

## Two component boson–fermion plasma at finite temperature

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We discuss thermodynamic stability of neutral real (quantum) matter from the point of view of a computer experiment at finite, nonzero, temperature. We perform (restricted) path integral Monte Carlo simulations of the two component plasma where the two species are both bosons, both fermions, and one boson and one fermion. We calculate the structure of the plasma and discuss about the formation of binded couples of oppositely charged particles. The purely bosonic case is thermodynamically unstable. In this case we find an undetermined size-dependent contact value unlike partial radial distribution function. For the purely fermionic case, we find a demixing transition with binding also of like species.

*Keywords:* Two component plasma; Monte Carlo simulation; finite temperature; restricted path integral; worm algorithm; fermions sign problem; structure; thermodynamic stability.

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### 1. Introduction

For matter to be stable it must be globally neutral. It is well known that in order for a system of an equal number  $N$  of oppositely charged point particles to be stable against collapse, quantum mechanics is required, and furthermore at least one of the species of particles must be a fermion. Without the exclusion principle, the ground state energy per particle of the system diverges as  $N^{7/5}$  and the thermodynamic limit is not well defined.<sup>1</sup> As a matter of fact, in the classical limit one is forced to introduce a short-range regularization (like an hard core or others)<sup>2</sup> of the pair-potential between the particles in order to prevent the collapse of the negative charges on the positive ones.<sup>3,4</sup> All this is at the heart of the fundamental question of whether the matter we live in is stable or not.

In this work, we want to explore the structure of a two-component mixture of particles with two opposite charge species. We will consider particles of charge  $\pm e$  with  $e$  the charge of an electron. Furthermore, we will assume that the two species both have the mass of an electron  $m$ . We will consider explicitly the cases where

both species have spin 1/2 (purely fermionic), when they both have spin 1 (purely bosonic) and when one species has spin 1/2 and one species has spin 1 (fermions–bosons mixture). In all cases, we assume that each species has polarization equal to 1. Doing so, we will be able to determine the thermodynamic instability of the purely bosonic case as opposed to the other two cases. We will work at high temperatures and intermediate densities, when the quantum effects are not very important. The path integral Monte Carlo computer experiment is only exact in the purely bosonic case apart from the usual finite size and imaginary time discretization errors. For the other two cases, it is necessary to resort to an approximation due to the *fermions sign problem*.<sup>5,6</sup> We will choose the restricted path integral approximation with a restriction based on the nodes of the ideal density matrix, which is known to perform reasonably well for the one component (Jellium) case from the pioneering work of Brown *et al.*<sup>7,8</sup> Other methods have been implemented recently in order to reach high densities: Bonitz *et al.*<sup>9,10</sup> combine configuration path integral Monte Carlo and permutation blocking path integral Monte Carlo. Malone *et al.*<sup>11</sup> agrees well with the one of Bonitz at high densities and the direct path integral Monte Carlo one of Filinov *et al.*<sup>12</sup> that agrees well with Brown at low density and moderate temperature. Our method is alternative to all previously employed ones.

In our simulations, we use the *worm algorithm*<sup>13,14</sup> which is able to sample the necessary permutations of the indistinguishable particles without the need of explicitly sampling the permutations' space treating the paths as “worms” with a tail (*Masha*) and a head (*Ira*) in the  $\beta$ -periodic imaginary time, which can be attached one with the other in different ways or swap some of their portions. We explicitly and efficiently applied the restriction to the worms and this allowed us to treat the fermionic or mixed case explicitly, albeit only approximately. The approximation is expected to become better at low density and high temperature, i.e. when correlation effects are weak.

Possible physical realizations of interest to our work for the case of both species of spin 1/2 are a nonrelativistic electron–positron plasmas created in the laboratory<sup>15</sup> or an electron–hole plasma which is important in the realm of low-temperature semiconductor physics. Conduction electrons and holes in semiconductors interact with Coulomb force and can have very similar effective masses.<sup>16,17</sup>

The work is organized as follows: In Sec. 2, we describe the physical model we want to study, in Sec. 3, we describe the computer experiment method and techniques, in Sec. 4, we describe our numerical results, and Sec. 5 is for final remarks.

## 2. The Model

Setting lengths in units of the Bohr radius  $a_0 = \hbar^2/me^2$  and energies in Rydberg's units,  $\text{Ry} = \hbar^2/2ma_0^2$ , where  $m$  is the electron mass, the Hamiltonian of the two

component nonrelativistic electron–positron mixture is

$$\mathcal{H} = \mathcal{T} + \mathcal{V} = -\lambda \sum_{i=1}^{N_+} \nabla_{\mathbf{r}_i^+}^2 - \lambda \sum_{i=1}^{N_-} \nabla_{\mathbf{r}_i^-}^2 + V(R), \quad (2.1)$$

$$V = 2 \left( \sum_{i < j}^{N_+} \frac{1}{|\mathbf{r}_i^+ - \mathbf{r}_j^+|} + \sum_{i < j}^{N_-} \frac{1}{|\mathbf{r}_i^- - \mathbf{r}_j^-|} - \sum_{i=1}^{N_+} \sum_{j=1}^{N_-} \frac{1}{|\mathbf{r}_i^+ - \mathbf{r}_j^-|} \right), \quad (2.2)$$

where  $\lambda = \hbar^2/2ma_0^2 = Ry$ ,  $R = (\mathbf{r}_1^+, \dots, \mathbf{r}_{N_+}^+, \mathbf{r}_1^-, \dots, \mathbf{r}_{N_-}^-)$  with  $\mathbf{r}_i^+$  the coordinates of the  $i$ th positron and  $\mathbf{r}_i^-$  the ones of the  $i$ th electron. We will choose  $N_+ = N_- = N$ , since the system must be neutrally charged in order to be thermodynamically stable. We will not introduce any short-range regularization of the Coulomb potential. And we will treat the Coulomb long-range potential using the Ewald sums technique<sup>18</sup> in order to treat it in the periodic box of side  $L$  of the simulation.

We will treat explicitly the electron–positron case where the two particles are both fermions, the case where both species are bosons, and the case where only one species is a fermion. Of course, there is no charged boson in nature with the mass and the charge of the electron, so this will remain a speculative analysis, to explore the thermodynamic stability and statistical properties of the mixture.

We will carry on a grand canonical simulation at fixed chemical potentials of the two species  $\mu^+, \mu^-$ , volume  $\Omega = L^3$ , and absolute temperature  $T = 1/k_B\beta$ , with  $k_B$  the Boltzmann constant.

### 3. Simulation Method

We carry on a (restricted) path integral Monte Carlo computer experiment<sup>19</sup> using the *worm algorithm*<sup>13,14</sup> to simulate the behavior of the quantum mixture at finite temperature.

The *density matrix* of a system of many distinguishable bodies at temperature  $k_B T = \beta^{-1}$  can be written as an integral over all paths  $\{R_t\}$

$$\rho(R_\beta, R_0; \beta) = \oint_{R_0 \rightarrow R_\beta} dR_t \exp(-S[R_t]). \quad (3.1)$$

The path  $R_t$  begins at  $R_0$  and ends at  $R_\beta$ . For nonrelativistic particles interacting with a potential  $V(R)$ , the *action* of the path,  $S[R_t]$ , is given by the Feynman–Kac formula

$$S[R_t] = \int_0^\beta dt \left[ \frac{1}{4\lambda} \left| \frac{dR_t}{dt} \right|^2 + V(R_t) \right]. \quad (3.2)$$

Thermodynamic properties, such as the radial distribution function (RDF), are related to the diagonal part of the density matrix, so that the path returns to its starting place after a time  $\beta$ .

To perform Monte Carlo calculations of the integrand, one makes imaginary thermal time discrete with a *time step*  $\tau$ , so that one has a finite (and hopefully small)

number of time slices and thus a classical system of  $N$  particles in  $M = \beta/\tau$  time slices; an equivalent  $NM$  particle classical system of “polymers”.<sup>19</sup>

Thermodynamic properties are averages over the thermal  $2N$ -body density matrix which is defined as a thermal occupation of the exact eigenstates  $\phi_i(R)$

$$\rho(R, R'; \beta) = \sum_i \phi_i^*(R) e^{-\beta E_i} \phi_i(R'). \quad (3.3)$$

The partition function is the trace of the density matrix

$$Z(\beta) = e^{-\beta F} = \int dR \rho(R, R; \beta) = \sum_i e^{-\beta E_i}, \quad (3.4)$$

with  $F$  Helmholtz’s free energy. Other thermodynamic averages are obtained as

$$\langle \mathcal{O} \rangle = Z(\beta)^{-1} \int dR dR' \langle R | \mathcal{O} | R' \rangle \rho(R', R; \beta). \quad (3.5)$$

Path integrals are constructed using the product property of density matrices

$$\rho(R_2, R_0; \beta_1 + \beta_2) = \int dR_1 \rho(R_2, R_1; \beta_2) \rho(R_1, R_0; \beta_1), \quad (3.6)$$

which holds for any sort of density matrix. If the product property is used  $M$  times, we can relate the density matrix at a temperature  $\beta^{-1}$  to the density matrix at a temperature  $M\beta^{-1}$ . The sequence of intermediate points  $\{R_1, R_2, \dots, R_{M-1}\}$  is the path, and the *time step* is  $\tau = \beta/M$ . As the time step gets sufficiently small, the Trotter theorem tells us that we can assume that the kinetic  $\mathcal{T}$  and potential  $\mathcal{V}$  operator commute so that:  $e^{-\tau \mathcal{H}} = e^{-\tau \mathcal{T}} e^{-\tau \mathcal{V}}$  (strictly speaking this is only possible when  $\mathcal{V}$  is bounded from below<sup>20</sup> but this is always satisfied by our simulation since we use a radial discretization of the pair Coulomb potential) and the *primitive approximation* for the Boltzmann density matrix is found<sup>19</sup>

$$\rho(R_0, R_M; \beta) = \int dR_1 \dots dR_{M-1} \exp \left[ - \sum_{m=1}^M S^m \right], \quad (3.7)$$

$$K^m = \frac{3N}{2} \ln(4\pi\lambda\tau) + \frac{(R_{m-1} - R_m)^2}{4\lambda\tau}, \quad (3.8)$$

$$S^m - K^m \approx U_{\text{primitive}}^m = \frac{\tau}{2} [V(R_{m-1}) + V(R_m)]. \quad (3.9)$$

The Feynman–Kac formula for the Boltzmann density matrix results from taking the limit  $M \rightarrow \infty$ . The price we have to pay for having an explicit expression for the density matrix is additional integrations; all together  $3N(M - 1)$ . Without techniques for multidimensional integration, nothing would have been gained by expanding the density matrix into a path. Fortunately, simulation methods can accurately treat such integrands. It is feasible to make  $M$  rather large, say in the hundreds or thousands, and thereby systematically reduce the time-step error. The leading error of the primitive approximation goes like  $\sim \lambda\tau^2$ .<sup>19</sup>

In addition to sampling the path, one also needs to sample all the various necessary permutations of the indistinguishable particles (bosons or fermions) and this is accomplished on the fly through the use of the worm algorithm.<sup>13,14</sup>

When we are dealing with bosons or fermions  $\rho_{B,F}(R_\beta, R_0; \beta) = \mathcal{A}_\mathcal{P} \rho(R_\beta, \mathcal{P}R_0; \beta)$  is the density matrix corresponding to some set of quantum numbers which are obtained by using the projection operator  $\mathcal{A}_\mathcal{P} = \frac{1}{N!} \sum_{\mathcal{P}} \varphi(\pm)^\mathcal{P}$ , where  $\mathcal{P}$  is a permutation of particle labels and the permutation sign is a plus for bosons ( $B$ ) and a minus for fermions ( $F$ ), on the distinguishable particle density matrix. Then, for bosons we can carry on the Monte Carlo calculation without further approximations, but for fermions the following *Restricted Path Integral* approximation is also necessary in order to overcome the ubiquitous sign problem<sup>5,6</sup>

$$\rho_F(R_\beta, R_0; \beta) = \int dR' \rho_F(R', R_0; 0) \oint_{R' \rightarrow R_\beta \in \gamma_T(R_0)} dR_t e^{-S[R_t]}, \quad (3.10)$$

where the subscript means that we restrict the path integration to paths starting at  $R'$ , ending at  $R_\beta$  and avoiding the nodes (the zeroes) of a known *trial density matrix*,  $\rho_T$ , assumed to have nodes,  $\partial\gamma_T$ , close to the true ones. The weight of the walk is  $\rho_F(R', R_0; 0) = (N!)^{-1} \sum_{\mathcal{P}} \varphi(-)^\mathcal{P} \delta(R' - \mathcal{P}R_0)$ . It is clear that the contribution of all the paths for a single element of the density matrix will be of the same sign, thus avoiding the sign problem. On the diagonal, the density matrix is positive and on the path restriction  $\rho_F(R, R_0; \beta) > 0$ , then, only even permutations are allowed since  $\rho_F(R, \mathcal{P}R; \beta) = (-)^\mathcal{P} \rho_F(R, R; \beta)$ . It is then possible to use a bosonic calculation to get the approximate fermionic case.

The restriction is implemented choosing as the trial density matrix the ideal density matrix: we just reject the move (*remove*, *close*, *wiggle* and *displace* in the  $Z$ -sector, and *advance* and *swap* in the  $G$ -sector),<sup>13,14</sup> whenever the proposed path is such that the ideal fermionic or fermionic-bosonic density matrix calculated between the reference point and any of the time slices subject to newly generated particles positions has a negative value.

The ideal fermionic or fermionic–bosonic density matrix is given by

$$\rho_0(R, R'; t) \propto \mathcal{A} \begin{pmatrix} e^{-\frac{(r_i^+ - r_j^+)^2}{4\lambda t}} & e^{-\frac{(r_i^+ - r_k^-)^2}{4\lambda t}} \\ e^{-\frac{(r_l^- - r_j^+)^2}{4\lambda t}} & e^{-\frac{(r_l^- - r_k^-)^2}{4\lambda t}} \end{pmatrix}, \quad (3.11)$$

where  $\lambda = \hbar^2/2m$  and  $\mathcal{A}$  is the (anti)symmetrization operator for the positive and negative species (purely fermionic mixture) or for the positive species only (fermionic–bosonic mixture). We expect this approximation to be best at high temperatures and low densities when the correlation (the particles coupling and their quantum nature) effects are weak. Clearly in a simulation of the ideal gas ( $V = 0$ ), this restriction returns the exact result for fermions, otherwise, it is just an approximation.

The restriction or the fixed nodes path integral may have an influence on the thermodynamic stability of the fluid under study, especially at low temperatures

when quantum effects become more relevant. On the other hand, if this were the case, it would have an influence on the stability of the fluid under all thermodynamic states which we can clearly exclude since as soon as we include at least one fermionic species in the binary mixture, the system becomes thermodynamically stable even at moderately low temperatures when the restriction is not very effective.

#### 4. Results

In our simulations, we chose  $k_B T = 10 \text{ Ry}$  and  $L = 5a_0$ . Going to lower temperatures, the contact value for the unlike partial RDF tends to increase since the

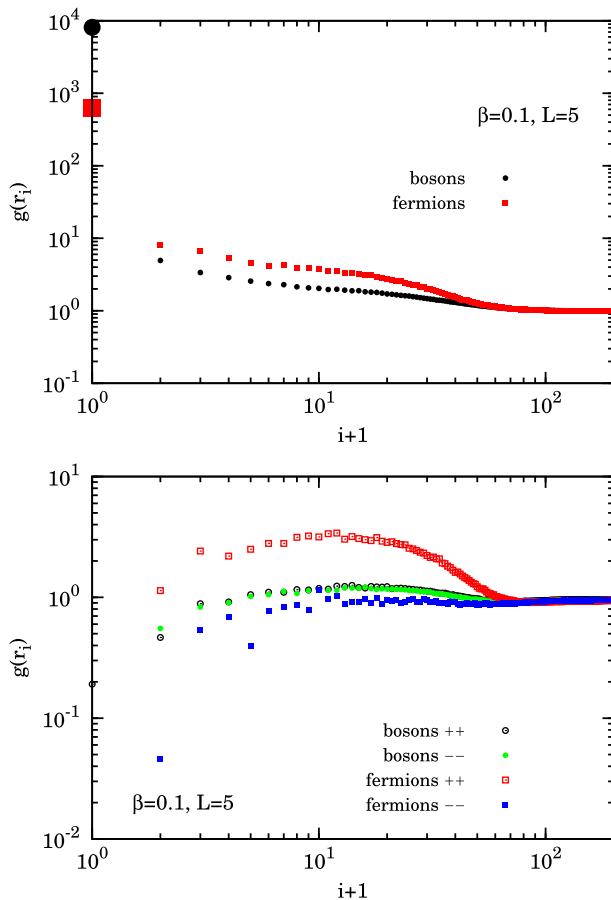


Fig. 1. (Color online) We show the partial RDF on a log–log scale. For the mixture of bosons and the fluid with one bosonic species and one fermionic species, we show  $g_{+-}(r_i)$  in the upper panel and  $g_{++}(r_i)$ ,  $g_{--}(r_i)$  in the bottom panel. In all cases, we have  $L/2 = r_{\text{cut}} a_0 = 2.5a_0$  and the RDF are calculated on 200 radial points  $r_i = idr$  with  $dr = r_{\text{cut}}/200$ . The simulation was carried on at  $\beta = 0.1 \text{ Ry}^{-1}$  with  $M = 10$  time slices and an average of approximately 36 particles for the fermions case and 39 for the bosons case. The simulation was 15 000 blocks of 500 steps taking averages every 100 moves. But  $g_{+-}(0)$  for the purely bosonic case continued to grow afterwards.

binding between a positive and a negative charge increases. This is because the coupling constant of the mixture is  $\Gamma = \beta e^2/a_0$ . For the purely bosonic case, the contact value never reaches an equilibrium during the simulation evolution unlike for the purely fermionic case or the fermions–bosons mixture where a positive charge binds with a negative charge in a stable way at low densities.<sup>21</sup>

It is also useful to introduce a degeneracy temperature  $\Theta = T/T_F$ , where  $T_F = T_D 2\pi^2/\alpha_3^{2/3}$  is the Fermi temperature, here  $\alpha_3 = 4\pi/3$ , and

$$T_D = \frac{2n^{2/3}}{k_B} \text{Ry}, \quad (4.1)$$

with  $n = Na_0^3/V$ , the density is the degeneracy temperature. For temperatures higher than  $T_D$ , as in our simulations, quantum effects are less relevant. For this reason, we chose  $M = 10$  in all cases giving a  $\tau = 0.01 \text{Ry}^{-1}$ . So the primitive approximation is a good one.

Another relevant parameter is the Wigner–Seitz radius  $r_s = (3/4\pi n)^{1/3}$  which in the degenerate regime  $\Theta \ll 1$  regulates whether the system of particles is dominated by the potential energy or by the kinetic energy. At high  $r_s$ , the potential energy dominates and the system tends to crystallize.<sup>17</sup>

From Fig. 1, we see how the binary mixture is stable when the particles are fermions and unstable when they are bosons. This is manifested by a contact value of the unlike partial RDF, for the purely bosonic case, which is one order of magnitude higher than the one for the purely fermionic case. It varies wildly during the simulation evolution, with variations of one or more orders of magnitudes upon

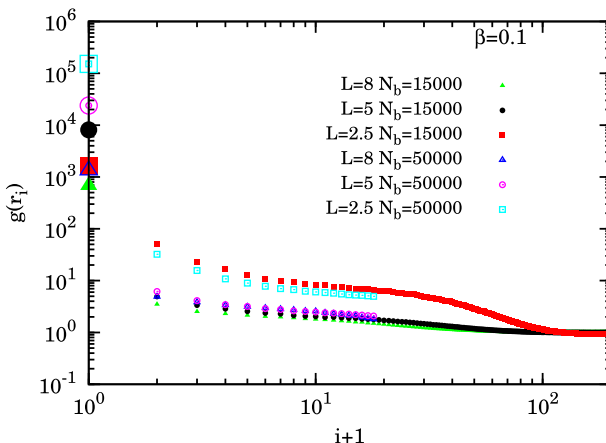


Fig. 2. (Color online) We show the unlike partial RDF on a log–log scale for the purely bosonic case at three different values of  $L/2 = r_{\text{cut}}a_0$  and approximately same density and at two times during the simulation, after  $N_b = 15\,000$  blocks (of 50 000 worm moves) and after  $N_b = 50\,000$  blocks. The RDF are calculated on 200 radial points  $r_i = idr$  with  $dr = r_{\text{cut}}/200$ . The simulation was carried on at  $\beta = 0.1 \text{Ry}^{-1}$  with  $M = 10$  time slices. The simulation was 15 000 blocks of 500 steps taking averages every 100 moves. But  $g_{+-}(0)$  continued to grow afterwards.

inspections of the simulation at different time intervals of 10 000 blocks of 50 000 worm moves each. The like partial RDF for the purely fermionic case shows a spontaneous symmetry breaking, where the positive–positive RDF differs from the negative–negative one and presents a broad shoulder near the origin which suggests the formation of like positive pairs. The contact value in the bosonic case has huge variations upon changes of the size of the system as shown by Fig. 2. This also means that there is no well-defined thermodynamic limit of the RDF which in turn is a manifestation of the system instability.<sup>1</sup> This does not occur when at least one of the two species is a fermion. In this case, a slight shoulder near the origin in the

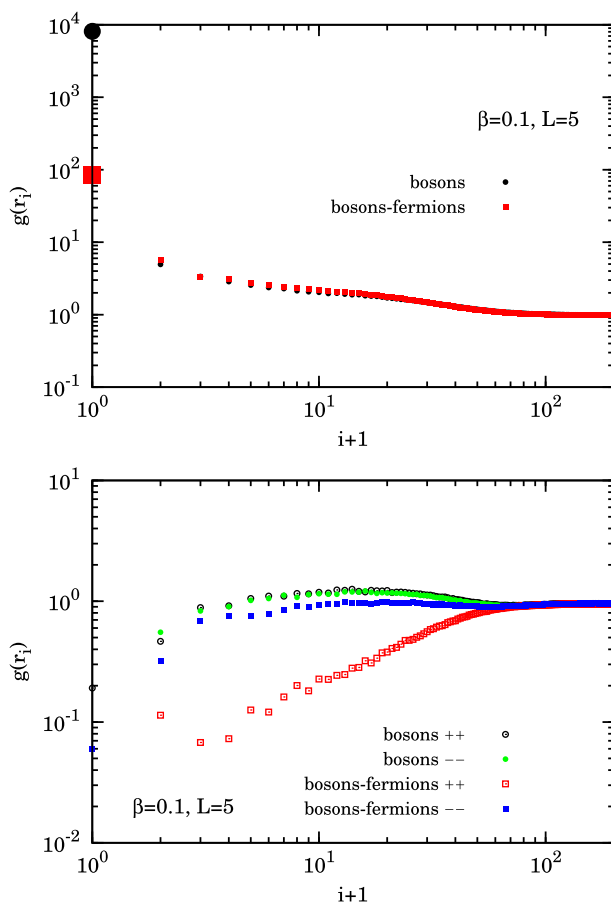


Fig. 3. (Color online) We show the partial RDF on a log–log scale. For the mixture of bosons and the fluid with one bosonic species and one fermionic species, we show  $g_{+-}(r_i)$  in the upper panel and  $g_{++}(r_i), g_{--}(r_i)$  in the bottom panel. In all cases, we have  $L/2 = r_{\text{cut}} a_0 = 2.5 a_0$  and the RDF are calculated on 200 radial points  $r_i = i dr$  with  $dr = r_{\text{cut}}/200$ . The simulation was carried on at  $\beta = 0.1 \text{ Ry}^{-1}$  with  $M = 10$  time slices and an average of approximately 38 particles for the mixed fermionic–bosonic case and 39 for the purely bosonic case. The simulation was 15 000 blocks of 500 steps taking averages every 100 moves. But  $g_{+-}(0)$  for the purely bosonic case continued to grow afterwards.



unlike partial RDF indicates the stable pairing between a positive and a negative charge. The shoulder grows at lower temperature and lower density.

In order to have stability, it is sufficient to have at least one of the two particle species to be a fermion as is shown in Fig. 3. In this case, the like partial RDF for the bosonic species is comparable with the one of the purely bosonic case and the one for the fermionic component is lower. No like pair formation is visible from the structure analysis. The unlike partial RDF is superposed to the one of the purely fermionic case but presents an on top value two orders of magnitudes smaller.

The difference between the purely fermionic mixture and the fermions–bosons had to be expected also from the point of view of the fact that our spin polarized fermions, unlike the bosons, do not have a state with zero total angular momentum.

## 5. Conclusions

In conclusion, we carried on some computer experiments for the binary mixture of oppositely charged pointwise particle species when both species are bosons, both fermions, and one boson and one fermion. We chose the charge and the mass equal to the ones of the electron and only considered fully polarized species. We used the worm algorithm to perform (restricted) path integral Monte Carlo simulations, at finite temperatures.

We simulated the mixture with a weak degree of degeneracy  $\Theta \sim 1.4$  and a weak coupling  $\Gamma = 0.2$ . The Wigner–Seitz radius for each species was  $r_s \sim 1$ .

During the simulations, we measured the radial distribution function of the three mixtures and found that the purely bosonic one is thermodynamically unstable toward the collapse of oppositely charged particles upon the others. Whereas, in the other two mixtures, the Pauli exclusion principle restores the stability producing stable bindings: like pairs form for the purely fermionic case as a result of a spontaneous symmetry breaking in a demixing transition and unlike pairs form in both cases. The instability manifests itself through a pronounced peak in the contact value of the unlike partial RDF which is strongly size-dependent in the experiment and keeps growing as the simulation evolves without ever reaching convergence towards a stable value. This observation tells us that the fermionic character of the simplest constituent of matter is essential in nature to be able to have a stable matter. On the other hand, if one uses nonquantum statistical mechanics, one must regularize the Coulomb potential at short range, for example through the addition of a hard core to the otherwise pointwise particles.<sup>3,4</sup> Even if in the relativistic regime it is plausible to talk about an electron radius, attempts to model the electron as a nonpoint particle are considered ill-conceived and counter-pedagogic.<sup>22</sup>

In order to have a stable matter, it is necessary that it is globally neutral and that it is made up of at least one fermionic species. Physical realizations of our model are nonrelativistic electron–positron plasma produced in the laboratory<sup>15</sup> and electron–hole plasma in semiconductors.<sup>16</sup> Of course, in the numerical experiment we do not have the physical limitations that occur in a laboratory. This allowed us to inquire

into also the mixture with one bosonic or even both bosonic components. Another interesting issue where our study could become relevant is atom and molecule formation. In its simplest setting it involves the study of an electron–proton mixture. Since the mass of an electron is three orders of magnitude smaller than the mass of a proton, the degeneracy temperature of the electron species is three orders of magnitude smaller than the one of the nuclei, at a given density. Therefore, it is very unlikely that an electron, with a world-line with many particle exchanges will bind to a nucleus which has a world-line with many less particle exchanges. In order for this to occur we have to go down to temperatures  $k_B T_I \sim e^2/2a_0 = 1 \text{ Ry}$  and electron densities such that  $T_F \sim T_I$ , i.e.  $n \sim 0.048$  or  $r_s \sim 1.7$ .<sup>21</sup> Molecules may form at even lower temperatures. Nonetheless in our stable purely fermionic mixture with an equal species mass, we see already at the chosen thermodynamic state, the unlike species binding and a spontaneous symmetry breaking for like species bindings in a demixing transition.<sup>23–25</sup>

We intend to adopt this method to simulate the two-component plasma in a curved surface<sup>26–29</sup> in the near future. For example, it could be interesting to study the two-component plasma on the surface of a sphere with a magnetic monopole at the center.<sup>30</sup>

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