUU) [1–8] and its relativistic version (RBUU), which is formulated within the relativistic mean-field theory [9–15]. Quantum molecular dynamics (QMD) [16–22] and its relativistic version (RQMD) [23–28] follow the spacetime evolution of the N -body phase-space distribution, enabling event-by-event simulations of heavy-ion collisions. RQMD models incorporating relativistic mean-field theory have also been developed [29–31]. Furthermore, antisymmetrized molecular dynamics (AMD) [32,33] takes into account the fermionic nature of the nucleons.

These microscopic transport approaches include a Boltzmann-type collision term and the mean-field propagation to describe the nonequilibrium dynamics of nuclear reactions in a semiclassical way. For detailed comparisons of these

transport models, we refer the reader to the series of TMEP collaboration papers [34–39].

In this work, we focus on the development of the mean-field propagation in transport models. The BUU-type approach solves the time evolution of the one-body phase-space distribution function by using the test particle method, in which the distribution function is represented by an ensemble of oversampled particles [5]. These test particles follow Hamilton's equations of motion (EoMs). In the limit of an infinite number of test particles, the numerical solution converges to the exact solution. In practical numerical implementations of the BUU approach, a spatial grid is often introduced to evaluate the local density and its derivatives. However, due to the limited number of test particles, unphysical numerical fluctuations can arise, necessitating additional smearing of the particle distribution [6,40,41]. In the QMD approach, particles are represented by Gaussian wave packets, and their centroid coordinates and corresponding momenta evolve in time following the canonical EoMs. In the QMD approach, the total momentum is exactly conserved by construction in each event. However, in the traditional QMD calculations, an approximation is introduced in the evaluation of the density-dependent potential for nonlinear terms. This approximation results in a weaker gradient of the repulsive mean-field potential [37,39]. Consequently, the equation of state (EoS) of nuclear matter may not be accurately reflected during the dynamical evolution of the system in QMD. Several methods are proposed to improve the

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treatment of the density dependence of the potential in QMD [18,21,22].

In both the BUU and QMD approaches, more accurate calculation methods have been developed. In the BUU framework, the lattice Hamiltonian method [42–45] was introduced to solve the EoMs for the test particles, in which excellent energy and momentum conservation are achieved. For QMD models, the density-dependent potential is calculated exactly by numerical integration as implemented in ImQMD-L [46] and AMD [47]. However, no such calculations have been performed within relativistic models.

In this work, we propose a new consistent formulation of Lorentz-covariant EoMs with the finite-size Gaussian wave packets interacting via the scalar and vector potentials based on the manifestly covariant variational principle. Instead of imposing the mass-shell constraints on the centroids of the wave packets, we impose the mass-shell constraints in a weak form where each mass-shell constraint is satisfied after the phase-space integration over the Gaussian profile of the corresponding wave packet. This choice of the mass-shell constraints enables us to derive the consistent form of EoMs throughout different levels of treatment of the mean fields: We first derive the EoMs in the case of the mean fields being externally specified as external fields in Sec. III A and show that the dynamical-field case produces consistent EoMs in Sec. III B. This produces the “BUU-like” covariant EoMs. In Sec. III C, by explicitly considering the field part of the action including the effective self-interaction of the fields, we obtain the “BUU-like” EoMs also in the case of the mean fields determined by local densities through the self-consistent equations.

We also show that a “BUU-like” EoM, which is written with weighted spatial integration of a potential (typically a single-particle potential), can be transformed into “QMD-like” covariant EoMs, which is written with spatial integration of density derivatives of an integrated potential per particle (typically a one-particle potential energy [48]), in the case that the mean fields are evaluated from local densities. Since this is equivalent transformation, the “QMD-like” EoMs maintain energy-momentum conservation of the total system explicitly. The density-dependent potential written by spatial integration in the “QMD-like” EoMs will accurately be calculated by applying the Monte Carlo integration with the relativistic Gaussian weight. This establishes a basis for a better estimation of the EoS than previous RQMD approaches.

Based on this, to reduce the computational cost of the Monte Carlo integration in evaluating the forces for each particle at every time step, we propose an approximation to the spatial integration in the EoMs while controlling the approximation error. We demonstrate that the approximation provides a good agreement with the exact solution obtained through numerical integration. We note that our EoMs can also be used to propagate test particles in the BUU and RBUU models.

Although it is not the primary purpose of this work, another important aspect in telling the history of RQMD is the choice of the time fixations of temporal coordinates appearing in the formulation. In the RQMD-type approach, quantum dynamics is approximated using a finite number of degrees

of freedom, while an infinite number of local degrees such as dynamical fields are integrated out. To formulate relativistic N -particle system in a covariant manner, an $8N$ -dimensional phase space is introduced. To extract physical trajectories, $2N$ constraints are imposed, consisting of N -mass shell constraints and N -time fixation conditions. The time fixations fix the temporal coordinates of particles, but their choice is not unique. Ideally, since the choice of the time fixations is gauge degrees of freedom of specifying temporal coordinates of particles, it should not affect the physics, which is the time-reparametrization invariance. However, the idea of RQMD describing a system with a finite number of interacting degrees of freedom is explicitly incompatible with relativity and prohibits the exact time-reparametrization invariance because the interaction cannot be local with a finite number of degrees of freedom located on different spatial points.

In this perspective, one of the interests in formulating RQMD has been the design of reasonable time fixations that effectively capture the dynamics of real systems, while keeping violation of time-reparametrization invariance numerically small. Different prescriptions for determining the time fixations correspond to different models of RQMD. In the original RQMD approach [23,24], the time fixations are defined so that when two particles are close in space, their times coincide in their center-of-mass frame. Although the EoMs are formally given under this condition, issues with this formulation become clear in numerical implementations [27,49]. For example, at each two-body collision or decay, time-fixation conditions are violated, requiring the solution of a set of N -dimensional nonlinear equations. Such equations do not always admit solutions, or even when solutions exist, unphysical backward evolution may occur. Consequently, actual implementations are forced to introduce ad hoc modifications [24,49] at the EoM level. Later, simpler time-fixation schemes were proposed in Ref. [25], which yields results similar to those obtained with the original constraints [23], and have been widely adopted in subsequent studies [26–28,30,31,48]. In these schemes, the times of all particles are set equal in the global center-of-mass frame.

In the present paper, we introduce the spacetime foliation. A foliation is the family of spacelike hypersurfaces that defines simultaneity. The time-fixation condition is implemented as the constraint that assigns the particle coordinates to one hypersurface in the chosen foliation. Different choices of foliation may lead to residual foliation dependence.

It is useful to distinguish three related but different concepts. First, Lorentz covariance means that the EoMs retain the same form under Lorentz transformations when all four-vector quantities, including the particle coordinates, momenta, and the foliation vector, are transformed consistently. Second, Lorentz symmetry refers to the invariance of the physical dynamics under Lorentz transformations without changing the prescription that defines the theory. Third, the dependence on the choice of spacetime foliation is conceptually distinct from both Lorentz covariance and Lorentz symmetry. A formulation may, in general, exhibit a residual dependence on the chosen foliation while remaining Lorentz covariant.

The prescriptions of Sorge [23,24] and others [27,50–52] define the time-fixation condition through dynamical variables, although they have other well-known drawbacks such as difficulties with cluster separability or practical implementation. Maruyama's prescription [25] provides a simpler alternative by employing an externally specified foliation vector. Consequently, the resulting dynamics depends on the chosen foliation.

In the present work, we adopt the time-fixation prescription of Maruyama. The EoMs are Lorentz covariant in the sense that all four-vector quantities, including the foliation vector, are transformed consistently under Lorentz transformations and the equations retain the same form in any inertial frame. In interpretations where the foliation vector is regarded as an externally specified background structure, the residual foliation dependence corresponds to a violation of Lorentz symmetry. The present work does not attempt to construct a completely foliation-independent formulation. Instead, our objective is to establish a Lorentz-covariant formulation for a specified foliation and to quantify the residual foliation dependence. To this end, we perform a quantitative study of the foliation dependence and show that it remains weak for physically reasonable choices of the foliation. This residual foliation dependence should therefore be regarded as a controlled model dependence.

A covariant cascade method has been developed to simulate the Boltzmann-type collision term based on the constrained Hamiltonian formulation in Ref. [49]. Combining this covariant cascade method with the new mean-field EoMs enables us to perform event-by-event simulations of the space-time evolution of heavy-ion collisions in a fully covariant way within the RQMD approach. We have implemented our new EoMs into the event generator JAM2 [53], and performed simulations of heavy-ion collisions, which are compared with the results from the previous RQMD.

This paper is organized as follows. In Sec. II, we introduce the new QMD EoMs, which provide a good approximation to full integration and exactly conserve total momentum. In Sec. III, we derive the covariant EoMs based on the variational principle. After briefly summarizing the EoMs in Sec. IV A, the covariant EoMs are applied to the σ - ω type relativistic mean-field theory in Sec. IV B and Lorentz-vector Skyrme-type potentials in Sec. IV D. We present the results of our RQMD simulations for Au + Au collisions in Secs. IV C and IV E. Finally, a summary is provided in Sec. V.

II. MEAN-FIELD PART OF QUANTUM MOLECULAR DYNAMICS

We first discuss the nonrelativistic case. We consider the system of N nucleon system interacting with the density n -dependent single-particle potential $U(n)$ by the following Hamiltonian:

$$H = \frac{g_N}{(2\pi)^3} \int d^3x d^3p \frac{\mathbf{p}^2}{2m} f(\mathbf{x}, \mathbf{p}) + \int d^3x \int_0^{n(\mathbf{x})} U(n) dn, \quad (1)$$

where g_N is the degeneracy factor for spin and isospin, and we assume the Skyrme-type single-particle potential,

$$U(n) = \alpha \frac{n}{n_0} + \beta \left(\frac{n}{n_0} \right)^\gamma. \quad (2)$$

In the QMD approach [17,18,18–20], the total N -body wave function is assumed to be a direct product of Gaussian wave packets. Hamilton's EoMs of the N -body system are obtained from the variational principle. The zero-point kinetic energy appears due to Gaussian wave packets satisfying the uncertainty principle. In QMD, this zero-point kinetic energy is often dropped, which means that the Gaussian in the momentum space is replaced by the δ function [54]. We take the distribution function to be the sum of a Gaussian wave packet,

$$f(\mathbf{x}, \mathbf{p}) = \frac{(2\pi)^3}{g_N} \sum_{i=1}^N g(\mathbf{x} - \mathbf{x}_i) \delta(\mathbf{p} - \mathbf{p}_i). \quad (3)$$

The Gaussian for a particle is defined as

$$g(\mathbf{x} - \mathbf{x}_i) = \left(\frac{1}{2\pi L} \right)^{3/2} \exp \left(- \frac{[\mathbf{x} - \mathbf{x}_i(t)]^2}{2L} \right). \quad (4)$$

The local density $n(\mathbf{x})$ in Eq. (1) is evaluated by the sum of Gaussian profiles,

$$n(\mathbf{x}) = \frac{g_N}{(2\pi)^3} \int d^3p f(\mathbf{x}, \mathbf{p}) = \sum_{i=1}^N g(\mathbf{x} - \mathbf{x}_i). \quad (5)$$

Hamilton's equation for the i th particle yields

$$\frac{d\mathbf{x}_i}{dt} = \frac{\mathbf{p}_i}{m_i}, \quad \frac{d\mathbf{p}_i}{dt} = - \int d^3x U(n(\mathbf{x})) \frac{\partial g(\mathbf{x} - \mathbf{x}_i)}{\partial \mathbf{x}_i}. \quad (6)$$

After integrating Eq. (6) by parts or taking the differentiation of the Gaussian, the equation can be viewed as an integral with the Gaussian weight. In the harmonic approximation [13], the integration of a function $F(\mathbf{x})$ with a Gaussian weight is estimated by the value of the function at the center of the Gaussian:

$$\int d^3x F(\mathbf{x}) g(\mathbf{x} - \mathbf{x}_i) \approx F(\mathbf{x}_i). \quad (7)$$

This approximation yields the *BUU-like* equation within the QMD framework

$$\frac{d\mathbf{p}_i}{dt} = - \sum_{j=1}^N \frac{dU(n(\mathbf{x}_i))}{dn} \frac{\partial g(\mathbf{x}_i - \mathbf{x}_j)}{\partial \mathbf{x}_i}. \quad (8)$$

This EoM is the same as the one in the relativistic Landau-Vlasov method [13] in the nonrelativistic limit. In this approach, a particle's momentum changes by the mean-field potential $U(n)$ at its position.

We now consider the QMD framework. The key part of this study includes a new method to evaluate the potential integral in Eq. (6) numerically. Different existing models of QMD and BUU can be concisely summarized as the respective methods to evaluate the potential integral. After reviewing the existing methods, we propose an efficient and accurate way to evaluate the potential integral.

We first note that Eq. (6) includes the self-interaction of the i th particle through $n(\mathbf{x})$. In the Hartree-Fock method,

where the wave function for fermions is antisymmetrized, the self-interaction vanishes due to the cancellation of the Hartree and Fock terms. This is not enforced in the QMD framework, where the wave function is given by a direct product of Gaussian wave packets. To partially take account of the antisymmetrization of the fermion wave function, the self-interaction is typically excluded by hand,¹ replacing $n(\mathbf{x})$ with $n(\mathbf{x}) - g(\mathbf{x} - \mathbf{x}_i) = \sum_{j \neq i} g(\mathbf{x} - \mathbf{x}_j)$ in Eq. (6). However, this manual tweak of the EoMs introduces a subtlety in extension to the relativistic case. The fact that each particle feels a distinct density $n(\mathbf{x}) - g(\mathbf{x} - \mathbf{x}_i) = \sum_{j \neq i} g(\mathbf{x} - \mathbf{x}_j)$ ($i = 1, \dots, N$) implies that there are effectively N -independent local densities, which is incompatible with the relativistic picture of the interaction mediated by common dynamical fields as discussed in Sec. IV B. To avoid subtleties arising from the manual tweak and to be more consistent with the dynamical-field case, we fully consider the self-interaction in the main part of this study following the approach of the ImQMD model [55,56].

The QMD model uses the one-particle potential $V(n)$ [48], which is related with the single-particle potential by [57,58]

$$V(n) = \frac{1}{n} \int U(n) dn. \quad (9)$$

Using this one-particle potential, the Hamiltonian (1) can be rewritten as

$$H = \frac{g_N}{(2\pi)^3} \int d^3x d^3p \frac{\mathbf{p}^2}{2m} f(\mathbf{x}, \mathbf{p}) + \int d^3x n V(n). \quad (10)$$

In the traditional QMD, the potential term in the Hamiltonian (10) is evaluated by what we refer to as the *QMD approximation*. In this approximation, the spatial integral of the density-dependent potential becomes

$$\int d^3x n V(n) = \sum_{i=1}^N \int d^3x g(\mathbf{x} - \mathbf{x}_i) V(n) \approx \sum_{i=1}^N V(\langle n \rangle_i), \quad (11)$$

where the *interaction density* $\langle n \rangle_i$ is defined as the sum of Gaussian overlap,

$$\langle n \rangle_i = \sum_{j \neq i} \int d^3x g(\mathbf{x} - \mathbf{x}_i) g(\mathbf{x} - \mathbf{x}_j) = \sum_{j \neq i} g_{ij}, \quad (12)$$

where

$$g_{ij} = \frac{1}{(4\pi L)^{3/2}} \exp \left[-\frac{(\mathbf{x}_i - \mathbf{x}_j)^2}{4L} \right]. \quad (13)$$

The approximation (11) is symbolically stated as $\langle n^\gamma \rangle \approx \langle n \rangle^\gamma$, with $\langle A \rangle := \int d^3x' g(\mathbf{x}' - \mathbf{x}) A(\mathbf{x}')$, for a term in $V(n)$ proportional to n^γ (see also Eq. (44) of Ref. [48] and Eq. (11) of

Ref. [22]). Within this QMD approximation, the QMD EoM for the i th particle leads to

$$\frac{d\mathbf{p}_i}{dt} = - \sum_{j \neq i}^N \left[\left. \frac{dV(n)}{dn} \right|_{n=\langle n \rangle_i} + \left. \frac{dV(n)}{dn} \right|_{n=\langle n \rangle_j} \right] \frac{\partial g_{ij}}{\partial \mathbf{x}_i}. \quad (14)$$

The QMD EoMs take the form of the symmetric interaction between two particles so that the total momentum is exactly conserved. However, the density-dependent potential is not correctly estimated due to the approximation $\langle n^\gamma \rangle \approx \langle n \rangle^\gamma$ in the nonlinear case $\gamma \neq 1$.

In this paper, “BUU-like” EoMs are defined as the ones using the single-particle potential $U(n)$, such as Eqs. (6) and (8), while “QMD-like” EoMs are defined as the ones using the one-particle potential $V(n)$, such as Eqs. (14), (17), and (18).

It is practically possible to integrate the EoM (6) numerically. The lattice-Hamiltonian method in the BUU approach [42] divides the coordinate space into cells Δx and evaluates the derivatives as

$$\int d^3x U(n) \frac{\partial g(\mathbf{x} - \mathbf{x}_i)}{\partial \mathbf{x}_i} \approx \sum_{\alpha} (\Delta x)^3 U(n_{\alpha}) \frac{\partial g(\mathbf{x}_{\alpha} - \mathbf{x}_i)}{\partial \mathbf{x}_i}, \quad (15)$$

where α is a grid label, and n_{α} is the density in the grid cell α . The lattice-Hamiltonian method typically uses a triangle profile for $g(\mathbf{x} - \mathbf{x}_i)$. The energy-momentum has been confirmed to be conserved well in this method [42,43]. Within the QMD approaches, the numerical integration with the Gauss-Legendre quadrature was performed in ImQMD-L [46]. The Monte Carlo integration is used in the AMD model [47]. The Monte Carlo integration of Eq. (6) can be performed as

$$\begin{aligned} \frac{d\mathbf{p}_i}{dt} &= - \int d^3x U(n(\mathbf{x})) \frac{\mathbf{r} - \mathbf{r}_i}{L} g(\mathbf{x} - \mathbf{x}_i) \\ &\approx - \frac{1}{N_{\text{MC}}} \sum_{k=1}^{N_{\text{MC}}} U(n(\mathbf{x}_k)) \frac{\mathbf{r}_k - \mathbf{r}_i}{L}, \end{aligned} \quad (16)$$

where we sample the coordinates $\mathbf{x}_k$ according to the Gaussian distribution $g(\mathbf{x} - \mathbf{x}_i)$, and N_{MC} is the number of Monte Carlo sampling points.

Since the integration is numerically expensive, we consider another approximation for the potential integration. Instead of using the single-particle potential in Eq. (6), we use one-particle potential: from the Hamiltonian (10), we obtain

$$\frac{d\mathbf{p}_i}{dt} = - \int d^3x \left[V(n) + n \frac{dV(n)}{dn} \right] \frac{\partial g(\mathbf{x} - \mathbf{x}_i)}{\partial \mathbf{x}_i}. \quad (17)$$

After integrating the first term by parts and replacing the total density $n(\mathbf{x})$ by the sum of the Gaussian (5), we obtain

$$\begin{aligned} \frac{d\mathbf{p}_i}{dt} &= - \sum_{j=1}^N \int d^3x \left[\frac{dV(n)}{dn} \frac{\partial g(\mathbf{x} - \mathbf{x}_j)}{\partial \mathbf{x}} g(\mathbf{x} - \mathbf{x}_i) \right. \\ &\quad \left. + \frac{dV(n)}{dn} \frac{\partial g(\mathbf{x} - \mathbf{x}_i)}{\partial \mathbf{x}_i} g(\mathbf{x} - \mathbf{x}_j) \right]. \end{aligned} \quad (18)$$

We now approximate the derivatives of the potential term at the center of the Gaussian, and then take the Gaussian overlap

¹The actual EoMs are unaffected by this replacement only in the case of linear $U(n)$ [i.e., $\beta = 0$ in Eq. (2)]. In general, the exclusion of the self-interaction affects the EoMs in the presence of the non-linear potential term, which originates in microscopic three-body (or many-body) forces.

integration, which yields the EoMs,

$$\frac{d\mathbf{p}_i}{dt} \approx - \sum_{j=1}^N \left[\frac{dV(n(\mathbf{x}_i))}{dn} + \frac{dV(n(\mathbf{x}_j))}{dn} \right] \frac{\partial g_{ij}}{\partial \mathbf{x}_i}. \quad (19)$$

We refer to this procedure as the *QMD2 approximation*. These equations may be regarded as a variant of the Monte Carlo sampling with two sample points, where the points are fixed to be the representative points in Eq. (18), $\mathbf{x}_i$ and $\mathbf{x}_j$. These equations have the same structure as the EoMs for the traditional QMD approximation (14). They have the interaction term from the position of the other particles, and the total momentum is exactly conserved. These equations are exact for $\gamma = 1$, and as shown below, a good approximation for the density-dependent potential term is achieved for $\gamma \neq 1$. We note that the derivative of the one-particle potential is obtained by

$$\frac{dV(n)}{dn} = \frac{1}{n} [U(n) - V(n)]. \quad (20)$$

For the potential $U = n^\gamma$, the traditional QMD EoM becomes

$$\frac{d\mathbf{p}_i}{dt} = - \sum_{j \neq i}^N \frac{\gamma}{\gamma + 1} (\langle n \rangle_i^{\gamma-1} + \langle n \rangle_j^{\gamma-1}) \frac{\partial g_{ij}}{\partial \mathbf{x}_i}. \quad (21)$$

The difference between the traditional QMD EoM and our EoM is the following. The traditional QMD approach uses the interaction density (12), while we use the particle density (5). Thus, for the potential $U = n^\gamma$, the explicit expression of our EoM (19) is obtained by replacing the interaction density $\langle n \rangle_i$ in Eq. (21) with the particle density $n(\mathbf{x}_i)$:

$$\frac{d\mathbf{p}_i}{dt} = - \sum_{j \neq i}^N \frac{\gamma}{\gamma + 1} [n(\mathbf{x}_i)^{\gamma-1} + n(\mathbf{x}_j)^{\gamma-1}] \frac{\partial g_{ij}}{\partial \mathbf{x}_i}. \quad (22)$$

In Fig. 1, we compare the ratio of the absolute value of the force to the results from the numerical integration (16) for the potential $U(n) = n^\gamma$ in a two-particle system for QMD (21) and a new QMD (QMD2) (22). The traditional QMD significantly underestimates the absolute value of force for large γ , mainly because of the absence of self-interaction (i.e., the contribution from the wave packet of itself in the density evaluation), which is relevant in the two-particle system. Indeed, when self-interaction is included in the evaluation of the density in QMD, the ratio improves significantly from about 0.2 to 0.8 in the $\gamma = 2$ case. In contrast, our method, denoted by “QMD2,” provides a good approximation, as confirmed by comparison with numerical integration using the Monte Carlo integration with the Gaussian weight (16). We have checked that the Monte Carlo integration yields results practically identical to those obtained with the Gauss-Legendre quadrature method, while the Monte Carlo integration is much faster than the Gauss-Legendre quadrature method.

In the case of heavy-ion collisions such as Au + Au collisions, the total number of nucleons is typically 400. To mimic such situations, we sample 400 nucleons inside a sphere, where the density of the system is controlled by the radius of the sphere. Figure 2 represents the baryon density dependence of the ratio of the absolute value of the force to the

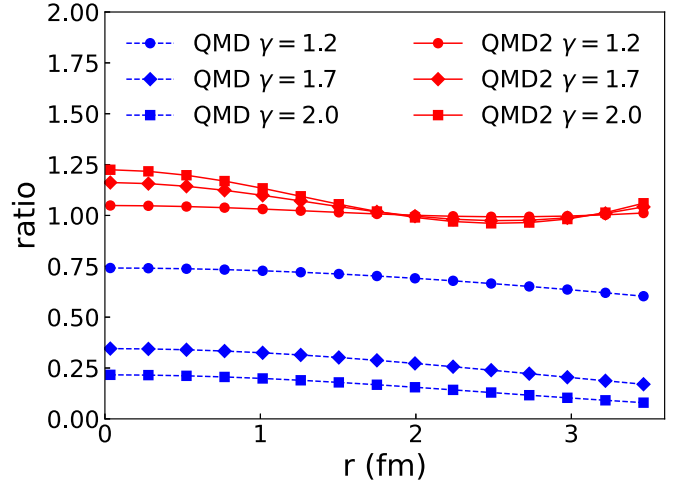


FIG. 1. Ratios of the absolute value of the force for the potential $U(n) = n^\gamma$ to the numerical integration in the two-particle case are plotted as a function of the separation between two Gaussians. The results from the traditional QMD are shown by the dashed lines, while those from the new method (denoted as QMD2) are shown by the solid lines. A Gaussian width $L = 2.0 \text{ fm}^2$ is used. The circles, diamonds, and squares correspond to results for $\gamma = 1.2$, 1.7 , and 2.0 , respectively.

Monte Carlo integration result for the 400-nucleon system. We randomly chose one particle and computed its force and average over events. We compare the traditional QMD results with our results. Our formula is found to provide a good approximation over a wide range of densities. We have checked that when particles are chosen from the center or surface, our approximation method still performs well. The traditional QMD results agree well with the exact solution for $\gamma = 1.2$, which corresponds to the value typically used for a soft EoS. However, for larger values of γ , the traditional QMD underestimates by about 20%, in contrast to the two-particle system. This is because the self-interaction is less relevant in systems

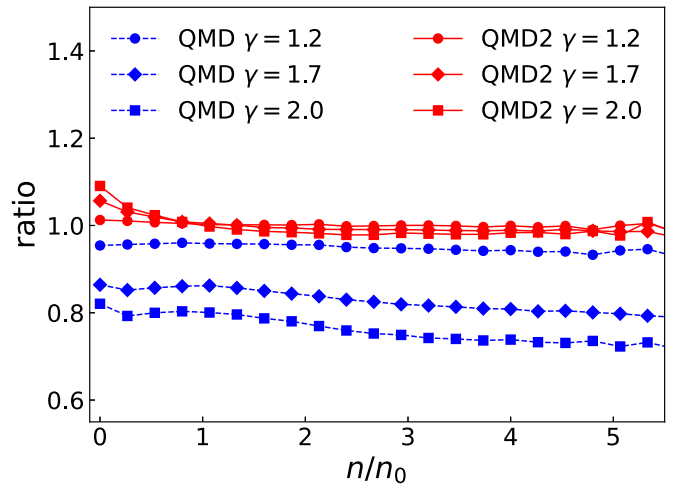


FIG. 2. Same as Fig. 1 but as a function of normalized baryon density for a system of 400 particles sampled randomly inside a sphere.

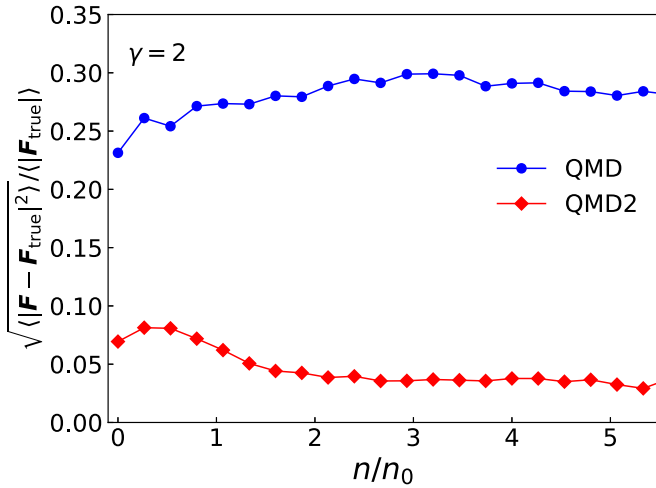


FIG. 3. Same as Fig. 2 but the root-mean-square deviation of the force is plotted.

with a large number of particles. When self-interaction is included in QMD, the results does not change much for the 400 particle case. The main reason for the underestimation in the QMD model is the use of the interaction density when evaluating the local density. Note that the Gaussian width of the interaction density (12) is $\sqrt{2}$ times larger than that of the local density (5).

To further see the accuracy of the approximation, we plot in Fig. 3, the relative root-mean-square deviation (RMSD),

$$\frac{\sqrt{\langle |\mathbf{F} - \mathbf{F}_{\text{true}}|^2 \rangle}}{\langle |\mathbf{F}_{\text{true}}| \rangle}, \quad (23)$$

as a function of the baryon density for the potential parameter $\gamma = 2$. One can see that the event-by-event deviation observed with the QMD approximation of the spatial integral is significantly reduced by the new QMD2 approximation.

III. VARIATIONAL FORMULATION OF RQMD

We present a new covariant formulation of the mean-field part of the EoMs in RQMD, which extends QMD to systems of relativistically interacting wave packets via the scalar and vector potentials.

In this work, we provide a manifestly covariant formulation of RQMD based on the variational principle. Specifically, we adopt the modified Hamilton's principle (also known as the Weiss action principle), which is the variational principle within the Hamiltonian formalism to ensure Lorentz covariance. A more detailed discussion of this formulation, including its relation to the standard Hamiltonian formulation and Dirac's constrained Hamiltonian method, will be presented in a separate paper.

For simplicity, we consider a single species of particles; however, the extension to multispecies is straightforward. We study an N -particle system interacting through the single-particle Lorentz scalar and vector potentials, $U_s(x, p)$ and $U^\mu(x, p)$, which generally depend on the eight-dimensional phase space (x, p) , where x^μ and p^μ are the spacetime coordinates and the corresponding canonical momentum. The

effective mass $m^*(x, p)$ and kinetic momentum $p^*(x, p)$ are defined as

$$m^*(x, p) = m + U_s(x, p), \quad (24)$$

$$p^{*\mu}(x, p) = p^\mu - U^\mu(x, p), \quad (25)$$

where m is the bare mass. We discuss three different treatments of the single-particle potentials: the cases with “external fields,” “dynamical fields,” and “local density approximation” in Secs. III A–III C. The actual meanings of the three terms will be explained in the respective sections.

A. External fields

For the external-field case, we assume the following form of the Weiss action for an interacting N -particle system:

$$S_{\text{part}}[\{x_i, p_i\}_i] = \sum_{i=1}^N \int p_i(s) \cdot \frac{dx_i(s)}{ds} ds - \int d^4x d^4p W(x, p) f(x, p), \quad (26)$$

where $W(x, p)$ is the *generalized potential* [11]:

$$W(x, p) = \frac{p^{*2}(x, p) - m^{*2}(x, p)}{2}. \quad (27)$$

The physical state of $f(x, p)$ is constrained by the mass-shell condition [11, 12] as

$$W(x, p) f(x, p) = 0, \quad \text{for any } x, p \in \mathbb{R}^{3,1}, \quad (28)$$

which requires $f(x, p)$ to vanish outside the physical hypersurface specified by $W(x, p) = 0$. However, Eq. (28) is too strong when we approximate the distribution function $f(x, p)$ with a parametrized form such as the Gaussian form. Equation (28) imposes an infinite number of constraints, which cannot be satisfied in general by adjusting only a finite number of parameters $\{x_i, p_i\}_i$, unless the parametrized form is intentionally designed to satisfy Eq. (28) in advance. Later in this section, we will find a weaker form of the mass-shell constraints (44).

The action (26) is a functional of the phase-space particle trajectories $\{x_i(s), p_i(s)\}_{i=1}^N$, where the particle trajectories are the functions of a Lorentz-invariant evolution parameter s . In the Weiss action principle, independent variations of four-coordinates $x_i(s)$ and four-momenta $p_i(s)$ are considered. It is straightforward to extend the action for the case of multiple particle species by giving S_{part} as the sum over the different species: $\sum_B S_{\text{part}}^B$.

To formulate the dynamics based on the variational principle for the action (26), we first specify the phase-space density $f(x, p)$ as a functional of the phase-space trajectories $\{x_i(s), p_i(s)\}_i$. We assume that the distribution function $f(x, p)$ is expressed by a sum of single-particle distributions:

$$f(x, p) = \sum_{i=1}^N f_i(x, p). \quad (29)$$

Here, we define the single-particle phase-space density $f_i(x, p)$ for the i th particle as a functional of its phase-space

trajectory $(x_i(s), p_i(s))$:

$$f_i(x, p) = \int ds \lambda_i(s) G(x, p; x_i(s), p_i(s)), \quad (30)$$

with

$$G(x, p; x_i, p_i) := \delta(\hat{s}(x) - \hat{s}(x_i)) g(x, p; x_i, p_i), \quad (31)$$

where $\hat{s}(x)$ is a Lorentz-scalar field² externally specified to foliate spacetime into a series of spacelike equal-time hypersurfaces: $\Sigma_s = \{x \in \mathbb{R}^{3,1} \mid \hat{s}(x) = s\}$. The foliation dependence of the resulting dynamics will be discussed later in Sec. III D. The proper choice of the functional form of the particle profile $g(x, p; x_i, p_i)$ depends on the choice of $\hat{s}(x)$, as the normalization must hold on each hypersurface Σ_s :

$$\int d^4x d^4p \delta(\hat{s}(x) - s) g(x, p; x', p') = 1, \quad (32)$$

for any $s \in \mathbb{R}$, $p' \in \mathbb{R}^{3,1}$, and $x' \in \Sigma_s$. The undetermined coefficient $\lambda_i(s)$ will be specified later to ensure that $x_i^\mu(s)$ lies on the hypersurface Σ_s of the same time s , i.e., $\hat{s}(x_i(s)) = s$.³ The form (30) of the distribution function can be regarded as an extension of the one in Ref. [13], with the identification $\hat{s}(x) = x \cdot u_i$, but an important difference is that we use a single common time function $\hat{s}(x)$ for all the particles to foliate the spacetime consistently in the presence of interaction between particles.

As in Sec. IV for the application, the particle profile is often taken to be the Lorentz-contracted Gaussian form (75)–(78), which depends on the velocity of the particle u_i . In the non-interacting case, the velocity can be written as $u_i^\mu = p_i^\mu / m_i$, where $m_i = \sqrt{p_i^\mu p_{i\mu}}$. However, in the interacting case, the expression of the velocity u_i as a function of (x_i, p_i) is unknown until we obtain EoMs, which implies the necessity of the special treatment of the u_i dependence of the profile $g(x - x_i, p - p_i; u_i)$ in the derivation step of the EoMs. A full treatment of the u_i dependence would require the modification in the variational principle because the “Hamiltonian” becomes a function of the velocity $\dot{x}_i$ in addition to x_i and

p_i . In the present study, we ignore the u_i dependence of the profile in the derivation step, as if we already know the expression of the velocity in terms of (x_i, p_i) . As will be discussed in Sec. IV, this approximate treatment leaves a small problem in the derived EoMs, but it is expected to be negligible in the slow-acceleration regime. A full treatment of the variation with explicit velocity dependence is left for future studies.

The principle of least action yields the following Hamilton’s EoMs for the i th particle:

$$\frac{dx_i^\mu}{ds} = \frac{\partial H}{\partial p_{i\mu}}, \quad \frac{dp_i^\mu}{ds} = -\frac{\partial H}{\partial x_{i\mu}}, \quad (33)$$

where the Hamiltonian is identified as

$$H(\{x_i, p_i\}) = \sum_{i=1}^N \lambda_i \bar{W}(x_i, p_i), \quad (34)$$

$$\bar{W}(x_i, p_i) = \int d^4x d^4p W(x, p) G(x, p; x_i, p_i). \quad (35)$$

Thus, the EoMs can be transformed into

$$\frac{dx_i^\mu}{ds} = \lambda_i \bar{\Pi}_i^\mu, \quad \frac{dp_i^\mu}{ds} = -\lambda_i \bar{Q}_i^\mu, \quad (36)$$

where

$$\bar{\Pi}_i^\mu := \int d^4x d^4p W(x, p) \frac{\partial G(x, p; x_i, p_i)}{\partial p_{i\mu}}, \quad (37)$$

$$\bar{Q}_i^\mu := \int d^4x d^4p W(x, p) \frac{\partial G(x, p; x_i, p_i)}{\partial x_{i\mu}}. \quad (38)$$

The coefficients λ_i are determined to satisfy

$$\hat{s}(x_i(s)) = s, \quad (39)$$

i.e., $d\hat{s}(x_i(s))/ds = 1$:

$$\lambda_i = \frac{1}{\bar{\Pi}_i \cdot a_i}, \quad a_i^\mu := \frac{\partial \hat{s}(x_i)}{\partial x_{i\mu}}, \quad (40)$$

where we note that a_i^μ forms a contravariant Lorentz vector.⁴

To solve the dynamics as an initial-value problem consistently, it is practically necessary to use the above form of EoMs (36), which are expressed with the common evolution parameter s . Nevertheless, it is useful to examine the form of the EoMs that uses the proper time of each particle, $\tau_i = \int \sqrt{dx_i^\mu dx_{i\mu}}$:

$$\frac{dx_i^\mu}{d\tau_i} = \frac{\bar{\Pi}_i^\mu}{\bar{m}_i} \equiv u_i^\mu, \quad \frac{dp_i^\mu}{d\tau_i} = -\frac{\bar{Q}_i^\mu}{\bar{m}_i}, \quad (41)$$

²The statement that $\hat{s}(x)$ is a Lorentz-scalar field means that the scalar field $\hat{s}(x)$ experiences the proper transformation $\hat{s}(x) \mapsto \hat{s}'(x') = \hat{s}(\Lambda^{-1}x')$ on the coordinate transformation for the change of the reference frame $x \mapsto x' = \Lambda x$, where Λ is a Lorentz transformation. It also means that the field $\hat{s}(x)$ undergoes the proper transformation $\hat{s}(x) \mapsto \hat{s}'(x') = \hat{s}(x - \epsilon)$ for the translation transformation $x^\mu \mapsto x'^\mu = x^\mu + \epsilon^\mu$, with ϵ^μ being a constant displacement. In this sense, strictly speaking, it may be more appropriate to call it a Poincaré-scalar field instead of a Lorentz-scalar field, but we here simply refer to it as a Lorentz-scalar field by convention.

³Using this dynamical constraint $\hat{s}(x_i(s)) = s$ retroactively, one might think it would be useful to simplify the δ function in Eq. (30) as $\delta(\hat{s}(x) - s)$, and thus $f_i(x, p) = \lambda(\hat{s}(x)) g(x, p; x_i(\hat{s}(x)), p_i(\hat{s}(x)))$. However, if such rewriting is performed on $f_i(x, p)$ in the action, then it breaks the dynamics because it effectively introduces an explicit dependence on the time parameter s into the Hamiltonian, i.e., temporal translation symmetry is broken. For example, the weak mass-shell constraint (44) is broken by an extra term $\partial \bar{W}_i / \partial s$ in Eq. (45).

⁴The statement that a_i^μ is a contravariant Lorentz vector specifically means that a_i^μ transforms as a contravariant Lorentz vector under changes of the reference frame. This is by construction because the field $\hat{s}(x)$ is defined to be a Lorentz-scalar field and the derivative with respect to the coordinates $x_{i\mu}$ with the lower Lorentz index, $\partial/\partial x_{i\mu}$, forms a contravariant vector.

where $\bar{m}_i = \sqrt{\bar{\Pi}_i^\mu \bar{\Pi}_{i\mu}}$, and $u_i^\mu = dx_i^\mu/d\tau_i$ is the four-velocity of the i th particle. Here, $\bar{\Pi}_i^\mu$ and $\bar{m}_i$ are the *generalized momentum and mass*, respectively. When the potentials do not depend on the momentum, they are identical to the kinetic ones, $\bar{\Pi}_i = p_i^*$ and $\bar{m}_i = m_i^*$ within the harmonic approximation (7) of Eq. (35). Using

$$\frac{d\tau_i}{ds} = \sqrt{\frac{dx_i^\mu}{ds} \frac{dx_{i\mu}}{ds}} = \lambda_i \bar{m}_i = \frac{1}{u_i \cdot a_i}, \quad (42)$$

we may obtain another representation of the EoMs:

$$\frac{dx_i^\mu}{d\tau_i} = u_i \cdot a_i \frac{\partial H}{\partial p_{i\mu}}, \quad \frac{dp_i^\mu}{d\tau_i} = -u_i \cdot a_i \frac{\partial H}{\partial x_{i\mu}}. \quad (43)$$

If we choose the time function to be the time in the inertial frame of the i th particle (i.e., $\hat{s}(x) = u_i \cdot x$), then the factor $u_i \cdot a_i$ reduces to unity. If we choose the time function to be the time in the reference frame (i.e., $\hat{s}(x) = x_{\text{ref}}^0$), then the factor $u_i \cdot a_i$ reduces to the Lorentz factor u_i^0 .

A weak form of the mass-shell constraints (28),

$$\bar{W}(x_i, p_i) = 0, \quad (i = 1, \dots, N), \quad (44)$$

is satisfied for any time s for the solution of EoMs if we assume it holds at the initial time s_0 because

$$\begin{aligned} \frac{d\bar{W}_i}{ds} &= [H, \bar{W}_i] \\ &= \sum_{j=1}^N ([\lambda_j, \bar{W}_i] \bar{W}_j + \lambda_j [\bar{W}_j, \bar{W}_i]) = 0, \end{aligned} \quad (45)$$

where the Poisson bracket is defined as

$$[A, B] = \sum_{i=1}^N \left(\frac{\partial A}{\partial p_i} \cdot \frac{\partial B}{\partial x_i} - \frac{\partial A}{\partial x_i} \cdot \frac{\partial B}{\partial p_i} \right). \quad (46)$$

Similar to the constrained Hamiltonian formulation [23,50–52], the $2N$ -constraints (39) and (44) reduce the phase space from $8N$ dimensions to the physical $6N$ dimensions.

B. Dynamical fields

In the dynamical-field case, the action is written as the sum of the particle part (26) and the field part S_{field} :

$$S[\{x_i, p_i\}_i, \Sigma] = S_{\text{part}}[\{x_i, p_i\}_i, \Sigma] + S_{\text{field}}[\Sigma]. \quad (47)$$

This is a functional of the phase-space particle trajectories $\{x_i(s), p_i(s)\}_i$ and the field degrees of freedom collectively denoted by $\Sigma(x)$. The actual set of fields in Σ depends on the system. For example, in the case of the σ - ω model (which we will discuss in Sec. IV B), the dynamical fields are identified to be the scalar and vector fields: $\Sigma(x) = (\sigma(x), \omega_\mu(x))$. Consequently, $p^*[\mathbf{x}, p, \Sigma]$, $m^*[\mathbf{x}, p, \Sigma]$, $W[\mathbf{x}, p, \Sigma]$, and $\bar{W}[\mathbf{x}, p, \Sigma]$ become functionals of Σ . The particle part S_{part} is given by Eq. (26) and includes their interaction with the fields, where $U_s(x, p)$ and $U_\mu(x, p)$ appearing in $m^*(x, p)$ and $p^*(x, p)$ of $W(x, p)$ are given by the field degrees $\Sigma(x)$. The field part $S_{\text{field}}[\Sigma]$ is a normal action

for the fields times an extra negative sign;⁵ we consider the Weiss action principle for the particle part and the normal variation for the dynamical fields $\Sigma(x)$. The field part contains only the self-interactions of the fields. In this section, we omit the explicit form of the field part of the action because it is irrelevant in deriving the EoMs for particles.

The EoMs for the particles turn out to be identical to the EoMs (36)–(40) derived for the external-field case. This is because the new term $S_{\text{field}}[\Sigma]$ in the action does not depend on the particle degrees of freedom, and thus it does not contribute to the variation with respect to $\delta x_i(s)$ and $\delta p_i(s)$.

Consequently, the discussions regarding the particle EoMs for the external-field case in Sec. III A remain valid for the dynamical-field case, except for the weak mass-shell constraints (44). The original proof (45) of the weak mass-shell constraints in the external-field case is no longer applicable because the field degrees of freedom are involved. The proof for the dynamical-field case is the following: First, we note that

$$\frac{d\bar{W}_i}{ds} = \int d^4x d^4p W(x, p) \frac{dG_i}{ds}, \quad (48)$$

with $G_i := G(x, p; x_i, p_i)$ being defined in Eq. (31). It should be noted that $dW(x, p)/ds = 0$ because the evolution parameter in the generalized potential $W(x, p)$ ⁶ is specified by the integral variable x through $\hat{s}(x)$ and is independent of the evolution parameter s specified externally. Since G_i is a function of x_i and p_i and independent of the field degrees of freedom Σ , its time derivative can be expanded as

$$\frac{dG_i}{ds} = \frac{dx_i^\mu}{ds} \frac{\partial G_i}{\partial x_i^\mu} + \frac{dp_i^\mu}{ds} \frac{\partial G_i}{\partial p_i^\mu}. \quad (49)$$

Plugging this into Eq. (48) and using EoMs (36), we obtain

$$\begin{aligned} \frac{d\bar{W}_i}{ds} &= \frac{dx_i^\mu}{ds} \int d^4x d^4p W(x, p) \frac{\partial G_i}{\partial x_i^\mu} \\ &\quad + \frac{dp_i^\mu}{ds} \int d^4x d^4p W(x, p) \frac{\partial G_i}{\partial p_i^\mu} \\ &= (\lambda_i \bar{\Pi}_i^\mu) \bar{Q}_{i\mu} + (-\lambda_i \bar{Q}_i^\mu) \bar{\Pi}_{i\mu} = 0, \end{aligned} \quad (50)$$

and hence $\bar{W}_i \equiv 0$ if it initially vanishes.

Finally, we note that one can recover the same EoMs in the RBUU approach when the harmonic approximation is applied to both the coordinate and momentum parts of the particle profile. In this case, the weak mass-shell constraints (44) become exact at the center of the profile:

$$W(x_i, p_i) = 0, \quad (51)$$

⁵The extra negative sign is present to be consistent with the sign in S_{part} written by $\bar{W}_i$; the mass-shell constraint W_i for the i th particle in the current action effectively has a negative sign relative to the single-particle energy E_i in the normal Hamiltonian, as observed in $(1/E_i^*) \partial W_i / \partial p_i \sim -p_i^* / E_i^*$ and $\partial E_i / \partial p_i \sim p_i^* / E_i^*$.

⁶ $W(x, p)$ is written in terms of $p^*(x, p)$ and $m^*(x, p)$. Then, $p^*(x, p)$ and $m^*(x, p)$ are determined by the field degrees of freedom Σ , and Σ is determined by field EoMs as a function of the evolution parameter s in the dynamical-field case.

which leads to the EoMs,

$$\frac{dx_i^\mu}{d\tau_i} = \frac{\Pi^\mu(x_i, p_i)}{\tilde{m}_i}, \quad \frac{dp_i^\mu}{d\tau_i} = -\frac{Q^\mu(x_i, p_i)}{\tilde{m}_i}, \quad (52)$$

where $\tilde{m}_i = \sqrt{\Pi^\mu(x_i, p_i)\Pi_\mu(x_i, p_i)}$. These equations are identical to those derived in the RBUU approach in Ref. [11]. Furthermore, they extend the equations presented in Ref. [13] by including the momentum-dependent potential.

C. Local density approximation

In the previous section, Sec. III B, we have considered the dynamical-field case, where the particle and field degrees of freedom, $\{x_i, p_i\}_i$ and $\Sigma(x)$, are independent variables. The single-particle potentials, $U_s(x, p)$ and $U_\mu(x, p)$, appearing in $m^*(x, p)$ (24) and $p_\mu^*(x, p)$ (25), are determined by $\Sigma(x)$ but do not directly depend on $\{x_i, p_i\}_i$.

However, in the numerical implementation, the derivatives of the meson fields, namely, the kinetic terms of the fields, are often neglected. As a result, the meson fields are determined from the present configuration of particles, $\{x_i, p_i\}_i$. This approximation is called the local density approximation [11]. In other words, to formulate the dynamics purely in terms of the particle degrees of freedom, we may specify $U_s(x, p)$ and $U_\mu(x, p)$ using the local quantity determined by the particle degrees of freedom $\{x_i, p_i\}_i$. In this work, we consider the general case of the local density approximation, where the effective mass and the kinetic momentum depend not only on the local scalar and vector densities but also on the local momentum distribution $f(x, p)$ because of the momentum-dependent potential [11].

Under the local density approximation, $U_s(x, p)$ and $U_\mu(x, p)$ are functions of phase-space variables of particles, $\{x_i, p_i\}$, and subject to variation by the particle trajectories. We first introduce the free-energy functional $F[\phi, \phi_\mu]$ to give $U_s(x, p)$ and $U_\mu(x, p)$ consistently. We then show that the form of the particles' EoMs matches the dynamical-field case, Eqs. (33)–(35). This owes to the exact cancellation of the contributions from the variation of $U_s(x, p)$ and $U_\mu(x, p)$ and that of the field energy.

To define the free-energy functional, we first introduce new fields, the scalar and vector distributions, $\phi(x, p)$ and $\phi_\mu(x, p)$, with $x, p \in \mathbb{R}^{3,1}$, and $\mu = 0, 1, 2, 3$. We consider the free energy functional $F[\phi, \phi_\mu]$ as an arbitrary functional of $\phi(x, p)$ and $\phi_\mu(x, p)$. This generalizes the total potential energy in the nonrelativistic case in Refs. [5, 48] (see Eq. (E.2) of Ref. [5] and Eq. (9) in Ref. [48]) to the relativistic case.

Using the free-energy functional $F[\phi, \phi_\mu]$, the single-particle potentials are written as

$$U_s(x, p) = \frac{\delta F[\phi, \phi_\mu]}{\delta \phi(x, p)}, \quad (53)$$

$$U_\mu(x, p) = g_{\mu\nu} \frac{\delta F[\phi, \phi_\mu]}{\delta \phi_\nu(x, p)}, \quad (54)$$

where $\phi(x, p)$ and $\phi_\mu(x, p)$ are determined by solving the self-consistent equations,

$$\phi(x, p) = m^*(x, p)f(x, p), \quad (55)$$

$$\phi_\mu(x, p) = p_\mu^*(x, p)f(x, p), \quad (56)$$

combined with Eqs. (24), (25), (53), and (54). The distribution function $f(x, p)$ is specified externally but can optionally depend on $m^*(x, p)$ and $p_\mu^*(x, p)$ in solving the self-consistent equations.

To consider the N -particle dynamics, we give the distribution function $f(x, p)$ in terms of the phase-space variables $\{x_i, p_i\}_{i=1}^N$. In this case, $m^*(x, p)$, $p_\mu^*(x, p)$, $\phi(x, p)$, and $\phi_\mu(x, p)$ become functions of $\{x_i, p_i\}_i$. We give the action by

$$S[\{x_i, p_i\}_i] = S_{\text{part}}[\{x_i, p_i\}_i] + S_{\text{field}}[\{x_i, p_i\}_i], \quad (57)$$

with the particle part S_{part} being Eq. (26). The field part of the action is identified⁵ as

$$S_{\text{field}} = V_{\text{field}}, \quad (58)$$

with the field potential functional V_{field} being the Legendre transform of the free-energy functional:

$$V_{\text{field}}[\phi, \phi_\mu] = F[\phi, \phi_\mu] - \int d^4x d^4p \times \left\{ \phi(x, p) \frac{\delta F[\phi, \phi_\mu]}{\delta \phi(x, p)} + \phi_\mu(x, p) \frac{\delta F[\phi, \phi_\mu]}{\delta \phi_\mu(x, p)} \right\}. \quad (59)$$

It should be noted that the fields $\Sigma(x)$ in Eq. (26) are no longer dynamical degrees in this setup and determined by the particle degrees of freedom, $\{x_i, p_i\}_i$.

The variation of the action is expressed as

$$\delta S = \delta \int ds \sum_i p_i \cdot \frac{dx_i}{ds} - \int d^4x d^4p W(x, p) \delta f(x, p) - \int d^4x d^4p \delta W(x, p) f(x, p) + \delta V_{\text{field}}. \quad (60)$$

The first line matches the variation of the action with respect to the particle degrees discussed in Sec. III B. The second line corresponds to the variation through the fields specified by the particle degrees. We can show that two terms on the second line exactly cancel with each other (see Appendix A):

$$- \int d^4x d^4p \delta W(x, p) f(x, p) + \delta V_{\text{field}} = 0. \quad (61)$$

As a result, the substantial part of the variation of the action is only the first line of Eq. (60), which matches the variation of the particle part of the action in the external-field case.

For this reason, with the local density approximation, the least action principle yields exactly the same form of EoMs as Eqs. (36)–(40) for the external- and dynamical-field cases in Secs. III A and III B. The only difference is that the potentials $U_s(x, p)$ and $U_\mu(x, p)$ are given by the particle degrees, while they are given independently of the particle degrees in Sec. III B.

This result is reasonable: If we first derive the EoMs for the dynamical-field case and then take the limit where the kinetic terms of the dynamical fields vanish, the form of the particle EoMs remains unchanged during taking the limit. Therefore, it is not surprising that we obtain the same form of the EoMs even when we instead first apply the local density approximation to the action and then derive the EoMs for the particles.

Finally, we shall check the weak mass-shell constraints (44) in the case of the local density approximation. Since the EoMs have the same structure as the dynamical-field case, Eqs. (48)–(50) also apply to the present case with the local density approximation. Thus, the weak form of the mass-shell constraint (44) is preserved by the local density approximation.

D. Foliation dependence and uniform foliation

We finally discuss the foliation dependence of the obtained dynamics. So far, we discussed the formalism with the general foliation $\hat{s}(x)$. However, we shall note that the dynamics depends on the choice of the foliation $\hat{s}(x)$ in this formulation in general, which means that different physics results may be obtained for different choices of the foliation. We have discussed the time-fixation dependence of the RQMD frameworks in the introduction. The foliation dependence is the manifestation of the time-fixation dependence within the present formulation, and this explicitly breaks the time-reparametrization invariance of the dynamics despite the covariant forms of the EoMs. This comes from effective nonlocal interactions in the RQMD framework, where interaction happens between two spatially distant coordinates on a time hypersurface in the current choice of the foliation. As discussed in the introduction, this is an unavoidable consequence of in relativistic N -body particle dynamics of a finite number of degrees of freedom interacting with each other [50]. In practical applications, it needs to be checked that the results do not largely depend on different choices of reasonable foliations, as will be done in Sec. IV F in the present study. It is noted that the foliation dependence is eliminated in the limit of the δ particle profile with an infinite number of test particles as in the RBUU approach or in the case of the point particles interacting through dynamical fields.

To perform actual calculations, we need to specify an appropriate foliation that roughly traces the proper time of the matter. In the subsequent discussions, motivated by the time-fixation conditions used in Refs. [25–28,30,31,48], we suppose the uniform foliation $\hat{s}(x) = \hat{a} \cdot x$ with $\hat{a}^\mu$ normalized as $\hat{a}^\mu \hat{a}_\mu = 1$. However, it should be emphasized here that we define $\hat{a}^\mu$ as a Lorentz vector⁷ so that $\hat{s}(x)$ is a Lorentz-scalar field. This choice implies that the times x_i^0 of all particles are the same in the specific inertial frame in which $\hat{s}(x) = \hat{a} \cdot x = x^0$ is satisfied.⁸ In other words, we impose the N time-fixation

conditions:

$$\hat{a} \cdot x_i - s = 0, \quad (i = 1, \dots, N), \quad (62)$$

where s is the Lorentz invariant evolution parameter. The normal vector $\hat{a}^\mu$ can be chosen arbitrarily in principle, depending on the concrete setup. With this choice of time function, a_i^μ in Eq. (40) becomes constant $a_i^\mu \equiv \hat{a}^\mu$, and thus the EoMs read

$$\frac{dx_i^\mu}{ds} = \frac{\bar{\Pi}_i^\mu(x_i, p_i)}{\bar{\Pi}_i \cdot \hat{a}}, \quad \frac{dp_i^\mu}{ds} = -\frac{\bar{Q}_i^\mu(x_i, p_i)}{\bar{\Pi}_i \cdot \hat{a}}, \quad (63)$$

which has the same structure as obtained in the constrained Hamiltonian formulation [49]. We note that the free particle version of the EoMs (63) is used for the Lorentz covariant cascade method proposed in Ref. [49].

Under this spatially uniform foliation, we may consider the translationally invariant particle profile:

$$G(x, p; x_i, p_i) = G(x - x_i, p - p_i), \quad (64)$$

where the dependence on the positions and momenta appears in the combinations $x - x_i$ and $p - p_i$. With this particle profile, Eqs. (37) and (38) can be explicitly written down as

$$\bar{\Pi}_i^\mu = \int d^4x d^4p \Pi^\mu(x, p) G(x - x_i, p - p_i), \quad (65)$$

$$\bar{Q}_i^\mu = \int d^4x d^4p Q^\mu(x, p) G(x - x_i, p - p_i), \quad (66)$$

where the derivatives of the generalized potential are defined as

$$\Pi^\mu(x, p) := \frac{\partial W(x, p)}{\partial p_\mu}, \quad (67)$$

$$Q^\mu(x, p) := \frac{\partial W(x, p)}{\partial x_\mu}. \quad (68)$$

We also comment on energy-momentum conservation in the present framework. Because of the presence of the externally specified foliation $\hat{s}(x)$, if the foliation is not considered subject to the translation, the translational symmetry of the system is apparently broken in general. However, the translational symmetry of the system is preserved at least when the uniform foliation in the form $\hat{s}(x) = \hat{a} \cdot x$ is considered, in which case the energy-momentum conservation holds. In other cases, the energy-momentum conservation is not necessarily satisfied by simply considering the momenta of the particles and mean fields. Detailed discussions for the implication will be discussed in future studies.

IV. APPLICATIONS

In this section, for the numerical demonstration with physical setups, we shall apply our RQMD formulation to the interaction by the relativistic mean field and the Skyrme-type potentials implemented as a Lorentz vector. We assume the uniform foliation $\hat{s}(x) = \hat{a} \cdot x$ with $\hat{a}_\mu \hat{a}^\mu = 1$.

Let us first summarize the covariant equations (63) formulated in Secs. III B and III C:

$$\frac{dx_i^\mu}{ds} = \frac{\bar{\Pi}_i^\mu}{\bar{\Pi}_i \cdot \hat{a}}, \quad \frac{dp_i^\mu}{ds} = -\frac{\bar{Q}_i^\mu}{\bar{\Pi}_i \cdot \hat{a}}, \quad (69)$$

⁷The statement that $\hat{a}^\mu$ is defined to be a Lorentz vector means that $\hat{a}^\mu$ transforms as a Lorentz vector properly under changes of the reference frame. This definition of $\hat{a}^\mu$ is chosen to be consistent with the Lorentz vector a_i^μ in Eq. (40) so that a_i^μ becomes uniform in the spacetime: $a_i^\mu = \hat{a}^\mu$.

⁸The apparently noncovariant expression $\hat{s}(x) = \hat{a} \cdot x = x^0$ is only valid in a specific frame, and this does not imply $\hat{a}$ is fixed to be (1, 0, 0, 0) in an arbitrary reference frame. The function $\hat{s}(x)$ and the vector $\hat{a}$ are still considered to transform appropriately as a Lorentz-scalar field and a Lorentz-vector, respectively, under changes of the reference frame.

where

$$\bar{\Pi}_i^\mu = \int d^4x d^4p \Pi^\mu(x, p) G(x - x_i, p - p_i), \quad (70)$$

$$\bar{Q}_i^\mu = \int d^4x d^4p Q^\mu(x, p) G(x - x_i, p - p_j), \quad (71)$$

and the derivatives of the generalized potential are defined as

$$\begin{aligned} \Pi^\mu(x, p) &= \frac{\partial W(x, p)}{\partial p_\mu} \\ &= p^*(x, p) \cdot \frac{\partial p^*(x, p)}{\partial p_\mu} - m^*(x, p) \frac{\partial m^*(x, p)}{\partial p_\mu}, \end{aligned} \quad (72)$$

$$\begin{aligned} Q^\mu(x, p) &= \frac{\partial W(x, p)}{\partial x_\mu} \\ &= p^*(x, p) \cdot \frac{\partial p^*(x, p)}{\partial x_\mu} - m^*(x, p) \frac{\partial m^*(x, p)}{\partial x_\mu}. \end{aligned} \quad (73)$$

In the numerical implementation, we assume the factorization of the particle profile into the spatial and momentum parts, and the momentum-space profile is taken to be a δ function:

$$G(x, p; x_i, p_i) = G(x - x_i) \delta(p - p_i), \quad (74)$$

as in the QMD case in Sec. II. We also assume the following Lorentz-contracted Gaussian for the particle profile:

$$G(x - x_i; u_i) = (u_i \cdot \hat{a}) \tilde{G}(x - x_i; u_i), \quad (75)$$

$$\tilde{G}(x - x_i; u_i) = \delta((x - x_i) \cdot \hat{a}) \tilde{g}(x - x_i; u_i), \quad (76)$$

$$\tilde{g}(x - x_i; u_i) = \frac{1}{(2\pi L)^{3/2}} \exp \frac{R(x - x_i; u_i)^2}{2L}, \quad (77)$$

$$R(x - x_i; u_i)^\mu = \Delta_i^{\mu\nu} (x_\nu - x_{i\nu}), \quad (78)$$

where L is the Gaussian width parameter, and $\Delta_i^{\mu\nu} = g^{\mu\nu} - u_i^\mu u_i^\nu$ is the spatial projector orthogonal to the velocity u_i^μ of the i th particle. As already discussed in Sec. III A, this form of the profile $G(x - x_i; u_i)$ has an additional dependence on $u_i = dx_i/d\tau_i$, which was not taken into account when deriving the EoMs (69) and obtaining the expressions (70) and (71). Although the Lorentz-contracted Gaussian (75)–(78) violates the weak mass-shell constraints (44) due to the u_i dependence, this violation is expected to be small in the slow-acceleration regime ($du_i/d\tau_i \ll 1/L$). In the subsequent discussions, unless we intend to emphasize, we omit the explicit dependence on u_i in the argument of $G(x - x_i)$ (75), $\tilde{G}(x - x_i)$ (76), $\tilde{g}(x - x_i)$ (77), $g(x, p; x_i, p_i) = (u_i \cdot \hat{a}) g(x - x_i) \delta(p - p_i)$, but they implicitly depend on u_i , where i shall be identified by the symbol x_i appearing in an explicit argument.

Under this approximation, Eqs. (70) and (71) are evaluated by

$$\bar{\Pi}_i^\mu = \int d^4x \Pi^\mu(x, p_i) G(x - x_i), \quad (79)$$

$$\bar{Q}_i^\mu = \int d^4x Q^\mu(x, p_i) G(x - x_i). \quad (80)$$

Since $G(x - x_i; u_i)$ is a normalized Gaussian profile, Eqs. (79) and (80) can be evaluated by the Monte Carlo integration as

$$\bar{\Pi}_i^\mu = \frac{1}{N_{\text{MC}}} \sum_{k=1}^{N_{\text{MC}}} \Pi_i^\mu(x_k, p_i), \quad (81)$$

$$\bar{Q}_i^\mu = \frac{1}{N_{\text{MC}}} \sum_{k=1}^{N_{\text{MC}}} Q_i^\mu(x_k, p_i), \quad (82)$$

with N_{MC} being the number of Monte Carlo points for the coordinates x_k , which are sampled according to the relativistic Gaussian distribution $G(x - x_i; u_i)$. The detailed procedure can be found in Appendix B.

The EoMs are explicitly written as

$$\begin{aligned} \frac{dx_i^\mu}{ds} &= \int d^4x (u_i \cdot \hat{a}) \frac{p^{*\mu}(x, p_i)}{\bar{\Pi}_i \cdot \hat{a}} \tilde{G}(x - x_i) \\ &\quad - \int d^4x \frac{m^*(x, p_i)}{\bar{m}_i} \frac{\partial m^*(x, p_i)}{\partial p_{i\mu}} \tilde{G}(x - x_i) \\ &\quad - \int d^4x \frac{p^{*\nu}(x, p_i)}{\bar{m}_i} \frac{\partial U_\nu(x, p_i)}{\partial p_{i\mu}} \tilde{G}(x - x_i), \end{aligned} \quad (83)$$

$$\begin{aligned} \frac{dp_i^\mu}{ds} &= \int d^4x \frac{m^*(x, p_i)}{\bar{m}_i} \frac{\partial m^*(x, p_i)}{\partial x_\mu} \tilde{G}(x - x_i) \\ &\quad + \int d^4x \frac{p^{*\nu}(x, p_i)}{\bar{m}_i} \frac{\partial U_\nu(x, p_i)}{\partial x_\mu} \tilde{G}(x - x_i). \end{aligned} \quad (84)$$

The scalar and vector potentials are determined by the scalar density and the vector current,⁹

$$\rho_s(x) = \int d^4p m^*(x, p) f(x, p), \quad (85)$$

$$J^\mu(x) = \int d^4p p^{*\mu}(x, p) f(x, p). \quad (86)$$

To solve the EoMs, we need to evaluate the distribution function $f(x, p)$ appearing in the scalar density (85) and baryon current (86). The distribution function (30) involves the time integration from the past to the future, which would be inconvenient in solving the EoMs. However, within the current setup, using the dynamical constraint $\hat{s}(x_i(s)) = s$, the time integration in Eq. (30) can be eliminated as

$$f_i(x, p) = \lambda_i(\hat{s}(x)) g(x, p; x_i(\hat{s}(x)), p_i(\hat{s}(x))). \quad (87)$$

In the case of the Gaussian (75) for the coordinate space and the δ function for the momentum space, the distribution function is given by

$$\begin{aligned} f_i(x, p) &= \frac{u_i \cdot \hat{a}}{\bar{\Pi}_i \cdot \hat{a}} \tilde{g}(x - x_i(\hat{s}(x))) \delta(p - p_i(\hat{s}(x))) \\ &= \frac{1}{\bar{m}_i} \tilde{g}(x - x_i(\hat{s}(x))) \delta(p - p_i(\hat{s}(x))), \end{aligned} \quad (88)$$

⁹We note that the conserved current may be given by $J^\mu(x) = \int d^4p \Pi^\mu(x, p) f(x, p)$, when momentum-dependent potentials are included.

where $u_i = \tilde{\Pi}_i/\tilde{m}_i$ was used. Then, the scalar density and the vector current are evaluated by the following expressions:

$$\rho_s(x) = \sum_{i=1}^N \frac{m^*(x, p_i)}{\tilde{m}_i} \tilde{g}(x - x_i(\hat{s}(x))), \quad (89)$$

$$J(x) = \sum_{i=1}^N \frac{p^*(x, p_i)}{\tilde{m}_i} \tilde{g}(x - x_i(\hat{s}(x))). \quad (90)$$

A. Numerical implementation

In the first numerical implementation, we make simplifications,

$$\frac{m^*(x, p_i)}{\tilde{m}_i} \approx 1, \quad (91)$$

$$\frac{p^*(x, p_i)}{\tilde{m}_i} \approx \frac{p^*(x, p_i)}{\sqrt{p^{*2}(x, p_i)}} =: u(x, p_i), \quad (92)$$

to avoid numerical complications in solving the RQMD EoM. Then, the EoMs become

$$\frac{dx_i^\mu}{ds} = \frac{p_i^\mu}{\Pi_i \cdot \hat{a}} - \int d^4x \left[\frac{\partial m^*(x, p_i)}{\partial p_{i\mu}} + u^v(x, p_i) \frac{\partial U_v(x, p_i)}{\partial p_{i\mu}} \right] \tilde{G}(x - x_i), \quad (93)$$

$$\frac{dp_i^\mu}{ds} = \int d^4x \left[\frac{\partial m^*(x, p_i)}{\partial x_\mu} + u^v(x, p_i) \frac{\partial U_v(x, p_i)}{\partial x_\mu} \right] \tilde{G}(x - x_i), \quad (94)$$

where the first term of Eq. (93) is obtained by using the harmonic approximation that the argument x of $p^*(x, p_i)$ and $m^*(x, p_i)$ is replaced by the coordinates of the center of the Gaussian, i.e., x_i . Also, u_i in the Gaussian profile is approximated by $u_i \approx u(x_i, p_i)$. Accordingly, the scalar density and vector current become

$$\rho_s(x) = \sum_{i=1}^N \tilde{g}(x - x_i), \quad J^\mu(x) = \sum_{i=1}^N u_i^\mu \tilde{g}(x - x_i). \quad (95)$$

In the next sections, we apply these equations to the relativistic mean-field theory and the Skyrme-type potentials.

The relativistic molecular dynamics (RQMD) model combines the Boltzmann-type collision term for hadrons and the propagation of hadrons according to the mean-field potential. We implemented the covariant EoMs derived in the following sections in the Monte Carlo event generator JAM2 [53]. JAM2 is a C++ version of JAM1 [59]. The collision term includes the hadronic resonance and string excitation and their decay to simulate particle production processes. JAM2 uses Pythia8 [60,61] for the string fragmentation with the formation time. During the formation time, hadrons from strings do not scatter, but the leading hadrons (which carry original constituent quarks) can scatter within the formation time with reduced cross sections.

B. RQMD for the relativistic mean-field theory (RQMD.RMF2)

We now apply the formulation for the system of interacting wave packets via the relativistic mean fields. Specifically, we consider the σ and ω meson exchange. The Lagrangian density is given by

$$\mathcal{L} = \sum_B \bar{\psi}_B \{ \gamma^\mu [i\partial_\mu - U_{B,\mu}(\omega)] - m_B^*(\sigma) \} \psi_B + \frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma - V_\sigma(\sigma) - \frac{1}{4} \omega_{\mu\nu} \omega^{\mu\nu} + V_\omega(\omega_\mu), \quad (96)$$

where B runs over different baryon species, $U_{B,\mu} := g_{\omega,B} \omega_\mu$, $m_B^*(\sigma) := m_B + U_{\sigma,B}(\sigma)$, and $\omega_{\mu\nu} := \partial_\mu \omega_\nu - \partial_\nu \omega_\mu$. In the case of the Walecka-type model, the single-particle scalar potential is given by $U_{\sigma,B} = -g_{\sigma,B} \sigma$.

In the σ - ω model, the following potentials are often used:

$$V_\sigma(\sigma) = \frac{m_\sigma^2}{2} \sigma^2 + \frac{g_2}{3} \sigma^3 + \frac{g_3}{4} \sigma^4, \quad (97)$$

$$V_\omega(\omega_\mu) = \frac{m_\omega^2}{2} \omega_\mu \omega^\mu + \frac{c_4}{4} (\omega_\mu \omega^\mu)^2. \quad (98)$$

We assume the mean-field approximation, where the meson-field operators are replaced by the expectation value of the field. Furthermore, we take the positive energy solutions of the Dirac equations (the no-sea approximation). A variation of the Lagrangian density with respect to the fields σ and ω yields the following EoMs:

$$\partial_\mu \partial^\mu \sigma + \frac{\partial V_\sigma}{\partial \sigma} = \sum_B y_B(x) \rho_{s,B}, \quad (99)$$

$$\partial_\nu \omega^{\nu\mu} + \frac{\partial V_\omega}{\partial \omega_\mu} = \sum_B g_{\omega,B} J_B^\mu, \quad (100)$$

where $y_B(x) = -\partial m_B^*/\partial \sigma = -\partial U_{\sigma,B}/\partial \sigma$. The scalar density and the baryon current are given by the expectation values of the field operators: $\rho_{s,B} = \langle \bar{\psi}_B \psi_B \rangle$ and $J_B^\mu = \langle \bar{\psi}_B \gamma^\mu \psi_B \rangle$.

In the transport description of a system, one switches to the phase space picture [11,12], and within the RQMD approach, the scalar density and the vector current are given by the sum of the Gaussian,

$$\sum_B y_B(x) \rho_{s,B}(x) = \sum_{j=1}^N y_j \tilde{g}(x - x_j) \equiv n_s(x), \quad (101)$$

$$\sum_B g_{\omega,B} J_B^\mu(x) = \sum_{j=1}^N g_{\omega,j} u_j^\mu \tilde{g}(x - x_j) \equiv j^\mu(x), \quad (102)$$

where the summation index j runs over N particles of all species, and $g_{\omega,j} = g_{\omega,B_j}$ ¹⁰ with B_j being the baryon species of the i th particle. Here, we made the same approximations as in Eq. (95): $y_{B_j}(x) \approx y_{B_j}(x_j) =: y_j$ and $u(x, p_j) \approx u_j$. The spatial part of the BUU-like EoM (94) becomes

$$\frac{dp_i}{ds} = \int d^4x \left[y_i \frac{\partial \sigma(x)}{\partial x} - g_{\omega,i} u_i^\mu \frac{\partial \omega_\mu(x)}{\partial x} \right] \tilde{G}(x - x_i), \quad (103)$$

¹⁰Here, we do not consider the contributions from antibaryons.

where we replaced $y_{B_i}(x)$ and $u(x, p_i)$ with y_i and u_i .

Below, we assume the local density approximation that neglects the kinetic terms of the meson fields in the field EoMs (99) and (100). The field potential (59) is given by

$$V_{\text{field}}[\sigma, \omega] = \int d^4x [V_\sigma(\sigma(x)) - V_\omega(\omega_\mu(x))]. \quad (104)$$

The corresponding free-energy functional (in the formulation of Sec. III C) is found to be

$$\begin{aligned} F[\rho_{s,B}, J_B^\mu] &= V_{\text{field}} + \sum_B \int d^4x (\rho_{s,B} U_{\sigma,B} + J_B^\mu \cdot U_{B\mu}) \\ &= V_{\text{field}} + \int d^4x \left(\sum_B \rho_{s,B} U_{\sigma,B} + \omega \cdot j \right). \end{aligned} \quad (105)$$

We follow the same approach as done in the previous sections to obtain the QMD-like EoMs from the BUU-like ones. In a similar way to Sec. II, we consider rewriting Eq. (103) by defining “one-particle” scalar and vector fields:

$$\tilde{\sigma} = \frac{1}{n_s} \int \sigma dn_s, \quad \tilde{\omega}_\mu = \frac{j_\mu}{n^2} \int \omega \cdot dj, \quad (106)$$

where $n = \sqrt{j_\mu j^\mu}$. One can show that the integral $\int \omega \cdot dj$ is well-defined using the fact that the vector current can be expressed by the ω^μ field as

$$j^\mu = \frac{\partial V_\omega}{\partial \omega_\mu} = 2 \frac{\partial V_\omega}{\partial (\omega_\mu \omega^\mu)} \omega^\mu \equiv f(\omega_\mu \omega^\mu) \omega^\mu. \quad (107)$$

Since ω^2 can be solved as a function of n using $n^2 = j^2 = f(\omega^2) \omega^2$, $\omega \cdot dj = [n/f(\omega^2)] dn$ is integrable. The one-particle scalar field is evaluated as

$$\tilde{\sigma} = \frac{1}{n_s} \left(\sigma n_s - \int n_s d\sigma \right) = \sigma - \frac{V_\sigma}{n_s}, \quad (108)$$

and the derivative of the $\tilde{\sigma}$ may be evaluated as

$$\frac{\partial \tilde{\sigma}}{\partial n_s} = \frac{V_\sigma}{n_s^2}. \quad (109)$$

In the same way, $\tilde{\omega}$ is expressed by the function of ω field

$$\tilde{\omega}_\mu = \frac{j_\mu}{n^2} \left(\omega \cdot j - \int j \cdot d\omega \right) = \omega_\mu - \frac{j_\mu}{n^2} V_\omega. \quad (110)$$

The derivative of $\tilde{\omega}$ with respect to the vector current reads

$$\frac{\partial \tilde{\omega}_\mu}{\partial j^\nu} = \frac{\partial \omega_\mu}{\partial j^\nu} - \frac{j_\mu}{n^2} \left(j^\lambda \frac{\partial \omega_\lambda}{\partial j^\nu} - \frac{2V_\omega}{n^2} j_\nu \right) - \frac{V_\omega}{n^2} g_{\mu\nu}. \quad (111)$$

As worked out in Appendix D, the derivative of the vector field with respect to the vector current for the quartic interaction (98) is evaluated as

$$\frac{\partial \omega_\mu}{\partial j^\nu} = \frac{1}{m^2 + c\omega^2} \left(g_{\mu\nu} - \frac{2c\omega_\mu \omega_\nu}{m^2 + 3c\omega^2} \right). \quad (112)$$

We are now in a position to rewrite the BUU-like EoMs (103) to derive the QMD-like EoMs for the scalar and vector fields. The EoM for the momentum is written as the sum of

two forces from the scalar and vector potentials:

$$\frac{d\mathbf{p}_i}{ds} = \mathbf{F}_{\sigma,i} + \mathbf{F}_{\omega,i}. \quad (113)$$

After replacing the σ and ω fields with the $\tilde{\sigma}$ and $\tilde{\omega}$ fields by using the relations,

$$\sigma = \frac{\partial(n_s \tilde{\sigma})}{\partial n_s} = \tilde{\sigma} + n_s \frac{\partial \tilde{\sigma}}{\partial n_s}, \quad (114)$$

$$\omega_\mu = \frac{\partial(\tilde{\omega} \cdot j)}{\partial j^\mu} = \tilde{\omega}_\mu + j^\nu \frac{\partial \tilde{\omega}_\nu}{\partial j^\mu}, \quad (115)$$

and replacing the scalar density and vector current by the sum of the Gaussian using Eqs. (101) and (102), we obtain

$$\begin{aligned} \mathbf{F}_{\sigma,i} &= \sum_{j=1}^N \int d^4x y_{ij} \left[\frac{\partial \tilde{\sigma}(x)}{\partial n_s} \frac{\partial \tilde{g}(x-x_j)}{\partial \mathbf{x}} \tilde{G}(x-x_i) \right. \\ &\quad \left. + \frac{\partial \tilde{\sigma}(x)}{\partial n_s} \frac{\partial \tilde{G}(x-x_i)}{\partial \mathbf{x}_i} \tilde{g}(x-x_j) \right], \end{aligned} \quad (116)$$

and

$$\begin{aligned} \mathbf{F}_{\omega,i} &= - \sum_{j=1}^N \int d^4x u_{ij}^{\mu\nu} \left[\frac{\partial \tilde{\omega}_\mu(x)}{\partial j^\nu} \frac{\partial \tilde{g}(x-x_j)}{\partial \mathbf{x}} \tilde{G}(x-x_i) \right. \\ &\quad \left. + \frac{\partial \tilde{\omega}_\nu(x)}{\partial j^\mu} \frac{\partial \tilde{G}(x-x_i)}{\partial \mathbf{x}_i} \tilde{g}(x-x_j) \right], \end{aligned} \quad (117)$$

where $y_{ij} = y_i y_j$ and $u_{ij}^{\mu\nu} = g_{\omega,i} g_{\omega,j} u_i^\mu u_j^\nu$. We approximate the integral by the QMD2 approximation (19), which replaces the argument x of the potential in the integral with the center of a Gaussian wave packet and performs the integral for the overlap of two Gaussians. Then, we obtain EoMs that are symmetric (in the sense of the law of action and reaction for each particle pair) and exactly conserve the total momentum, with the scalar part of the force being

$$\mathbf{F}_\sigma = \sum_{j=1}^N y_{ij} \left[\frac{V_\sigma(x_i)}{n_s^2(x_i)} + \frac{V_\sigma(x_j)}{n_s^2(x_j)} \right] \frac{\partial \tilde{g}_{ij}}{\partial \mathbf{x}_i}, \quad (118)$$

and the vector part being

$$\mathbf{F}_{\omega,i} = - \sum_{j=1}^N u_{ij}^{\mu\nu} \left[\frac{\partial \tilde{\omega}_\mu(x_i)}{\partial j^\nu} + \frac{\partial \tilde{\omega}_\nu(x_j)}{\partial j^\mu} \right] \frac{\partial \tilde{g}_{ij}}{\partial \mathbf{x}_i}. \quad (119)$$

The symbol $\tilde{g}_{ij}$ denotes the relativistic Gaussian overlap integral:

$$\begin{aligned} \tilde{g}_{ij} &:= \int d^4x \delta((x-x_i) \cdot \hat{a}) \tilde{g}(x-x_i) \tilde{g}(x-x_j) \\ &= \frac{1}{(4\pi L)^{3/2} \sqrt{d}} \exp \frac{(x_i-x_j)^T A (x_i-x_j)}{4L}, \end{aligned} \quad (120)$$

where

$$A^{\mu\nu} = g^{\mu\nu} - \frac{u_{ij}^{\mu\nu}}{2d}, \quad (121)$$

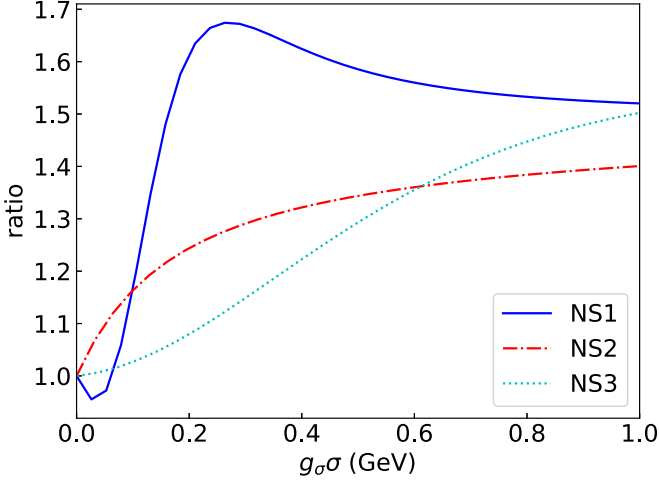


FIG. 4. Ratio of Eq. (128) to Eq. (129) as a function of σ for the parameter sets of NS1, NS2, and NS3 taken from Ref. [31].

with

$$u_{ij}^{\mu\nu} = bu_i^\mu u_j^\nu + au_j^\mu u_i^\nu + c(u_i^\mu u_j^\nu + u_j^\mu u_i^\nu), \quad (122)$$

$$a = 1 + \frac{1}{2}[(u_i \cdot \hat{a})^2 - u_i^2], \quad (123)$$

$$b = 1 + \frac{1}{2}[(u_j \cdot \hat{a})^2 - u_j^2], \quad (124)$$

$$c = \frac{1}{2}[(u_i \cdot \hat{a})(u_j \cdot \hat{a}) - u_i \cdot u_j], \quad (125)$$

$$d = ab - c^2. \quad (126)$$

A derivation of the above expressions is given in Appendix C. We finally note that the exact energy conservation is not maintained by the QMD2 approximation in general unlike the momentum conservation, and thus the violation of the energy conservation based on these EoMs should be checked carefully as we do in Sec. IV F.

In the previous RQMD.RMF model [30,31], the mass-shell condition is taken to be

$$(m_i + V_s)^2 - (p_i - V_i)^2 = 0, \quad (127)$$

and we simply assumed $V_s = -g_\sigma \sigma / 2$ and $V_i = g_\omega \omega / 2$ to symmetrize the EoMs to conserve total momentum. When fields do not contain the nonlinear terms, these choices are identical to the one-particle fields $\tilde{\sigma}$ and $\tilde{\omega}$. In the previous RQMD.RMF model, the relevant term for the scalar part of the EoMs is $\partial \sigma / \partial n_s = (\partial^2 V_\sigma / \partial \sigma^2)^{-1}$. Thus, it is interesting to compare the differences of the present and previous models. We compare them for the scalar potential (97)

$$\frac{V_\sigma}{n_s^2} = V_\sigma \left(\frac{\partial V_\sigma}{\partial \sigma} \right)^{-2} = \frac{\frac{m_\sigma^2}{2} + \frac{g_2}{3} \sigma + \frac{g_3}{4} \sigma^2}{(m_\sigma^2 + g_2 \sigma + g_3 \sigma^2)^2}, \quad (128)$$

and

$$\frac{1}{2} \left(\frac{\partial^2 V_\sigma}{\partial \sigma^2} \right)^{-1} = \frac{1}{2} (m_\sigma^2 + 2g_2 \sigma + 3g_3 \sigma^2)^{-1}. \quad (129)$$

In Fig. 4, we compare the ratio of Eq. (128) to Eq. (129) as a function of σ field for the EoS parameter sets of NS1, NS2,

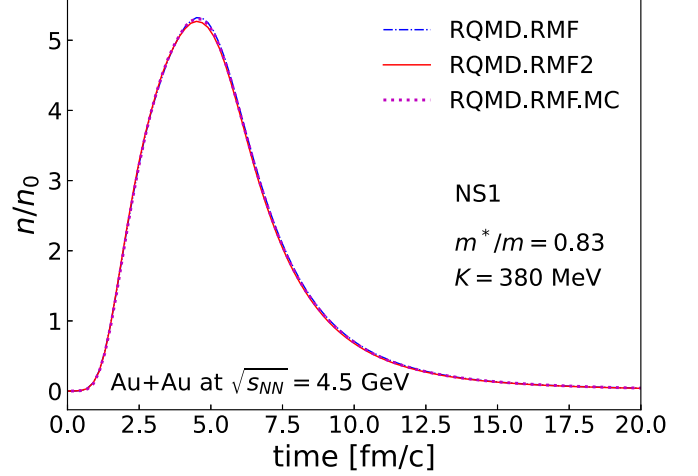


FIG. 5. Time evolution of the baryon density at the center of mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV from the RQMD with the σ - ω model. Impact parameter range of $4.6 < b < 9.4$ fm is selected. The RQMD.RMF model results are compared with the new model, RQMD.RMF2, and the RQMD using the Monte Carlo integration (RQMD.RMF.MC).

and NS3 taken from Ref. [31]. It is seen that the new approach predicts larger values than the previous model for all parameter sets at the large σ field. We may make an order estimate for the typical values of σ field by neglecting the nonlinear term in the σ field, which yields $g_\sigma \sigma = (g_\sigma / m_\sigma)^2 n_s \approx 0.18, 0.27$, and 0.3 GeV for NS1, NS2, and NS3 at the normal nuclear density, respectively. In this range of the σ field, the difference is within 30%.

C. Application to heavy-ion collisions with RQMD.RMF2

To investigate the effects of different treatments in the nonlinear term for the scalar interaction, the time evolution of the central density in mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV is shown in Fig. 5 for the NS1 EoS. For the specific calculations in this subsection, we have chosen the uniform foliation with $\hat{a} = (1, 0, 0, 0)$ in the initial global CM frame defined by the initial total momentum. The impact parameter range is selected as $4.6 < b < 9.4$ fm, which approximately corresponds to the 10–40% centrality class in STAR experiments. The results are compared for three models: the previous model (dubbed RQMD.RMF, shown by the dash-dotted line), the new model (RQMD.RMF2, the solid line), and the Monte Carlo integration (RQMD.RMF.MC, the dotted line), where we solve Eqs. (93) and (94).

The comparison reveals no significant differences in the density evolution among the three models. We also note that no significant differences are observed in the 0–5% central Au + Au collisions.

The directed flow $v_1 = \langle \cos \phi \rangle$ is considered to be a sensitive probe of the EoS, where ϕ is the azimuthal angle with respect to the reaction plane. Figure 6 shows the time

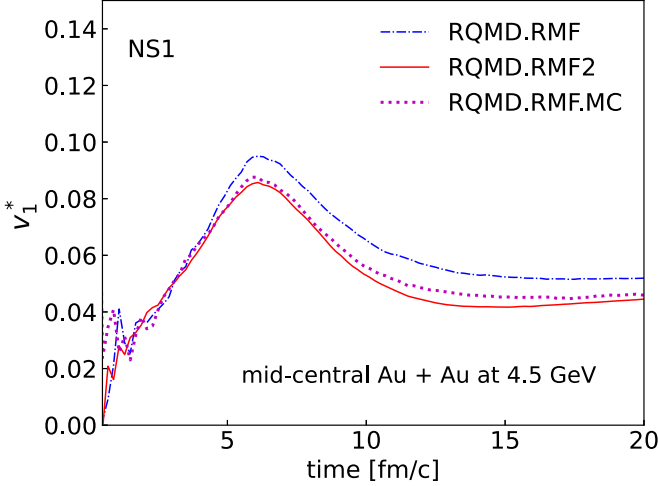


FIG. 6. Time evolution of the sign-weighted directed flow v_1^* in mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV are shown from the RQMD with the σ - ω model. The RQMD.RMF model results are compared with the new model, RQMD.RMF2, and the RQMD using the Monte Carlo integration (RQMD.RMF.MC).

evolutions of the sign-weighted directed flow of baryons defined as

$$v_1^* = \frac{\int_{-1}^1 dy \int d\phi \frac{dN}{dyd\phi} \cos \phi \operatorname{sgn} y}{\int_{-1}^1 dy \int d\phi \frac{dN}{dyd\phi}}, \quad (130)$$

where the range of the integration is taken to be $|y| < 1$. As pointed out in Ref. [48], the directed flow at mid-rapidity increases during the compression stage of the collisions and then decreases in the expansion stages due to a tilted shape of the matter, which is also observed with the interaction by the relativistic mean-field. We observe that RQMD.RMF2 provides a good approximation to RQMD.RMF.MC. RQMD.RMF predicts a larger directed flow than the new models due to a less attractive scalar potential.

In Fig. 7, we compare the rapidity dependence of the proton v_1 among the three models in mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV. We select “free” protons using nuclear coalescence with the phase space cutoff parameters $r_0 < 3$ fm and $p_0 < 0.3$ GeV/c at the simulation time of 40 fm/c. We do not observe any significant differences among the three models. It is seen at high rapidity region that the RQMD.RMF2 results are in good agreement with the RQMD.RMF.MC results. We note that this agreement is also seen in the rapidity distribution. In these models, the treatment of the ω field is the same, because only the linear dependence on the baryon density is included. The effects of the nonlinear density dependence in the vector potential will be examined in the next section.

We have checked that the main differences between the old model and the new models for density evolution and directed flow from other parametrization of NS2 and NS3 predictions are the same as those of NS1.

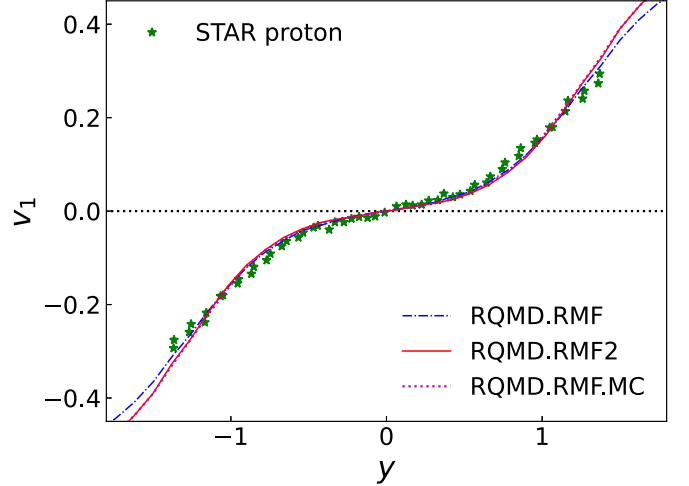


FIG. 7. Rapidity dependence of directed flow for protons with transverse momentum $0.4 < p_T < 2.0$ GeV in mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV is compared with three models within RQMD with the σ - ω potential. The result from the RQMD.RMF model is shown as a dash-dotted line, the RQMD.RMF2 result is plotted by a solid line, and the RQMD.RMF.MC result is plotted by a dotted line. STAR data were taken from Ref. [62].

D. RQMD for Skyrme potentials (RQMDs2 and RQMDv2)

In this section, we consider the Skyrme-type density-dependent potential together with the Lorentzian-type momentum-dependent potential. In the following discussion, we consider the specific structure of the free-energy functional:

$$F[\phi, \phi_\mu] = \int d^4x \mathcal{F}(x), \quad (131)$$

with

$$\begin{aligned} \mathcal{F}(x) = & \int_0^{\rho_s[\phi(x,p)]} U_s^d(z) dz + \int_0^{\rho[\phi_\mu(x,p)]} U_v^d(z) dz \\ & + \frac{C}{2\rho_0} \int d^4p d^4p' D(p-p') \phi(x,p) \phi(x,p') \\ & + \frac{C}{2\rho_0} \int d^4p d^4p' D(p-p') \phi_\mu(x,p) \phi^\mu(x,p'), \end{aligned} \quad (132)$$

where C is fixed by fitting the optical potential and ρ_0 is the normal nuclear density. The functions $U_s^d(z)$ and $U_v^d(z)$ specify the density-dependent parts of the potential, and $D(p-p')$ specifies the momentum-dependent part. The functional form of the momentum-dependence is taken to be

$$D(p-p') = \frac{1}{1 - (p-p')^2/\mu^2}, \quad (133)$$

where μ is a parameter for the momentum width. The scalar density $\rho_s[\phi]$ and the current density $\rho[\phi_\mu]$ are given by

$$\rho_s(x) = \int d^4p \phi(x,p), \quad (134)$$

$$J_\mu(x) = \int d^4p \phi_\mu(x,p), \quad (135)$$

$$\rho(x) = \sqrt{J^\mu(x)J_\mu(x)}. \quad (136)$$

The single-particle potentials are obtained as

$$U_s(x, p) = U_s^d(\rho_s(x)) + U_s^{\text{MD}}(x, p), \quad (137)$$

$$U_\mu(x, p) = U_\mu^d(J^\mu(x)) + U_\mu^{\text{MD}}(x, p), \quad (138)$$

with Skyrme-type density-dependent single-particle potential as

$$U_{s,v}^d(n(x)) = \alpha \frac{n(x)}{\rho_0} + \beta \left[\frac{n(x)}{\rho_0} \right]^\gamma, \quad (139)$$

where $n(x)$ can be either the scalar density or the baryon density corresponding to the notations $U_s(\rho_s)$ and $U_v(\rho)$, respectively. The density-dependent part of the vector potential is defined as $U_\mu^d := (J_\mu/\rho)U_v^d(\rho)$. According to Eqs. (53) and (54), the single-particle momentum-dependent potentials become

$$\begin{aligned} U_s^{\text{MD}}(x, p) &= \frac{C}{\rho_0} \int d^4 p' D(p - p') \phi(p') \\ &= \frac{C}{\rho_0} \sum_{i=1}^N D(p - p_i) \tilde{g}(x - x_i), \end{aligned} \quad (140)$$

$$\begin{aligned} U_\mu^{\text{MD}}(x, p) &= \frac{C}{\rho_0} \int d^4 p' D(p - p') \phi_\mu(p') \\ &= \frac{C}{\rho_0} \sum_{i=1}^N u_{i,\mu} D(p - p_i) \tilde{g}(x - x_i), \end{aligned} \quad (141)$$

where we make simplifications as stated in Sec. IV A: $\bar{m}_i = m^*(x, p_i)$ and $u_i = p^*(x, p_i)/m^*(x, p_i)$. We here note that in general the kernel $D(p - p')$ appearing in the single-particle momentum-dependent potentials (140) and (141) need to be symmetric with respect to its arguments, $D(p - p') = D(p' - p)$, which is required to ensure conservation laws of current and energy-momentum [11]. In the present formulation starting with the free energy functional (132), the kernel $D(p - p')$ in the free energy functional does not have this restriction for the symmetry because the kernel in Eqs. (140) and (141) becomes $[D(p - p') + D(p' - p)]/2$, which automatically satisfies the symmetry. For simplicity, we replaced $[D(p - p') + D(p' - p)]/2$ with $D(p - p')$ using the symmetry of Eq. (133), $D(p - p') = D(p' - p)$. The field potential is given by

$$V[\phi, \phi_\mu] = \int d^4 x \mathcal{V}_{\text{field}}(x), \quad (142)$$

with

$$\begin{aligned} \mathcal{V}_{\text{field}}(x) &= \rho_s U_s^d(\rho_s) - \int_0^{\rho_s} U_s^d(z) dz \\ &+ \rho U_v^d(\rho) - \int_0^\rho U_v^d(z) dz \\ &+ \frac{1}{2} \int d^4 p \phi(x, p) U_s^{\text{MD}}(x, p) \\ &+ \frac{1}{2} \int d^4 p \phi^\mu(x, p) U_\mu^{\text{MD}}(x, p). \end{aligned} \quad (143)$$

We now consider the QMD2 approximation (19) of the spatial integral. We apply the same procedure as discussed in the previous section for the integration of Eqs. (93) and (94) to obtain the covariant QMD-like EoMs. We eliminate the p^0 dependence of the momentum-dependent potentials $U_s^{\text{MD}}(x, p)$ and $U_\mu^{\text{MD}}(x, p)$ by substituting the mass-shell constraint for p^0 so that $\Pi_i^0 = p_i^{*0}$. In the center-of-mass frame where $\hat{a} = (1, 0, 0, 0)$, $\Pi_i \cdot \hat{a} = p_i^{*0}$. Let us consider below in the Lorentz frame specified by $\hat{a} = (1, 0, 0, 0)$, where the times of all particles are the same $t = x_i^0$. The time integration can be trivially done, and the Gaussian becomes the following form:

$$\begin{aligned} \tilde{g}(\mathbf{x}; u_i) &= \int dx^0 \tilde{G}(x) \\ &= \frac{1}{(2\pi L)^{3/2}} \exp \left[-\frac{\mathbf{x}^2 + (\mathbf{x} \cdot \mathbf{u}_i)^2}{2L} \right]. \end{aligned} \quad (144)$$

It is sufficient to propagate the spatial components of momentum $\mathbf{p}_i$, since the time component p_i^0 can be determined by the mass-shell constraint. In this work, we use a mass-shell condition within the harmonic approximation for simplicity, i.e., p_i^0 is determined by solving $W(x_i, p_i) = 0$ instead of $\bar{W}(x_i, p_i) = 0$.

The EoMs (93) and (94) receive contributions from the four terms in the scalar and vector potentials (137) and (138):

$$\frac{d\mathbf{x}_i}{dt} = \frac{\mathbf{p}_i^*}{p_i^{*0}} + \mathbf{E}_{s,i}^{\text{MD}} + \mathbf{E}_{v,i}^{\text{MD}}, \quad (145)$$

$$\frac{d\mathbf{p}_i}{dt} = \mathbf{F}_{s,i}^d + \mathbf{F}_{v,i}^d + \mathbf{F}_{s,i}^{\text{MD}} + \mathbf{F}_{v,i}^{\text{MD}}, \quad (146)$$

where $\mathbf{F}_{s,i}^d$ and $\mathbf{F}_{v,i}^d$ denote the forces from the density-dependent parts of the scalar and vector potentials, respectively. The symbols $\mathbf{F}_{s,i}^{\text{MD}}$ and $\mathbf{F}_{v,i}^{\text{MD}}$ denote the forces from the momentum-dependent parts, while $\mathbf{E}_{s,i}^{\text{MD}}$ and $\mathbf{E}_{v,i}^{\text{MD}}$ denote similar contributions to the spatial part of the EoM.

To obtain the density-dependent parts of the EoM, we introduce one-particle potentials for the density-dependent potential defined as

$$V_s(x) = \frac{1}{\rho_s} \int U_s^d(\rho_s) d\rho_s, \quad (147)$$

$$V^\mu(x) = \frac{J^\mu}{\rho^2} \int U_\alpha^d(\rho) dJ^\alpha = \frac{J^\mu}{\rho^2} \int U_v^d(\rho) d\rho. \quad (148)$$

Then, the single-particle potentials can be replaced with the one-particle potentials by using the relations

$$U_s^d(x) = V_s + \rho_s \frac{\partial V_s}{\partial \rho_s}, \quad U_\mu^d(x) = V_\mu + J^\alpha \frac{\partial V_\alpha}{\partial J^\mu}. \quad (149)$$

The density-dependent scalar potential part of the EoMs is given by

$$\mathbf{F}_{s,i}^d = - \int d^3 x \frac{\partial U_s^d(x)}{\partial \mathbf{x}} \tilde{g}(x - x_i). \quad (150)$$

We replace the single-particle potential $U_s^d(x)$ with the one-particle potential $V_s(x)$, and replace the total scalar density

$\rho_s(x)$ with the sum of the Gaussian profiles. We obtain

$$\mathbf{F}_{s,i}^d = - \sum_{j=1}^N \left[\int d^3x \frac{dV_s(x)}{d\rho_s} \frac{\partial \tilde{g}(x - x_j)}{\partial \mathbf{x}} \tilde{g}(x - x_i) + \int d^3x \frac{dV_s(x)}{d\rho_s} \frac{\partial \tilde{g}(x - x_i)}{\partial \mathbf{x}_i} \tilde{g}(x - x_j) \right]. \quad (151)$$

We approximate this integral by replacing the argument of the potential by the center of the Gaussian x_i and x_j , and perform integration, which yields

$$\mathbf{F}_{s,i}^d \approx - \sum_{j=1}^N \left[\frac{dV_s(x_i)}{d\rho_s} + \frac{dV_s(x_j)}{d\rho_s} \right] \frac{\partial \tilde{g}_{ij}}{\partial \mathbf{x}_i}, \quad (152)$$

where

$$\tilde{g}_{ij} = \int d^3x \tilde{g}(x - x_i) \tilde{g}(x - x_j). \quad (153)$$

Similarly, the vector potential part is obtained as

$$\mathbf{F}_{v,i}^d \approx - \sum_{j=1}^N u_{i\mu} u_{j\nu} \left[\frac{\partial V^\mu(x_i)}{\partial J_\nu} + \frac{\partial V^\nu(x_j)}{\partial J_\mu} \right] \frac{\partial \tilde{g}_{ij}}{\partial \mathbf{x}_i}. \quad (154)$$

The derivative of the vector potential can be evaluated by using $V^\mu = V_v(\rho) J^\mu / \rho$, with $V_v(\rho) = (1/\rho) \int U_v^d(\rho) d\rho$,

$$\frac{\partial V^\mu}{\partial J_\nu} u_\nu = \left[\frac{\partial V_v(\rho)}{\partial \rho} - \frac{V_v(\rho)}{\rho} \right] \frac{J^\nu u_\nu}{\rho} \frac{J^\mu}{\rho} + \frac{V_v(\rho)}{\rho} u^\mu. \quad (155)$$

The contributions from the momentum-dependent scalar potentials are expressed as

$$\mathbf{E}_{s,i}^{\text{MD}} = \frac{C}{\rho_0} \sum_{j=1}^N \frac{\partial D(p_i - p_j)}{\partial \mathbf{p}_i} \tilde{g}_{ij}, \quad (156)$$

$$\mathbf{F}_{s,i}^{\text{MD}} = - \frac{C}{\rho_0} \sum_{j=1}^N D(p_i - p_j) \frac{\partial \tilde{g}_{ij}}{\partial \mathbf{x}_i}. \quad (157)$$

For the momentum-dependent vector potential, we have the expression

$$\mathbf{E}_{v,i}^{\text{MD}} = \frac{C}{\rho_0} \sum_{j=1}^N (u_i \cdot u_j) \frac{\partial D(p_i - p_j)}{\partial \mathbf{p}_i} \tilde{g}_{ij}, \quad (158)$$

$$\mathbf{F}_{v,i}^{\text{MD}} = - \frac{C}{\rho_0} \sum_{j=1}^N (u_i \cdot u_j) D(p_i - p_j) \frac{\partial \tilde{g}_{ij}}{\partial \mathbf{x}_i}. \quad (159)$$

In the numerical simulation, to evaluate the momentum-dependent function $D(p_i - p_j)$, we use the relative momentum $p_i - p_j$ seen in the two-particle center-of-mass system:

$$(\mathbf{p}_i - \mathbf{p}_j)_{\text{c.m.}}^2 = -(\mathbf{p}_i - \mathbf{p}_j)^2 + \frac{[(\mathbf{p}_i - \mathbf{p}_j) \cdot (\mathbf{p}_i + \mathbf{p}_j)]^2}{(\mathbf{p}_i + \mathbf{p}_j)^2}. \quad (160)$$

To summarize, RQMD2 EoMs are obtained as

$$\frac{dx_i^\mu}{ds} = \frac{p_i^*}{\Pi_i \cdot \hat{a}} - \frac{C}{\rho_0} \sum_{j=1}^N (u_i \cdot u_j + 1) \frac{\partial D(p_i - p_j)}{\partial p_{i\mu}} \tilde{g}_{ij}, \quad (161)$$

$$\frac{dp_i^\mu}{ds} = \sum_{j=1}^N (u_{i\mu} u_{j\nu} V_{ij}^{\mu\nu} + V_{ij}^s) \frac{\partial \tilde{g}_{ij}}{\partial x_{i\mu}}, \quad (162)$$

where

$$V_{ij}^s = \frac{\partial V_s(x_i)}{\partial n_s} + \frac{\partial V_s(x_j)}{\partial n_s} + \frac{C}{\rho_0} D(p_i - p_j), \quad (163)$$

$$V_{ij}^{\mu\nu} = \frac{\partial V^\mu(x_i)}{\partial J_\nu} + \frac{\partial V^\nu(x_j)}{\partial J_\mu} + \frac{C}{\rho_0} D(p_i - p_j) g^{\mu\nu}. \quad (164)$$

We define RQMDs2 to be the version only with the scalar part of the Skyrme potential in Eqs. (161) and (162), and RQMDv2 to be the version only with the vector part.

E. Application to heavy-ion collisions with RQMDv2

In this section, we focus on the vector potentials as they have a stronger influence on the dynamics than the scalar potentials [48]. We compare the results of the previous RQMDv approach [48] with those obtained using the newly proposed equations of motion (RQMDv2), as well as with the exact solutions calculated via numerical integration using the Monte Carlo method with a Gaussian weight (RQMDv.MC, which solves Eqs. (93) and (94) by simulating Au + Au collisions with the JAM2 event generator.

In Fig. 8, we plot the time evolution of baryon density at the center of the matter in mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV. For the calculations in this subsection, we have chosen the uniform foliation with $\hat{a} = (1, 0, 0, 0)$ in the initial global CM frame the same as in Sec. IV C. We compare two different EoS taken from Ref. [48]. The hard momentum-dependent Skyrme EoS (MH1) uses a repulsive density-dependent potential (139) with the exponent $\gamma = 2.273$, while the soft Skyrme EoS (MS1) uses $\gamma = 1.109$. The left and right panels show the results from the MH1 and MS1, respectively. For the MH1 EoS, the numerical estimate by the Monte Carlo integration (RQMDv.MC) suppresses the density compared with the traditional RQMD results, indicating that the traditional QMD approximation underestimates the repulsive density-dependent potential. This is consistent with the findings in Ref. [39]. We observe in Fig. 8 that our new approximation method for computing the density-dependent potential (RQMDv2) reproduces the RQMDv.MC results, confirming that RQMDv2 can be reliably used for the simulations of heavy-ion collisions, which is numerically much more efficient than the Monte Carlo integration. However, in the case of the MS1 EoS, there is no significant difference among the three models, because the density dependence in the vector potential is nearly linear in the MS1 EoS.

Figure 9 shows the time evolutions of the sign-weighted directed flow v_1^* (130) of baryons integrated in the rapidity range $|y| < 1$. We also confirm that RQMDv2 results are in good agreement with the RQMDv.MC results for the directed

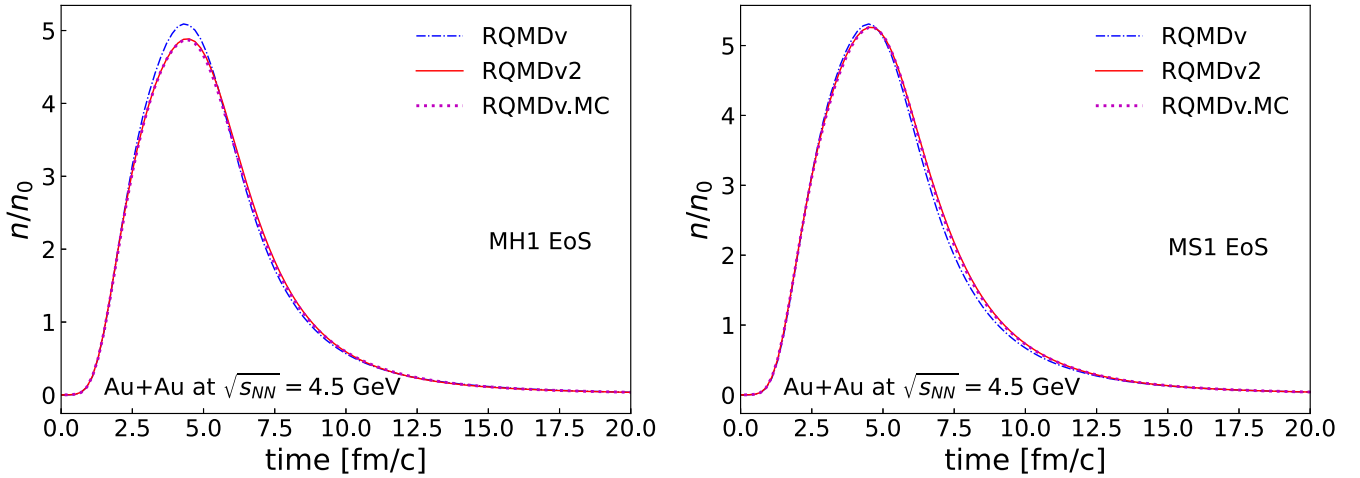


FIG. 8. Time evolution of the density at the center of mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV from RQMD with the Skyrme vector potential. The left panel shows the results from hard momentum-dependent EoS (MH1) and the right panel shows the results from the soft momentum-dependent EoS (MS1). The dashed-dotted line corresponds to the result from the previous RQMDv model. The RQMDv2 model prediction is shown by the solid line, and the RQMDv.MC result is shown by the dashed line.

flow, while the traditional RQMDv predicts a smaller directed flow compared to the RQMDv.MC.

Finally, we show in Fig. 10 the rapidity dependence of the proton directed flow v_1 in mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV, compared with the STAR data [62]. For the MS1 EoS, it is seen that all approaches are in good agreement, and the directed flow is not sensitive to the treatment of the density-dependent potential, as expected when the value of γ is close to unity. However, for the MH1 EoS, which uses a large γ value, the differences are observed between the RQMDv and RQMDv2 results. For a large γ , RQMDv2 remains a good approximation to RQMDv.MC for describing the rapidity dependence of the directed flow.

F. Frame dependence, foliation dependence, and energy conservation

To validate the Lorentz covariance of the present formulation, we first demonstrate that the calculated results are independent of the choice of inertial frame for a fixed foliation. Furthermore, we also check the extent of the violation of the time-reparametrization invariance and energy conservation by the new formulation and the approximations.

As discussed earlier, we employ a uniform foliation $\hat{s}(x) = \hat{a} \cdot x$ with the Lorentz vector $\hat{a} = (1, 0, 0, 0)$ defined in the initial global center-of-mass (CM) frame [25]. In this setup, the global CM frame is shown to remain to be the initial global CM frame at later times after deriving the EoS; we will simply call this frame the global CM frame hereafter. When changing the reference frame, the components of $\hat{a}$ must be Lorentz-transformed accordingly to ensure the Lorentz covariance.

Figure 11 shows the rapidity distributions of protons and negative pions in central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV obtained using the RQMDv2 model to demonstrate reference-frame independence. We have confirmed the same behavior with the RQMD.RMF2 model. The label “(cm,cm)” denotes the case where both $\hat{a}$ and the computational frame

are the global CM frame, shown by the blue curves. In contrast, “(cm,lab)” corresponds to calculations performed in the laboratory frame—where one gold nucleus is initially at rest—while keeping $\hat{a}$ fixed to $(1, 0, 0, 0)$ in the global CM frame and Lorentz transformed to laboratory frame. These results are shown by the red curves. The two sets of calculations coincide exactly, demonstrating frame independence for the same specified foliation. This frame independence should be distinguished from the residual dependence on the choice of foliation, which is investigated in the following subsection.

Having established reference-frame independence for a fixed foliation, we now examine the dependence on the choice of foliation. The foliation $\hat{s}(x)$ is a concept independent of the computational reference frame. Different choices of foliation are possible as long as it satisfies certain requirements within the covariant formulation, but the dynamics itself may change because different foliations define different evolution hypersurfaces. A physically reasonable foliation should be determined by the physics so that it effectively captures the dynamics of a real system. For the foliation $\hat{s}(x) = \hat{a} \cdot x$, a natural choice for the Lorentz vector $\hat{a}$ is the inertial frame of the global CM system which ensures synchronization of particle clocks in the global CM frame [25–27]. It is shown by Refs. [25,49] that this foliation reproduces the results obtained with Sorge’s method given by the original RQMD paper [23], in which the evolution parameters of particles are determined by reflecting the velocities of surrounding particles.

Although the foliation dependence is unavoidable as far as the system is described by the N -body particle coordinates, it is important to examine results obtained with different foliations to check that the extent of the violation of the time-reparametrization invariance within the new formulation is not large. In Fig. 12, we present results obtained by choosing a foliation $\hat{s}(x) = \hat{a}' \cdot x$ with $\hat{a}' = (1, 0, 0, 0)$ in the laboratory frame.

The resulting rapidity distributions remain similar to those in Fig. 11, but are no longer perfectly symmetric, reflecting the foliation dependence of the RQMD framework written by

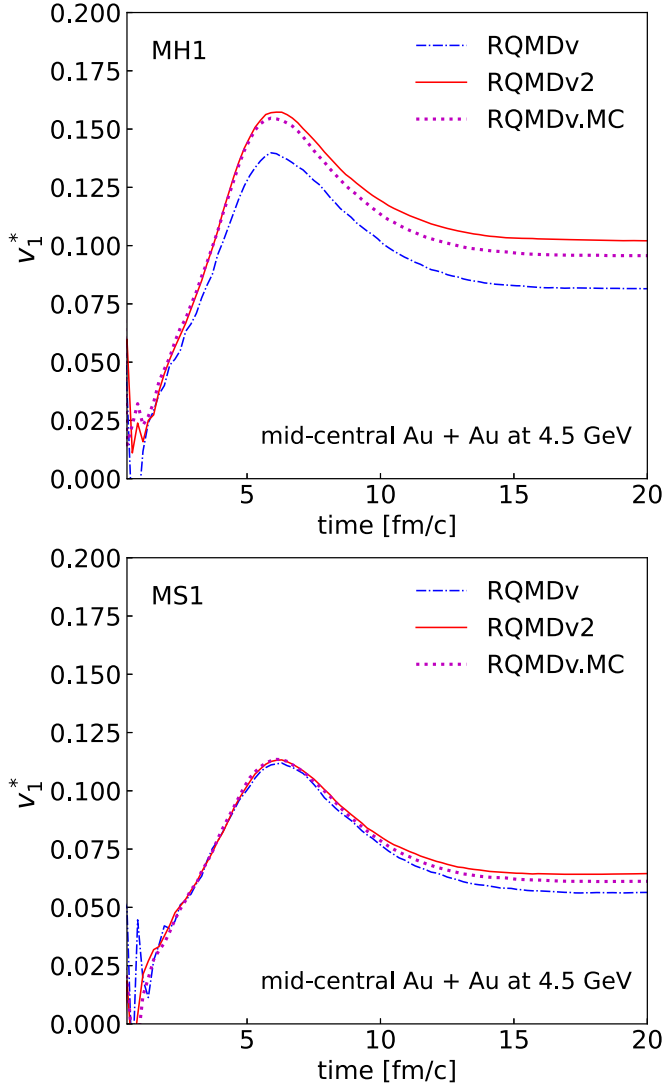


FIG. 9. Time evolution of sign-weighted directed flows v_1^* of baryons in mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV is compared with different models. Rapidity cut for the integration of the directed flow is $|y| < 1.0$. The meaning of the lines is the same as in Fig. 8.

a finite number of degrees of freedom. It is noted that the violation is not a reference-frame artifact, as confirmed by observing that results computed for a given foliation remain invariant under the change of the reference frame between the red solid and blue dot-dashed lines in Fig. 12. This clearly distinguishes the residual foliation dependence from the reference-frame independence demonstrated in Fig. 11. This also implies that the cluster separability can be approximately maintained by determining the frame for each cluster [49] because the results are not largely affected by whether $\hat{a}$ is determined based on the global CM frame or the cluster frame.

In our formulation, momentum is conserved independent of time step size, because of the strict implementation of action-reaction law in our model. We now turn to the validation of total energy conservation. Although our EoMs with the

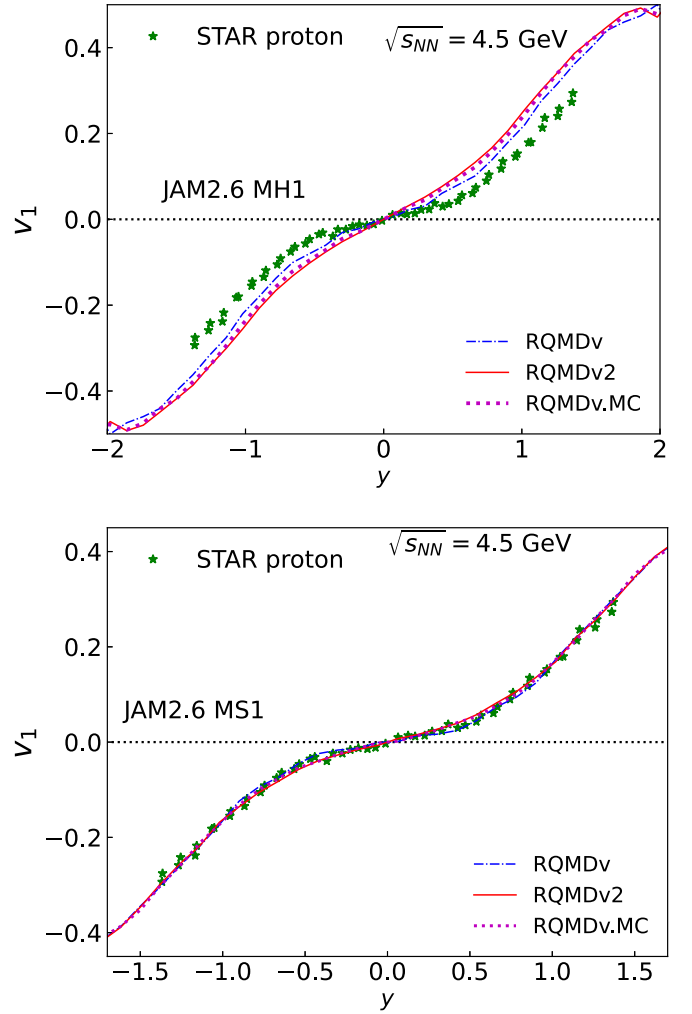


FIG. 10. Directed flows of protons in mid-central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV are compared with different models. The upper panel shows results obtained with the MS1 EoS, while the lower panel shows results from the MH1 EoS. STAR data were taken from Ref. [62]. The meaning of the lines is the same as in Fig. 8.

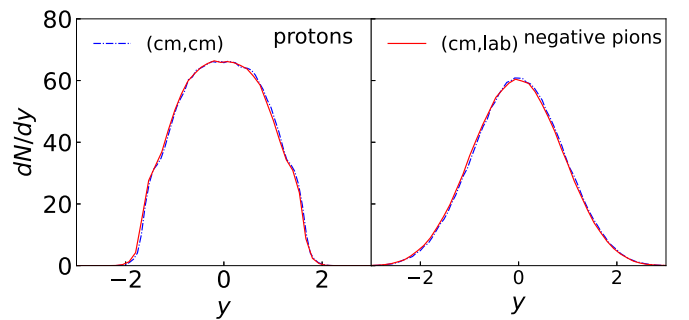


FIG. 11. Rapidity distributions of the protons (left panel) and negative pions (right panel) in central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV are compared for different reference frames: the global CM frame (blue lines) and the laboratory frame (red lines). The impact parameters are chosen as $0 < b < 3.0$ fm.

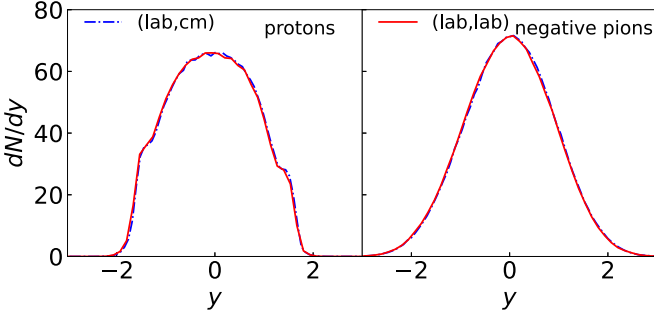


FIG. 12. Same as Fig. 11, but the $\hat{a}$ is chosen to be (1,0,0,0) in the laboratory frame.

QMD2 approximation exactly conserve momentum, exact energy conservation is not guaranteed due to the approximation of the spatial integral in the EoMs. Thus, we need to check the degree of violation of the total energy conservation. Since our approximation to the force has been shown to reproduce well the results of spatial integration, and since density evolution and directed flow are consistent with the numerical integration, we expect good energy conservation. To see the degree of the total energy conservation, the relative error of the total energy E from its initial value E_{ini} ,

$$\frac{\Delta E}{E_{\text{ini}}} = \frac{\langle E - E_{\text{ini}} \rangle}{\langle E_{\text{ini}} \rangle}, \quad (165)$$

is plotted in Fig. 13 as a function of the evolution time in central Au + Au collisions at $\sqrt{s_{NN}} = 4.5$ GeV with impact parameter $b = 1.0$ fm. The results from RQMDv2 (RQMD.RMF2) are shown in the left (right) panel for three different time-step sizes: $dt = 0.2, 0.1$ and 0.05 fm/c. Even with a larger time-step size of $dt = 0.2$ fm/c, the relative error remains within 1%. It is seen that the total energy is conserved within 0.25% when using $dt = 0.1$ fm/c. The accuracy of the energy conservation is even better for mid-central collisions. We also confirm that physical observables such as dN/dy and v_1 do not change when varying the time-step size. We finally mention that the relative RMSD

$$\frac{\sqrt{\langle (E - E_{\text{ini}})^2 \rangle}}{\langle E_{\text{ini}} \rangle} \quad (166)$$

agrees with the relative error (165) except the sign, which means that event-by-event fluctuations in the energy conservation are small. In fact, we confirmed that the standard deviation of $E - E_{\text{ini}}$ is small compared to the typical size of $E - E_{\text{ini}}$.

G. Difference between RQMD and RQMD2

Finally, we mention the differences between the previous RQMD approach [30,31,48] and the new one. In the previous RQMD approach, the EoMs at the center-of-mass frame are obtained by the Hamiltonian using one-particle potentials,

$$H = \sum_{j=1}^N \sqrt{(m_j + V_{s,j})^2 + (\mathbf{p}_j - \mathbf{V}_j)^2} + V_j^0, \quad (167)$$

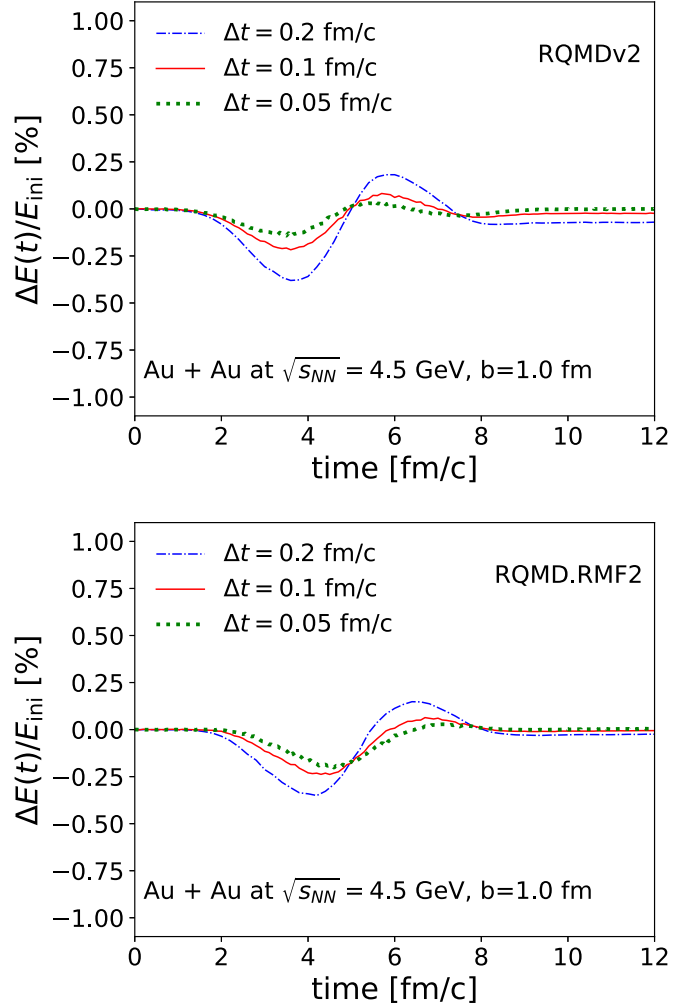


FIG. 13. Relative error to the initial total energy as a function of time is plotted for RQMDv2 (upper panel) and RQMD.RMF2 (lower panel) in Au + Au collision at $\sqrt{s_{NN}} = 4.5$ GeV, and $b = 1.0$ fm. The three different time step-sizes of $dt = 0.2, 0.1$ and 0.05 fm/c are compared.

where m_j is the mass of the j th particle, and the scalar and vector one-particle potentials, $V_{s,j} := V_s(x_j)$ and $V_j^\mu := V^\mu(x_j)$, are defined by Eqs. (147) and (148) using the interaction density with the relativistic Gaussian. The momentum-dependent one-particle potential is given by half of the single-particle potential in Eqs. (140) and (141). See Ref. [48] for the details. The structure of the EoMs for RQMD is similar to that of the new approach (RQMD2). Their main difference is the same as the QMD case; the density of the potential is evaluated by the real particle density in the new approach instead of the interaction density in the RQMD approach. There are two differences in the relativistic approaches: the RQMD uses the relativistic Gaussian for the interaction density, while the new approach explicitly computes the overlap of the relativistic Gaussian. The new RQMD2 uses the mass-shell condition with the single-particle potential, while the previous one uses the one-particle potential. We will see that the difference in the mass-shell condition does not affect much

the dynamics of heavy-ion collisions. However, the mass-shell condition with the single-particle potential may become relevant when chiral models are used to generate effective mass.

V. SUMMARY

We have presented a novel formulation for the mean-field propagation part of RQMD based on the variational principle for interacting Gaussian wave packets for the first time. We derived new covariant canonical EoMs for an N -body system interacting via Lorentz scalar and vector potentials. We have first derived BUU-like EoMs, which are expressed by the single-particle potentials, in the external and dynamical fields cases. Then, assuming the local density approximation described in Sec. III C, we have rewritten the EoMs to obtain QMD-like EoMs, which are expressed by the one-particle potentials. Furthermore, we proposed a new approximation for the spatial integral, and showed that it provides an excellent approximation to the full integral.

The main differences from the previous approaches are as follows: (1) Our approach imposes mass-shell constraints with the single-particle potential, whereas previous approaches employed one-particle potentials. (2) Our method uses the overlap of relativistic Gaussians. (3) It provides an accurate estimation of the underlying EoS.

We have implemented these equations into the event generator JAM2 to perform event-by-event simulations of heavy-ion collisions. These covariant EoMs enable numerical simulation of heavy-ion collisions with computational costs comparable to those of nonrelativistic quantum molecular dynamics. We demonstrated that the new EoMs accurately simulate density-dependent potential in heavy-ion collisions by comparing the results with Monte Carlo integration for the three-dimensional spatial integral.

In this work, we assumed the local density approximation to evaluate the scalar and vector potentials in the numerical implementation. As a future extension, dynamical meson fields must be included by solving explicitly the spacetime evolution of meson fields.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [53].

APPENDIX A: PROOF OF EQ. (61)

In this appendix, we show Eq. (61). We first consider the contribution of the variation of the generalized potential

$\delta W(x, p)$:

$$\begin{aligned} & \int d^4x d^4p \delta W(x, p) f(x, p) \\ &= \int d^4x d^4p [\delta p^{*\mu}(x, p) p_\mu^*(x, p) \\ & \quad - \delta m^*(x, p) m^*(x, p)] f(x, p) \\ &= \int d^4x d^4p [-\delta U(x, p) \phi_\mu(x, p) - \delta U_s(x, p) \phi(x, p)]. \end{aligned} \quad (\text{A1})$$

In the second equality, we used Eqs. (24) and (25) to rewrite $\delta p^*(x, p)$ and $\delta m^*(x, p)$ and Eqs. (55) and (56) to obtain $\phi(x, p)$ and $\phi_\mu(x, p)$.

The variation of the field energy can be rewritten as

$$\begin{aligned} \delta V_{\text{field}} &= \delta F[\phi, \phi_\mu] - \int d^4x d^4p \left\{ \delta \phi(x, p) \frac{\delta F[\phi, \phi_\mu]}{\delta \phi(x, p)} \right. \\ & \quad \left. + \delta \phi_\mu(x, p) \frac{\delta F[\phi, \phi_\mu]}{\delta \phi_\mu(x, p)} \right\} \\ & \quad - \int d^4x d^4p \left\{ \phi(x, p) \delta \frac{\delta F[\phi, \phi_\mu]}{\delta \phi(x, p)} \right. \\ & \quad \left. + \phi_\mu(x, p) \delta \frac{\delta F[\phi, \phi_\mu]}{\delta \phi_\mu(x, p)} \right\} \\ &= - \int d^4x d^4p [\phi(x, p) \delta U_s(x, p) + \phi_\mu(x, p) \delta U^\mu(x, p)]. \end{aligned} \quad (\text{A2})$$

In the second equality, we used the fact that the first and second terms cancel with each other, and the third term was rewritten in terms of $U_s(x, p)$ and $U^\mu(x, p)$ using Eqs. (53) and (54).

It is now clear that Eqs. (A1) and (A2) cancel with each other.

APPENDIX B: MONTE CARLO INTEGRATION WITH A RELATIVISTIC GAUSSIAN WEIGHT

In this appendix, we explain how we perform the Monte Carlo integration of the integral:

$$I_i = \int d^4x f(x) G(x - x_i; u_i), \quad (\text{B1})$$

where $f(x)$ is an arbitrary function of the coordinates x , and $G(x - x_i; u_i)$ is the relativistic Gaussian (75).

Without loss of generality, we may choose new coordinates x'^μ in the rest frame of $\hat{a}$ so that the particle position is the origin, $x'_i = 0$. This can be achieved by performing the following Poincaré transformation:

$$x^\mu \mapsto x'^\mu = \Lambda^\mu_\nu (x^\nu - x_i^\nu), \quad (\text{B2})$$

where Λ is the Lorentz boost with the four-velocity $\hat{a}^\mu = (a^0, \mathbf{a})^T$:

$$\Lambda = \left(\begin{array}{c|c} a^0 & -\mathbf{a}^T \\ \hline -\mathbf{a} & \mathbb{1} + \frac{\mathbf{a}\mathbf{a}^T}{a^0+1} \end{array} \right), \quad (\text{B3})$$

where $\mathbb{1}$ is the 3×3 identity matrix. The integral is written as

$$I_i = \int d^4x' f(\Lambda^{-1}x' + x_i) \delta(x' \cdot \hat{a}') \frac{u' \cdot \hat{a}'}{(2\pi L)^{3/2}} e^{x'_\mu \Delta_i'^{\mu\nu} x'_\nu / 2L} \\ = \int d^3x' f(\Lambda^{-1}x' + x_i)|_{x^0=0} \frac{\gamma_i}{(2\pi L)^{3/2}} e^{-x'^a A^{ab} x'^b / 2L}, \quad (\text{B4})$$

where $\hat{a}' = (1, 0, 0, 0)$, $\gamma_i = u'_i \cdot \hat{a}' = u_i^0$, $\Delta_i'^{\mu\nu} = g^{\mu\nu} - u_i^\mu u_i^\nu$, $A^{ab} = -\Delta_i'^{ab}$, and

$$u'^\mu = \begin{pmatrix} a^\mu u_{i\mu} \\ -u_i^0 \mathbf{a} + (1 + \frac{\mathbf{a}\mathbf{a}^\top}{a^0+1}) \mathbf{u}_i \end{pmatrix}. \quad (\text{B5})$$

Next, we complete the square for the quadratic form in the exponent by diagonalizing the 3×3 coefficient matrix A^{ab} , ($a, b = 1, 2, 3$). The matrix can be decomposed into the components of its eigenspaces as

$$A = P_\perp + \gamma_i^2 P_u, \quad (\text{B6})$$

using the projectors,

$$(P_\perp)^{ab} = \delta^{ab} - (P_u)^{ab}, \quad (P_u)^{ab} = \hat{u}_i^a \hat{u}_i^b, \quad (\text{B7})$$

with $\hat{u}_i^a := u_i^a / \sqrt{\gamma_i^2 - 1}$. In the following argument, duplicate indices a, b , or c appearing in a term imply the sum over 1, 2, 3. Using the properties of the projectors,

$$P_\perp^2 = P_\perp, \quad P_\perp P_u = 0, \quad P_u^2 = P_u, \quad (\text{B8})$$

one can confirm that the square root of the matrix A and its inverse become

$$(A^{1/2})^{ab} = (P_\perp + \gamma_i P_u)^{ab}, \quad (\text{B9})$$

$$(A^{-1/2})^{ab} = \left(P_\perp + \frac{P_u}{\gamma_i} \right)^{ab} = \delta^{ab} - \frac{u_i^a u_i^b}{\gamma_i(\gamma_i + 1)}. \quad (\text{B10})$$

Noting that $\det(A^{-1/2}) = 1/\gamma_i$, we may simplify the expression of the integral I_i by the change of variables, $\mathbf{x}' \mapsto \mathbf{x}' = \sqrt{L} A^{-1/2} \tilde{\mathbf{x}}$:

$$I_i = \int d^3\tilde{x} f(T(\tilde{x}; x_i, u_i)) \frac{1}{(2\pi)^{3/2}} e^{-\tilde{x}^2/2}, \quad (\text{B11})$$

where

$$T(\tilde{x}; x_i, u_i) = x_i + \sqrt{L} \Lambda^{-1} \begin{pmatrix} 0 \\ A^{-1/2} \tilde{\mathbf{x}} \end{pmatrix}. \quad (\text{B12})$$

Based on the above consideration, we implement the Monte Carlo integration in the following procedure: First, we sample the coordinates $\tilde{\mathbf{x}} = (\tilde{x}_1, \tilde{x}_2, \tilde{x}_3)$ according to the Gaussian distribution $\exp(-\tilde{x}^2/2)$ and transform it as

$$\tilde{x}^a = \sqrt{L} (A^{-1/2})^{ab} \tilde{x}^b = \sqrt{L} \left[\delta^{ab} - \frac{u_i^a u_i^b}{\gamma_i(\gamma_i + 1)} \right] \tilde{x}^b. \quad (\text{B13})$$

To obtain the n th Monte Carlo sample point $x_{(n)}^\mu$ in the computational frame, we perform the Poincaré transformation:

$$x_{(n)}^0 = x_i^0 + \hat{a}^a \tilde{x}^a, \\ x_{(n)}^a = x_i^a + \left(\delta^{ab} + \frac{\hat{a}^a \hat{a}^b}{\hat{a}^0 + 1} \right) \tilde{x}^b. \quad (\text{B14})$$

We repeat this procedure N_{MC} times and take the average to obtain a value for the integral:

$$I_i \approx \frac{1}{N_{\text{MC}}} \sum_{n=1}^{N_{\text{MC}}} f(x_{(n)}). \quad (\text{B15})$$

APPENDIX C: GAUSSIAN OVERLAP INTEGRAL

We evaluate the integral of the overlap of two relativistic Gaussians,

$$\tilde{g}_{ij}(x_i - x_j) = \int d^4x \delta((x - x_i) \cdot \hat{a}) \tilde{g}(x - x_j) \tilde{g}(x - x_i), \quad (\text{C1})$$

where

$$\tilde{g}(x - x_i) = \frac{1}{(2\pi L)^{3/2}} \exp \frac{R(x - x_i; u_i)^2}{2L}. \quad (\text{C2})$$

Note that because of the translational invariance, $\tilde{g}_{ij}$ is a function of the relative distance $x_i - x_j$. We go to the frame $\hat{a} = (1, 0, 0, 0)$ so that the temporal components vanish: $x^0 - x_i^0 = x^0 - x_j^0 = 0$. The Gaussian overlap (C1) becomes

$$\tilde{g}_{ij}(0, \mathbf{r}) = \frac{1}{(2\pi L)^3} \int d^3x e^{-\frac{1}{2L} Q}, \quad (\text{C3})$$

where $\mathbf{r} = \mathbf{x}_i - \mathbf{x}_j$,

$$Q = (\mathbf{x} - \mathbf{r})^T A (\mathbf{x} - \mathbf{r}) + \mathbf{x}^T B \mathbf{x}, \quad (\text{C4})$$

and

$$A = \mathbb{1} + \mathbf{u}_i \mathbf{u}_i^T, \quad B = \mathbb{1} + \mathbf{u}_j \mathbf{u}_j^T, \quad (\text{C5})$$

with $\mathbb{1}$ being the 3×3 identity matrix.

The square in Q with respect to $\mathbf{x}$ may be completed as

$$Q = [\mathbf{x} - (A + B)^{-1} A \mathbf{r}]^T (A + B) [\mathbf{x} - (A + B)^{-1} A \mathbf{r}] \\ + \mathbf{r}^T A \mathbf{r} - \mathbf{r}^T A (A + B)^{-1} A \mathbf{r} \\ = [\mathbf{x} - (A + B)^{-1} A \mathbf{r}]^T (A + B) [\mathbf{x} - (A + B)^{-1} A \mathbf{r}] \\ + \mathbf{r}^T A (A + B)^{-1} B \mathbf{r}. \quad (\text{C6})$$

The relative kernel can be integrated as

$$\tilde{g}_{ij}(\mathbf{r}, 0) = \frac{e^{-\frac{1}{2L} \mathbf{r}^T A (A + B)^{-1} B \mathbf{r}}}{(2\pi L)^{3/2} \det(A + B)^{1/2}}. \quad (\text{C7})$$

Let us consider the explicit form of $(A + B)^{-1}$ and $A(A + B)^{-1}B$. The 3×3 matrices A and B can be written as

$$A := \mathbb{1} + a^2 \pi_a, \quad B := \mathbb{1} + b^2 \pi_b, \quad (\text{C8})$$

with $a = |\mathbf{u}_i|$ and $b = |\mathbf{u}_j|$, and the projectors onto the direction of $\mathbf{u}_i$ and $\mathbf{u}_j$:

$$\pi_a := \frac{\mathbf{u}_i \mathbf{u}_i^T}{a^2}, \quad \pi_b := \frac{\mathbf{u}_j \mathbf{u}_j^T}{b^2}. \quad (\text{C9})$$

Those projectors satisfy $\pi_a^2 = \pi_a$ and $\pi_b^2 = \pi_b$ but are not orthogonal to each other, $\pi_a \pi_b \neq 0$. We define the

anticommutator of the projectors as

$$\rho := \pi_a \pi_b + \pi_b \pi_a = c \frac{\mathbf{u}_i \mathbf{u}_j^T + \mathbf{u}_j \mathbf{u}_i^T}{ab}, \quad (\text{C10})$$

where $c := \cos \theta = \mathbf{u}_i \cdot \mathbf{u}_j / ab$ with θ being the angle between $\mathbf{u}_i$ and $\mathbf{u}_j$. It is useful to define

$$X = \frac{A+B}{2} = \mathbb{1} + \frac{a^2 \pi_a + b^2 \pi_b}{2}. \quad (\text{C11})$$

To write down the components of X , we choose the basis as $\mathbf{e}_1 = \hat{\mathbf{u}}_i = \mathbf{u}_i/a$ and $\mathbf{e}_2 \propto (1 - \pi_a)\hat{\mathbf{u}}_j$. Here, $\mathbf{u}_i$ and $\mathbf{u}_j$ are written as

$$\mathbf{u}_i = a \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{u}_j = b \begin{pmatrix} c \\ s \\ 0 \end{pmatrix}, \quad (\text{C12})$$

where

$$c := \cos \theta = \frac{\mathbf{u}_i^T \mathbf{u}_j}{ab}, \quad s := \sin \theta = \sqrt{1 - c^2}, \quad (\text{C13})$$

and θ is the angle between $\mathbf{u}_i$ and $\mathbf{u}_j$. In this basis, X is written as

$$X = \begin{pmatrix} 1 + \frac{a^2+b^2c^2}{2} & \frac{b^2cs}{2} & 0 \\ \frac{b^2cs}{2} & 1 + \frac{b^2s^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (\text{C14})$$

Now, we consider the Cayley-Hamilton theorem for a 3×3 matrix X :

$$X^3 - tX^2 + uX - d\mathbb{1} = 0, \quad (\text{C15})$$

where t , u , and d are the coefficients of the characteristic equation $\det(\lambda\mathbb{1} - X) = 0$:

$$t = \text{tr}X = 3 + \frac{a^2 + b^2}{2}, \quad (\text{C16})$$

$$\begin{aligned} d = \det X &= 1 + \frac{a^2 + b^2}{2} + \frac{a^2 b^2 s^2}{4} \\ &= \left(1 + \frac{a^2}{2}\right) \left(1 + \frac{b^2}{2}\right) - \frac{a^2 b^2 c^2}{4}, \end{aligned} \quad (\text{C17})$$

$$\begin{aligned} u &= \begin{vmatrix} 1 + \frac{a^2+b^2c^2}{2} & \frac{b^2cs}{2} \\ \frac{b^2cs}{2} & 1 + \frac{b^2s^2}{2} \end{vmatrix} + \begin{vmatrix} 1 + \frac{b^2s^2}{2} & 0 \\ 0 & 1 \end{vmatrix} \\ &\quad + \begin{vmatrix} 1 & 0 \\ 0 & 1 + \frac{a^2+b^2c^2}{2} \end{vmatrix} \\ &= d + X_{11} + X_{22} = d + t - 1. \end{aligned} \quad (\text{C18})$$

The inverse of X can be obtained using Eq. (C15):

$$\begin{aligned} X^{-1} &= \frac{1}{d}(X^2 - tX + u\mathbb{1}) \\ &= \mathbb{1} + \frac{1}{d}[X^2 - \mathbb{1} + t(X - \mathbb{1})] \\ &= \mathbb{1} + \frac{1}{d}(X - \mathbb{1})[X + (1-t)\mathbb{1}] \\ &= \mathbb{1} + \frac{a^2 \pi_a + b^2 \pi_b}{2d} \left[\frac{a^2 \pi_a + b^2 \pi_b}{2} - \left(1 + \frac{a^2 + b^2}{2}\right) \mathbb{1} \right] \end{aligned}$$

$$\begin{aligned} &= \mathbb{1} - \frac{1}{2d} \left[a^2 \pi_a + b^2 \pi_b + \frac{a^2 b^2}{2} (\pi_a + \pi_b - \rho) \right] \\ &= \mathbb{1} - \frac{1}{2d} \tau + \frac{a^2 b^2}{4d} \rho. \end{aligned} \quad (\text{C19})$$

We next consider $A - A(A+B)^{-1}A = (1/2)AX^{-1}B$. Since the result is a symmetric matrix by definition, we can calculate it ignoring the difference of the antisymmetric part and pick up the symmetric part of the final result, i.e., $M = M^T + (M - M^T) \equiv M^T$ for an arbitrary matrix M , where the symbol “ $\equiv$ ” represents equivalence ignoring antisymmetric differences. For example, we can use the relations $M_1 M_2 \equiv M_2^T M_1^T$ and $\pi_a \pi_b \equiv \rho/2$.

$$\begin{aligned} AX^{-1}B &\equiv \underbrace{(\mathbb{1} + a^2 \pi_a + b^2 \pi_b)}_{2X - \mathbb{1}} X^{-1} + a^2 b^2 \pi_a X^{-1} \pi_b \\ &= 2\mathbb{1} - X^{-1} + a^2 b^2 \pi_a X^{-1} \pi_b. \end{aligned} \quad (\text{C20})$$

Applying $\pi_a(\pi_a, \pi_b, \rho)\pi_b = (1, 1, 1 + c^2)\pi_a \pi_b$ to the second last line of Eq. (C19), we obtain

$$\begin{aligned} \pi_a X^{-1} \pi_b &= \pi_a \pi_b \left\{ 1 - \frac{1}{2d} \left[a^2 + b^2 + \frac{a^2 b^2}{2} (1 - c^2) \right] \right\} \\ &= \pi_a \pi_b \frac{2d - a^2 - b^2 - a^2 b^2 s^2 / 2}{2d} \\ &= \pi_a \pi_b \frac{2}{2d} \equiv \frac{\rho}{2d}. \end{aligned} \quad (\text{C21})$$

Substituting Eq. (C21) in Eq. (C20), we obtain

$$\begin{aligned} AX^{-1}B &\equiv 2\mathbb{1} - X^{-1} + \frac{a^2 b^2}{2d} \rho \\ &= \mathbb{1} + \frac{1}{2d} \tau + \frac{a^2 b^2}{4d} \rho. \end{aligned} \quad (\text{C22})$$

The right-hand side is already in a symmetric form, so it matches $AX^{-1}B$.

Finally, since $(A+B)^{-1} = 2^{-1}[(A+B)/2]^{-1}$, we get

$$(A+B)^{-1} = \frac{1}{2}X^{-1}, \quad (\text{C23})$$

$$A(A+B)^{-1}B = \frac{1}{2}AX^{-1}B. \quad (\text{C24})$$

Using those matrices, $(A+B)^{-1}$ and $A(A+B)^{-1}B$ can be written as

$$(A+B)^{-1} = \frac{1}{2} \left[\mathbb{1} + \frac{1}{2d} \left(-\tau + \frac{a^2 b^2}{2} \rho \right) \right], \quad (\text{C25})$$

$$A(A+B)^{-1}B = \frac{1}{2} \left[\mathbb{1} + \frac{1}{2d} \left(\tau + \frac{a^2 b^2}{2} \rho \right) \right], \quad (\text{C26})$$

where

$$\tau := \left(1 + \frac{b^2}{2}\right) a^2 \pi_a + \left(1 + \frac{a^2}{2}\right) b^2 \pi_b. \quad (\text{C27})$$

The exponent is obtained as

$$\begin{aligned} & -\frac{1}{2L} \mathbf{r}^T A(A+B)^{-1} B \mathbf{r} \\ & = -\frac{1}{4L} \left\{ -r^2 + \frac{1}{2d} \left[\left(1 + \frac{b^2}{2} \right) t_a^2 \right. \right. \\ & \quad \left. \left. + \left(1 + \frac{a^2}{2} \right) t_b^2 + abct_a t_b \right] \right\}, \end{aligned} \quad (\text{C28})$$

where $r^2 = -\mathbf{r}^T \mathbf{r}$, $t_a = -\mathbf{r}^T \mathbf{u}_i$, and $t_b = -\mathbf{r}^T \mathbf{u}_j$. Note that $d = \det[(A+B)/2]$, thus $\det(A+B) = 2^3 d$.

When we perform a simulation with the constraints $x_i \cdot \hat{a} = s$, we can define the relative kernel in the $\hat{a}$ frame [i.e., the inertial frame in which $\hat{a} = (1, 0, 0, 0)^T$]. Since $r^0 = x_i^0 - x_j^0 = s - s = 0$ in the $\hat{a}$ frame, we may write $\mathbf{r}^T \mathbf{v}$ (with v^μ being an arbitrary Lorentz vector) in a covariant form as $\mathbf{r}^T \mathbf{v} = -(r^0 v^0 - \mathbf{r}^T \mathbf{v}) = -r^\mu v_\mu$. Therefore, we can evaluate the exponent (C28) in a covariant way using

$$\begin{aligned} a^2 & = -(g_{\mu\nu} - \hat{a}_\mu \hat{a}_\nu) u_i^\mu u_i^\nu \\ & = -u_i^2 + (u_i \cdot \hat{a})^2, \end{aligned} \quad (\text{C29})$$

$$\begin{aligned} b^2 & = -(g_{\mu\nu} - \hat{a}_\mu \hat{a}_\nu) u_j^\mu u_j^\nu \\ & = -u_j^2 + (u_j \cdot \hat{a})^2, \end{aligned} \quad (\text{C30})$$

$$\begin{aligned} c & = -(g_{\mu\nu} - \hat{a}_\mu \hat{a}_\nu) u_i^\mu u_j^\nu / ab \\ & = \frac{-u_i \cdot u_j + (u_i \cdot \hat{a})(u_j \cdot \hat{a})}{ab}, \end{aligned} \quad (\text{C31})$$

$$r^2 = \mathbf{r} \cdot \mathbf{r}, \quad (\text{C32})$$

$$t_a = \mathbf{r} \cdot \mathbf{u}_i, \quad (\text{C33})$$

$$t_b = \mathbf{r} \cdot \mathbf{u}_j. \quad (\text{C34})$$

APPENDIX D: NONLINEAR VECTOR POTENTIAL

We consider the vector potential of the form

$$V(\omega) = -\frac{m_\omega^2}{2} \omega^2 - \frac{c_4}{4} \omega^4. \quad (\text{D1})$$

The gap equation is

$$m_\omega^2 \omega^\mu + c_4 \omega^2 \omega^\mu = g_\omega J^\mu. \quad (\text{D2})$$

The differentiation with respect to x_i yields

$$\left[(m_\omega^2 + c_4 \omega^2) g^{\mu\nu} + 2c_4 \omega^\mu \omega^\nu \right] \frac{\partial \omega_\nu}{\partial x_i} = g_\omega \frac{\partial J^\mu}{\partial x_i}. \quad (\text{D3})$$

The inverse is given by

$$\begin{aligned} & [(m^2 + c\omega^2) g^{\mu\nu} + 2c\omega^\mu \omega^\nu]^{-1} \\ & = \frac{(m^2 + 3c\omega^2) g_{\mu\nu} - 2c\omega_\mu \omega_\nu}{(m^2 + 3c\omega^2)(m^2 + c\omega^2)} \\ & = \frac{1}{m^2 + 3c\omega^2} \left[g_{\mu\nu} + \frac{2c(\omega^2 g_{\mu\nu} - \omega_\mu \omega_\nu)}{m^2 + c\omega^2} \right], \end{aligned} \quad (\text{D4})$$

or by another expression,

$$\begin{aligned} & [(m^2 + c\omega^2) g^{\mu\nu} + 2c\omega^\mu \omega^\nu]^{-1} \\ & = \frac{1}{m^2 + c\omega^2} \left(g_{\mu\nu} - \frac{2c\omega_\mu \omega_\nu}{m^2 + 3c\omega^2} \right), \end{aligned} \quad (\text{D5})$$

which is obtained by separating the transverse and longitudinal component. When a matrix is decomposed into the transverse component a and the longitudinal component b ,

$$A^{\mu\nu} = a \left(g^{\mu\nu} - \frac{k^\mu k^\nu}{k^2} \right) + b \frac{k^\mu k^\nu}{k^2}, \quad (\text{D6})$$

and its inverse is given by

$$A_{\mu\nu}^{-1} = \frac{1}{a} \left(g_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right) + \frac{1}{b} \frac{k_\mu k_\nu}{k^2}. \quad (\text{D7})$$

One can confirm $A^{\mu\lambda} A_{\lambda\nu}^{-1} = g^{\mu\lambda} g_{\lambda\nu}$. In our case, $a = m_\omega^2 + c_4 \omega^2$ and $b = m_\omega^2 + 3c_4 \omega^2$. Thus, the derivative of the ω field is expressed as the linear combination of the current:

$$\frac{\partial \omega_\mu}{\partial x_i} = \frac{g_\omega}{m^2 + 3c\omega^2} \left[g_{\mu\nu} + \frac{2c(\omega^2 g_{\mu\nu} - \omega_\mu \omega_\nu)}{m^2 + c\omega^2} \right] \frac{\partial J^\nu}{\partial x_i}. \quad (\text{D8})$$

The derivative with respect to J_λ yields

$$\left[(m_\omega^2 + c_4 \omega^2) g^{\mu\nu} + 2c_4 \omega^\mu \omega^\nu \right] \frac{\partial \omega_\nu}{\partial J_\lambda} = g_\omega \frac{\partial J^\mu}{\partial J_\lambda} = g_\omega g^{\mu\lambda}, \quad (\text{D9})$$

$$\begin{aligned} \frac{\partial \omega_\nu}{\partial J_\lambda} & = \frac{g_\omega}{m^2 + c\omega^2} \left(g_{\mu\nu} - \frac{2c\omega_\mu \omega_\nu}{m^2 + 3c\omega^2} \right) g^{\mu\lambda} \\ & = \frac{g_\omega}{m^2 + c\omega^2} \left(\delta_\nu^\lambda - \frac{2c\omega^\lambda \omega_\nu}{m^2 + 3c\omega^2} \right). \end{aligned} \quad (\text{D10})$$

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