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Derivation and Classical Limit of the Mean-Field Equation for a Quantum Coulomb System: Maxwell–Boltzmann Statistics

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The mean-field density matrix of a charged plasma of quantum particles with Maxwell–Boltzmann statistics in a confining external potential is obtained as a limit of the N-body canonical states for suitably scaled charges. Also, it is shown that the density profile of the quantum mean-field theory converges to the solution of the classical mean-field equation when the Planck's constant tends to zero.

KEY WORDS: Quantum Coulomb system; Maxwell–Boltzmann statistics; Feynman–Kac formula; mean-field approximation; classical limit.

1. INTRODUCTION

Consider a plasma of identical charged quantum particles obeying the Maxwell–Boltzmann statistics in thermal equilibrium, in the presence of a confining external potential. In the Hartree approximation, the state of the system is described by a density matrix $\hat{\rho}$, given by the following self-consistent equation:

$$\hat{\rho} = \frac{e^{(\varepsilon/2)\Delta - V * n - V_e}}{\operatorname{Tr} e^{(\varepsilon/2)\Delta - V * n - V_e}} \tag{1.1}$$

where V is the Coulomb interaction

$$V(x) = 1/4\pi\, |x| \tag{1.2}$$

$$V * n(x) := \int V(x-y)\, n(y)\, dy \tag{1.3}$$

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V_e is the external potential, chosen such that $\mathrm{Tr}\, e^{(\varepsilon/2)\Delta - V_e} < \infty$; and n is the particle density:

$$n(x) = \rho(x, x) \tag{1.4}$$

where $\rho(x, y)$ is the kernel of $\hat{\rho}$; finally, $\varepsilon = \hbar^2/m$, where m is the mass of the particles and, for the sake of notational simplicity, we have taken the inverse temperature $\beta = 1$.

In a recent paper Markowich[1] proved existence and uniqueness of solutions to (1.1) and the classical limit, namely that, for $\varepsilon \searrow 0$, the particle density (1.4) approaches the solution of the classical mean-field equation:

$$n(x) = \frac{e^{-V * n(x) - V_e(x)}}{\int dy\, e^{-V * n(y) - V_e(y)}} \tag{1.5}$$

In this paper we deal with the problem of obtaining the quantum mean-field theory by a limiting procedure from the original N-body equilibrium state. More precisely, we shall prove that $\hat{\rho}^N$, the density matrix for the N-particle system with suitably scaled charges ($\sim N^{-1/2}$), is close, for large N, to the N-fold tensor product of the solution of (1.1). Incidentally, our result ensures the existence of solutions of (1.1), providing a simpler alternative to the proof given in ref. 1. The corresponding classical problem has been considered by Messer and Spohn[2] for bounded interaction and by Caglioti *et al.*[3] and Kiessling[4] for Coulomb interaction, to which we refer for further motivation.

The basic idea of the analysis is the use of the Feynman–Kac formula and the Ginibre formalism,[5,6] by which the problem is reduced to a classical one on a suitable space of trajectories. This allows us to transfer to this context many ideas used for the classical problem.[2–4] Moreover, the same formalism is well suited for the study of the classical limit of the solution of (1.1), and we use it to extend a previous result obtained in ref. 1. In fact, the only assumption we need on the external potential V_e is

$$V_e \text{ is bounded below, continuous, and } e^{-V_e} \in L_1(R^3) \tag{1.6}$$

The present analysis covers only the case of Maxwell–Boltzmann statistics; the physically relevant case of Fermi–Dirac statistics requires further consideration.

In ref. 7 the same problem was considered for any statistics, but for interaction potential of a special kind. We finally notice that the positive-temperature Thomas–Fermi limit has been considered by various authors. See the monographs,[8,9] the references quoted therein, and ref. 10.

2. THE MEAN-FIELD LIMIT: STATEMENT OF THE PROBLEM AND RESULTS

Consider the N-particle system in R^3 described by the following Hamiltonian:

$$H_N = -\frac{\varepsilon}{2}\sum_{i=1}^{N} \Delta_i + \frac{1}{2N}\sum_{\substack{i,j=1\\ i\neq j}}^{N} V(x_i - x_j) + \sum_{i=1}^{N} V_e(x_i) \tag{2.1}$$

where Δ_i is the Laplacian associated to the ith particle, V is given by (1.2), and V_e satisfies (1.6). Under such conditions $\exp(-H_N)$ is a positive trace-class operator in $L_2(R^{3N})$. We denote

$$\hat{\rho}^N = Z_N^{-1} e^{-H_N}; \qquad Z_N = \operatorname{Tr} e^{-H_N} \tag{2.2}$$

the density matrix, and $\rho^N(X^N, Y^N)$ its kernel, where $X^N = (x_1,..., x_N)$, $Y^N = (y_1,..., y_N) \in R^{3N}$. The j-particle reduced density matrices ρ_j^N are defined by

$$\rho_j^N(X^j, Y^j) = \int dZ^{N-j}\, \rho^N(X^j \cup Z^{N-j}, Y^j \cup Z^{N-j}) \tag{2.3}$$

By the Feynman–Kac formula[5,6] we have the following representation of the kernel of $\exp(-H_N)$:

$$\exp(-H_N)(X^N, Y^N) = \int P^{\varepsilon}_{X^N, Y^N}(d\omega^N) \exp\left[-\frac{1}{\varepsilon}\int_0^{\varepsilon} U_N(\omega^N(t))\, dt\right] \tag{2.4}$$

where $\omega^N = (\omega_1,..., \omega_N)$, ω_i: $[0, \varepsilon] \to R^3$ are (continuous) Brownian paths;

$$P^{\varepsilon}_{X^N, Y^N}(d\omega^N) = \prod_{i=1}^{N} P^{\varepsilon}_{x_i, y_i}(d\omega_i) \tag{2.5}$$

where $P^{\varepsilon}_{x,y}(d\omega)$ is the conditional Wiener measure given $\omega(0) = x$, $\omega(\varepsilon) = y$; and, finally,

$$U_N(X^N) = \frac{1}{2N}\sum_{\substack{i,j=1\\ i\neq j}}^{N} V(x_i - x_j) + \sum_{i=1}^{N} V_e(x_i) \tag{2.6}$$

Also, we shall use the short-hand notation

$$\bar{U}^{\varepsilon}_N(\omega^N) = \frac{1}{\varepsilon}\int_0^{\varepsilon} U_N(\omega^N(t))\, dt \tag{2.7}$$

Inserting this representation into (2.2), (2.3), we have

$$\rho_j^N(X^j, Y^j) = \int P^\varepsilon_{X^j, Y^j}(d\omega^j)\, \rho_j^N(\omega^j) \tag{2.8}$$

with

$$\rho_j^N(\omega^j) = \int dZ^{N-j} \int P^\varepsilon_{Z^{N-j}, Z^{N-j}}(d\eta^{N-j})\, Z_N^{-1} \exp[-\bar{U}^\varepsilon_N(\omega^j \cup \eta^{N-j})] \tag{2.9}$$

$$Z_N = \int dX^N \int P^\varepsilon_{X^N, X^N}(d\omega^N) \exp[-\bar{U}^\varepsilon_N(\omega^N)] \tag{2.10}$$

The quantum statistical mechanics problem can thus be formulated in terms of purely "classical" objects: trajectories of time interval ε. Namely, the space of continuous closed paths

$$\Omega_\varepsilon = \{\omega: \omega \in C([0, \varepsilon]; R^3); \omega(0) = \omega(\varepsilon)\} \tag{2.11}$$

which is a complete separable metric space with distance given by

$$d(\omega, \eta) = \|\omega - \eta\|_\infty := \sup_{t \in [0,\varepsilon]} |\omega(t) - \eta(t)| \tag{2.12}$$

is endowed with the measure

$$\underline{d}\omega = dx\, P^\varepsilon_{x,x}(d\omega) \tag{2.13}$$

Then, (2.9), (2.10) show that $\rho_j^N(\omega^j)\, \underline{d}\omega^j$ ($\underline{d}\omega^j = \prod_{s=1}^j \underline{d}\omega_s$) is a probability measure on $(\Omega_\varepsilon)^j$, which is in fact the j-particle marginal of the "classical" Gibbs measure on $(\Omega_\varepsilon)^N$:

$$\rho_N^N(\omega^N)\, \underline{d}\omega^N = Z_N^{-1} \exp[-\bar{U}^\varepsilon_N(\omega^N)]\, \underline{d}\omega^N \tag{2.14}$$

As in classical statistical mechanics, ρ_N^N minimizes the free-energy functional, defined on probability densities μ on $((\Omega_\varepsilon)^N, \underline{d}\omega^N)$ by

$$F_N(\mu) = \frac{1}{N} \int \mu(\omega^N) \log \mu(\omega^N)\, \underline{d}\omega^N + \frac{1}{N} \int \mu(\omega^N)\, \bar{U}^\varepsilon_N(\omega^N)\, d\omega^N \tag{2.15}$$

The following bound on ρ_j^N is crucial to investigate the limit $N \to \infty$:

Proposition 2.1. There exists a constant $K > 0$ such that for all $N \geq 1$, $1 \leq j \leq N$, $\varepsilon > 0$, and $\omega^j \in (\Omega_\varepsilon)^j$:

$$\rho_j^N(\omega^j) \leq K^j \varepsilon^{3j/2} \exp\left[-\sum_{i=1}^j \bar{V}^\varepsilon_e(\omega_i)\right] \tag{2.16}$$

The proof will be given in the next section. The above proposition makes the following statement almost obvious.

Proposition 2.2. For every $j \geqslant 1$, the sequence $\{\rho_j^N(\omega^j)\, \underline{d}\omega^j\}_{N \geqslant j}$ of probability measures on $(\Omega_\varepsilon)^j$ is tight, therefore precompact. Every cluster point is absolutely continuous, i.e., of the form $\rho_j(\omega^j)\, \underline{d}\omega^j$, and ρ_j satisfies the bound (2.16).

We are now in a position to formulate the main results of this section:

Theorem 2.1. For all $j \geqslant 1$, the sequence $\{\rho_j^N(\omega^j)\, \underline{d}\omega^j\}_{N \geqslant j}$ converges weakly to a probability measure $\rho_j(\omega^j)\, \underline{d}\omega^j$ on $(\Omega_\varepsilon)^j$, i.e., for all bounded continuous φ: $(\Omega_\varepsilon)^j \to R$:

$$\lim_{N \to \infty} \int \varphi(\omega^j)\, \rho_j^N(\omega^j)\, \underline{d}\omega^j = \int \varphi(\omega^j)\, \rho_j(\omega^j)\, \underline{d}\omega^j \tag{2.17}$$

Moreover, $\rho_j(\omega^j)$ factorizes:

$$\rho_j(\omega^j) = \prod_{i=1}^{j} \rho(\omega_i) \tag{2.18}$$

where ρ: $\Omega_\varepsilon \to R_+$ minimizes the functional

$$\begin{aligned} f_\varepsilon(\rho) = &\int \rho(\omega) \log \rho(\omega)\, \underline{d}(\omega) \\ &+ \tfrac{1}{2} \int \underline{d}\omega_1\, \underline{d}\omega_2\, \rho(\omega_1)\, \rho(\omega_2)\, \bar{V}^\varepsilon(\omega_1 - \omega_2) \\ &+ \int \underline{d}\omega\, \rho(\omega)\, \bar{V}_e^\varepsilon(\omega) \end{aligned} \tag{2.19}$$

under the constraints $\rho(\omega) > 0$, $\int \rho(\omega)\, \underline{d}\omega = 1$. In fact, ρ is the unique minimizer of f_ε and satisfies the equation

$$\rho(\omega) = N(\rho)^{-1} \exp[-\overline{V * n}^\varepsilon(\omega) - \bar{V}_e^\varepsilon(\omega)], \qquad \omega \in \Omega_\varepsilon \tag{2.20}$$

where $N(\rho)$ is the normalizing factor and

$$n(x) = \int P_{x,x}^\varepsilon(d\omega)\, \rho(\omega) \tag{2.21}$$

The proof will be presented in the next section. Notice that Theorem 2.1 asserts only the convergence of the restriction $\rho_j^N(\Omega_\varepsilon)^j$ (i.e., to closed trajectories), implying apparently only the convergence of the diagonal part of the reduced density matrices. The following theorem will achieve the convergence problem.

Theorem 2.2. Pointwise in $R^{3j} \times R^{3j}$:

$$\lim_{N \to \infty} \rho_j^N(X^j, Y^j) = \prod_{i=1}^{j} \rho(x_i, y_i) \tag{2.22}$$

where $\rho(x, y)$ is the kernel of the trace-class positive operator $\hat{\rho}$:

$$\hat{\rho} = \frac{e^{(\varepsilon/2)\Delta - V * n_\varepsilon - V_e}}{\operatorname{Tr} e^{(\varepsilon/2)\Delta - V * n_\varepsilon - V_e}} \tag{2.23}$$

Again, the proof is relegated to the next section.

We conclude this section with a few remarks on related results which can be obtained using the same formalism.

Remark 1. All results in this section extend, with minor modifications, to the case where the system is confined to a bounded domain $\Lambda \subset R^3$ with smooth boundary and V_e is a continuous function on $\bar{\Lambda}$. In this case, Δ_i in (2.1) should be supplemented with boundary conditions making it a positive self-adjoint operator in $L_2(\Lambda)$. The integral representation (2.4) still holds with $P^\varepsilon_{x,y}$ replaced by the adequate Wiener-type measure.[11] For example, for Dirichlet boundary conditions one has to use $\alpha_\Lambda(\omega) P^\varepsilon_{x,y}(d\omega)$, where $\alpha_\Lambda(\omega) = 1$, if $\omega([0, \varepsilon]) \subset \Lambda$, and $=0$ otherwise. Depending on the physical properties of the boundary, one also has to modify the interaction potential. For example, if the boundary is perfectly conducting, then $V(x_i - x_j)$ in (2.1) should be replaced by $V_\Lambda(x_i, x_j) =$ the fundamental solution of the Poisson equation in Λ with Dirichlet boundary conditions. As the latter is known to have the same local singularity as the Coulomb potential and is smooth outside the diagonal, the proof goes through. One recovers in this case the equation for the bounded case considered in ref. 1.

Remark 2. As already mentioned in the Introduction, Theorem 2.2 ensures the existence of solutions to Eqs. (1.1)–(1.4): these can be obtained as the limit of $\rho_1^N(x, y)$. It may be worth at this point to say that the functional integration formalism and the variational principle associated to the "free energy" (2.19) can be used to settle directly the existence and uniqueness problems of Eq. (1.1).

Indeed, every solution of Eq. (1.1) is seen to be a positive trace-one operator, the kernel of which is positive and has the form

$$\rho(x, y) = \int P^\varepsilon_{x,y}(d\omega)\, \rho(\omega) \tag{2.24}$$

with some bounded, positive $\rho(\omega)$; this is so because the r.h.s. of Eq. (1.1) has this property, once $n(x)=\rho(x, x)$ is known, with

$$\rho(\omega)=N(\rho)^{-1}\exp[-\overline{V*n}^{\varepsilon}(\omega)-\bar{V}_e^{\varepsilon}(\omega)] \tag{2.25}$$

for all Brownian paths ω. In particular, a solution ρ of (2.25) restricted to Ω_ε is a solution of Eq. (2.20), which extends by (2.25) to a measurable function on all Brownian paths. Conversely, every solution of Eq. (2.20) provides, via the extension (2.25) and Eq. (2.24), a solution of Eq. (1.1). Thus, it is sufficient to settle existence and uniqueness for Eq. (2.20).

Now, by the positivity of V, any solution of Eq. (2.20) has an *a priori* bound $N(\rho)^{-1}\exp[-\bar{V}_e^{\varepsilon}(\omega)]$, which ensures finiteness of $f_\varepsilon(\rho)$. So, if ρ_1, ρ_2 were solutions, then $\varphi(t)=f_\varepsilon(t\rho_1+(1-t)\rho_2)$ would be differentiable on $[0, 1]$, with $\varphi'(0+)=\varphi'(1-)=0$, which is impossible due to the strict convexity (of f_ε and hence) of φ. Existence of a solution is ensured by f_ε being positive and with compact levels, implying that it attains its infimum on some ρ, which is a solution of Eq. (2.20) (this latter fact needs a discussion of the differentiability of f_ε around ρ).

3. PROOFS

The proofs are similar to those in the classical case,[2-4] with some additional probability estimates.

We shall include, for convenience, the external potential factor into the measure, i.e., define the probability measure on Ω_ε:

$$d\mu(\omega)=Z_e^{-1}\exp[-\bar{V}_e^{\varepsilon}(\omega)]\,\underline{d}\omega \tag{3.1}$$

and denote, as well, by $d\mu(\omega^j)$ the product measure on $(\Omega_\varepsilon)^j$. Notice that, by assumption (1.6), the definition (3.1) makes sense, i.e., the normalizing factor Z_e is finite; indeed, by Jensen's inequality and Lemma 3.1

$$\begin{aligned} Z_e &= \int \exp[-\bar{V}_e^{\varepsilon}(\omega)]\,\underline{d}\omega \\ &\leqslant \frac{1}{\varepsilon}\int_0^\varepsilon dt \int e^{-V_e(\omega(t))}\,\underline{d}\omega \\ &= \int e^{-V_e(\omega(0))}\,\underline{d}\omega \\ &= (2\pi\varepsilon)^{-3/2}\,\|e^{-V_e}\|_{L_1} \end{aligned} \tag{3.2}$$

We have used here the following elementary property:

Lemma. Consider the mapping $T_r: \Omega_\varepsilon \to \Omega_\varepsilon$ defined by

$$(T_r\omega)(t) = \omega((t+r) \text{ modulo } \varepsilon) \tag{3.3}$$

Then, for all $f \in L_1(\Omega_\varepsilon, \underline{d}\omega)$,

$$\int f(T_r\omega)\,\underline{d}\omega = \int f(\omega)\,\underline{d}\omega \tag{3.4}$$

Proof. It is sufficient to prove (3.4) for cylindrical functions

$$f(\omega) = G(\omega(t_1),..., \omega(t_n)), \qquad G \in C(R^n), \quad \text{bounded} \tag{3.5}$$

This is done by inspection, making explicit use of the definition of $\underline{d}\omega$. ∎

Proof of Proposition 2.1. In terms of the measure (3.1), the definition (2.9) of ρ_j^N is written as

$$\rho_j^N(\omega^j) = Z_e^{-j} \exp[-\bar{V}_e^\varepsilon(\omega^j)] \frac{\int d\mu(\eta^{N-j}) \exp[-\bar{W}_N^\varepsilon(\omega^j \cup \eta^{N-j})]}{\int d\mu(\eta^N) \exp[-\bar{W}_N^\varepsilon(\eta^N)]} \tag{3.6}$$

where we used the notation (2.7) and defined

$$W_N(X^k) = \frac{1}{2N} \sum_{\substack{i,j=1 \\ i \neq j}}^{k} V(x_i - x_j), \qquad 1 \leqslant k \leqslant N \tag{3.7}$$

[So, $W_N(X^N)$ is the interaction part of the total potential energy $U_N(X^N)$.]

Putting

$$\theta_N(k) = \int d\mu(\omega^k) \exp[-\bar{W}_N^\varepsilon(\omega^k)] \tag{3.8}$$

we have, by the positivity of V,

$$\rho_j^N(\omega^j) \leqslant Z_e^{-j}\{\exp[-\bar{V}_e^\varepsilon(\omega^j)]\} \frac{\theta_N(N-j)}{\theta_N(N)} \tag{3.9}$$

The bound (2.16) follows at once from the two inequalities below:

There exist constants $M, C > 0$ such that, for all $\varepsilon > 0$, all $M \geqslant 1$, and all $1 \leqslant k \leqslant N-1$,

$$\theta_N(k) \leqslant M\theta_N(k+1) \tag{3.10}$$

and

$$Z_e \geqslant C\varepsilon^{-3/2} \tag{3.11}$$

To prove (3.10), we start from the obvious inequality

$$\theta_N(k) \leqslant \theta_N(k+1) \Big/ \inf_{\omega^k} \int d\mu(\eta) \exp\left[-\frac{1}{2N} \sum_{i=1}^{k} \bar{V}^\varepsilon(\omega_i - \eta)\right] \tag{3.12}$$

By Jensen's inequality

$$\begin{aligned} &\int d\mu(\eta) \exp\left[-\frac{1}{2N} \sum_{i=1}^{k} \bar{V}^\varepsilon(\omega_i - \eta)\right] \\ &\qquad \geqslant \exp\left[-\frac{1}{2N\varepsilon} \int_0^\varepsilon dt \sum_{i=1}^{k} \int d\mu(\eta)\, V(\omega_i(t) - \eta(t))\right] \\ &\qquad \geqslant \exp\left[-\frac{k}{2N} \frac{1}{\varepsilon} \int_0^\varepsilon dt \sup_\omega \int d\mu(\eta)\, V(\omega(t) - \eta(t))\right] \end{aligned} \tag{3.13}$$

On the other hand, using again Jensen's inequality and Lemma 3.1,

$$\begin{aligned} &\int d\mu(\eta)\, V(z - \eta(t)) \\ &\quad = Z_e^{-1} \int dx \int P_{00}^\varepsilon(d\eta) \left\{ \exp\left[-\frac{1}{\varepsilon} \int_0^\varepsilon V_e(x + \eta(t'))\, dt'\right]\right\} V(z - x - \eta(t)) \\ &\quad \leqslant Z_\varepsilon^{-1} \frac{1}{\varepsilon} \int_0^\varepsilon dt' \int P_{00}^\varepsilon(d\eta) \\ &\qquad \times \int dx\, e^{-V_e(x)} V(z - x - (T_{-t'}\eta))(t) \\ &\quad \leqslant Z_e^{-1} (2\pi\varepsilon)^{-3/2} \sup_{z \in R^3} \int dx\, e^{-V_e(x)} V(z - x) \end{aligned} \tag{3.14}$$

The sup in the last line is finite, because $e^{-V_e} \in L_1 \cap L_\infty$ and $V \in L_{1,\mathrm{loc}}$. By (3.11), the bound is uniform in ε. Inserting this into (3.13) and then into (3.12), one obtains (3.10).

Finally, we prove (3.11). Let Λ be a ball in R^3; we obtain a lower bound to Z_e by restricting the integration to trajectories contained in Λ:

$$\begin{aligned} Z_e &= \int \underline{d}\omega \exp[-\bar{V}_e^\varepsilon(\omega)] \\ &\geqslant \int \underline{d}\omega\, \alpha_\Lambda(\omega) \exp[-\bar{V}_e^\varepsilon(\omega)] \\ &\geqslant \{\exp[-\sup_{x \in \Lambda} V_e(x)]\} \int \underline{d}\omega\, \alpha_\Lambda(\omega) \end{aligned} \tag{3.15}$$

Now

$$\int \underline{d}\omega\, \alpha_\Lambda(\omega) = \operatorname{Tr} e^{(\varepsilon/2)\Delta_\Lambda} \geqslant \text{const} \cdot \varepsilon^{-3/2} \tag{3.16}$$

as follows by a simple scaling argument. ∎

Proof of Proposition 2.2. By (3.9) and (3.10),

$$\rho_j^N(\omega^j)\, \underline{d}\omega^j \leqslant M^j\, d\mu(\omega^j) \tag{3.17}$$

As $d\mu(\omega^j)$ is a probability measure on $(\Omega_\varepsilon)^j$, hence almost concentrated on a compact, the tightness follows easily. The bound (2.16) yields at once the absolute continuity of—and is satisfied by—any cluster point. ∎

Proof of Theorem 2.1. This is essentially a rephrasing of the classical case,[2-4] but we include it here for the sake of completeness.

Let $\rho_j(\omega^j)\, \underline{d}\omega^j$ be a cluster point, $j \geqslant 1$. By the usual diagonal trick we can find a unique subsequence $\{N_k\}$, the j-marginals of which converge to $\rho_j(\omega^j)\, \underline{d}\omega^j$ for all j. By the Hewitt–Savage theorem[12] there exists a Borel probability measure ν on $M_{+,1}(\Omega_\varepsilon)$ such that

$$\rho_j(\omega^j)\, \underline{d}\omega^j = \int \nu(d\rho)\, \rho(d\omega_1) \cdots \rho(d\omega_j), \qquad j \geqslant 1 \tag{3.18}$$

In fact, ν is supported by absolutely continuous measures $\rho(\omega)\, \underline{d}\omega$ with $\rho \in L_1 \cap L_\infty(\Omega_\varepsilon, \underline{d}\omega)$, because applying (3.18) to $\prod_{i=1}^j f(\omega_i)$ for positive f and using (2.16), we have

$$\int \nu(d\rho) \left[\int f(\omega)\, \rho(\omega)\, \underline{d}\omega \right]^j \leqslant M^j \left[\int f(\omega)\, d\mu(\omega) \right]^j$$

from which

$$\left\| \int f(\omega)\, \rho(\omega)\, \underline{d}\omega \right\|_{L_\infty(\nu)} \leqslant M\, \| f \|_{L_1(d\mu)}$$

Thus, ρ itself satisfies (2.16).

For every ν associated via (3.18) to a sequence $\{\rho_j\}_{j=1}^\infty$ we define the free energy functional

$$f(\nu) = s(\nu) + e(\nu) \tag{3.19}$$

where, as is well known,[13]

$$s(\nu) := \lim_{j\to\infty} \frac{1}{j} \int \rho_j(\omega^j) \log \rho_j(\omega^j)\, \underline{d}\omega^j$$

$$= \int \nu(d\rho) \int \rho(\omega) \log \rho(\omega)\, \underline{d}\omega \tag{3.20}$$

$$e(\nu) := \frac{1}{2} \int \nu(d\rho) \int \rho(\omega_1)\, \rho(\omega_2)\, \bar{V}^{\varepsilon}(\omega_1 - \omega_2)\, \underline{d}\omega_1\, \underline{d}\omega_2$$

$$+ \int \nu(d\rho) \int \rho(\omega)\, \bar{V}_e^{\varepsilon}(\omega)\, \underline{d}\omega \tag{3.21}$$

Notice that $s(\nu)$ is the kinetic entropy, which is minus the usual physical entropy.

We now prove that the free energy $F_N(\rho_N^N)$, Eq. (2.15), converges along the chosen subsequence to $f(\nu)$. By Propositions 2.1, 2.2 we easily obtain

$$\lim_N \frac{1}{N} \int \rho_N^N(\omega^N)\, U_N(\omega^N)\, \underline{d}\omega^N = e(\nu) \tag{3.22}$$

By convexity and subadditivity of the entropy

$$\frac{1}{j} \int \rho_j(\omega^j) \log \rho_j(\omega^j)\, \underline{d}\omega^j$$

$$\leqslant \liminf_N \frac{1}{j} \int \rho_j^N(\omega^j) \log \rho_j^N(\omega^j)\, \underline{d}\omega^j$$

$$\leqslant \liminf_N \frac{1}{N} \int \rho_N^N(\omega^N) \log \rho_N^N(\omega^N)\, \underline{d}\omega^N \tag{3.23}$$

and hence

$$f(\nu) \leqslant \liminf_N F_N(\rho_N^N) \tag{3.24}$$

On the other hand, by the variational principle for F_N,

$$F_N(\rho_N^N) \leqslant F_N(\rho_N)$$

Hence, with an easy calculation using the particular form (3.18) of ρ_N

$$\limsup_N F_N(\rho_N^N) \leqslant f(\nu) \tag{3.25}$$

We now prove that ν is concentrated on those ρ minimizing the functional f_ε, Eq. (2.19). Indeed, if $\tilde{\nu}$, $\{\tilde{\rho}_j\}$ is another pair connected by (3.18), we have again $F_N(\rho_N^N) \leqslant F_N(\tilde{\rho}_N)$, implying $f(\nu) \leqslant f(\tilde{\nu})$. As $f(\nu) = \int \nu(d\rho) f_\varepsilon(\rho)$ by (3.19)–(3.21), the claim is proved.

The strict convexity of f_ε implies a unique minimizer ρ, hence $\nu = \delta_\rho$ and the factorization property (2.18) holds. Moreover, the uniqueness of the limit allows us to pass from subsequence to sequence.

Finally, we show that ρ fulfills Eq. (2.20), which formally means that the minimum point ρ is a stationary point of f_ε. In order to avoid discussing differentiability of $f_\varepsilon: M_{+,1}(\Omega_\varepsilon) \to [0, \infty]$ around ρ_ε, we provide a direct proof, exploiting that $\rho = \lim_N \rho_1^N$.

We start with Eq. (3.6) for $j = 1$, which can be written using (3.8) as

$$\rho_1^N(\omega) = Z_e^{-1} \exp[-\bar{V}_e^\varepsilon(\omega)] \frac{\theta_N(N-1)}{\theta_N(N)} \int \exp\left[-\frac{1}{N} \sum_{i=1}^{N-1} \bar{V}^\varepsilon(\omega - \eta_i)\right] \times \bar{\rho}_{N-1}^{N-1}(\eta^{N-1})\, d\mu(\eta^{N-1}) \tag{3.26}$$

where the probability density $\bar{\rho}_{N-1}^{N-1}$ on $((\Omega_\varepsilon)^{N-1}, d\mu(\eta^{N-1}))$ is given by

$$\bar{\rho}_{N-1}^{N-1}(\eta^{N-1}) = \theta_N(N-1)^{-1} \exp\left[-\left(1 - \frac{1}{N}\right) \bar{W}_{N-1}^\varepsilon(\eta^{N-1})\right] \tag{3.27}$$

By the same proof as for Proposition 2.1, the marginal distributions of $\bar{\rho}_N^N$, say $\bar{\rho}_j^N$, satisfy the same kind of bound, Eq. (3.9), as ρ_j^N, and the proof for ρ_j^N can be easily adapted to conclude convergence of $\bar{\rho}_j^N$ to the same limit as ρ_j^N [it is sufficient to replace the "inverse temperature" $1 - 1/(N+1)$ instead of 1 whenever necessary]. Moreover, the ratio $C_N = \theta_N(N-1)/\theta_N(N)$ is bounded by (3.10), so

$$\bar{c} := \limsup_N C_N < \infty$$

Using Jensen's inequality in (3.26), we have the lower bound

$$\rho_1^N(\omega) \geqslant Z_e^{-1} \exp[-\bar{V}_e^\varepsilon(\omega)] \times C_N \exp\left[-\frac{1}{\varepsilon} \int_0^\varepsilon dt \int d\mu(\eta)\, \bar{\rho}_1^{N-1}(\eta)\, V(\omega(t) - \eta(t))\right] \tag{3.28}$$

yielding, by the discussion above,

$$\rho(\omega) \geqslant \bar{c} Z_e^{-1} \exp[-\bar{V}_e^\varepsilon(\omega) - \overline{V * n}^\varepsilon(\omega)] \tag{3.29}$$

On the other hand, putting

$$V_\delta(x) = \begin{cases} V(x) & \text{if } |x| > \delta \\ V(\delta) & \text{if } |x| \leqslant \delta \end{cases} \tag{3.30}$$

we have, expanding the exponential,

$$\begin{aligned} \rho_1^N(\omega) &\leqslant C_N Z_e^{-1} \exp[-\bar{V}_e^\varepsilon(\omega)] \int d\mu(\eta^{N-1})\, \bar{\rho}_{N-1}^{N-1}(\eta^{N-1}) \\ &\quad \times \exp\left[-\frac{1}{N}\sum_{i=1}^{N-1} \bar{V}_\delta^\varepsilon(\omega-\eta_i)\right] \\ &\leqslant C_N Z_e^{-1} \exp[-\bar{V}_e^\varepsilon(\omega)] \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \\ &\quad \times \sum_{j_1,\dots,j_n=1}^{N-1} \int d\mu(\eta^{N-1})\, \bar{\rho}_{N-1}^{N-1}(\eta^{N-1}) \\ &\quad \times \prod_{i=1}^{n} \bar{V}_\delta^\varepsilon(\omega-\eta_{j_i}) \\ &= C_N Z_e^{-1} \exp[-\bar{V}_e^\varepsilon(\omega)] \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left\{ \frac{(N-1)\cdots(N-n+1)}{N^n} \right. \\ &\quad \left. \times \left[\int d\mu(\eta)\, \bar{\rho}_1^{N-1}(\eta)\, \bar{V}_\delta^\varepsilon(\omega-\eta)\right]^n + R_N^n(\delta) \right\} \end{aligned} \tag{3.31}$$

In the last term we just split the contribution of $(j_1,\dots, j_n)$ with at least two equal indices into $R_N^n(\delta)$. It is easy to see that $R_N^n(\delta) = O(N^{-1})$ for every n and δ. Therefore, the nth term of the series (3.31) converges as $N \to \infty$ to

$$\frac{(-1)^n}{n!} [\overline{V_\delta * n_\varepsilon}^\varepsilon(\omega)]^n$$

and is uniformly bounded by $1/(n!\, \delta^n)$. Letting $N \to \infty$ and then $\delta \searrow 0$, we have

$$\rho(\omega) \leqslant \underline{c} Z_e^{-1} \exp[-\bar{V}_e^\varepsilon(\omega) - \overline{(V*n)}^\varepsilon(\omega)] \tag{3.32}$$

where $\underline{c} := \liminf_N C_N$. Equations (3.22) and (3.29) prove (2.20). We notice that, along the way, we proved the convergence of C_N:

$$\lim_N \frac{\theta_N(N-1)}{\theta_N(N)} = N(\rho)^{-1} \quad \blacksquare \tag{3.33}$$

Proof of Theorem 2.2. It is sufficient to remark that the bounds (3.28) and (3.31) hold true for all (not necessarily closed) Brownian paths ω. As we have already proved the convergence as $N \to \infty$ of the r.h.s. of these equations, we have, after letting $\delta \searrow 0$,

$$\limsup_N \rho_1^N(\omega) = \liminf_N \rho_1^N(\omega) = N(\rho)^{-1} Z_e^{-1} \exp[-\bar{V}_e^\varepsilon(\omega) - (\overline{V * n^\varepsilon})(\omega)] \tag{3.34}$$

for all paths ω. By a similar argument, one obtains the pointwise convergence of $\rho_j^N(\omega^j)$ to $\prod_{i=1}^j \rho(\omega_i)$. As also the bound (3.9) holds for arbitrary paths ω^j, the dominated convergence theorem applied to (2.8) accomplishes the proof. ∎

4. THE CLASSICAL LIMIT

In this section we shall explore the limit $\varepsilon \searrow 0$ and prove the convergence of the particle density of the quantum mean-field theory, which is the solution of Eqs. (2.20), (2.21), to the solution of the corresponding classical problem, Eq. (1.5). In doing this we use a compactness argument in conjunction with the uniqueness of the solution of Eq. (1.5).

Theorem 4.1. Let $\rho_\varepsilon, n_\varepsilon$ be the unique solution of Eqs. (2.20), (2.21), and n_0 be the unique solution of Eq. (1.5). The probability measures $\{n_\varepsilon(x)\,dx\}_{\varepsilon>0}$ on R^3 converge weakly to $n_0(x)\,dx$ as $\varepsilon \searrow 0$. Moreover, $n_\varepsilon \to n_0$ in $H^{-1}(R^3)$ and pointwise.

Proof. We start by proving the tightness of the family $n_\varepsilon(x)\,dx$, $\varepsilon \in (0, 1]$. To this aim, using the scaling property of Wiener measure and Jensen's inequality, we obtain from (2.16)

$$\begin{aligned} n_\varepsilon(x) &\leqslant K\varepsilon^{3/2} \int P_{xx}^\varepsilon(d\omega) \exp[-\bar{V}_e^\varepsilon(\omega)] \\ &= K \int P_{00}^1(d\omega) \exp\left[-\int_0^1 dt\, V_e(x + \sqrt{\varepsilon}\,\omega(t))\right] \\ &\leqslant K \int_0^1 dt \int P_{00}^1(d\omega) \exp[-V_e(x + \sqrt{\varepsilon}\,\omega(t))] \end{aligned} \tag{4.1}$$

Hence, separating the contribution of paths which do not leave the ball of radius $(R/\varepsilon)^{1/2}$, we have

$$\int_{|x|>R} n_\varepsilon(x)\,dx$$

$$\leqslant K\int_0^1 dt \int P_{00}^1(d\omega)\int_{|x|>R} dx \exp[-V_e(x+\sqrt{\varepsilon}\,\omega(t))]$$

$$\leqslant K\bigg[P_{00}^1(\{\omega\colon \|\omega\|_\infty \geqslant (R/\varepsilon)^{1/2}\})\,\|e^{-V_e}\|_1$$

$$+(2\pi)^{-3/2}\int_{|x|>R-\sqrt{R}} e^{-V_e(x)}\,dx\bigg]$$

where we used $|x+\sqrt{\varepsilon}\,\omega(t)|>R-\sqrt{R}$, for $|x|>R$ and $|\omega(t)|<(R/\varepsilon)^{1/2}$. Therefore,

$$\sup_{\varepsilon\in(0,1]}\int_{|x|>R} n_\varepsilon(x)\,dx \leqslant K\bigg[P_{00}^1(\{\omega\colon \|\omega\|_\infty \geqslant \sqrt{R}\})\,\|e^{-V_e}\|_1$$

$$+(2\pi)^{-3/2}\int_{|x|>R-\sqrt{R}} e^{-V_e(x)}\,dx\bigg] \tag{4.2}$$

converges to zero as $R\to\infty$, proving tightness.

Next, we show that any limit point of $n_\varepsilon(x)\,dx$ as $\varepsilon\to 0$ is of the form $\bar{n}(x)\,dx$, with $\bar{n}$ solution of Eq. (1.5). The bound (4.1) implies

$$\|n_\varepsilon\|_\infty \leqslant (2\pi)^{-3/2}\,Ke^{-\min V_e} := M \tag{4.3}$$

and then the absolute continuity of any limit point. By (2.20), (2.21), and scaling, we have for every $\varepsilon>0$

$$n_\varepsilon(x) = N_\varepsilon^{-1}\int (2\pi)^{3/2}\,P_{00}^1(d\omega)$$

$$\times \exp\left\{-\int_0^1 [V * n_\varepsilon(x+\sqrt{\varepsilon}\,\omega(t)) + V_e(x+\sqrt{\varepsilon}\,\omega(t))]\,dt\right\} \tag{4.4}$$

$$N_\varepsilon = \int dx \int (2\pi)^{3/2}\,P_{00}^1(d\omega)$$

$$\times \exp\left\{-\int_0^1 [V * n_\varepsilon(x+\sqrt{\varepsilon}\,\omega(t)) + V_e(x+\sqrt{\varepsilon}\,\omega(t))]\,dx\right\} \tag{4.5}$$

If $\varepsilon_k \searrow 0$ and $n_{\varepsilon_k}\to\bar{n}$, in the sense of the weak convergence of measures, then

$$\lim_{\varepsilon_k} V * n_{\varepsilon_k}(x) = V * \bar{n}(x), \qquad \forall x\in R^3 \tag{4.6}$$

Indeed, with V_δ defined in Eq. (3.30) and using (4.3), we have

$$V_\delta * n_{\varepsilon_k}(x) \leqslant V * n_{\varepsilon_k}(x) \leqslant V_\delta * n_{\varepsilon_k}(x) + M \int_{|y| < \delta} V(y)\, dy$$

and hence

$$\begin{aligned} V_\delta * \bar{n}(x) &\leqslant \liminf_{\varepsilon_k} V * n_{\varepsilon_k}(x) \\ &\leqslant \limsup_{\varepsilon_k} V * n_{\varepsilon_k}(x) \\ &\leqslant V_\delta * \bar{n}(x) + O(\delta^2) \end{aligned}$$

which implies (4.6) by the arbitrariness of δ.

We shall show below that there exists a constant A such that

$$\sup_{x \in R^3} |V * n_\varepsilon(x + \sqrt{\varepsilon}\, u) - V * n_\varepsilon(x)| \leqslant A \sqrt{\varepsilon}\, |u|, \qquad \forall u \in R^3, \quad |u| \sqrt{\varepsilon} \leqslant 1 \tag{4.7}$$

Combining (4.6), (4.7), and the positivity of V, we obtain, by Lebesgue's theorem, the convergence as $\varepsilon_k \searrow 0$ of the numerator in the r.h.s. of (4.4) to $\exp[-V * \bar{n}(x) - V_e(x)]$. In the same way also N_{ε_k} converges to the normalization factor of the limit, implying that $\bar{n}$ is a solution of Eq. (1.5). By the uniqueness of the latter, the weak convergence follows. Finally, by (4.6) also pointwise convergence follows.

To prove (4.7), let D_1 be the ball of center x and radius $(\sqrt{\varepsilon}\, |u|)^{1/2}$, and D_2 be the ball of center x and radius 2. Then

$$\begin{aligned} &\left| \int [V(x - y + \sqrt{\varepsilon}\, u) - V(x - y)]\, n_\varepsilon(y)\, dy \right| \\ &\quad \leqslant M \int_{D_1} [V(x - y + \sqrt{\varepsilon}\, u) + V(x - y)]\, dy \\ &\qquad + \left(\int_{D_2 \setminus D_1} + \int_{R^3 \setminus D_2} \right) |V(x - y + \sqrt{\varepsilon}\, u) - V(x - y)|\, n_\varepsilon(y)\, dy \end{aligned} \tag{4.8}$$

For $y \in D_1$, both $|x - y + \sqrt{\varepsilon}\, u|$ and $|x - y|$ are less than $2(\sqrt{\varepsilon}\, |u|)^{1/2}$, so the first term in (4.9) is dominated by $2M\, |u| \sqrt{\varepsilon}$. Outside D_1 we use Lagrange's theorem:

$$|V(x - y + \sqrt{\varepsilon}\, u) - V(x - y)| = \frac{\sqrt{\varepsilon}\, u}{4\pi\, |x - y + \theta \sqrt{\varepsilon}\, u|^2}, \qquad \theta \in (0, 1)$$

For $y \in D_2 \backslash D_1$, $|x - y + \theta\sqrt{\varepsilon}\, u| \leqslant 2 + |u|\sqrt{\varepsilon}$, so the second integral is majorized by

$$M\sqrt{\varepsilon}\,|u| \int_{|y| \leqslant 3} \frac{1}{4\pi\,|y|^2}\,dy$$

Finally, on $R^3 \backslash D_2$ we exploit boundedness of $|x - y + \theta\sqrt{\varepsilon}\, u|^{-2} \leqslant 1$, and

$$\int_{R^3 \backslash D_2} n_\varepsilon(y)\,dy \leqslant 1$$

We now prove convergence in H^{-1}. To this aim, we argue that $\rho_\varepsilon(\omega)$, besides minimizing f_ε, Eq. (2.19), also maximizes the concave functional

$$g_\varepsilon(\rho) = -\tfrac{1}{2} \int n(x)\,n(y)\,V(x-y)\,dx\,dy$$
$$-\log \int \underline{d}\omega\, \exp[-\overline{V * n}^{\varepsilon}(\omega) - \bar{V}_e^{\varepsilon}(\omega)] \qquad (4.9)$$

where again n is the particle density of ρ, Eq. (2.21). The advantage of using g_ε is that it depends on ρ only through n; we shall write $g_\varepsilon(n)$ from now on.

We also consider the classical functional

$$g_0(n) = -\frac{1}{2} \int n(x)\,n(y)\,V(x-y)\,dx\,dy$$
$$-\log \int \frac{dx}{(2\pi\varepsilon)^{3/2}}\, e^{-V * n(x) - V_e(x)} \qquad (4.10)$$

which is maximized by n_0. [The factor $(2\pi\varepsilon)^{-3/2}$ is inserted to take into account the kinetic energy as in the quantum case; notice that formally $g_0 + \frac{3}{2}\log\varepsilon$ is the $\varepsilon \searrow 0$ limit of $g_\varepsilon + \frac{3}{2}\log\varepsilon$.]

For an arbitrary probability density n in the domain of g_ε, we have with $\delta n = n - n_\varepsilon$, and using Eq. (2.20) for n_ε,

$$g_\varepsilon(n_\varepsilon) - g_\varepsilon(n) = \tfrac{1}{2} \int \delta n(x)(V * \delta n)(x)\,dx$$
$$+ \int n_\varepsilon(x)(V * \delta n)(x)\,dx$$
$$+ \log \int \underline{d}\omega\, \rho_\varepsilon(\omega)\, \exp[-\overline{V * \delta n}^{\varepsilon}(\omega)] \qquad (4.11)$$

By Jensen's inequality and Lemma 3.1

$$\log \int \underline{d}\omega\, \rho_\varepsilon(\omega) \exp[-\overline{V * \delta n}^{\varepsilon}(\omega)]$$

$$\geqslant -\frac{1}{\varepsilon} \int_0^\varepsilon dt \int \underline{d}\omega\, \rho_\varepsilon(\omega)(V * \delta n)(\omega(t))$$

$$- \int n_\varepsilon(x)(V * \delta n)(x)\, dx$$

implying

$$g_\varepsilon(n_\varepsilon) - g_\varepsilon(n) \geqslant \tfrac{1}{2} \int \delta n(x)\, V * \delta n(x)\, dx = \tfrac{1}{2} \|\delta n\|^2_{-1} \tag{4.12}$$

Similarly,

$$g_0(n_0) - g_0(n) \geqslant \tfrac{1}{2} \|n - n_0\|^2_{-1} \tag{4.13}$$

Hence

$$\|n_\varepsilon - n_0\|^2_{-1} \leqslant [g_\varepsilon(n_\varepsilon) - g_0(n_\varepsilon)] + [g_0(n_0) - g_\varepsilon(n_0)] \tag{4.14}$$

Finally, the square brackets in (4.14) both converge to zero for $\varepsilon \searrow 0$ by the dominated convergence theorem, e.g.,

$$\begin{aligned} &g_\varepsilon(n_\varepsilon) - g_0(n_\varepsilon) \\ &\quad = \log \int dx \exp[-V * n_\varepsilon(x) - V_e(x)] \\ &\quad\quad - \log \int dx \int P^1_{00}(d\omega) \exp\left[-\frac{1}{\varepsilon}\int_0^\varepsilon dt\, (V * n_\varepsilon + V_e)(x + \sqrt{\varepsilon}\, \omega(t))\right] \end{aligned} \tag{4.15}$$

in which both terms converge to $\log \int dx \exp[-V * n_0(x) - V_e(x)]$, as in the first part of the proof.

5. CONCLUDING REMARKS

The results in Section 2 can be regarded as providing a mathematical basis for the Hartree approximation, that is, a rigorous derivation of Eq. (1.1) in terms of particle systems. We treated here the simplest case of repulsive interactions and classical statistics. More interesting, both physically and mathematically, would be the case of Fermi–Dirac statistics and/or attractive (gravitational) forces, which, as far as we know, have not been treated rigorously in the literature.

Scaling charges as $N^{-1/2}$ at fixed temperature is clearly unphysical, as the ratio charge/mass approaches zero as $N \to \infty$. Other, physically more reasonable interpretations of the result are, however, possible: e.g., in a bounded domain and with $V_e = 0$ the same convergence holds when scaling temperature like $N^{1/3}$, and both mass and charge like $N^{-1/3}$, which would be "close" for large N to a hot, dense plasma. Though not much insight is gained in this way concerning the range of applicability of the mean-field approximation, it is, however, conforting to see that the latter has some relation to a genuine N-body problem.

Another advantage of presenting Hartree's theory as a limit is that it provides a constructive approach to the existence problem for the mean-field equation from physical considerations and, in cases of nonuniqueness, it should give criteria for selecting relevant solutions.

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