van der Waals Interactions in Hadron Resonance Gas: From Nuclear Matter to Lattice QCD

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An extension of the ideal hadron resonance gas (HRG) model is constructed which includes the attractive and repulsive van der Waals (VDW) interactions between baryons. This VDW-HRG model yields the nuclear liquid-gas transition at low temperatures and high baryon densities. The VDW parameters a and b are fixed by the ground state properties of nuclear matter, and the temperature dependence of various thermodynamic observables at zero chemical potential are calculated within the VDW-HRG model. Compared to the ideal HRG model, the inclusion of VDW interactions between baryons leads to a qualitatively different behavior of second and higher moments of fluctuations of conserved charges, in particular in the so-called crossover region $T \sim 140$–190 MeV. For many observables this behavior resembles closely the results obtained from lattice QCD simulations. This hadronic model also predicts nontrivial behavior of net-baryon fluctuations in the region of phase diagram probed by heavy-ion collision experiments. These results imply that VDW interactions play a crucial role in the thermodynamics of hadron gas. Thus, the commonly performed comparisons of the ideal HRG model with the lattice and heavy-ion data may lead to misconceptions and misleading conclusions.

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The thermodynamic properties of strongly interacting matter at zero chemical potential and finite temperature have been computed using Monte Carlo simulations in lattice QCD [1,2]. A crossover is observed [3] in the temperature range of 140–190 MeV. At lower temperatures, $T \sim 100$–150 MeV, QCD exhibits features similar to simple ideal hadron resonance gas (IHRG) which successfully reproduces many lattice observables [4–7]. In the crossover region, however, the agreement between IHRG and lattice QCD deteriorates. The breakdown of the IHRG model especially concerns the higher order fluctuations and correlations of conserved charges [8], resulting in statements that hadrons melt quickly and are basically absent at $T > 160$ MeV [9]. In this Letter, it is shown that these conclusions are inconclusive. van der Waals (VDW) interactions between baryons play a crucial role for the thermodynamics of hadron fluid at sufficiently high temperatures. As a result, the qualitative features of the thermodynamics of interacting HRG appear to be close to lattice results in the crossover region. The results also have important phenomenological relevance for heavy-ion collision experiments where measurements of conserved charges fluctuations have been suggested as probes for chemical freeze-out [10,11] or the QCD critical point [12].

The IHRG model does not capture the VDW nature of nucleon-nucleon interaction and, thus, fails to describe the properties of nuclear matter at small temperatures and large baryon densities. This shortcoming of this common HRG model is usually considered to be of minor significance when applied to ultrarelativistic heavy-ion collisions or to lattice data, although recently possible relevance for fluctuations was pointed out [13]. The repulsive part of VDW interactions had often been included into HRG by means of an excluded-volume (EV) procedure [14], usually assuming identical EV interactions between all hadron pairs [15]. The grand canonical ensemble formulation of the full VDW equation with both attractive and repulsive interactions, and including quantum statistics, was developed in Refs. [16–18] for single-component systems. In these works, the basic features of nuclear matter have been successfully described by the VDW equation with Fermi statistics for nucleons. The VDW parameters a and b were uniquely fixed by reproducing the saturation density $n_0 = 0.16$ fm^{-3} and binding energy $E/A = -16$ MeV of the ground state of nuclear matter. For nucleons the values $a = 329$ MeV fm^3 and $b = 3.42$ fm^3 were obtained in Ref. [18], and also later in Ref. [19]. The resulting model predicts a liquid-gas first-order phase transition in symmetric nuclear matter with a critical point located at $T_c \simeq 19.7$ MeV and $\mu_c \simeq 908$ MeV ($n_c \simeq 0.07$ fm$^3 = 0.45 n_0$).

In the following a minimal extension of IHRG model, which includes the VDW interactions between (anti)baryons, is described. We refer to this model as VDW-HRG and it is based on the following assumptions:

(1) VDW interactions are assumed to exist between all pairs of baryons and between all pairs of antibaryons. The VDW parameters a and b for all (anti)baryons are assumed to be equal to those of nucleons, as obtained from the fit to the ground state of nuclear matter.

(2) The baryon-antibaryon, meson-meson, and meson-(anti)baryon VDW interactions are neglected.

In a sense the present VDW-HRG model is a "minimal-interaction" extension of the IHRG model, which describes the basic properties of nuclear matter. Whether significant VDW interactions exist between hadron pairs other than (anti)baryons is not clearly established. For instance, it has been argued that short-range interactions between baryons and antibaryons may be dominated by annihilation processes and not by repulsion [20], and this is our motivation to exclude VDW terms for them in this study. The presence of significant mesonic eigenvolumes, comparable to those of baryons, leads to significant suppression of thermodynamic functions in the crossover region at $\mu_B = 0$, which is at odds with lattice data (see Refs. [20,21]). The attractive interactions involving mesons, on the other hand, normally lead to resonance formation [22], which are already included in HRG by construction. For these reasons, we neglect the meson-related VDW interactions in this study. The VDW-HRG consists of three subsystems: Noninteracting mesons, VDW baryons, and VDW antibaryons. The total pressure reads

$$p(T,\boldsymbol{\mu}) = P_M(T,\boldsymbol{\mu}) + P_B(T,\boldsymbol{\mu}) + P_{\bar{B}}(T,\boldsymbol{\mu}), \qquad (1)$$

with

$$P_M(T,\boldsymbol{\mu}) = \sum_{j\in M} p_j^{\mathrm{id}}(T,\mu_j), \qquad (2)$$

$$P_B(T,\boldsymbol{\mu}) = \sum_{j\in B} p_j^{\mathrm{id}}(T,\mu_j^{B*}) - a n_B^2, \qquad (3)$$

$$P_{\bar{B}}(T,\boldsymbol{\mu}) = \sum_{j\in \bar{B}} p_j^{\mathrm{id}}(T,\mu_j^{\bar{B}*}) - a n_{\bar{B}}^2, \qquad (4)$$

where M stands for mesons, B for baryons, and $\bar{B}$ for antibaryons, p_j^{id} is the Fermi or Bose ideal gas pressure, $\boldsymbol{\mu} = (\mu_B, \mu_S, \mu_Q)$ are the chemical potentials which regulate the average values of net baryon number B, strangeness S, electric charge Q, $\mu_j^{B(\bar{B})*} = \mu_j - bP_{B(\bar{B})} - abn_{B(\bar{B})}^2 + 2an_{B(\bar{B})}$, and n_B and $n_{\bar{B}}$ are, respectively, total densities of baryons and antibaryons.

The calculation of mesonic pressure $P_M(T,\boldsymbol{\mu})$ is straightforward. The shifted chemical potentials $\mu_j^{B(\bar{B})*}$ of (anti) baryons depend explicitly on (anti)baryon pressure $P_{B(\bar{B})}$ and on total (anti)baryon density $n_{B(\bar{B})}$. By taking the derivatives of $P_{B(\bar{B})}$ with respect to the baryochemical potential one obtains additional equations for $n_{B(\bar{B})}(T,\boldsymbol{\mu})$,

$$n_{B(\bar{B})} = (1 - bn_{B(\bar{B})}) \sum_{j\in B(\bar{B})} n_j^{\mathrm{id}}(T,\mu_j^{B(\bar{B})*}). \qquad (5)$$

At given T and $\boldsymbol{\mu}$, Eqs. (2)–(5) are solved numerically, giving $P_{B(\bar{B})}(T,\boldsymbol{\mu})$ and $n_{B(\bar{B})}(T,\boldsymbol{\mu})$. Entropy density is calculated as $s = (\partial p/\partial T)_\mu$, and energy density is obtained from Gibbs relation.

The present calculations include all established strange and nonstrange hadrons which are listed in the Particle Data Tables [23], with the exception of σ and κ mesons [24,25]. The finite widths of the resonances are included by means of an additional mass integration over their Breit-Wigner shapes. We employ the HRG code used in Refs. [26,27], modified to include the VDW interactions between (anti) baryons. The temperature dependence of the scaled pressure p/T^4, energy density ε/T^4, and the speed of sound squared $c_s^2 = dp/d\varepsilon$ calculated at $\boldsymbol{\mu} = 0$ within IHRG and VDW-HRG models is compared to the lattice data in Fig. 1. To clarify the role of attractive and repulsive interactions, we also show the calculations, denoted as EV-HRG, where the VDW attraction was "switched off," i.e., $a = 0$. Since

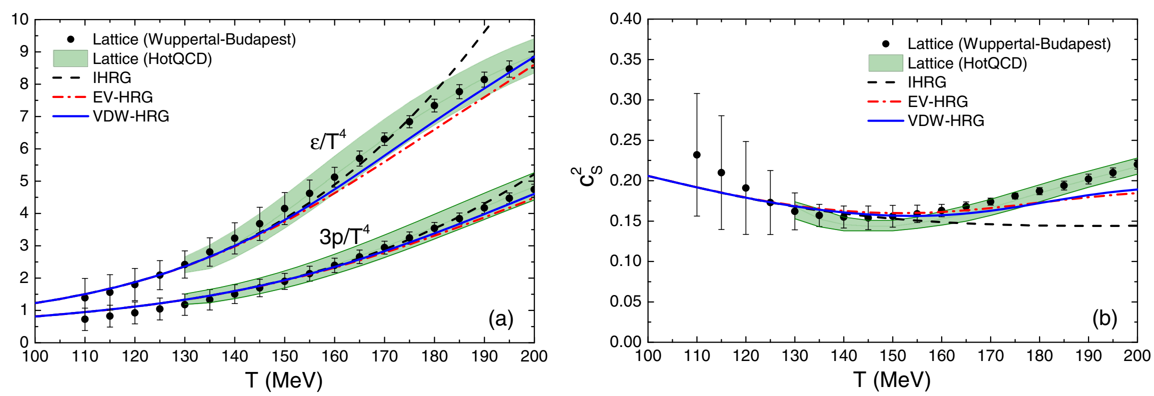

FIG. 1. The temperature dependence of (a) scaled pressure and energy density, and of (b) the square of the speed of sound at zero chemical potential, as calculated within IHRG (dashed black lines), EV-HRG with $b = 3.42$ fm^3 (dash-dotted red lines), and VDW-HRG with $a = 329$ MeV fm^3 and $b = 3.42$ fm^3 (solid blue lines). Lattice QCD results of Wuppertal-Budapest [1] and HotQCD [2] Collaborations are shown, respectively, by symbols and green bands.

the matter is meson dominated at $\mu_B = 0$, and the mesons are modeled as noninteracting, no significant suppression of thermodynamic functions is seen, in contrast to earlier studies [20,21], where constant EV interactions between all hadrons were assumed. The energy density is somewhat below the lattice data at $T > 160$ MeV for VDW-HRG. This may be explained by missing heavy Hagedorn states which add a significant contribution to the energy density [21]. The temperature dependence of the speed of sound squared, c_s^2, is consistent with lattice data and shows a minimum at $T \sim 155$–160 MeV, in contrast to the IHRG where c_s^2 decreases slowly and monotonically.

In addition to the thermodynamical functions, the VDW-HRG model allows us to calculate the fluctuations of conserved charges:

$$\chi_{lmn}^{BSQ} = \frac{\partial^{l+m+n} p/T^4}{\partial(\mu_B/T)^l \partial(\mu_S/T)^m \partial(\mu_Q/T)^n}. \qquad (6)$$

The fluctuations of the net number of light quarks $L = (u+d)/2 = (3B+S)/2$ are also considered.

The temperature dependencies of the second order susceptibilities are shown in Fig. 2. These include (a) net number of light quarks χ_2^L, (b) net baryon number χ_2^B, (c) net strangeness χ_2^S, and (d) baryon-electric charge correlator χ_{11}^{BQ}. The χ_2^L calculated within the VDW-HRG model shows a very different behavior compared to IHRG at $T > 160$ MeV, and agrees well with the lattice data [4] up to $T = 180$ MeV. A qualitatively similar picture is obtained for χ_2^B. The qualitative difference between IHRG and VDW-HRG models appears to be driven by the EV interaction terms between (anti)baryons, while the inclusion of VDW attraction leads to an improved agreement with the lattice data. The strangeness susceptibility χ_2^S is described fairly well by the IHRG model, but appears to be underestimated by the VDW-HRG model. We have also found that the baryon-strangeness correlator (not shown in plots) is rather notably underestimated by all considered HRG models. Does this reflect the presence of hitherto undiscovered strange hadrons? The inclusion of such states was shown to improve the agreement between lattice data and IHRG [28,29]. The correlator χ_{11}^{BQ} between the net baryon number and net electric charge has a very different temperature dependence in IHRG and VDW-HRG. In the IHRG model the χ_{11}^{BQ} increases rapidly at $T > 150$ MeV, in stark contrast to the lattice data. In the VDW-HRG model, this correlator has a broad bump with a maximum at $T \sim 160$–190 MeV, showing a behavior which is in qualitative agreement with the correlator obtained on the lattice.

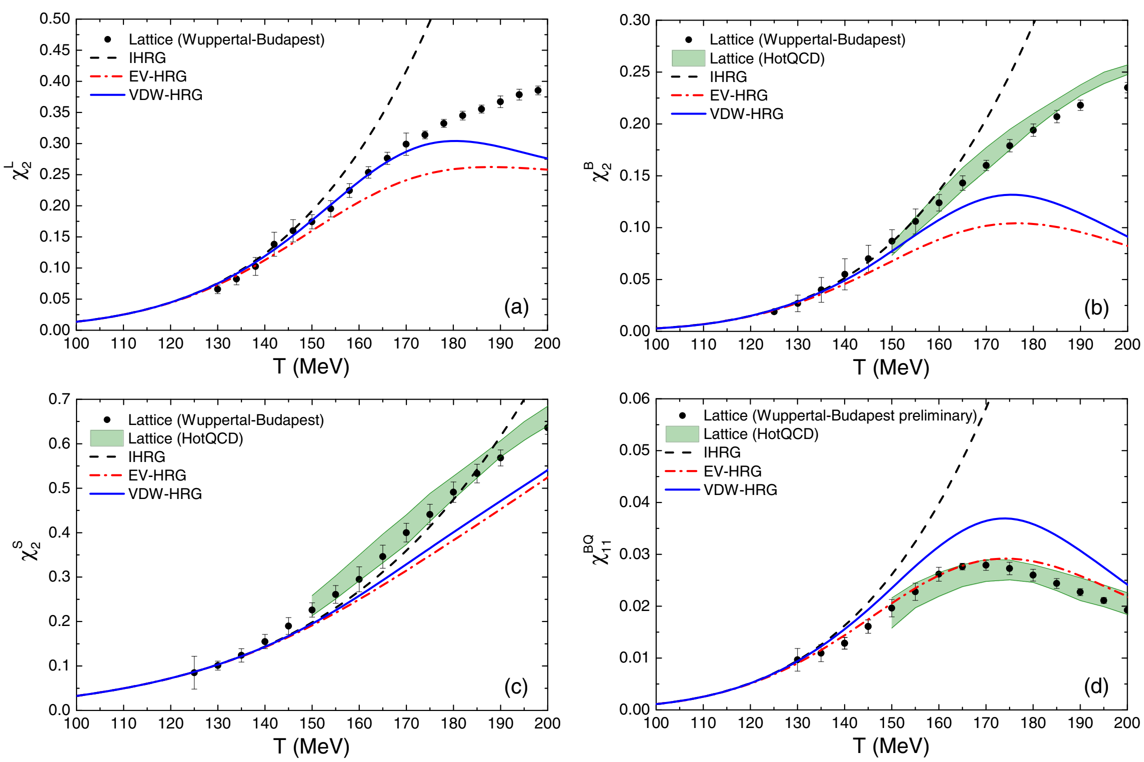

FIG. 2. The temperature dependence of the second order susceptibilities of conserved charges. These include (a) net number of light quarks χ_2^L, (b) net baryon number χ_2^B, (c) net strangeness χ_2^S, and (d) baryon-electric charge correlator χ_{11}^{BQ}. Calculations are done within IHRG (dashed black lines), EV-HRG (dash-dotted red lines), and VDW-HRG (solid blue lines). Lattice QCD results of the Wuppertal-Budapest [4,7] (for χ_{11}^{BQ} preliminary results [30,31] are used) and HotQCD [5] Collaborations are shown, respectively, by symbols and green bands.

The higher order fluctuations are also analyzed and exhibited in Fig. 3. All considered observables show very different behavior between IHRG and VDW-HRG. The net-light number χ_4^L/χ_2^L monotonically increases in the IHRG model and overshoots the lattice data at $T \sim 140$ MeV. The VDW-HRG model, in contrast, yields a nonmonotonic behavior with a wide peak at $T \sim 120$–145 MeV, resembling the lattice data [7], which peaks at slightly higher temperature. The peak in the T dependence of net strangeness χ_4^S/χ_2^S is relatively well reproduced within the VDW-HRG model. In contrast, the IHRG model shows no maximum at all. It is remarkable that our model shows flavor hierarchy: The peak for net-light number χ_4/χ_2 is at smaller temperatures as compared to the peak in net strangeness. The same result is seen in the lattice data. It was argued that this observation is related to the flavor separation in the deconfinement transition in QCD [7]. Since the VDW-HRG model has only hadronic degrees of freedom, the present results cast doubt on this interpretation to trace back to deconfinement the observed flavor dependence in χ_4/χ_2, as well as the presence of the peaks themselves. Turning to higher-order fluctuations of net-baryon number: The net-baryon kurtosis, χ_4^B/χ_2^B, shows the expected Skellam behavior for IHRG model with values very close to unity. The VDW-HRG model, on the other hand, shows a stark decrease at $T = 130$–165 MeV, i.e., in the so-called "crossover region," even though the VDW-HRG model does not contain any transition to the quark-gluon degrees of freedom. The χ_4^B/χ_2^B even turns negative at $T > 165$ MeV. This decrease of χ_4^B/χ_2^B is also seen on the lattice [6], although it starts at higher $T = 145$ MeV and χ_4^B/χ_2^B does not become negative. Also, the temperature dependence of the sixth order cumulant ratio χ_6^B/χ_2^B is predicted: The VDW-HRG model exhibits very strong variations and nonmonotonic behavior in the crossover region. Will a similarly dramatic T-dependent behavior be observed in corresponding lattice simulations?

Finally, the kurtosis of net-baryon fluctuations at finite baryon density is explored [Fig. 3(d)]. For simplicity it is assumed that $\mu_S = \mu_Q = 0$. The region of negative χ_4^B/χ_2^B at small μ_B is smoothly connected to the region of the liquid-vapor phase transition in nuclear matter, and seems relevant for "chemical freeze-out" in heavy-ion collisions (see dashed line). The VDW-HRG model suggests nonmonotonic behavior of χ_4/χ_2 with respect to collision energy, in stark contrast to IHRG [32]. This implies that nontrivial fluctuations of net-baryon number in heavy-ion collisions [33–35] may simply be a manifestation of the nuclear

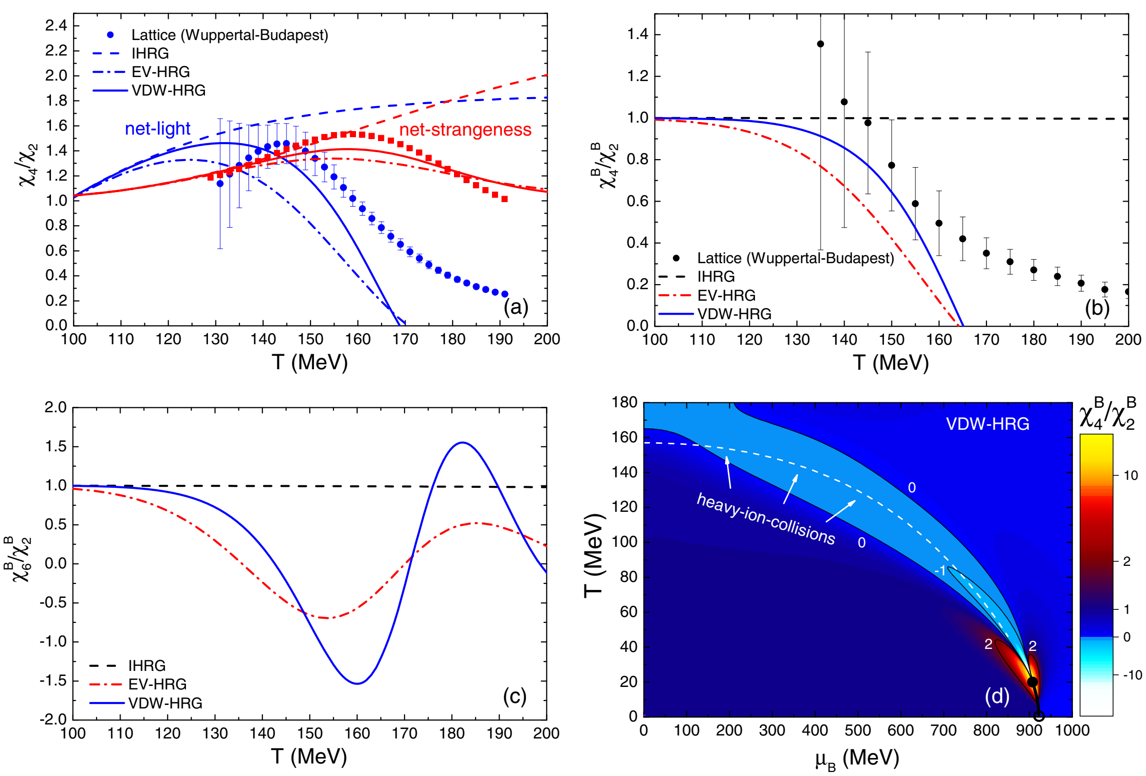

FIG. 3. The temperature dependence of the χ_4/χ_2 cumulant ratio for (a) net number of light or strange quarks, (b) net baryon number, and the (c) χ_6/χ_2 for net baryon number. Calculations are done within IHRG (dashed lines), EV-HRG (dash-dotted lines), and VDW-HRG (solid lines). The lattice QCD results of the Wuppertal-Budapest Collaboration [6,7] are shown by symbols. (d) The χ_4^B/χ_2^B ratio in VDW-HRG in the T-μ_B plane. The possible chemical freeze-out line in heavy-ion collisions taken from Ref. [27] is sketched by the dashed line.

liquid-gas phase transition (see also Refs. [13] and [36]). As VDW interactions also affect the thermal fits [26,37], this question demands further study.

For many observables, the *quantitative* agreement of the VDW-HRG model calculations presented here with the lattice data in the crossover region is not perfect. This is hardly surprising. Indeed, we have modeled the VDW interactions between baryons in the simplest way possible: It is assumed that the VDW interactions between all baryons are the same as those between nucleons, as obtained from nuclear matter properties at $T = 0$. Conceptually, the VDW-HRG model is quite different from an underlying fundamental QCD theory. Still, the presented analysis is essentially parameter-free, in the sense that no new parameters which could be adjusted to lattice data were introduced. Indeed, the two VDW parameters had been fixed by reproducing the saturation properties of nuclear matter [17,19], independently from any lattice data. While there are other model parameters, e.g., the hadron list and its properties, they are known and fixed experimentally. It is feasible that VDW parameters are different for different baryon pairs. In the course of calculations, it was noticed that the agreement of the VDW-HRG with the lattice data is improved by taking smaller values of the nucleon or baryon EV parameter, $b \simeq 2$–$3\ \mathrm{fm}^3$. Such modification does not necessarily break down the existing agreement of our model with the properties of nuclear matter: As suggested in Ref. [38], the heavier and/or strange baryons may have smaller eigenvolumes, thus reducing the average b. The present VDW-HRG model leaves plenty of room for improvement. Owing to the expectation that possible meson-related VDW interactions are considerably weaker than the baryon-baryon VDW interactions, we do not expect major qualitative changes to the results presented in this Letter for baryon number susceptibilities. This, however, may not be the case for other observables and should be carefully explored in future works.

To summarize, a minimal extension of the IHRG model is presented which includes both attractive and repulsive VDW interactions between baryons, with parameters a and b taken from previous fits to the ground state of nuclear matter. Compared to the usually used IHRG model, the VDW-HRG model shows a qualitatively different behavior of most fluctuations and correlations of conserved charges in the crossover region at zero chemical potential. This behavior resembles closely the lattice QCD results. These results hint towards the crucial importance of the VDW interactions in hadron gas, and indicate that commonly performed comparisons of IHRG with the lattice data may result in misleading conclusions. Particularly, our results suggest that hadrons do not melt quickly with increasing temperature, as one could conclude on the basis of the IHRG. It is feasible that the nuclear liquid-gas phase transition manifests itself into significant nontrivial fluctuations of net-baryon number in heavy-ion collisions. The influence of VDW interactions on thermal fits to hadron yield data from heavy-ion collisions is another possibility which will be explored.

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