Equilibrium properties of the Vlasov functional: The generalized Poisson-Boltzmann-Emden equation

François Bavaud

*Department of Mathematics, Heriot-Watt University, Edinburgh EH14 4AS, Scotland**

This article investigates in a systematic way the properties of the classical continuous mean-field theory governed by the generalized Poisson-Boltzmann-Emden equation $\rho(x)=A\exp[-\beta\int_\Lambda dy\,\rho(y)V(x-y)]$ together with the associated variational problem $\inf_\rho \frac{1}{2}\int_\Lambda dx\int_\Lambda dy\,\rho(x)\rho(y)V(x-y)+kT\int_\Lambda dx\,\rho(x)\ln\rho(x)$. Origins of the theory are traced back. Past studies (freezing theories, electrostatic and self-gravitating systems) are relocated in a broader framework. New results concerning the thermodynamic limit, phase transitions, metastability, and the shape of density profiles are provided. In particular, the question of ground states (in relationship to condensation and wetting phenomena) is illustrated by numerous explicit solutions.

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I. INTRODUCTION AND SCOPE OF THE PAPER

The central equation we shall deal with in this article is the nonlinear integral equation for $\rho(x)$:

$$\rho(x)=A\ \exp(-\beta\phi(x))\quad \forall x\in\Lambda\ , \tag{1}$$

where

$$\phi(x):=\int_\Lambda dy\,\rho(y)V(x-y)\ ,\qquad A:=\frac{N}{\int_\Lambda dy\,\exp(-\beta\phi(y))}\ . \tag{2}$$

$\rho(x)$ is a positive measure normalized to N with support in the container $\Lambda\subset\mathbf{R}^\nu$, $V(x)$ is the two-body interaction potential, and $\phi(x)$ is the potential induced by the density profile $\rho(x)$. Equation (1) is known in the literature as the Poisson-Boltzmann equation in the case of Coulomb systems (Hill, 1956; Davidson, 1962) or the Emden equation for isothermal gas spheres (Emden, 1907; Chandrasekhar, 1967) in the case of self-gravitating systems. We shall subsequently refer to it as the *generalized Poisson-Boltzmann-Emden* (GPBE) *equation.* Equation (1) is the Euler-Lagrange equation associated with the minimization of the functional

$$F[\rho]:=U[\rho]-TS[\rho]\ , \tag{3}$$

where

$$U[\rho]:=\tfrac{1}{2}\int_\Lambda dx\int_\Lambda dy\,\rho(x)\rho(y)V(x-y)\ ;\qquad -TS[\rho]:=kT\int_\Lambda dx\,\rho(x)\ln\rho(x)\ . \tag{4}$$

$U[\rho]$ is the energy part and $-TS[\rho]$ (that is, the *negative* of the entropy) is the entropy part of the functional $F[\rho]$, which we shall refer to as the *Vlasov functional.* $F[\rho]$ is a mapping from $\mathcal{R}(\Lambda,N)$ to $\mathbf{R}$, where

$$\mathcal{R}(\Lambda,N):=\{\rho\,|\,\rho(x)\geq 0,\ \mathrm{supp}(\rho)\subset\Lambda,\ \int_\Lambda dx\,\rho(x)=N\} \tag{5}$$

is the set of admissible densities. The presence of the entropy term allows us to consider absolutely continuous densities only.

Provided a minimizing profile $\rho^0(x)\in\mathcal{R}(\Lambda,N)$ exists, the corresponding value of the Vlasov functional $F^0(\Lambda,N):=F[\rho^0]$ will be called the (*equilibrium*) Vlasov free energy.

As a general rule, we have attempted to concentrate on

*New address: Institut de Mathématiques Appliquées, Université de Lausanne, BFSH2, CH-1015 Lausanne, Switzerland.

the study of the GPBE equation and the Vlasov functional *for their own sake,* that is, without seeking to model a specific phenomenon or treating the former as byproducts resulting from an approximate treatment of some exact theory. (In Sec. II, however, we describe the classical routes leading to the GPBE equation, and in Sec. III we investigate the relationship existing between Vlasov and ordinary free energies; the N-body formalism will not otherwise be considered.)

This approach allows for a greater unity and homogeneity in the presentation and provides a natural cutoff to the scope of what should or should not be included. The generality of results is also enhanced. On the other hand, standard and new physical applications (such as freezing, metastability, wetting, condensation, etc.) emerge so to speak naturally in their direct relation to mathematical questions (such as unicity and stability of stationary solutions, location of their support, existence of a singular part, etc.).

The study of the thermodynamic limit in Sec. IV entails a natural taxonomy of interactions: positive definite, nonpositive definite and stable, unstable. The second class turns out to be only of thermodynamic interest.

The existence of a solution is demonstrated in Sec. V; the question of uniqueness is investigated and solved for some situations. Bifurcation from the uniform profile has been widely used in previous theories of freezing. An exactly solvable model undergoing such a transition is described in Sec. VI.

Section VII gathers basic facts concerning Newtonian and Coulombic potentials. A criterion for the stability of self-gravitating systems is proposed.

Section VIII deals with the dependence of the density profile on both container and potential. We pay particular attention to the rotational invariance of the former. The relationship between pressure and density at the boundary (the wall theorem) is derived in Sec. IX.

Finally, in Sec. X, systems at zero temperature are studied. In the absence of an entropy part, minimizing profiles (ground states) might possess a singular part (condensation). Simple criteria (involving the value of the slope of the potential at the origin) are shown to provide direct information on the existence of condensation, as well as on the presence of wetting (defined as the presence of fluid in immediate proximity to the boundary of the container). The exact ground states associated with typical potentials (Yukawa, cosine, Gaussian, Morse, rectangular, etc.) are determined, thus illustrating condensation and wetting phenomena.

As far as we are aware, Secs. IV, VI, VIII, IX, and X (X.A excepted) are entirely new. In particular, the study of ground states (which appears to have been neglected in the past) presumably constitutes a promising field for future investigations.

II. DERIVATION OF THE GPBE EQUATION

As a general rule, the GPBE equation has been used by previous workers as an approximate, simple tool for extracting information on some underlying, more complex, "true" system. Having said that, we must remark that the different approaches, techniques, and results of relevance we have so far been able to identify constitute a strongly inhomogeneous class: this mainly reflects a wide variety of motivations in previous studies.

The pure Coulombic and Newtonian cases expected (see Hill, 1956; Davidson, 1962; Chandrasekhar, 1967; and references therein), the first-principles derivations of the GPBE equation (1) and its associated Vlasov functional can be fit into the following three main categories.

A. Classical mechanics

Consider a system of N classical point particles of identical masses m, interacting through a smooth pair potential $V(x)$ and enclosed in a container $\Lambda \subset \mathbf{R}^\nu$. In the *mean-field limit* (Spohn, 1980), the particle number and the potential are rescaled, respectively, as $N(\epsilon)=N/\epsilon$ and $V(\epsilon,x)=\epsilon V(x)$, with $\epsilon \to 0$. Let

$$\mu(\epsilon,x,p,t):=\epsilon \sum_{i=1}^{N(\epsilon)} \delta(x-x_i(t))\delta(p-p_i(t)) \tag{6}$$

be the one-point distribution function (normalized to N), where $x_i(t)$ and $p_i(t)$ are the position and the momentum of particle i at time t, evolving in the rescaled potential. Neunzert (1978) and, independently, Braun and Hepp (1977) have established that if, initially,

$$\lim_{\epsilon \to 0} \mu(\epsilon,x,p,0)=r(x,p,0) \tag{7}$$

weakly on $\mathbf{R}^{2\nu}$, then

$$\lim_{\epsilon \to 0} \mu(\epsilon,x,p,t)=r(x,p,t) \tag{8}$$

for all subsequent times $t \geq 0$, where $r(x,p,t)$ satisfies the *Vlasov equation* (Vlasov, 1938)

$$\frac{\partial r(x,p,t)}{\partial t} = -\frac{p_\alpha}{m}\frac{\partial r(x,p,t)}{\partial x_\alpha} + \frac{\partial r(x,p,t)}{\partial p_\alpha} \int_\Lambda dy \int_{R^\nu} d\tilde{p}\, r(y,\tilde{p},t) \frac{\partial V(x-y)}{\partial x_\alpha} \tag{9}$$

with initial condition $r(x,p,0)$.

Equation (9) is clearly time-reversible and, unless a collision term is added (Gogny and Lions, 1989; Bouchut, 1990; Desvillettes and Dolbeault, 1990), there is no possible relaxation towards any kind of equilibrium: typically, solutions will behave in an oscillatory or (in the absence of a container) indefinitely expanding way, as explicitly illustrated by Kurth (1978) in an astrophysical context (see also Batt *et al.*, 1986). (In the case of strongly attractive potentials, the collapse of the system remains of course

another possibility.)

In fact, the metaphorical "equilibrium properties" appearing in the title of this paper actually refer to the capacity of stationary solutions of the Vlasov equations to mimic (sometimes surprisingly well) some of the properties encountered in ordinary statistical mechanics, i.e., in N-body systems. This is the essence of mean-field theories. In this spirit, let us consider a stationary solution $r(x,p)$ of Eq. (9) with a Maxwellian distribution of momentum, at temperature $kT=\beta^{-1}$. The density profile $\rho(x)=\int dp\, r(x,p)$, normalized to N, then satisfies

$$\frac{\partial\rho(x)}{\partial x_\alpha}=-\beta\rho(x)\int_\Lambda dy\,\rho(y)\frac{\partial V(x-y)}{\partial x_\alpha}\ , \tag{10}$$

whose integrated form is nothing but the GPBE equation (1).

The GPBE equation can also be derived directly from ordinary equilibrium statistical mechanics. With the rescaling $N(\epsilon)=1/\epsilon$ (corresponding to $N=1$), $V(\epsilon,x)=\epsilon V(x)$, Battle (1977), in the C^*-algebras framework, and Messer and Spohn (1982), in a more classical context, show that the $N(\epsilon)$-point canonical distribution function tends in the limit $\epsilon\to 0$ towards a symmetric superposition of products of one-point distribution functions which turn out to be global minimizers of the Vlasov functional [Eq. (3)] (with $N=1$). Were the minimizer unique, the resulting state would be completely factorized. This is the static expression of *molecular chaos*. It can be compared to the dynamical result (Braun and Hepp, 1977) that an initially factorized state remains factorized for all subsequent times, in the limit $\epsilon\to 0$.

B. Functional expansion of the partition function

In an astrophysical context, Horwitz and Katz (1977) obtain a mean-field formalism by saddle-point expansion of the functional-integral expression of the partition function. More directly, Cally and Monaghan (1981) show the potential $\mathbf{W}_0=\sum_i\phi(x_i)$ [where $\phi(x)$ is the induced potential (2)] to be [up to $O(N^{-1})$ corrections] the best one-body approximation to the two-body potential $\mathbf{V}=\sum_{i<j}V(x_i-x_j)$, in the sense that, among all one-body potentials $\mathbf{W}$, $\mathbf{W}_0$ best minimizes the right-hand side of the Gibbs-Bogoliubov inequality (Falk, 1969)

$$F_{\mathbf{V}}\le F_{\mathbf{W}}+\langle\mathbf{V}-\mathbf{W}\rangle_{\mathbf{W}}\ . \tag{11}$$

C. Truncation of higher-order correlations

We regroup here several approaches initiated by Kirkwood and Monroe (1941), all sharing the following common features: they seek to model the freezing transition as a bifurcation problem governed by a nonlinear integral equation. This equation is obtained by means of an approximation eliminating the higher-order correlations, and most of the time it coincides with our GPBE equation (1) with a (possibly nontranslationally invariant) effective potential $V^*(x,y)$, generally differing from the interaction potential $V(x-y)$:

$$\rho(x)=A\exp\left[-\beta\int_\Lambda dy\ V^*(x,y)\rho(y)\right]\ . \tag{12}$$

For instance, Eq. (12) is exact (Kirkwood and Monroe, 1941; Hill, 1956; Jancovici, 1965) with

$$V^*(x,y)=V(x-y)\int_0^1 d\xi\, g(x,y;\xi)\ , \tag{13}$$

where $\xi\in[0,1]$ is a parameter coupling the interaction between the particle located at x to all the other particles ($\xi=1$ for the real system); $g(x,y;\xi)$ is the corresponding correlation function. $V^*(x,y)$ can be further approximated by using the Percus-Yevick or hypernetted-chain equation (Jancovici, 1965); alternatively, the "indirect coupling" method (Weeks *et al.*, 1970) yields $V^*(x,y)=g(x,y)\beta^{-1}[\exp(\beta V(x-y))-1]$ or, at high temperatures (Brout, 1963), $V^*(x,y)=g(x,y)V(x-y)$. It is also possible (Raveché and Stuart, 1975; Lovett, 1977; Raveché and Kayser, 1978; Jacobs, 1983) to start from the (exact) first BBGKY equation

$$\nabla_x\rho(x)=-\beta\rho(x)\int_\Lambda dy\, g(x,y)\rho(y)\nabla_x V(x-y)\ , \tag{14}$$

corresponding to Eq. (10) with $\nabla_x V^*(x,y)=g(x,y)\nabla_x V(x-y)$. In the aforementioned approaches, the correlation function $g(x,y)$ generally undergoes further approximations. For instance, the functional form of $g(x,y)$ is restricted (for all temperatures and densities) to a form corresponding to the uniform phase. A typical output (Raveché and Stuart, 1979; Raveché and Kayser, 1978) is $V^*(x,y)=\beta^{-1}g(a)\theta(x-a)$ for a system of hard spheres of radius a, where $\theta(\cdot)$ is the unit-step potential.

Finally, the so-called density-functional theory (see, for example, Baus, 1987; Jones and Gunnarsson, 1989, and references therein) leads in practice (despite the view sometimes advocated by its zealots) to very close approaches. In numerical applications, the excess free energy $\Delta F[\rho]=F[\rho]-F[\rho_u]$, where $\rho_u=$const. is the uniform profile, is approximated as

$$\Delta F[\rho]=-\tfrac{1}{2}kT\int_\Lambda dx\int_\Lambda dy\, c(x,y)[\rho(x)-\rho_u][\rho(y)-\rho_u]$$
$$+kT\int_\Lambda dx\,\rho(x)\ln\left[\frac{\rho(x)}{\rho_u}-1\right]\ , \tag{15}$$

where $c(x,y)$ is the fluid direct correlation function. To first order in density (Stell, 1964)

$$c(x,y)\approx\exp[-\beta V(x-y)]-1\ . \tag{16}$$

At high temperatures and low densities, the variational problem associated with Eq. (15) then becomes identical to the GPBE equation (1) with the same interaction potential.

As a general comment, one should be well aware of the

necessity for the Vlasov potential to be *integrable*. Otherwise, functionals like Eq. (4) are simply not defined. Of course, this requirement does not apply to the bare interaction potential appearing in situations depicted above, in which the Vlasov potential stands as a mesoscopic, effective potential.

III. BOUNDS FOR THE *N*-BODY FREE ENERGY

We first address the question of the relationship between the Vlasov functional and the *ordinary* free-energy functional of the N-body problem. Using the notation $\underline{x}_N := \{x_1, \ldots, x_N\}$, we find that the latter is

$$\mathcal{F}[n_N] := \int_{\Lambda^N} d\underline{x}_N \, n_N(\underline{x}_N) \left[\sum_{i<j} V(x_i - x_j) + kT \ln[n_N(\underline{x}_N)] \right] + kT \ln N! \,, \tag{17}$$

where $n_N(\underline{x}_N)$ is the N-point distribution function, normalized to unity. $n_1(x)$ and $n_2(x,y)$ stand for the corresponding one- and two-point distribution functions, normalized to N, and $N(N-1)$, respectively. The minimum of the free-energy functional under the constraints

$$\begin{aligned} & n_N(\underline{x}_N) \geq 0 \,, \\ & \mathrm{supp}(n_N) \subseteq \Lambda \,, \\ & \int_{\Lambda^N} d\underline{x}_N \, n(\underline{x}_N) = 1 \,, \end{aligned} \tag{18}$$

is the (*equilibrium*) *free energy* and will be denoted by $\mathcal{F}^0(\Lambda, N)$. $\mathcal{F}[n_N]$ being a convex functional of n_N, its minimizer n_N^0 (the normalized Boltzmann factor) is unique.

Given a one-point density $\rho(x)$, together with a partition $\{\omega_i\}_{i=1,\ldots,N}$ of $\Lambda = \bigcup_{i=1}^N \omega_i$, satisfying $\int_{\omega_i} dx \, \rho(x) = 1$ for $i = 1, \ldots, N$, one constructs the trial N-body distribution functions:

$$\begin{aligned} n_N^a(\underline{x}_N) &:= \frac{1}{N^N} \prod_{i=1}^N \rho(x_i) \,, \\ n_N^b(\underline{x}_N) &:= \begin{cases} 0 & \text{if any cell is empty} \,, \\ \dfrac{1}{N!} \displaystyle\prod_{i=1}^N \rho(x_i) & \text{otherwise} \,. \end{cases} \end{aligned} \tag{19}$$

Here $n_N^b(\underline{x}_N)$ is a classical analog of the Hartree-Fock wave function (Conlon, 1984). It is a simple matter to show

$$\mathcal{F}[n_N^a] = \left(1 - \frac{1}{N}\right) U[\rho] - TS[\rho] + kT \ln(N! N^{-N}) \,, \tag{20}$$

$$\mathcal{F}[n_N^b] = U[\rho] - TS[\rho] - \tfrac{1}{2} \sum_{i=1}^N \int_{\omega_i} dx \int_{\omega_i} dy \, \rho(x) \rho(y) \, V(x-y) \,, \tag{21}$$

where $U[\rho]$ and $-TS[\rho]$ are the functionals introduced in Eq. (3). Let us emphasize the fact that the N- and 1-point correlation functions appearing in Eqs. (20) and (21) are by no means supposed to be solutions of a minimization problem. Evidently, $\mathcal{F}[n_N^0] \leq \mathcal{F}[n_N^a], \mathcal{F}[n_N^b] \leq \mathcal{F}[n_N^b]$. $\mathcal{F}[n_N^a]$ coincides with $\mathcal{F}[n_N^0]$ for noninteracting systems $[V(x) \equiv 0]$ for $\rho(x) = \text{const}$, whereas $\mathcal{F}[n_N^b]$ is worth considering for potentials strongly repulsive at the origin. It is instructive at this stage to consider the Gibbs-Bogoliubov inequality (11) with $\mathbf{W} = \mathbf{W}_0$. Explicit calculation yields

$$\mathcal{F}[n_N^0] \leq \left(1 - \frac{1}{N}\right) U[\rho^0] - TS[\rho^0] + kT \ln(N! N^{-N}) \,, \tag{22}$$

which again expresses $\mathcal{F}[n_N^0] \leq \mathcal{F}[n_N^a]$.

Before introducing lower bounds on the N-body free energy, let us recall (see, for example, Dobrushin, 1964; Fisher and Ruelle, 1965; Ruelle, 1969; Lewis *et al.*, 1984; Gielerak, 1989) that the (real, even) potential $V(x)$ is called stable if, for each bounded *positive* measure μ on R^ν,

$$\int \int V(x-y) \mu(dx) \mu(dy) \geq 0 \,. \tag{23}$$

The potential is said to be *of positive type* (see, for example, Dixmier, 1964; Dobrushin, 1964; Fisher and Ruelle, 1965; Ruelle, 1969; Lewis, 1984) if the same inequality holds for each bounded *signed* measure μ, which, by Bochner's theorem, amounts to saying that the Fourier transform $\tilde{V}(k) := \int dx \, V(x) \exp(ikx)$ of the potential is almost everywhere non-negative. [Bochner's theorem can be shown to hold for "slowly increasing" distributions also (Schwartz, 1966); more severely singular situations like the one-dimensional Coulomb potential must, however, be excluded.] Clearly, any positive-type potential is stable, but the converse generally does not hold.

When $V(x)$ is of positive type, any pair of one- and two-point correlation functions $n_1(x), n_2(x,y)$ satisfies (Conlon, 1984)

$$\int_\Lambda dx \int_\Lambda dy \, V(x-y) n_2(x,y) \geq \int_\Lambda dx \int_\Lambda dy \, V(x-y) n_1(x) n_2(y) - NV(0) \,. \tag{24}$$

We turn now to lower bounds for the N-body entropy. For a system of N particles endowed with a *symmetric* probability density $f(\underline{x}_N)$ normalized to unity, the N-body entropy (up to the Boltzmann constant) is defined as

$$S[f_N] := -\int d\underline{x}_N \, f(\underline{x}_N) \ln f(\underline{x}_N) \,. \tag{25}$$

We consider also the k-point entropy ($k \leq N$):

$$S[f_k]:=-\int d\underline{x}_k\, f_k(\underline{x}_k)\ln f_k(\underline{x}_k) \tag{26}$$

with

$$f_k(\underline{x}_k):=\int dx_{k+1}\ldots dx_N f(\underline{x}_N)\ . \tag{27}$$

For $k>j$, the following inequality holds (see, for example, Kullback, 1968; Falk, 1969):

$$\int d\underline{x}_k\, f_k(\underline{x}_k)\ln\frac{f_k(\underline{x}_k)}{f_j(\underline{x}_j)f_{k-j}(\underline{x}_{k-j})}\geq 0\ . \tag{28}$$

The equality is attained if and only if

$$f_k(x_1,\ldots,x_k)=f_{k-j}(x_1,\ldots,x_{k-j})f_j(x_{k-j+1},\ldots,x_k)\ .$$

Therefore

$$S[f_k]\leq S[f_j]+S[f_{k-j}]\quad\text{for } j<k\ , \tag{29}$$

and generally

$$S[f_k]\leq\sum_i S[f_{k_i}]\quad\text{for }\sum_i k_i=k\ . \tag{30}$$

In information-theoretical language, the higher-order correlations contained in the state f_k and absent from the factorized state $\{f_{k_i}\}$ reduce its uncertainty with respect to the latter. In particular, $S[f_N]\leq N\,S[f_1]$; with $n_N:\equiv f_N$ and $n_1:\equiv N f_1$, this amounts to

$$\int_{\Lambda^N}d\underline{x}_N\, n_N(\underline{x}_N)\ln n_N(\underline{x}_N)\geq\int_\Lambda dx\, n_1(x)\ln n_1(x)-N\ln N \tag{31}$$

and therefore

$$\mathcal{F}[n_N]\geq U[n_1]-TS[n_1]-\frac{N}{2}V(0)+kT\ln(N!N^{-N})\ . \tag{32}$$

[We observe in passing that the superposition approximation (Fisher, 1964)

$$f_3^{\sup}(x,y,z):=\frac{f_2(x,y)f_2(x,z)f_2(y,z)}{f_1(x)f_1(y)f_1(z)} \tag{33}$$

does not satisfy the normalization condition. The alternative approximation

$$f_3^*(x,y,z):=\tfrac{1}{3}[f_2(x,y)f_1(z)+f_2(x,z)f_1(y)+f_2(y,z)f_1(x)] \tag{34}$$

does, but generally violates requirement (30): $S[f_3^*]\geq S[f_1]+S[f_2]$ by Jensen's inequality.]

IV. THERMODYNAMIC LIMIT

Consider an increasing nested sequence of containers $\Lambda(N)$ tending to infinity in Van Hove's sense (Ruelle, 1969), at constant density $\rho=N/\Lambda(N)$. Although we deal with a continuous fluid $\rho(x)$, it is convenient to refer to F/N, U/N, etc. as the free energy and energy *per particle*.

Theorem 1. *Let the potential be continuous and integrable. Then the Vlasov free energy per particle* $f(\rho):=\lim_{N\to\infty}F^0[\Lambda(N),N]/N$ *satisfies*

$$\begin{aligned}&f(\rho)=\tfrac{1}{2}\rho\tilde{V}(0)+kT\ln\rho\quad\text{if } V(x)\text{ is of positive type}\ ,\\ &kT\ln\rho\leq f(\rho)\leq\tfrac{1}{2}\rho\tilde{V}(0)+kT\ln\rho\quad\text{if } V(x)\text{ is stable}\ ,\\ &f(\rho)=-\infty\quad\text{if } V(x)\text{ is unstable}\ .\end{aligned} \tag{35}$$

Proof. The arguments entering the proof are standard (Ruelle, 1969; Lewis *et al.*, 1984): First of all, the entropy term attains its minimum $kT\ln\rho$ with the uniform profile $\rho_u(x)\equiv\rho$. In the stable case, the energy term is bounded below by 0. In any case, the free energy is bounded above by the free energy corresponding to the uniform profile. For a positive-type potential, the quadratic form $K[\rho,\rho]$ is positive definite, and therefore $K[\rho^0,\rho^0]\geq 2K[\rho^0,\rho_u]-K[\rho_u,\rho_u]$; on the other hand, $\lim_{N\to\infty}(1/N)(K[\rho^0,\rho_u]-K[\rho_u,\rho_u])=0$ for an integrable potential. Finally, if $V(x)$ is unstable, there exists an N_0 and a density $\tilde{\rho}(x)$ supported in the container $\Lambda(N_0)$ such that $K[\tilde{\rho},\tilde{\rho}]=-\epsilon<0$ and $-TS[\tilde{\rho}]<\infty$ (if necessary, the profile can always be slightly spread to get a finite entropy; the continuity of the potential ensures that this can be done while keeping the energy negative). By construction

$$f(\rho)\leq\lim_{N\to\infty}\frac{F\left[\frac{N}{N_0}\tilde{\rho}\right]}{N}=\lim_{N\to\infty}[-\tfrac{1}{2}\epsilon N+0(1)]=-\infty\ .\ \blacksquare \tag{36}$$

Corollary 1a. *The N-body free energy per particle* $\mathbf{f}(\rho):=\lim_{N\to\infty}(\mathcal{F}[n_N^0]/N)$ *of a system interacting through a positive-type pair potential* $V(x)$ *satisfies*

$$-kT-\tfrac{1}{2}V(0)\leq\lim_{\rho\to\infty}[\,\mathbf{f}(\rho)-\tfrac{1}{2}\rho\tilde{V}(0)-kT\ln\rho]\leq\min[-kT,\ -\tfrac{1}{2}V(0)]\ . \tag{37}$$

The lower bound stems from Eq. (32); equations (20) and (21) provide the upper bounds. Recall that a positive-type potential satisfies $|V(x)|\leq V(0)\ \forall x\in\mathbf{R}^\nu$. The bounds coalesce for a noninteracting system or, as already obtained by Conlon (1984), at zero temperature.

Corollary 1b. *In a Vlasov system interacting through a two-body positive-type potential, the pressure P, compressibility modulus* $B=\chi_T^{-1}$ *(χ_T is the isothermal compressibility), configurational energy per particle u, configurational specific heat at constant volume* c_V, *and configurational chemical potential* μ *are, respectively,*

$$P=\rho^2\frac{\partial f}{\partial\rho}=\tfrac{1}{2}\rho^2\tilde{V}(0)+\rho kT\ ,$$
$$B=\rho\frac{\partial P}{\partial\rho}=\rho^2\tilde{V}(0)+\rho kT\ ,$$
$$u=\frac{\partial(\beta f)}{\partial\beta}=\tfrac{1}{2}\rho\tilde{V}(0)\ , \tag{38}$$
$$c_V=-\beta^2\frac{\partial u}{\partial\beta}=0\ ,$$
$$\mu=f+\rho\frac{\partial f}{\partial\rho}=\rho\tilde{V}(0)+kT(\ln\rho+1)\ .$$

The principal merit of these expressions is to provide reference thermodynamic quantities for comparison when dealing with a *stable, nonpositive definite interaction,* which, according to Theorem 1, is the only case of interest as far as thermodynamics is concerned. A nice study of *finite, unstable N*-body and Vlasov systems can be found in Posch *et al.*, 1990.

V. EXISTENCE AND UNIQUENESS

A. Existence

In the thermodynamic limit, the GBPE equation (1) is always satisfied by $\rho(x)=$const., which of course might or might not be the global minimizer of the Vlasov functional. For finite systems, we shall now demonstrate the existence of a global minimizer $\rho^0\in\mathcal{R}(\Lambda,N)$ to the Vlasov functional. It follows that the associated Euler-Lagrange solution (the GPBE equation) always has a solution in $\mathcal{R}(\Lambda,N)$; this approach is known as the *variational method* (see, for example, Krasnosel'skii, 1963; Vainberg, 1973; Chow and Hale, 1982).

Assume the potential $V(x)$ to be bounded. Let $\{\rho_j\}$ be a minimizing sequence in $\mathcal{R}(\Lambda,N)$, i.e., $\lim_{j\to\infty}F[\rho_j]=\inf_{\rho\in\mathcal{R}}F[\rho]$. By hypothesis, $\sup_j F[\rho_j]<\infty$, and therefore $\sup_j -TS[\rho_j]<\infty$. On the other hand, the integrand in the functional $-TS[\rho]$ is superlinear; by the de la Valée-Poussin theorem (see, for example, Ekeland and Temam, 1974) $\{\rho_j\}$ then contains a subsequence converging weakly (in L_1) to $\rho_0\in\mathcal{R}$. It remains to check the lower semicontinuity of $F[\rho]$, i.e., to verify $F[\rho_0]=F[\lim_{j\to\infty}\rho_j]\le\lim_{j\to\infty}F[\rho_j]$. By convexity, the entropy part is lower semicontinuous. Consider now a sequence of profiles $\{\rho_j\}$ converging towards ρ_0. By equi-integrability, there exists, for each $\epsilon>0$, an $M(\epsilon)$ with the property $\int_{\rho_j\ge M}dx\,\rho_j(x)\le\epsilon$. Hence

$$2U[\rho_j]=\int dx\,\rho_j\phi_j=\int dx\,\rho_j\phi_0+\int_{\rho_j\ge M}dx\,\rho_j(\phi_j-\phi_0)+\int_{\rho_j<M}dx\,\rho_j(\phi_j-\phi_0)\ . \tag{39}$$

The first term goes to $2U[\rho_0]$. The remaining terms are bounded by $\epsilon\|\phi_j-\phi_0\|_\infty\to0$ and $M\|\phi_j-\phi_0\|_1\to0$, respectively. Therefore

Theorem 2. *For a bounded potential, the Vlasov free energy $F[\rho]$ attains its global minimum in $\mathcal{R}(\Lambda,N)$. The corresponding GPBE equation has at least one solution in $\mathcal{R}(\Lambda,N)$.* ■

Remark. The exponential form (1) of a density satisfying the GPBE equation makes any minimizer pointwise positive (or negative—in that case, one could make $F[\rho]$ even by taking $kT\int_\Lambda dx\,|\rho|\ln|\rho|$ as the entropy part). The unilateral constraint $\rho(x)\ge0$ can then be discarded.

B. Uniqueness

When many solutions to the GPBE equation are present, there are, besides the global minimizer of $F[\rho]$, other density profiles which might or might not be local minima. Physically, they correspond to metastable or unstable states, respectively. Uniqueness of a solution is known to hold *a priori* in two situations.

1. Convexity of the Vlasov functional

A sufficient condition for the uniqueness of the solution is the convexity of the Vlasov functional $F[\rho]$ on $\mathcal{R}(\Lambda,N)$, i.e.,

$$F[\lambda\rho_1+(1-\lambda)\rho_2]\le\lambda F[\rho_1]+(1-\lambda)F[\rho_2]\ ,\qquad\forall\lambda\in[0,1]\ . \tag{40}$$

The entropy part $-TS[\rho]$ is always convex. Let us introduce the notation

$$K[f_1,f_2]:=\int_\Lambda dx\int_\Lambda dy\,f_1(x)\,f_2(y)\,V(x-y)\ . \tag{41}$$

A sufficient condition for the energy part $U[\rho]=\frac{1}{2}K[\rho,\rho]$ to be convex is that the potential $V(x-y)$ be positive definite: In that case, the inequality $K[\rho_1-\rho_2,\ \rho_1-\rho_2]\ge0$ is equivalent to $K[\frac{1}{2}(\rho_1+\rho_2),\frac{1}{2}(\rho_1+\rho_2)]\le\frac{1}{2}K[\rho_1]+\frac{1}{2}K[\rho_2]$. Therefore systems interacting through a positive-type potential cannot sustain a metastable state, nor can they undergo phase transitions; this was already latent in Eq. (35). In the general case, the following holds.

Lemma 3. *$F[\rho]$ is convex in $\mathcal{R}(\Lambda,N)$ if and only if*

$$\inf_{g\in\mathcal{G}(\Lambda)}\frac{N^2}{2}K[g,g]+\frac{kTN}{2}[(1+\|g\|_1)\ln(1+\|g\|_1)+(1-\|g\|_1)\ln(1-\|g\|_1)]\ge0\ , \tag{42}$$

where $\mathcal{G}:=\{g\,|\,\mathrm{supp}(g)\subset\Lambda,\ \|g\|_1\le1,\ \int_\Lambda dx\,g(x)=0\}$ and $\|g\|_1:=\int dx\,|g(x)|$.

Proof: $F[\rho]$ is a convex functional if and only if

$$\inf_{\rho_1,\rho_2\in\mathcal{R}(\Lambda,N)}\Delta F[\rho_1,\rho_2]\geq 0\ ,$$

where

$$\Delta F[\rho_1,\rho_2]:=\tfrac{1}{2}F[\rho_1]+\tfrac{1}{2}F[\rho_2]-F[\tfrac{1}{2}\rho_1+\tfrac{1}{2}\rho_2]\ . \tag{43}$$

We set

$$f(x):=\frac{1}{N}\frac{\rho_1(x)+\rho_2(x)}{2},\quad g(x):=\frac{1}{N}\frac{\rho_1(x)-\rho_2(x)}{2} \tag{44}$$

to get

$$\Delta F[\rho_1,\rho_2]=:\Delta\tilde{F}[f,g]=\frac{N^2}{2}K[g,g]+\frac{kTN}{2}\int_\Lambda dx\left[(f+g)\ln\left[1+\frac{g}{f}\right]+(f-g)\ln\left[1-\frac{g}{f}\right]\right]\ . \tag{45}$$

We leave it to the reader to verify that the minimization of $\Delta\tilde{F}[f,g]$ over f for g fixed gives $f^0(x)=|g(x)|/\|g\|_1$. Provided we take $g\in\mathcal{G}(\Lambda)$ as required by Eq. (44), the ρ_1 and ρ_2 corresponding to g and f^0 both belong to $\mathcal{R}(\Lambda,N)$. Thus the minimization procedure is *a posteriori* justified. When we split Λ into $\Lambda_+:=\{x\in\Lambda|g(x)\geq 0\}$ and its complementary $\Lambda\setminus\Lambda_+$, the computation of $\Delta\tilde{F}[f^0,g]$ presents no difficulty and yields Eq. (42). ■

As it stands, the minimization problem (42) is no simpler than the original problem $\inf_{\rho\in\mathcal{R}(\Lambda,N)}F[\rho]$. It warrants some comments, however.

● The energy part in Eq. (42) has become the self-interaction of a *neutral* fluid $[\int_\Lambda dx\, g(x)=0]$. Alternatively, the energy part can be considered as the self-interaction of a charged fluid $[(g^*(x)\geq 0,\int_\Lambda dx\, g^*(x)=1]$ with the modified potential

$$V^*(x,y):=V(x-y)-\frac{1}{|\Lambda|}\int_\Lambda dz\,[V(x-z)+V(y-z)]+\frac{1}{|\Lambda|^2}\int_\Lambda dz\int_\Lambda dw\, V(z-w)\ . \tag{46}$$

By construction, $\int_\Lambda dy\, V^*(x,y)\equiv 0$. Equation (46) stems from the identity $K[g,g]=K[g^*-\langle g^*\rangle,g^*-\langle g^*\rangle]=K^*[g^*,g^*]$. In both cases, indications of the convexity of $F[\rho]$ are obtained from auxiliary density profiles, minimizers of a related variational problem. Neutral systems are most frequently encountered in electrostatics. However, a purely Coulombic potential (see Sec. VII) is positive definite, and the convexity problem does not arise in that context.

● The entropy part satisfies the estimates

$$\|g\|_1^2\leq(1+\|g\|_1)\ln(1+\|g\|_1)+(1-\|g\|_1)\ln(1-\|g\|_1)$$
$$\leq\|g\|_1^2+\tfrac{2}{3}\|g\|_1^4\ . \tag{47}$$

The lower bound is characteristic of information theory, where a similar result holds for the so-called Kullback-Leibler information number (see, for example, Devroye, 1987). On the other hand, the natural estimate for the energy is $K[g,g]\leq\lambda\int_\Lambda dx\, g^2(x)$ where λ is the lowest eigenvalue of the linear operator $L[f](x):=\int_\Lambda dy\, V(x-y)f(y)$. The inability of the L_1-norm to estimate the L_2-norm makes the entropy part unable to compete with the energy part as far as unicity of profiles is concerned. One could in that respect qualify the Vlasov functional of energy-dominated, in contrast to Cahn-Hilliard-type, theories (Penrose and Fife, 1990), whose functionals contain the Dirichlet integral $\int_\Lambda dx\,|\nabla g(x)|^2$ susceptible, via Sobolev's inequality, to estimate the L_2-norm of g.

● Finally, a straightforward consequence of Eq. (42) is the fact that uniqueness of a solution is more likely to hold for low densities and/or high temperatures (see next subsection).

2. Low densities, inverse temperatures, and fugacities

In a finite system, uniqueness of the solution $\rho(x)$ holds for sufficiently high temperatures and/or low densities. Consider the nonlinear operator $T:\mathcal{R}(\Lambda,N)\to\mathcal{R}(\Lambda,N)$,

$$T[f](x):=\frac{N\exp[-\beta(f*V)(x)]}{\int_\Lambda dy\exp[-\beta(f*V)(y)]}\ . \tag{48}$$

Under the proviso of convergence, successive approximations to the density profile can be numerically generated as $\rho_{n+1}(x)=T[\rho_n](x)$. We observe in passing that if we start the iteration by taking $\rho_0(x)$ as the energy minimizer in $\mathcal{R}(\Lambda,N)$, then $(\rho_0*V)=$const. in Λ (under the assumption that ρ_0 wets Λ everywhere; see Sec. IX), and therefore $\rho_1(x)=\rho=$const., i.e., the first iteration generates the entropy maximizer. This exemplifies the effects of successive applications of the operator T as a tennis game between energy and entropy, temperature playing the role of the arbiter. The following estimate, (Messer and Spohn, 1982; see also Battle, 1977)

$$\|T[\rho_a-\rho_b]\|_1 \le 2\beta N\|(\rho_a-\rho_b)*V\|_\infty \le 2\beta N\|V\|_\infty\|\rho_a-\rho_b\|_1 \quad (49)$$

ensures by contraction the uniqueness of the GPBE equation $\rho(x)=T[\rho](x)$ for $2\beta N\|V\|_\infty<1$. Note the presence of the factor N, which stems from the fact that $\rho(x)$ is a material density normalized to N, whereas $\rho(x)$ in Messer and Spohn (1982) represents a probability density normalized to 1. (Another contraction estimate involving the maximal and minimal values of the potential can be found in Posch *et al.*, 1990.)

An alternative approach consists in considering the function $\omega(x):=\ln[\rho(x)/A]=-\beta\phi(x)$ instead of $\rho(x)$. The former satisfies

$$\omega(x)+z\int_\Lambda dy\ V(x-y)\exp[\omega(y)]=0 \quad \forall x\in\Lambda\ , \quad (50)$$

where $z=\beta A$ depends on β,Λ,N through Eq. (2). Explicitly,

$$\frac{\partial z}{\partial N}=\frac{z}{N}(1+2\beta u)\ ,\qquad \frac{\partial z}{\partial \beta}=\frac{z}{\beta}(1-c_V+2\beta u)\ , \quad (51)$$

where $u=U/N$ is the energy per particle and c_V the specific heat at constant volume. The derivation of the first identity presents no difficulty; to get the second one, one can first substitute relationship (1) in the Vlasov functional, which yields $F(N,\beta)=-U(N,\beta)+N\beta^{-1}\ln A(N,\beta)$, and then apply on both sides the operator $\partial(\beta\cdots)/\partial\beta$, taking into account $z=\beta A(N,\beta)$, $c_V:=-\beta^2\partial u/\partial\beta$ as well as $\partial[\beta F(N,\beta)]/\partial\beta=U$ (see Sec. IX).

By Eq. (51), z is an increasing function of the density (for stable potentials) and a decreasing function of the temperature (at least for positive-type potentials; a more general proof is lacking at present).

Indeed, z plays very much the role of a fugacity in the "grand-canonical" description (50), to be compared with the equivalent "canonical" description of Eqs. (1) and (2).[1] In the latter, the density normalization N is given. In the former, the *family* $\{N,\beta\}$ corresponds to a given z and a given solution $\omega(x)$, with $N\beta=z\int_\Lambda dx\exp[\omega(x)]$. The possible existence of different solutions to Eq. (50) makes the question of the equivalence between the two descriptions delicate.

To avoid confusion, we shall in fact refer to Eq. (50) as "the Hammerstein description," (since that is the name under which this nonlinear integral equation is known in the mathematical literature) and reserve the appellation "grand canonical" to situations related to the minimization problem

$$\inf_{\{\rho(x)\ge 0,\ \mathrm{supp}(\rho)\in\Lambda\}}\{U[\rho]-TS[\rho]-\mu\int_\Lambda dx\,\rho(x)\}\ . \quad (52)$$

[An analysis of a variational problem close to Eq. (52) occurring in mean-field studies of boson gas can be found in Lewis *et al.* (1990) and Van den Berg *et al.* (1990). The main difference from Eq. (52) is the use of the boson entropy instead of the Bolzmann entropy (4). This allows for the possible existence of a singular part of the minimizer, even at finite temperatures, which is Bose-Einstein condensation (the density is here a distribution in energy rather than in configuration space).]

Coming back to Eq. (50), the latter satisfies a simple gauge invariance property: suppose $\omega(x)$ satisfies Eq. (50) for some given z and $V(x)$; then $\omega_c(x):=\omega(x)-\alpha c$ satisfies the same equation for $z_c=z\exp(\alpha c)$ and $V_c(x)=V(x)+c$, where $\alpha:=z\int_\Lambda dx\exp[\omega(x)]$. By comparison, the solutions $\rho(x)$ to the GBPE equation are of course invariant under the transformation $V(x)\to V_c(x)=V(x)+c$.

Mathematical properties of the Hammerstein equation (50) have been more extensively studied than those of the GPBE equation. Many relevant results are available in Dolph (1949), Tricomi (1957), Krasnosel'skii (1963), Amann (1976a), and Hudson and Pym (1980) [as well as in Gel'fand (1963) and Joseph and Lundgren (1973) for the case of a Newtonian interaction]. We shall here content ourselves with the following elementary contraction estimate: assume $V(x-y)$ to be pointwise positive for all $x,y\in\Lambda$. Then $\omega(x)$ satisfying Eq. (50) is pointwise negative, and $\|\omega_a-\omega_b\|_\infty\le z\sup_{x\in\Lambda}\int_\Lambda dy V(x-y)\|\omega_a-\omega_b\|_\infty$. Therefore, the uniqueness of the solution holds for $z\sup_{x\in\Lambda}\int_\Lambda dy V(x-y)<1$.

C. Stability of the uniform phase

As mentioned in Sec. I, the investigation of the *freezing transition* (i.e., the transition [uniform phase] $\to$[modulated phase]) has constituted one of the main motivations in past studies of the GPBE equation. The analysis of uniqueness and stability turns out to be dramatically simplified when applied on the uniform profile (for a reasonably smooth interaction):

Theorem 4. *In the thermodynamic limit, the uniform profile $\rho(x)=\rho=$const. is locally stable (i.e., is a local minimum of the Vlasov functional) if and only if*

$$\beta\rho\inf_q\tilde{V}(q)\ge -1\ . \quad (53)$$

Proof. The relevant quantity is the sign of the variations of the free energy $F(\epsilon):=F[\rho+\epsilon h(x)]$ in the neighborhood of $\epsilon=0$. We can restrict ourselves by choosing $h(x)$ to be periodic, with a period Ω that is as large as we wish: $h(x+\Omega)=h(x)$. The fixed-density constraint re-

[1] To be precise, the Vlasov chemical potential is $\mu:=\partial F(\beta,\Lambda,N)/\partial N=kT(1+\ln A)$ and, strictly speaking, the Vlasov fugacity should then be identified with $\exp(\beta\mu)=eA=e\beta^{-1}z$.

quires (using a self-explanatory notation) $\int_\Omega dx\, h(x)=0$. As observed before, the uniform profile satisfies the GPBE equation in the thermodynamic limit, and so $F'(0)=0$. The second variation $F''(0)$,

$$\int_\Omega dx \int_{\mathbf{R}^\nu} dy\, h(x)\,h(y)\,V(x-y)+\frac{kT}{\rho}\int_\Omega dx\, h^2(x)\ , \tag{54}$$

has its minimum governed by the eigenvalue problem

$$h(x)=-\beta\rho\int_{\mathbf{R}^\nu} dy\, h(y)\,V(x-y)\ . \tag{55}$$

[We note in passing that Eq. (55) yields $[1+\beta\rho\tilde{V}(0)]\int_\Omega dx\, h(x)=0$, and so $\int_\Omega dx\, h(x)=0$ because of the stability of $V(x)$]. The eigenfunctions of Eq. (55) are $h_q(x)=\cos\langle qx\rangle$ (with $\langle q\Omega\rangle\in 2\pi\mathbf{Z}$) with associated eigenvalues $\lambda_q=-\beta\rho\tilde{V}(q)$. Substituting this back into (54) completes the proof. ■

Let us note in passing that criterion (53) could also have been satisfied by the (N-body) Ornstein-Zernike equation, $\tilde{n}_2^T(k)=\rho^2\tilde{c}(k)/[1-\rho\tilde{c}(k)]$, for the truncated two-point correlation function (see, for example, Reichl, 1980), together with the high-temperature approximation for the structure factor (Stell, 1964), $c(x)\approx -\beta V(x)$.

As an example, consider the rectangular potential $V(x-y)=\gamma\theta(a-|x-y|)$, where $\gamma>0$, $a>0$ and $\theta(\cdot)$ is the unit step function. According to Theorem 4, the uniform phase ceases to be stable for $kT<kT_c=-\rho\min_q\tilde{V}(q)$, where

$$\tilde{V}(q)=\begin{cases}\dfrac{2\gamma a}{\eta}\sin\eta & \text{for } \nu=1\ ,\\ \dfrac{2\pi\gamma a^2}{\eta}J_1(\eta) & \text{for } \nu=2\ ,\\ \dfrac{4\pi\gamma a^3}{\eta^3}(\sin\eta-\eta\cos\eta) & \text{for } \nu=3\ ,\end{cases} \tag{56}$$

with $\eta=qa$. As mentioned in Sec. I, the mean-field freezing transition involving effective potentials of the form (56) has been analytically and numerically investigated (Kirkwood and Boggs, 1942; Weeks *et al.*, 1970; Raveché and Stuart, 1975, 1976; Co *et al.*, 1976; Lovett, 1977; Raveché and Kayser, 1978; Lovett and Buff, 1980; Feijoo and Rahman, 1982) in the hope of gaining some information concerning the (supposedly existing) freezing transition for N-body hard-core systems at $\nu=2$ and 3 dimensions, characterized by the two-body interaction

$$V(x)=\begin{cases}\infty & \text{for } |x|\le a\ ,\\ 0 & \text{otherwise}\ .\end{cases} \tag{57}$$

In those approaches (Weeks *et al.*, 1970; Raveché and Stuart, 1975), the factor γ in Eq. (56) is actually temperature- and density-dependent, in such a way that Theorem 4 cannot be invoked (as it must be) to justify a transition in the one-dimensional system.

Let us finally note that Theorem 4 does not exclude the possibility of the uniform phase's ceasing to be the *global* minimizer for temperatures lower than the critical temperature (53).

The next section illustrates the onset of freezing [for temperatures below the critical temperature defined in Eq. (53)] for an exactly solvable class of systems, enabling us to tackle the full nonlinear problem rather than its linearized version around $\epsilon=0$.

VI. A CLASS OF SYSTEMS UNDERGOING A SECOND-ORDER PHASE TRANSITION

We consider a one-dimensional infinite system at density ρ together with a band-limited pair potential $V(x)$, i.e., $\tilde{V}(q)=0$ for $|q|\ge q_0>0$. We look for even, periodic solutions $\rho(x+l)=\rho(x)$, with $l\le 4\pi/q_0$. Under those conditions, the induced potential (2) reads

$$\phi(x)=\rho\tilde{V}(0)+a\tilde{V}(k)\cos(kx)\ , \tag{58}$$

where $k:=2\pi/l$. Inserting Eq. (58) into Eq. (1), with $\Lambda=[0,l]$, we get

$$\rho(x)=\rho\frac{\exp[-\alpha\cos(kx)]}{I_0(\alpha)}\ , \tag{59}$$

where $\alpha:=\beta a\tilde{V}(k)$, and $I_0(\alpha)$ denotes the modified Bessel function of order zero. Finally, a in Eq. (58) must be the first Fourier coefficient of $\rho(x)$; this yields the consistency condition

$$\kappa\alpha=\frac{I_1(\alpha)}{I_0(\alpha)} \tag{60}$$

with

$$\kappa^{-1}:=-2\beta\rho\tilde{V}(k)\ . \tag{61}$$

The function $I_1(\alpha)/I_0(\alpha)$ is increasing, odd, with limits ± 1 for $\alpha\to\pm\infty$, strictly convex for $\alpha>0$, with a slope of $\frac{1}{2}$ at the origin. As a consequence, Eq. (60) possesses three distinct solutions, $-\alpha_0$, 0, and α_0, for $\kappa\in(0,\frac{1}{2})$, whereas only the trivial solution $\alpha=0$ is possible for $\kappa\le 0$ or $\kappa\ge\frac{1}{2}$. [Incidentally, the similarity of Eq. (60) to the magnetization equation in the Curie-Weiss model $\mu=\tanh(\beta J\mu)$ (Huang, 1963) is striking, emphasizing the common mean-field origin of both models.] Notice that $\alpha=0$ corresponds to the flat density profile $\rho(x)=\rho$, while the replacement of $\alpha_0>0$ by $-\alpha_0$ amounts to shifting the profile by half a period. The free energy per particle is evaluated by direct substitution of $\rho_{\alpha=\alpha_0}(x)$ in Eq. (3):

$$f_{\alpha=\alpha_0}(\rho)=\tfrac{1}{2}\rho\tilde{V}(0)+kT\ln\rho-kTK(\kappa) \tag{62}$$

with

$$K(\kappa):=\ln I_0[\alpha_0(\kappa)]-\tfrac{1}{2}\kappa\alpha_0^2(\kappa)\ . \tag{63}$$

One verifies easily [taking $K(\frac{1}{2})=0$, $\lim_{\kappa\to 0^+}2\kappa K(\kappa)$

$=1$, as well as $\partial K(\kappa)/\partial\kappa=-\alpha_0^2(\kappa)/2<0$ for $\kappa\in(0,\frac{1}{2})$ into account] that the free energy of the nontrivial phase satisfies

$$kT\ln\rho\le f_{\alpha=\alpha_0}(\rho)\le\tfrac{1}{2}\rho\tilde{V}(0)+kT\ln\rho \tag{64}$$

in accordance with Theorem 1.

By construction, $k=2\pi/l$ must verify $k\ge q_0/2$, but is otherwise arbitrary. The optimal choice for k is k_0, the value solving $\min_{q_0/2\le k\le q_0}\tilde{V}(k)$. Were $\tilde{V}(k_0)\ge -kT/\rho$, then $\kappa\notin(0,\frac{1}{2})$, and our nontrivial solution would cease to exist.

As $\lim_{\kappa\to 0^+}K(\kappa)=+\infty$, the free energy (61) can in principle be made arbitrarily low. However, at fixed density and temperature, the stability requirement of $V(x)$ (the absence of which makes the previous considerations pointless) implies a lower bound on $\tilde{V}(k)$ and therefore on κ. Actually the potential must satisfy $2\tilde{V}(k)\ge-\tilde{V}(0)$ as a consequence of Eq. (23) with $\mu(dx)=\sum_{n\in\mathbf{Z}}\delta(x-nl)dx$.

To discuss the thermodynamic properties of the modulate (nontrivial) phase, we take the uniform (trivial) phase as a reference system and consider the excess free energy $f_{\rm exc}(\rho):=f_{\alpha=\alpha_0}(\rho)-f_{\alpha=0}(\rho)=-kTK(\kappa)$. By Eq. (38), the excess pressure, compressibility modulus, energy, specific heat, and chemical potential are, for $\kappa\in(0,\frac{1}{2})$,

$$\begin{aligned}
P_{\rm exc}&=-\tfrac{1}{2}\rho kT\kappa\alpha_0^2(\kappa)<0\ ,\\
B_{\rm exc}&=\rho kT\kappa^2\alpha_0(\kappa)\frac{\partial\alpha_0(\kappa)}{\partial\kappa}<0\ ,\\
u_{\rm exc}&=-\tfrac{1}{2}kT\kappa\alpha_0^2(\kappa)<0\ ,\\
c_{\rm exc}&=-\tfrac{1}{2}\frac{\partial}{\partial\kappa}[\kappa\alpha_0(\kappa)]^2>0\ ,\\
\mu_{\rm exc}&=-kT[K(\kappa)+\tfrac{1}{2}\kappa\alpha_0^2(\kappa)]<0\ .
\end{aligned} \tag{65}$$

The physical picture is as follows: when isothermally compressed, the system reaches a critical density $\rho_c=-kT/\tilde{V}(k_0)$ beyond which it prefers to develop a periodic pattern, allowing it to lower its energy and pressure, become more compressible, and so on; in other words, the system manages to reduce its internal "stress" by partly adapting to external perturbations. As $K(\kappa)=4(\frac{1}{2}-\kappa)^2+0[(\frac{1}{2}-\kappa)^3]$ for $\kappa\in(0,\frac{1}{2})$, the transition turns out to be of second order. In particular, the compressibility modulus B jumps from the value $\rho^2[\tilde{V}(0)-\tilde{V}(k_0)]$ in the uniform phase to $\rho^2[\tilde{V}(0)+\tilde{V}(k_0)]$ in the modulated phase. Similarly, the (configurational) specific heat jumps from 0 to 2 (recall that its kinetic part is the constant $\frac{1}{2}$).

In conclusion, the above model is a tractable caricature of solidification, for which we are guaranteed that no other local minimizer of periodicity $l\le 4\pi/q_0$ can exist. Comparisons with profiles of larger periodicity would clearly necessitate more information on the potential and lack the same simplicity.

In a comparable approach, Messer and Spohn (1982), exemplifying the general setup of Battle (1977), have considered the one-dimensional system with potential $V(x-y)=\gamma\cos(x-y)$. For $\gamma>0$, the potential is of positive type and the GPBE equation has a unique solution. For $\gamma<0$, the potential is unstable and the system has no thermodynamic limit. In a finite container $\Lambda=[-\pi L,\pi L]$ and for $\gamma<0$, two cases need to be considered: for noninteger L, the GPBE equation has a unique solution. For integer L, the system undergoes a first-order phase transition (discontinuity of the pressure) from a uniform phase to a modulated phase, for $\beta>\beta_c=-2/N\gamma$.

VII. NEWTON AND COULOMB POTENTIALS

We denote by $C(x)$ the (ν-dimensional) Coulomb potential. Explicitly,

$$C(x)=\begin{cases}-\frac{1}{2}|x| & \text{for } \nu=1\ ,\\ -\dfrac{1}{2\pi}\ln|x| & \text{for } \nu=2\ ,\\ \dfrac{1}{(\nu-2)|\partial\omega_\nu|}\dfrac{1}{|x|^{\nu-2}} & \text{for } \nu\ge 3\ ,\end{cases} \tag{66}$$

where ω_ν denotes the ν-dimensional unit ball and $|\partial\omega_\nu|$ the measure of its boundary ($|\partial\omega_1|=2,|\partial\omega_2|=2\pi,|\partial\omega_3|=4\pi$). One can verify that, in the sense of distributions, $\tilde{C}(k):=\int dx\,\exp(ikx)C(x)=|k|^{-2}$, and

$$\Delta C(x)=-\delta(x)\quad\text{for } x\in\mathbf{R}^\nu\ . \tag{67}$$

Notice the equivalence of Eq. (67) to

$$\frac{\partial}{\partial x_\alpha}\frac{x_\alpha}{|x|^\nu}=|\partial\omega_\nu|\delta(x)\quad\text{for } x\in\mathbf{R}^\nu\ \ (\nu\ge 1)\ . \tag{68}$$

The equilibrium profile $\rho(x)$ of a self-interacting fluid with potential $\gamma C(x-y)$ satisfies [differentiating (1) twice]

$$\rho\Delta\rho=(\nabla\rho)^2+\beta\gamma\rho^3\ . \tag{69}$$

Here $\gamma<0$ corresponds to the attractive Newtonian gravitational potential, whereas $\gamma>0$ corresponds to the repulsive Coulombic electrostatic potential. The corresponding Hammerstein description [Eq. (50)] is

$$\Delta\omega(x)+\lambda e^{\omega(x)}=0\ , \tag{70}$$

where $\lambda:=-\gamma z$. Equation (70) is the Euler-Lagrange equation associated with the functional

$$J[\omega]:=\int_\Lambda dx\ (\tfrac{1}{2}[\nabla\omega(x)]^2-\lambda e^{\omega(x)})\ . \tag{71}$$

A. Newtonian systems

Newtonian potentials are unstable and so (Theorem 1) the thermodynamic limit does not exist. For rotationally invariant finite containers $\Lambda=B(0,R)$ [where $B(0,R)$ denotes a ball centered at the origin and radius R], a few

exact solutions are known; Theorem 7 below insures their radiality:

1. $\gamma<0$, $\nu=1$, $\Lambda=B(0,l)=[-l,l]$
(Camm, 1950; see also Rybicki, 1971)

$$\rho(x)=-\frac{2b^2}{\beta\gamma}\frac{1}{\cosh^2(bx)} \quad \text{with } b\tanh(bl)=\frac{-N\beta\gamma}{4}\ , \tag{72}$$

$$\phi(x)=2kT\ln\left[\frac{\cosh(bx)}{\cosh(bl)}\right]-\frac{N\gamma l}{2} \quad \text{for } |x|\le l\ . \tag{73}$$

For $x\ge l$, the potential obeys $\phi(x)=-\gamma Nx/2$ as a consequence of Newtonian screening. The solution exists for all density and temperature ranges.

2. $\gamma<0$, $\nu=2$, $\Lambda=B(0,R)$
(Liouville, 1853; Stodólkiewicz, 1963;
Ostriker, 1964; see also Padmanabhan, 1990)

$$\rho(x)=-\frac{8b^2}{\beta\gamma}\frac{1}{(|x|^2+b^2)^2} \quad \text{with } b^2=\left[-1-\frac{8\pi}{\beta\gamma N}\right]R^2\ , \tag{74}$$

$$\phi(x)=2kT\ln\left[\frac{|x|^2+b^2}{R^2+b^2}\right]-\frac{N\gamma}{2\pi}\ln R \quad \text{for } |x|\le R\ . \tag{75}$$

The solution (which is unique—see Bandle, 1975) exists for $kT>kT_c:=(-8\gamma N/\pi)$ only. For $kT\le kT_c$, the system collapses, its free energy diverging to $-\infty$. Note that the N-body system undergoes a similar collapse with the same critical temperature (Salzberg, 1965).

3. $\gamma<0$, $\nu\ge 3$, $\Lambda=B(0,R)$

No explicit solution is known, unless the external parameters satisfy the relation

$$2|\partial\omega_\nu|R^{\nu-2}=-N\beta\gamma\ . \tag{76}$$

In that case, the so-called singular solution

$$\rho(x)=\frac{-2(\nu-2)}{\beta\gamma|x|^2} \tag{77}$$

satisfies the GPBE equation for all $\nu\ge 3$. It should be said that any finite (obligatory radial) solution $\rho(x)$ is at most a local minimizer of the Vlasov functional $F[\rho]$, since $\inf_{\rho\in\mathcal{R}(\Lambda,N)}F[\rho]=-\infty$ for all temperatures and densities, when $\nu\ge 3$. This assertion is readily proved by considering the limit $\epsilon\to\infty$ of $F[\rho_\epsilon]$, where $\rho_\epsilon(x)$ is the constant profile in the ball $B(0,\epsilon)\subset\Lambda$. Then

$$F[\rho_\epsilon]=\frac{N^2\gamma\epsilon^{2-\nu}}{2(\nu+2)(\nu-2)|\omega_\nu|}+kTN\ln\left[\frac{N}{|\omega_\nu|\epsilon^\nu}\right]\ . \tag{78}$$

A presumably new criterion for the stability of solutions in $\Lambda=B(0,R)\subset\mathbf{R}^\nu$ is given in the following.

Lemma 5. *The profile $\rho(r)$ is stable or metastable [i.e., $\rho(x)$ is a local minimizer of the Vlasov functional] if and only if*

$$\inf_{H\in\mathcal{H}}\int_0^R\frac{dr}{r^{\nu-1}}\left[\beta\gamma H^2(r)+\frac{[H'(r)]^2}{\rho(r)}\right]\ge 0 \tag{79}$$

where $\mathcal{H}:=\{H\,|\,H(r)=0(r^{\nu-2}),H(R)=0,|H'(r)|\le\rho(r)\}$.

Proof. Taking Theorem 7 (below) into account, it is sufficient to check the sign of the second variation $F''(0)=(\partial^2F[\rho(r)+\epsilon h(r)]/\partial\epsilon^2)(\epsilon=0)$ for *radially symmetric* variations $h(r)$. One readily verifies that an admissible $H(r):=\int_0^r d\bar r\,\bar r^{\nu-1}h(\bar r)$ must belong to $\mathcal{H}$. Lemma 5 relies upon the Coulombic property

$$W(|x|,|y|):=\frac{1}{|\partial\omega_\nu|}\int_{\partial\omega_\nu}d\omega\,C(x-y_\omega)$$
$$=\min\{C(x),C(y)\}\ , \tag{80}$$

where y_ω denotes the image of y by the rotation ω. Equation (80) is a close relative of Gauss's law; its verification should present no difficulty. Using the argument of Sec. VIII.C below, one can substitute $W(x,y)$ for $C(x-y)$ in the expression for the second variation of the Vlasov free energy:

$$F''(0)=\gamma\int_\Lambda dx\int_\Lambda dy\,h(|x|)h(|y|)\,W(|x|,|y|)+kT\int_\Lambda dx\frac{h^2(|x|)}{\rho(|x|)}$$
$$=2\gamma|\partial\omega_\nu|^2\int_0^R dr\,h(r)\,C(r)\,r^{\nu-1}\int_0^r d\bar r\,\bar r^{\nu-1}h(\bar r)+kT\int_0^R dr\,r^{\nu-1}\frac{h^2(r)}{\rho(r)}$$
$$=|\partial\omega_\nu|kT\int_0^R\frac{dr}{r^{\nu-1}}\left[\beta\gamma H^2(r)+\frac{[H'(r)]^2}{\rho(r)}\right]\ . \tag{81}$$

The integration by parts implied by the last step is legitimized by the properties of $\mathcal{H}$. Use has been made of $\partial C(r)/\partial r = -|\partial\omega_\nu|^{-1} r^{1-\nu}$ as well. ■

As a simple application of Lemma 5, we show that the singular solution (77) is always unstable for $\nu \geq 3$. To that end, let us consider

$$H(r) = \begin{cases} cr & \text{for } 0 \leq r \leq R/2 \ , \\ c(R-r) & \text{for } R/2 \leq r \leq R \ , \end{cases} \tag{82}$$

where $c = -2(\nu-2)/\beta\gamma$. One can verify that $H(r) \in \mathcal{H}$ and that the value of the functional (79) is $-(3-\ln 16)Rc^2/2 < 0$.

Remarks. As far as stellar objects are concerned, one could argue that a constant energy-pressure ensemble would be better adapted than the above constant temperature-volume ensemble. Unfortunately, the question of equivalence between ensembles is rather delicate due to the instability of the gravitational interaction. See, for example, Lynden-Bell and Wood, 1968, Lynden-Bell and Lynden-Bell, 1977, for a discussion of the microcanonical ensemble and its relation to the canonical one. In the Hammerstein description, the situation goes as follows: Equation (70), supplemented by Dirichlet boundary conditions on $\partial\Lambda$, has two solutions for $0 < \lambda < \lambda_*$ in the case of a disk ($\nu = 2$), where λ_* is an explicitly known function of the external parameters (see, for example, Dancer, 1988, and references therein). One of the solutions is the global minimizer of the functional (71), the other being unstable (Amann, 1976b). Equation (70) has no solutions for $\lambda > \lambda_*$. In the case of a sphere ($\nu = 3$), there is also a λ_* beyond which no solutions exist; however, there are below λ_* many solutions in general, even an infinite number for the value of λ corresponding to the singular solution (77). More information is available in Gel'fand, 1963; Joseph and Lundgren, 1973; Bandle, 1975; Amann, 1976b; Dancer, 1988; and Suzuki and Nagasaki, 1988. Let us just mention that nonradially symmetric containers have been tackled in two dimensions by a complex-function method (Suzuki and Nagasaki, 1988) going back to Liouville (1853). See Dancer (1988) for the higher-dimensional case.

Lynden-Bell and Wood (1968), Horwitz and Katz (1977), Cally and Monaghan (1981), and Padmanabhan (1990) contain various (and variously rigorous) discussions on the stability of solutions. More on the classical (N-body/mean-field) relationship for gravitational systems can be found in Kiessling (1989, 1990). For the quantum case, see Baumgartner (1976), Messer (1981), and Lieb and Yau (1987) and references therein.

B. Coulombic systems

$\gamma > 0$ makes things much easier: The Vlasov functional being strictly convex, the unique solution to Eq. (69) is the global minimizer of the latter. By Theorem 1, a thermodynamic limit does not exist because of the long range [$\tilde{V}(0) = \infty$] of the Coulombic potentials. Exact solutions for finite systems are known in one and two dimensions:

1. $\gamma > 0$, $\nu = 1$, $\Lambda = B(0,l) = [-l,l]$

$$\rho(x) = \frac{2a^2}{\beta\gamma} \frac{1}{\cos^2(ax)} \quad \text{with} \begin{cases} a \tan al = N\beta\gamma/4 \\ 0 < al < \pi/2 \ . \end{cases} \tag{83}$$

2. $\gamma > 0$, $\nu = 2$, $\Lambda = B(0,R)$

$$\rho(x) = \frac{8a^2}{\beta\gamma} \frac{1}{(|x|^2 - a^2)^2} \quad \text{with } a^2 = \left[1 + \frac{8\pi}{\beta\gamma N}\right] R^2 \ . \tag{84}$$

This solution exists, as it must, for all ranges of temperature and density.

Note the obvious link between solutions for $\gamma > 0$ and their counterparts for $\gamma < 0$, as well as the impossibility of an analog of the singular solution (77) (for $\nu \geq 3$). Notice also that the value of the functional in Lemma 5 is always positive, as it must be.

For $\nu \geq 3$, explicit solutions are not available. In the case of *neutral* systems, i.e., those involving at least two kinds of particles or an external field induced by a neutralizing background (jellium), studies are generally carried on at this stage by linearizing $\exp(-\beta\phi) \approx 1 - \beta\phi$. This is the essence of the Debye-Hückel theory (Debye and Hückel, 1923; Hill, 1956; Davidson, 1962) of electrolytes and plasmas, which we clearly cannot develop further here. More on exact solutions to the GPBE equation for neutral and charged systems can be found in Garrett and Poladian (1988). See Kennedy (1984) and references therein for a derivation of the Poisson-Boltzmann equation in some appropriate mean-field limit for N-body neutral systems.

VIII. DENSITY PROFILES

At fixed temperature kT and density $\rho := N/|\Lambda|$, the shape of the minimizing density $\rho^0(x)$ is determined both by the potential $V(x)$ and by the shape of the container Λ. This section deals with general results characterizing this dependence.

A. Superharmonic potentials

Let us assume $V(x) = v(|x|)$, where $v(r)$ is $C^2(\mathbf{R}^+)$. Consequently (with $r := |x|$)

$$\Delta V(x) = -g\delta(x) + v''(r) + \frac{\nu-1}{r} v'(r)$$
$$\text{with } g := -|\partial\omega_\nu| \lim_{r \to 0^+} r^{\nu-1} v'(r) \ . \tag{85}$$

The occurrence of the δ function stems from Eq. (68). Differentiating Eq. (10) once more yields

$$\Delta\rho(x)=\rho^{-1}(x)[\nabla\rho(x)]^2+\beta g\rho^2(x) -\beta\rho(x)\int_\Lambda dy\,\rho(y)r^{-\nu+1}\frac{\partial}{\partial r}[r^{\nu-1}v'(r)]\ , \qquad (86)$$

where r now stands for $|x-y|$. Recall that a function f is called *subharmonic* (see, for example, Helms, 1975; Gilbarg and Trudinger, 1983; Doob, 1984) if $\Delta f(x)\geq 0$ and *superharmonic* if $-f$ is subharmonic. The value of a subharmonic function $f(x)$ does not exceed its mean value over any ball centered on x. A direct consequence of Eq. (86) is

Theorem 6. *If $V(x-y)$ is superharmonic in Λ [i.e., $\Delta V(x)\leq 0\ \forall x,|x|\leq\mathrm{diam}(\Lambda)$], then $\rho(x)$ is subharmonic in $\Lambda[\Delta\rho(x)\geq 0,\forall x\in\Lambda]$. In particular,*

$$\rho(x)\leq\frac{1}{|B(x,r)|}\int_{B(x,r)}dy\,\rho(y)\quad\forall B(x,r)\subset\Lambda\ . \qquad (87)$$

Observe that superharmonicity of the radial function $V(x)$ requires both $g\geq 0$ and $(r^{\nu-1}v'(r))'\leq 0$. Coulomb potentials [$g=1$ and $(r^{\nu-1}v'(r))'=0$] are superharmonic. In one dimension, superharmonicity and concavity are synonymous. The mean-value property (87) makes the fluid less dense far away from the boundary than near the boundary. In particular, the density attains its maximum on $\partial\Lambda$. The presence of the fluid in the interior of the container is uniquely due to entropic reasons: by Theorem 12 below, a system interacting with a superharmonic potential undergoes complete condensation on $\partial\Lambda$ at $kT=0$.

B. Attractive potentials

Another class of rather clear-cut situations is constituted by purely attractive potentials:

Theorem 7. *Let $V(x)$ be a nondecreasing radial function. Then*

(i) *when Λ is a ball, the minimizing density profile is a nonincreasing radial function,*

(ii) *among all containers Λ of fixed volume $|\Lambda|$, the Vlasov free energy is minimal when Λ is a ball.*

Proof. Theorem 7 is a direct consequence of Riesz's inequality,

$$\int_{\Lambda^2}dx\,dy\,f(x)\,g(x-y)\,h(y) \leq\int_{(\Lambda^*)^2}dx\,dy\,f^*(x)\,g^*(x-y)\,h^*(y)\ , \qquad (88)$$

which holds for non-negative functions f,g, and h. f^* is the *spherically decreasing rearrangement* of f, i.e., the (almost everywhere unique) radial decreasing function with the property that the sets $\{x|f(x)\geq\mu\}$ and $\{x|f^*(x)\geq\mu\}$ have the same Lebesgue measure for all $\mu>0$. Λ^* is a ball of volume $|\Lambda^*|=|\Lambda|$. (More on rearrangements can for instance be found in Hardy *et al.*, 1967; Luttinger, 1973; Lieb, 1977; Kawohl, 1985.) With $f(x)=h(x)=\rho(x)$, $g(x)=-V(x)$ and taking into account $g^*(x)=g(x)$, one finds that the energy part is lowered by the above rearrangement. On the other hand, the entropy part is left unchanged, and so $F_\Lambda[\rho]\geq F_{\Lambda^*}[\rho^*]$. ■

Let us notice, in the case of a radial *nonincreasing* potential, that the radial *increasing* rearrangement of $\rho(x)$ in Λ *does not* in general lower the value of the Vlasov functional: the "conjugate" to Theorem 7 does not hold, as can be seen in the one-dimensional example $V(x)=\theta(a-|x|)$, where $\theta(\cdot)$ is the unit-step function, and

$$\rho(x)=\begin{cases}c>0 & \text{for } r_1\leq|x|\leq r_2 \text{ and } r_3\leq|x|\leq r_4\ ,\\ 0 & \text{otherwise}\end{cases} \qquad (89)$$

in the container $\Lambda=[-R,R]$, with $a/2\leq r_1<r_2,r_2+a\leq r_3<r_4\leq R$. The symmetrically increasing rearrangement of the density

$$\rho_*(x)=\begin{cases}c>0 & \text{for } R+r_1+r_3-r_2-r_4\leq|x|\leq R\ ,\\ 0 & \text{otherwise}\end{cases} \qquad (90)$$

clearly enhances the energy.

C. Rotational invariance of density profiles

One might wonder at this stage if rotationally invariant containers $\Lambda=B(0,R)\subset\mathbf{R}^\nu$ and potentials $V(x)$ produce a rotationally invariant density profile. In what follows, $\langle f(x)\rangle_\omega$ will denote the angular average of the function $f(x)$, i.e.,

$$\langle f(x)\rangle_\omega:=\frac{1}{|\partial\omega_\nu|}\int_{\partial\omega_\nu}d\omega\,f(x_\omega)\ , \qquad (91)$$

where x_ω is the image of x by the rotation ω. The answer to the above question is positive in the case of

(i) nondecreasing potentials (Theorem 7),

(ii) positive definite potentials: $F[\langle\rho\rangle_\omega]\leq F[\rho]$ for all $\rho\in\mathcal{R}(\Lambda,N)$ by Jensen's inequality.

In the general case, we can show

Lemma 8. *Let the container and the potential be rotationally invariant. Then there exists a rotationally invariant solution to the GPBE equation.*

Proof. Consider

$$W(|x|,|y|):=\frac{1}{|\partial\omega_\nu|}\int_{\partial\omega_\nu}d\omega\,V(x-y_\omega)\ . \qquad (92)$$

By construction, any profile $\rho(x)$ satisfies

$$\int_\Lambda dx\,\rho(x)\int_\Lambda dy\,\rho(y)\,W(|x|,|y|) =\int_\Lambda dx\,\langle\rho(x)\rangle_\omega\int_\Lambda dy\,\langle\rho(y)\rangle_\omega\,V(x-y)\ . \qquad (93)$$

Let $\rho^0(x)$ be the minimizer of the modified Vlasov functional, where W has been substituted for V. $\rho^0(x)$, whose existence is ensured by Theorem 2, obeys the GPBE equation with W. On the other hand, the modified energy functional is insensitive to the angular averaging of the profiles, whereas the value of the entropy part, by convexity, is lowered. This shows $\rho^0(x)$ to be radial; therefore $W*\rho^0=V*\rho^0$, and so $\rho^0(x)$ obeys the GPBE equation with V. ■

It remains to be determined whether this radial solution $\rho^0(x)$ is the global minimizer of the Vlasov functional. Although the value of the entropy part is lowered by angular averaging, things are made delicate by the fact that the value of the energy part is enhanced.

Lemma 9. *For any rotationally invariant container and potential, and for any density $\rho(x)$,*

$$U[\langle\rho\rangle_\omega]\geq U[\rho]\ . \tag{94}$$

Proof. By Eq. (1),

$$(\rho(x)-\rho(y))(\phi(x)-\phi(y))\leq 0 \quad \text{for } x,y\in\Lambda\ . \tag{95}$$

By averaging the angular part in x we obtain

$$\langle\rho(x)\phi(x)\rangle_\omega+\rho(y)\phi(y)\leq\langle\rho(x)\rangle_\omega\phi(y)+\rho(y)\langle\phi(x)\rangle_\omega\ . \tag{96}$$

We now set $y=x$ and integrate over Λ:

$$\begin{aligned}4U[\rho]=2K[\rho,\rho]&\leq 2K[\rho,\langle\rho\rangle_\omega]\\&=K[\langle\rho\rangle_\omega,\langle\rho\rangle_\omega]=4U[\langle\rho\rangle_\omega]\ .\end{aligned} \tag{97}$$

■

In view of the last result and of the "energy-dominated" character of the Vlasov functional discussed in Sec. V.B.1, our final conclusion is that radial containers and potentials *do not* in general produce radial densities. The argument can be completed by considering the rectangular potential $V(x)=\theta(a-|x|)$ in two dimensions: for a certain range of densities and temperatures, one can show (Raveché and Stuart, 1975, as supported by numerical experiments of Raveché and Kayser, 1978; Feijoo and Rahman, 1982) that the minimizing profile has square planar symmetry in the thermodynamic limit. For a sufficiently big circular container, surface effects become negligible and the same (slightly distorted) nonradial pattern will constitute the global minimizer.

IX. WALL THEOREM

Another crucial feature of the density profile is its behavior near the boundary: as we shall show, the value of the density at the boundary $\partial\Lambda$ is directly related to the pressure of the system: this constitutes a "wall theorem," in close correspondence to the N-body theory (Lebowitz, 1960; Fisher, 1964; Siegert and Meeron, 1966; Bavaud, 1986).

Theorem 10. *The stress tensor $\tau_{\alpha\beta}$ is given by the formula*

$$\tau_{\alpha\beta}=\frac{-kT}{|\Lambda|}\int_{\partial\Lambda}d\sigma_\alpha x_\beta\rho(x)\ , \tag{98}$$

where $d\sigma_\alpha$ is the (outward oriented) surface element in $\partial\Lambda$. In the case of a density constant on $\partial\Lambda$, the pressure $P=-(1/\nu)\tau_{\alpha\alpha}$ satisfies

$$P=\rho(\partial\Lambda)\,kT\ . \tag{99}$$

Proof. In an N-body system, the pressure, stress tensor, and elastic modulus tensor are obtained by successive differentiation of the partition function with respect to the matrix elements $\epsilon_{\alpha\beta}$ parametrizing the homogeneous deformation (see, for example, Bavaud *et al.*, 1986, and references therein):

$$\tilde{x}_\alpha=x_\alpha+\epsilon_{\alpha\beta}x_\beta\ . \tag{100}$$

In the Vlasov case, direct differentiation with respect to ϵ [as done, for example, in Eq. (38)] is only possible when the ϵ dependence of the free energy is explicitly known. However, in the general situation, the free energy (3) depends on ϵ through $\rho^\epsilon(\tilde{x})$, the minimizing density in $\mathcal{R}(\tilde{\Lambda},N)$ where $\tilde{\Lambda}$ is the container obtained from Λ by the deformation (100). In the absence of explicit knowledge of ρ^ϵ, the following expedient can be used: Consider

$$\rho^{*\epsilon}(\tilde{x}):=\frac{1}{\det(\mathbf{1}+\epsilon)}\rho^0((\mathbf{1}+\epsilon)^{-1}\tilde{x})=\frac{1}{\det(\mathbf{1}+\epsilon)}\rho^0(x)\ , \tag{101}$$

where $\mathbf{1}$ is the unit $\nu\times\nu$ matrix. By construction, $\rho^{*\epsilon}$ belongs to $\mathcal{R}(\tilde{\Lambda},N)$ and satisfies $F[\rho^{*\epsilon}]\geq F[\rho^\epsilon]$. As $F[\rho^{*0}]=F[\rho^0]$, the tangents of the two functionals coincide at $\epsilon=0$ and

$$\tau_{\alpha\beta}:=\frac{1}{|\Lambda|}\frac{\partial F[\rho^\epsilon](\epsilon=0)}{\partial\epsilon_{\alpha\beta}}=\frac{1}{|\Lambda|}\frac{\partial F[\rho^{*\epsilon}](\epsilon=0)}{\partial\epsilon_{\alpha\beta}}\ . \tag{102}$$

As a consequence, the stress tensor $\tau_{\alpha\beta}$ and the pressure P are correctly evaluated by the right-hand side of Eq. (102), whereas an analogous computation involving the second derivatives of the free energy $F[\rho^{*\epsilon}]$ with respect to ϵ would lead to *upper bounds* for the elastic moduli $B_{\alpha\beta\gamma\delta}$ and the inverse compressibility B.

With an obvious change of variables,

$$\begin{aligned}F[\rho^{*\epsilon}]=&\tfrac{1}{2}\int_\Lambda dx\int_\Lambda dy\,\rho^0(x)\rho^0(y)V((\mathbf{1}+\epsilon)(x-y))\\&+kT\int_\Lambda dx\,\rho^0(x)\ln\rho^0(x)-kTN\ln\det(\mathbf{1}+\epsilon)\ .\end{aligned} \tag{103}$$

Consequently

$$\tau_{\alpha\beta}=\frac{1}{|\Lambda|}\int_\Lambda dx\,\rho^0(x)x_\beta\frac{\partial\phi^0(x)}{\partial x_\alpha}-\delta_{\alpha\beta}\rho kT\ . \tag{104}$$

Taking Eq. (1) into account and integrating by parts completes the proof. ■

Remark. Looking at the dependence in the temperature rather than in volume, we see that a similar procedure, involving a fake minimizer $\rho^{*\beta}$ (many possibilities exist), would show

$$\frac{\partial(\beta F[\rho^\beta])}{\partial\beta} = \tfrac{1}{2}K[\rho^\beta,\rho^\beta] = U[\rho^\beta] \ , \tag{105}$$

which is reassuring. A second differentiation of $F[\rho^{*\beta}]$ yields an upper bound for the specific heat.

X. GROUND STATES

At zero temperature, one deals with the minimization problem

$$\inf_{\rho\in\mathcal{R}(\Lambda,N)} \tfrac{1}{2}\int_\Lambda dx \int_\Lambda dy\, \rho(x)\rho(y)V(x-y) = :\inf_{\rho\in\mathcal{R}(\Lambda,N)} \tfrac{1}{2}K[\rho,\rho] =: \tfrac{1}{2}K[\rho^0,\rho^0] = U[\rho^0] \ , \tag{106}$$

whose solution(s) $\rho^0(x)$ will be referred to as *ground state(s)*. Here one can no longer exclude *a priori* the presence of a singular part in the density profile. Instead we shall consider (with an abuse of notation)

$$\rho(x) = \rho_a(x) + \rho_s(x) \ , \tag{107}$$

where ρ_a (of total mass N_a) is the absolutely continuous part of the profile, and ρ_s (of total mass N_b) its singular part ($N_a + N_s = N$). The nature of the singular part is intimately related to the nature of the potential: for instance, all ground states of a strictly increasing potential [i.e., $V(x) = v(|x|)$, $v'(r) > 0\ \forall r \geq 0$] are of the form $\rho(x) = N\delta(x - x_0)$ for some $x_0 \in \Lambda$. On the other hand, when the potential is decreasing, it is an easy matter to prove [with the help of Eq. (108) below] that it is always energetically favorable to spread any singularity *interior* to Λ. That is, the only possible singularities are located in the $(\nu-1)$-dimensional hypersurface $\partial\Lambda$, as is the case in electrostatics.

In general, a *necessary* condition for $\rho(x)$ to be a ground state is

$$\begin{aligned} &\phi(x) = 2u = \text{const.} \quad \forall x \in \text{supp}(\rho) \\ &\phi(x) \geq 2u \quad \forall x \in \Lambda \setminus \text{supp}(\rho) \ , \end{aligned} \tag{108}$$

where $\phi(x)$ is given by Eq. (2). In other words, the induced field $\phi(x)$ must attain its minimum value in Λ wherever $\rho(x) > 0$. Equation (108) now plays the role previously performed by (1). One can easily verify that when Eq. (108) does not hold, there is a way of redistributing the density $\rho(x)$ (while ensuring its global conservation and non-negativity) which lowers the energy. The constant u in Eq. (108) is actually the ground-state energy per particle,

$$U[\rho] = \tfrac{1}{2}\int_\Lambda dx\, \rho(x)\phi(x) = \tfrac{1}{2}\int_{\text{supp}(\rho)} dx\, \rho(x) 2u = Nu \ . \tag{109}$$

A. Positive-type potentials

Not surprisingly, it turns out that Eq. (108) is also a *sufficient* condition for positive-type potentials.

Theorem 11. *Let $V(x)$ be of positive type. $\rho^0(x)$ is a ground state if and only if it satisfies Eq. (108).*

Proof. By convexity, any admissible profile $\rho(x)$ satisfies

$$0 \leq \tfrac{1}{2}K[\rho^0-\rho,\rho^0-\rho] = U[\rho] + U[\rho^0] - K[\rho^0,\rho] \ . \tag{110}$$

On the other hand, from Eq. (108),

$$K[\rho^0,\rho] = \int_\Lambda dx\, \phi^0(x)\rho(x) \geq 2u\int_\Lambda dx\, \rho(x) = 2uN = 2U[\rho^0] \ , \tag{111}$$

and so $U[\rho] \geq U[\rho^0]$. ■

B. Superharmonic and Coulomb potentials

Theorem 12. *Let $V(x)$ be strictly superharmonic. Then $\text{supp}(\rho^0) \subset \partial\Lambda$. In particular $N_s = N$ and $N_a = 0$.*

Proof. Suppose the existence of a point x_0 interior to Λ with $\rho^0(x_0) > 0$. Let $B(x_0,r) \subset \Lambda$ for a sufficiently small r. This, together with strict superharmonicity and Eq. (108), entails the contradiction

$$\phi(x_0) > \frac{1}{|B(x_0,r)|}\int_{B(x_0,r)} dy\, \phi(y) \geq 2u = \phi(x_0) \ . \tag{112}$$

■

As a corollary to Theorem 12, the unique ground state of a strictly concave potential in the one-dimensional container $\Lambda = [-l,l]$ is $\rho^0(x) = (N/2)[\delta(x+l) + \delta(x-l)]$.

A celebrated consequence of Theorem 12 is the Faraday effect in the electrostatics: electric charges $[V(x) = C(x)]$ distribute themselves on the boundary of a conductor. By Eq. (109), the value of the electric potential on $\partial\Lambda$ is $2U[\rho^0]/N$. On the other hand, the *capacity* $\text{cap}(\Lambda)$ of a conductor Λ is defined as the ratio [total charge]/[value of the potential]. As a consequence

$$U[\rho^0] = \frac{1}{2}\frac{N^2}{\text{cap}(\Lambda)} \ . \tag{113}$$

For $\Lambda \in \mathbf{R}^\nu, \nu \geq 3$, the following equivalent characterization holds:

$$\text{cap}(\Lambda) = \inf_{\{f\in\mathcal{F}(\Lambda)\}}\int_{\mathcal{R}^\nu} dx\, |\nabla f(x)|^2 \ , \tag{114}$$

where $\mathcal{F}(\Lambda) := \{f \mid f(\partial\Lambda) = 1, \ \lim_{|x|\to\infty} f(x) = 0\}$. The equivalence stems from the following facts: by Eqs.

(108), (109), and (113), cap(Λ) is the total charge on $\partial\Lambda$ needed to create the induced potential $\phi^0(x)\equiv 1$ for $x\in\partial\Lambda$. On the other hand, $\phi^0(x)$ is harmonic outside $\partial\Lambda$, and therefore unique as the solution of a Dirichlet problem, and turns out to be the global minimizer in Eq. (114). The condition at infinity matches $\lim_{|x|\to\infty} C(x)=0$ for $\nu\geq 3$.

The concept of capacity (together with its relationship to potential theory, elliptic PDE's, and Brownian motion) has undergone considerable development in the mathematical literature. See, for example, Helms (1975), Gilbarg and Trudinger (1983), and Doob (1984). Among its basic properties are the following (for $\nu\geq 3$):

$$\begin{aligned}&\Lambda_1\subset\Lambda_2 \Longrightarrow \mathrm{cap}(\Lambda_1)\leq\mathrm{cap}(\Lambda_2)\ ,\\ &\mathrm{cap}(\Lambda_1\cup\Lambda_2)+\mathrm{cap}(\Lambda_1\cap\Lambda_2)\leq\mathrm{cap}(\Lambda_1)+\mathrm{cap}(\Lambda_2)\ ,\\ &\mathrm{cap}(\Lambda)\geq\mathrm{cap}(\Lambda^*)=(\nu-2)|\partial\omega_\nu|R^{\nu-2}\ ,\end{aligned} \tag{115}$$

where $\Lambda^*=B(0,R)$ is the symmetric rearrangement of Λ: $|\Lambda^*|=|\Lambda|$. In particular, among all containers of fixed volume $|\Lambda|$, the electrostatic ground-state energy is maximal when Λ is a ball.

C. Yukawa potential

We now turn to new types of situations. We consider first $V(x)=K_0(\gamma|x|)$, the modified Bessel function of order 0 ($\gamma>0$) in the two-dimensional disk $\Lambda=B(0,R)$. One recognizes in $\tilde{V}(k)=2\pi/(|k|^2+\gamma^2)$ the form of the (two-dimensional) Yukawa potential. By positive definiteness, one already knows the ground state $\rho^0(x)$ to be a radial function. Making the supposition that $\mathrm{supp}(\rho)=\Lambda$, and so $\phi(x)\equiv 2u$ in Λ, one is led [by deriving Eq. (108) twice] to the ansatz

$$\rho^0(x)=\frac{N_a}{\pi R^2}+\frac{N_s}{2\pi R}\delta(|x|-R)\ . \tag{116}$$

[Note that the structure (constant bulk density + homogeneous singular part on $\partial\Lambda$) holds for Yukawa potentials in any dimension, for instance $V(x)=\exp(-\gamma|x|)$ in dimension one.] The expression for the induced potential reads

$$\phi^0(x)=\frac{2N_a}{(\gamma R)^2}+\left[N_sK_0(\gamma R)-\frac{2N_a}{\gamma R}K_1(\gamma R)\right]I_0(\gamma|x|)\ . \tag{117}$$

Equation (108) will be satisfied (in which case we are guaranteed, by Theorem 11, to have determined the ground state) provided

$$N_s=\frac{2}{\gamma R}\frac{K_1(\gamma R)}{K_0(\gamma R)}N_a\ . \tag{118}$$

Equation (118), together with the condition $N_s+N_a=N=\rho\pi R^2$, determines the profile entirely. The energy and pressure of the system are

$$U[\rho^0]=\frac{\rho\pi N}{\gamma^2+\frac{2\gamma}{R}\frac{K_1(\gamma R)}{K_0(\gamma R)}}\ , \tag{119}$$

$$\begin{aligned}P=-\frac{\partial U[\rho^0]}{\partial(\pi R^2)}&=\frac{\pi\rho^2}{\gamma^2}\frac{K_1^2(\gamma R)}{K_0^2(\gamma R)}\frac{1}{\left[1+\frac{2}{\gamma R}\frac{K_1(\gamma R)}{K_0(\gamma R)}\right]^2}\\ &=\frac{N_s^2}{4\pi R^2}\ .\end{aligned} \tag{120}$$

In the thermodynamic limit, $u(\rho)=\rho\pi\gamma^{-2}$ and $P=\pi\rho^2\gamma^{-2}$, results which could have been obtained directly from Eqs. (35) and (38). The second expression for the pressure is by no means fortuitous, but a consequence of a "wall theorem for fluids completely wetting the boundary," which we shall now discuss.

D. Wetting and condensation

At zero temperature, Eq. (98) for the stress tensor

$$\tau_{\alpha\beta}=\frac{1}{|\Lambda|}\int_\Lambda dx\,\rho(x)x_\beta\frac{\partial\phi(x)}{\partial x_\alpha} \tag{121}$$

is still valid; however, Eq. (108) implies $\rho(x)\nabla\phi(x)=0$ for all x *interior* to Λ, whence

Lemma 13.

$$P>0\Longrightarrow\sup_{x\in\partial\Lambda}\rho(x)=\infty\ .$$

Lemma 13 was to be expected in view of the finite-temperature wall theorem (99), $P=\rho(\partial\Lambda)kT$. As $kT\to 0$, $\rho(\partial\Lambda)\to\infty$. This can essentially happen in two ways: when $\partial\Lambda$ supports the singular part $\rho_s(x)$, or when the absolutely continuous part $\rho_a(x)$ diverges on $\partial\Lambda$. In order to determine which of these possibilities prevails, we shall make at this stage the following assumptions:

(a1) $V(x)=v(|x|)$, where $v(r)$ is C^1 in $(0,\infty)$, and $V(x)$ is locally integrable.

(a2) Λ is a closed, convex subset of $\mathbf{R}^\nu$. Its boundary $\partial\Lambda$ is of class C^2.

(a3) The singular part of $\rho(x)$ (if existing) has support in $\partial\Lambda$. More precisely, $\rho_s(x)=\delta(\mathrm{dist}(x,\partial\Lambda))\mu(x)$, where the *hypersurface density* or *condensate* $\mu(x)$ does not itself undergo concentrations on $\partial\Lambda$: $\int_{\partial\Lambda}d\sigma\,\mu^2(x)<\infty$.

Without the local integrability condition in (a1), the energy diverges irrespective of the profile. One knows assumption (a3) to be true

(i) for strictly decreasing C^1 potentials [i.e., $v'(r)<0$],

(ii) for superharmonic potentials (by a refinement of Theorem 12),

(iii) for positive-type potentials, provided the ground state is unique [because of $V(0)\geq|V(x)|$]. A simple illustration of this point is provided by $V(x)=\cos(x)$ in the one-dimensional box $\Lambda=[-l,l]$. By convexity, the ground state $\rho(x)$ is an even (i.e., rotationally invariant in one dimension) function, whence

$$U[\rho]=\tfrac{1}{2}\left[\int_{-l}^{l} dx\,\rho(x)\cos(x)\right]^2 . \tag{122}$$

For $l\le(\pi/2)$, one can verify [using Eq. (108)] that the unique ground state is $\rho(x)=(N/2)(\delta(x+l)+\delta(x+l))$. For $l>(\pi/2)$, $\rho(x)=(N/2)(\delta[x+(\pi/2)]+\delta[x-(\pi/2)])$ is a ground state: the energy attains its lower bound zero. However, uniqueness does not hold, for the convolution of the latter profile with any even positive function of support in $[(\pi/2)-l,l-(\pi/2)]$ yields another ground state. Observe that the pressure satisfies $P>0$ in the first case and $P=0$ in the second (degenerate) case, in accordance with Lemma 13: the overall repulsive character of the interaction has been lost.

From now on, we assume the validity of assumptions (a1), (a2), and (a3). Equation (121) reads

$$\tau_{\alpha\beta}=\frac{1}{|\Lambda|}\int_{\partial\Lambda} d\sigma\,\mu(x)x_\beta\frac{\partial\phi(x)}{\partial x_\beta} . \tag{123}$$

Following a line of reasoning familiar in electrostatics (see, for example, Jackson, 1962), we see that the tangential components of $\nabla\phi(x)$ are continuous across $\partial\Lambda$, whereas its normal component is discontinuous. Explicitly, when x_- and x_+ are two points arbitrarily close together in the neighborhood of $\partial\Lambda$, with x_- and x_+ interior and exterior to Λ, respectively, the discontinuity is given by

$$\frac{\partial\phi(x_+)}{\partial x_\alpha}-\frac{\partial\phi(x_-)}{\partial x_\alpha}=-g\mu(x)\eta_\alpha(x) , \tag{124}$$

where $\eta_\alpha(x)$ is the outer normal at x, and g is given by Eq. (85). As far as the discontinuity of $\nabla\phi(x)$ across $\partial\Lambda$ is concerned, $V(x)$ can be replaced by the Coulombic potential $gC(x)$. We say the density profile $\rho(x)$ *completely wets the boundary* $\partial\Lambda$ is there is an $\epsilon>0$ such that

$$\left.\begin{array}{l} x\in\Lambda \\ \mathrm{dist}(x,\partial\Lambda)<\epsilon \end{array}\right\}\Longrightarrow\rho(x)>0 . \tag{125}$$

This condition, together with Eq. (108), makes $\phi(x)\equiv 2u$ in an interior layer of finite width ϵ parallel to $\partial\Lambda$, and therefore $\nabla\phi(x_-)=0$ in Eq. (124). Combining Eqs. (124) and (123), we have proven

Theorem 14. *Under assumptions (a1), (a2), and (a3), the stress tensor of a ground state that completely wets the boundary is given by the formula*

$$\tau_{\alpha\beta}=\frac{-g}{2|\Lambda|}\int_{\partial\Lambda} d\sigma_\alpha x_\beta\mu^2(x) , \tag{126}$$

where $g=-|\partial\omega_\nu|\lim_{r\to 0}r^{\nu-1}v'(r)$, *and* $\mu(x)$ *is the hypersurface density. When the latter is constant on* $\partial\Lambda$, *the pressure satisfies*

$$P=\frac{g\mu^2(\partial\Lambda)}{2}=\frac{gN_s^2}{2|\partial\Lambda|^2} . \tag{127}$$

Strictly speaking, a product of distributions is involved in the derivation of Eq. (126). The latter can be justified (together with the factor $\frac{1}{2}$) by a regularization procedure. One verifies that Eq. (120) is a particular case of Eq. (127) with $g=2\pi$. More generally, Eqs. (38) and (127) yield the following sum rule, to be satisfied in the thermodynamic limit for fluids that completely wet the boundary with a positive definite interaction:

$$\mu^2(\partial\Lambda)=\frac{\int_0^\infty d\bar r\,\bar r^{\,\nu-1}v(\bar r)}{-\lim_{r\to 0}r^{\nu-1}v'(r)}\rho^2 . \tag{128}$$

In addition to its intrinsic interest, Theorem 14 together with Lemma 13 provides a most effective characterization of ground states:

Corollary 14a. **(i)** *A system with* $g\le 0$ *cannot completely wet the boundary unless* $P=0$. **(ii)** *A system with* $g=\infty$ *cannot undergo condensation on the boundary [i.e.,* $\mu(x)\equiv 0$*], unless* $P=\infty$.

[Part (ii) of the corollary can also be understood from energetic considerations: $g=\infty$ is the mark of a potential that is strongly repulsive at the origin. Any condensation implied by $\rho_s(x)>0$ causes the energy to diverge.]

A simple illustration of part (ii) is provided by $V(x)=\cos(x)$ in one dimension. An application of part (i) of Corollary 14a consists of the result that one-dimensional systems in $\Lambda=[-l,l]$ interacting through the potentials $V_1(x):=1/(a^2+x^2)$ and $V_2(x):=\exp(-x^2/2a^2)$ *cannot* have ground states wetting the boundary, since $g=0$ (and $P>0$: the potentials are purely repulsive). Both potentials are of positive type, and strictly concave for $|x|\le a$. As a consequence of Theorem 11, Eq. (108) will be satisfied for $\rho(x)=(N/2)(\delta(x+l)+\delta(x-l))$ for sufficiently small l. When $l>0.71a$ for $V_1(x)$ or $l>0.86a$ for $V_2(x)$, the value of the potential $\phi(x)$ so induced becomes less at $x=0$ than on the walls, causing a certain amount of fluid previously condensed on the walls to be transported to the central region, until equalization of the wall and central-region potentials occurs. When l increases (at fixed N), so does N_a. However, $N_s=N-N_a$ remains strictly positive for $l<\infty$ by Lemma 13. Moreover, the central region and the wall always remain disconnected, by virtue of part (i) of Corollary 14a.

Let us now illustrate part (ii) with the two-dimensional example $V(x)=|x|^{-1}$, $\Lambda=B(0,R)$. The potential is integrable and $g=\infty$. As $\tilde V(k)=2\pi/|k|>0$, the ground state is, by convexity, radial. The guess $\rho(x)=c(R^2-|x|^2)^{-1/2}$ for $|x|\le R$ $(c=N/2\pi R)$ turns out to be a good one: the induced potential

$$\phi(x)=\begin{cases} c\pi^2 & \text{for } |x|\le R , \\ 2\pi c\,\mathrm{arccosec}\left[\dfrac{|x|}{R}\right] & \text{for } |x|\ge R \end{cases} \tag{129}$$

satisfies the necessary and sufficient condition (108). Moreover, $\rho(\partial\Lambda)=\infty$ in accordance with Lemma 13. Notice that the whole profile is absolutely continuous,

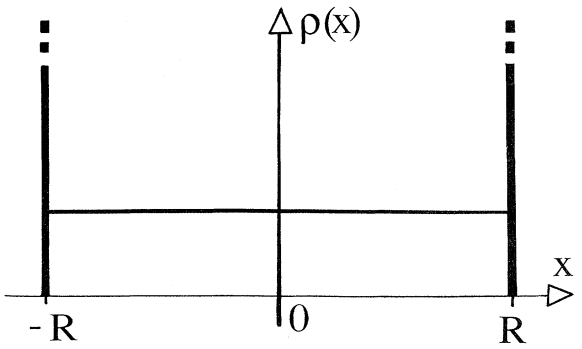

FIG. 1. $V(x)=K_0(\gamma|x|)$ (two-dimensional Yukawa potential) in the disk $B(0,R)$ (radial section).

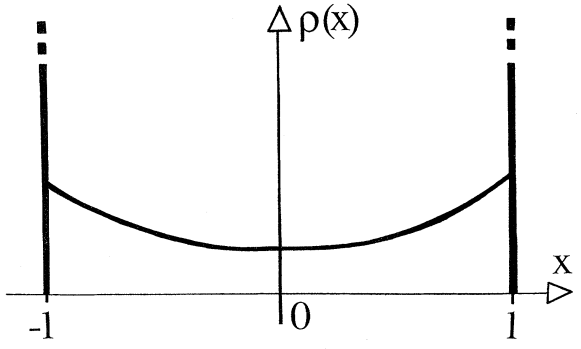

FIG. 2. $V(x)=\kappa\gamma\exp(-\gamma|x|)-\exp(-|x|)$ (one-dimensional Morse potential, $\kappa>1$).

i.e., no condensation occurs, as required by Corollary 14a.

A final consequence of Corollary 14a is the possibility that condensation and complete wetting may coexist, provided $0<g<\infty$, as in the case of the Yukawa potential. Another example is provided by the one-dimensional Morse potential

$$V(x)=\kappa\gamma\exp(-\gamma|x|)-\exp(-|x|) \tag{130}$$

for $\gamma>1$, $\kappa>\gamma^{-2}$. Then $g=2(\kappa\gamma^2-1)>0$. As

$$\tilde{V}(k)=\frac{(\kappa-1)\gamma^2+(g/2)k^2}{(\gamma^2+k^2)(1+k^2)}\ , \tag{131}$$

the Morse potential is positive definite for $\kappa\geq 1$. It is a somewhat tedious, but elementary, exercise to verify that condition (108) is satisfied for

$$\rho^0(x)=\begin{cases}\dfrac{\alpha_1}{2}[\delta(x-l)+\delta(x+l)]+\dfrac{\alpha_2}{2}\cosh(bx)+\dfrac{\alpha_3}{2} & \text{for } \kappa>1\ ,\\ \dfrac{\alpha_1}{2}[\delta(x-l)+\delta(x+l)]+\dfrac{\alpha_2}{2}x^2+\dfrac{\alpha_3}{2} & \text{for } \kappa=1\ ,\\ \dfrac{\alpha_1}{2}[\delta(x-l)+\delta(x+l)]+\dfrac{\alpha_2}{2}\cos(\tilde{b}x)+\dfrac{\alpha_3}{2} & \text{for } \kappa<1\ ,\end{cases} \tag{132}$$

for some strictly positive constants $\alpha_1=N_s,\alpha_2,\alpha_3,b$, and $\tilde{b}$.

Choquard and Rentsch (1986), who suggested to the author the above problem, have investigated the stability properties of the corresponding N-body system.

E. Rectangular potential

Finally, we investigate the ground states of the potential $V(x)=\theta(a-|x|)$. [We take $\theta(0)=0$ for convenience.] Although the potential is repulsive, assumption

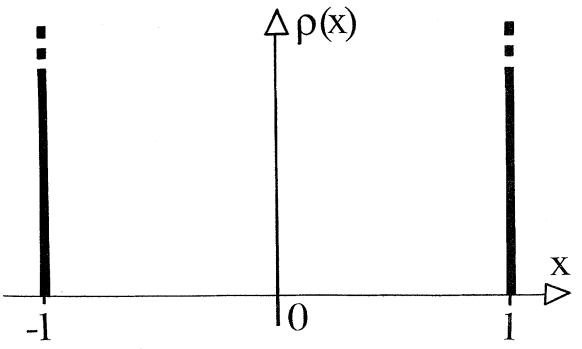

FIG. 3. $V(x)=\exp(-|x|^2/2a^2)$, with $l<0.86a$ (or any concave potential).

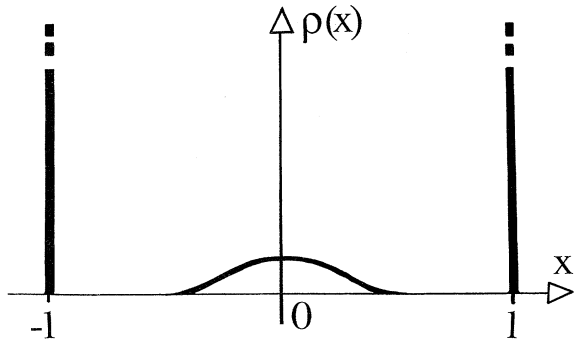

FIG. 4. $V(x)=\exp(-|x|^2/2a^2)$, with $l>0.86a$ (symbolic sketch of the central region).

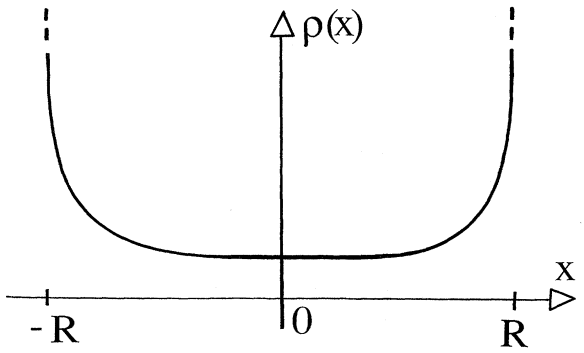

FIG. 5. $V(x)=|x|^{-1}$ in the disk $B(0,R)$ (radial section).

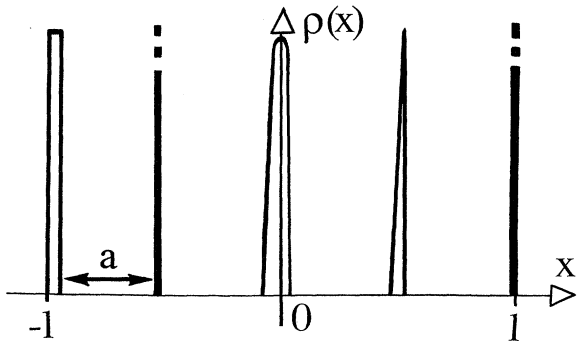

FIG. 7. $V(x)=\theta(a-|x|)$ (one-dimensional rectangular potential), with $2l=4.5a$ (degenerate ground state).

(a1) of Sec. IX.D does not hold, and a justification for (a3) is lacking. We suggest to the reader (if there are any left) spending a little while trying to guess the ground-state structure in the one-dimensional container $\Lambda=[0,L]$. When $L<a$, all admissible $\rho(x)\in\mathcal{R}(\Lambda,N)$ have the same energy $U[\rho]=N^2/2$. For $a<L<2a$, one finds that the minimizing profile consists of two drops of identical mass $N/2$ (but otherwise arbitrary shapes) at a distance greater than a apart. In the general case $L>a$, one first observes that $\mathrm{supp}(\rho)\neq\Lambda$, i.e., there must be holes in the fluid, for otherwise one would have $\phi(x)\equiv$const., and trying to satisfy this requirement for all $x\in[0,a]$ would imply, via Eq. (108), $\rho(x)=0$ almost everywhere in $[a,2a]$. There exists, therefore, a nonempty interval $[x_1,x_2]\subset\Lambda$ with $\rho(x)\equiv 0$ in $[x_1,x_2]$. If $x_1=0$ ($x_2=L$), displacing (without deforming) to the left (right) a fraction of the fluid creates a central hole without increasing the energy. One can then safely assume $0<x_1<x_2<L$. If $|x_2-x_1|>a$, a nondeforming displacement can be applied without energetic cost to an adjacent part of the fluid until a hole of size a is obtained; if $|x_2-x_1|<a$, one can condense the total amount of fluid contained in $[x_1-a,x_2-a]$ into a singular measure of the same mass concentrated at x_2-a (and similarly concentrate $[x_1+a,x_2+a]$ at x_1+a). In both cases, new holes are produced, to which the same displacement-condensation process can be applied. What is eventually left consists of $n'\leq n:=[L+a/a]$ Dirac peaks of respective masses $N_1, N_2, \ldots,$ separated by distances at least a. The energy

$$U[\rho]=\tfrac{1}{2}\sum_{i=1}^{n'}N_i^2 \quad \text{with} \quad \sum_{i=1}^{n'}N_i=N \tag{133}$$

is minimal for $n'=n$, $N_i=N/n$ for $i=1,\ldots,n$. The ground-state energy

$$U[\rho^0]=\frac{N^2}{2\left[\dfrac{L+a}{a}\right]} \tag{134}$$

is a discontinuous function of L: for $L=(n-1)a$, $n\in\mathbf{N}^*$, the ground state is unique and consists of n identical Dirac peaks at a distance a apart. For $(n-1)a<L<na$, these peaks can be slightly spread out while keeping their supports at mutual distances at least a apart, without modifying the energy: the ground state is strongly degenerate. At the transition, the pressure jumps from 0 (in accordance with Lemma 13) to ∞. We note in passing that part (i) of Corollary 14a remains valid.

One of the nice features of the above system is its ability to show how a *fluid can be turned into particles* (rather than the other way around!).

A similar behavior is likely to hold in higher dimensions; there will also be holes in the ground-state profile. However, the displacement-condensation argument requires a more cautious treatment. In any case, the upper bound

$$\min_{\rho(x)\in\mathcal{R}(\Lambda,N)}U[\rho]\leq\frac{N^2}{2n(a,\Lambda)} \tag{135}$$

is presumably close to optimum. $n(a,\Lambda)$ represents the maximum number of balls of radius a capable of being packed in the container $\Lambda_a:=\{x\in\mathbf{R}^\nu|\mathrm{dist}(x,\Lambda)\leq a\}$.

The energy per particle in the thermodynamic limit is $u=\frac{1}{2}\rho a$ for $\nu=1$ and $u\leq\frac{1}{3}\rho a^2$ for $\nu=2$. By comparison, the corresponding quantities with a uniform profile are $u_u=\rho a$ and $u_u=(\pi/2)\rho a^2$, respectively.

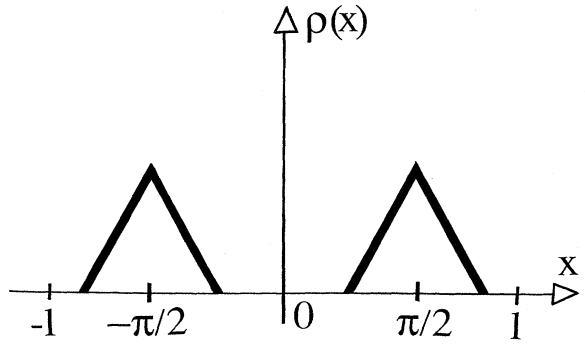

FIG. 6. $V(x)=\cos(x)$, with $l>\pi/2$ (degenerate ground state).

By way of conclusion, we give the plots of a series of ground-state profiles, in an effort to show graphically some of the phenomena encountered in this section. Unless otherwise stated, the container is $\Lambda=[-l,l]\subset\mathbf{R}$.

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