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The Equilibrium Statistical Mechanics of Self-gravitating Systems

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Abstract

The partition function and one- and two-particle distribution functions are calculated for a spherically symmetric self-gravitating system using a method which is exact except for terms of relative order N^{-1}. The results are in agreement with those found in the continuum approximation. First approximations to the correction terms are evaluated with particular emphasis on the form of the pair distribution as compared with the product of two one-particle distributions.

1. Introduction

Because of the long range forces involved, the investigation of the exact statistical mechanics of self-gravitating systems presents difficulties not normally encountered when studying their laboratory counterparts. Nevertheless, considerable progress has been made on the stability problem (e.g. Horwitz and Katz 1977, 1978; Cally and Monaghan 1980; see Section 2 below).

In this paper we are interested in the equilibrium structure of a spherically confined system consisting of a large number N of identical particles (cf. Horwitz and Katz 1977, 1978). (Some attention is also given to the analogous problems in one and two dimensions.) Using the optimal independent-particle potential found by Cally and Monaghan (1980), the canonical partition function Z and the one- and two-particle distribution functions $\nu_1(\boldsymbol{r}')$ and $\nu_2(\boldsymbol{r},\boldsymbol{r}')$ may be evaluated exactly to $O(1)$. In addition, approximations to the $O(N^{-1})$ correction terms may be found which suggest the form of the necessary modifications to the mean field results.

The purpose here is twofold. Firstly, we wish to verify that in the large N limit the thermodynamics and the distribution functions are as predicted by the continuum theory. This is of special interest partly because there must be some doubt about the applicability of the usual thermodynamic ideas to systems with long range forces. In particular the zeroth law (or cycle property), which assumes only thermal contact between neighbouring systems, is of dubious validity when gravitational interactions are also present. However, this 'law' is an important foundation in the axiomatic derivation of thermodynamics (Wilson 1960, p. 81). Therefore, to this approximation, we merely wish to show that all is as it should be.

Secondly, it is of interest to estimate the degree of deviation from the predictions of the mean field theory produced by finite N. This will be indicated not only by the modifications to Z and ν_1, but in particular by the accuracy of the Vlasov approximation

$$\nu_2(\boldsymbol{r},\boldsymbol{r}') = \nu_1(\boldsymbol{r})\,\nu_1(\boldsymbol{r}')\,, \tag{1}$$

and the extent to which it must be modified to take account of interparticle separation $|\boldsymbol{r}-\boldsymbol{r}'|$. (Rybicki (1971) and Monaghan (1978) have made some progress in this area for the one-dimensional case.) Another related point requires consideration: it is well known that self-gravitating systems of point masses have no true equilibrium state since total collapse into a singularity is more energetically favourable than any other configuration. However, the time scale of such an occurrence is far longer than any other relevant time scale, and a 'frozen equilibrium' is postulated and achieved mathematically, at least in principle, by modifying the interparticle potential at short range (see the discussion by Ipser 1974). We shall find in fact that many important features of our results do not depend on the nature of this modification, thereby increasing our confidence in the validity of simple point mass models in general.

Although the stability of the microcanonical model obviously differs from that of the canonical one, we might reasonably expect the broad features of the equilibrium structures to be similar. In any case, the mathematical difficulties inherent in the former appear prohibitive at present.

2. Preliminary Results

The stability of the system in question was investigated by Cally and Monaghan (1980) using a variational technique. We shall summarize the relevant details.

Letting m represent the mass of each particle, k Boltzmann's constant and T the temperature, the momentum part of the canonical partition function Z may be integrated immediately to give

$$Z = (2\pi mkT)^{3N/2}Q\,, \tag{2}$$

where Q is the configurational integral

$$Q = (1/N!)\int \exp(-\beta V)\,\mathrm{d}\Omega_s\,. \tag{3}$$

Here $\beta = 1/kT$, $\mathrm{d}\Omega_s = \mathrm{d}\boldsymbol{r}_1 \dots \mathrm{d}\boldsymbol{r}_N$ and V is the potential energy made up of the sum over all pairs of the two-particle interaction energies $F(|\boldsymbol{r}_i-\boldsymbol{r}_j|)$, that is,

$$V = \tfrac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} F(|\boldsymbol{r}_i-\boldsymbol{r}_j|)\,. \tag{4}$$

In the following we retain the general F, though specific attention is given to the three-dimensional self-gravitating system, for which

$$F(|\boldsymbol{r}-\boldsymbol{r}'|) = -Gm^2/|\boldsymbol{r}-\boldsymbol{r}'|\,. \tag{5a}$$

However, we also refer to the one- and two-dimensional systems where, respectively,

$$F(|x-x'|) = 2\pi Gm^2\,|x-x'|\,, \tag{5b}$$

$$F(|\boldsymbol{r}-\boldsymbol{r}'|) = 2Gm^2 \ln|\boldsymbol{r}-\boldsymbol{r}'|\,. \tag{5c}$$

The variational method is based on the introduction of a smooth (independent-particle) reference potential energy

$$U = \sum_{j=1}^{N} \phi(\boldsymbol{r}_j)\,, \tag{6}$$

where ϕ is initially unspecified. This allows us to rewrite the configurational integral in the form

$$Q = (1/N!) \int \exp(-\beta U) \exp\{-\beta(V-U)\} \, d\Omega_s \tag{7a}$$

$$= (1/N!) \int \exp(-\beta U) \, d\Omega_s . \langle \exp\{-\beta(V-U)\} \rangle , \tag{7b}$$

where the angle brackets denote an averaging with respect to the probability density

$$\exp(-\beta U) \Big/ \int \exp(-\beta U) \, d\Omega_s .$$

Noting Jensen's inequality for convex functions W (Hardy *et al.* 1959)

$$\langle W(f) \rangle \geqslant W(\langle f \rangle), \tag{8}$$

we find that equation (7b) yields

$$Q \geqslant K = (1/N!) \int \exp(-\beta U) \, d\Omega_s . \exp(-\beta \langle V-U \rangle). \tag{9}$$

The value of U is to be chosen so as to maximize the right-hand side of equation (9), i.e. so as to provide the best approximation to the configurational integral. To this end we perturb U by $\delta U = \sum_j \delta\phi(\boldsymbol{r}_j)$.

The condition that K be stationary decides the form of ϕ; it is found that

$$\phi(\boldsymbol{r}) = \{(N-1)/\zeta\} \int \exp\{-\beta\, \phi(\boldsymbol{r}')\} \, F(|\boldsymbol{r}-\boldsymbol{r}'|) \, d\tau' , \tag{10}$$

where $d\tau'$ is the ordinary volume element and

$$\zeta = \int \exp(-\beta\phi) \, d\tau . \tag{11}$$

Alternatively, for the three-dimensional system, equation (10) may be replaced by

$$\nabla^2 \phi = 4\pi G m^2 (N-1) \exp(-\beta\phi)/\zeta . \tag{12}$$

If we make the reasonable assumption that the mass density ρ is given by

$$\rho(\boldsymbol{r}) = Nm \exp(-\beta\phi)/\zeta \tag{13}$$

(see Section 3), equation (12) becomes

$$(kT/m) \nabla^2 (\ln \rho) = \{(N-1)/N\} 4\pi G \rho . \tag{14}$$

Apart from the unimportant factor $\{(N-1)/N\}$, this is just the equation of hydrostatic support for an isothermal perfect gas, and ϕ/m is the Emden potential for an isothermal gas sphere (see Chandrasekhar 1939).

Taking the analysis to second order (i.e. requiring that K be a maximum) yields the stability condition. This need not concern us here; it is sufficient to note that the system becomes unstable when the density contrast between centre and edge exceeds 32·125. (For the microcanonical ensemble the corresponding value is 708·61; see Horwitz and Katz 1978.)

3. Partition Function Expansion

We set $\Delta \equiv U-V$ in equation (7a) and rewrite Q as

$$Q = (1/N!)\exp(\beta\langle\Delta\rangle)\int \exp(-\beta U)\exp\{\beta(\Delta-\langle\Delta\rangle)\}\,\mathrm{d}\Omega_s. \tag{15}$$

Anticipating that $\beta(\Delta-\langle\Delta\rangle)$ is only $O(1)$ (see equation (26) below and the following discussion), we expand

$$\exp\{\beta(\Delta-\langle\Delta\rangle)\} = 1+\beta(\Delta-\langle\Delta\rangle)+(1/2!)\beta^2(\Delta-\langle\Delta\rangle)^2+\dots, \tag{16}$$

which, when inserted into equation (15), implies

$$Q = (1/N!)\exp(\beta\langle\Delta\rangle)\,\zeta^N\{1+(1/2!)\beta^2\langle(\Delta-\langle\Delta\rangle)^2\rangle+(1/3!)\beta^3\langle(\Delta-\langle\Delta\rangle)^3\rangle+\dots\}. \tag{17}$$

Note that the linear term disappears under the averaging. Equation (9) shows that the first term of (17) corresponds precisely to the stationary point found in the variational method. The expansion is therefore about that point.

The various averages are easily calculated. Firstly

$$\langle U\rangle = \zeta^{-N}\int \exp(-\beta U)\,U\,\mathrm{d}\Omega_s = (N/\zeta)\int \exp(-\beta\phi)\,\phi\,\mathrm{d}\tau = N\langle\phi\rangle, \tag{18}$$

and secondly

$$\langle V\rangle = \frac{N(N-1)}{2\zeta^2}\iint \exp(-\beta\phi-\beta\phi')\,F_{rr'}\,\mathrm{d}\tau\,\mathrm{d}\tau',$$

where $\phi' \equiv \phi(\boldsymbol{r}')$ and $F_{rr'} \equiv F(|\boldsymbol{r}-\boldsymbol{r}'|)$. Hence, by equation (10),

$$\langle V\rangle = \tfrac{1}{2}N\langle\phi\rangle, \tag{19}$$

and consequently

$$\langle\Delta\rangle = \tfrac{1}{2}N\langle\phi\rangle. \tag{20}$$

To calculate the second order correction term it is necessary to evaluate $\langle U^2\rangle$, $\langle UV\rangle$ and $\langle V^2\rangle$. Omitting the details, we find that these are given by

$$\langle U^2\rangle = N\langle\phi^2\rangle+N(N-1)\langle\phi\rangle^2, \tag{21}$$

$$\langle UV\rangle = N\langle\phi^2\rangle+\tfrac{1}{2}N(N-2)\langle\phi\rangle^2 \tag{22}$$

and

$$\langle V^2\rangle = \tfrac{1}{2}\langle\Lambda\rangle+\frac{N(N-2)}{N-1}\langle\phi^2\rangle+\frac{N(N-2)(N-3)}{4(N-1)}\langle\phi\rangle^2, \tag{23}$$

where

$$\Lambda(\boldsymbol{r}) = \{N(N-1)/\zeta\}\int \exp(-\beta\phi')\,F_{rr'}^2\,\mathrm{d}\tau'. \tag{24}$$

Noting that

$$\beta^2\langle(\Delta-\langle\Delta\rangle)^2\rangle = \beta^2(\langle\Delta^2\rangle-\langle\Delta\rangle^2) = \beta^2(\langle U^2\rangle-2\langle UV\rangle+\langle V^2\rangle-\langle\Delta\rangle^2), \tag{25}$$

we see that equations (20)–(23) imply

$$\beta^2\langle(\Delta-\langle\Delta\rangle)^2\rangle = \beta^2\left(\tfrac{1}{2}\langle\Lambda\rangle+\frac{N}{2(N-1)}\langle\phi\rangle^2-\frac{N}{N-1}\langle\phi^2\rangle\right) = \beta^2E_2 \quad \text{say}. \tag{26}$$

It is important to note that, although the individual terms in equation (25) are all of order N^2,* these terms cancel not only to order N^2 but also to order N, thus reducing the first correction term (26) to $O(1)$. Therefore, the 'width' of the distribution $\beta\Delta = \beta(U-V)$ in phase space is $\sim O(1)$, whilst the widths of U and V individually are $\sim O(N)$. This is a verification that the chosen form of the approximating potential energy function U mimics the behaviour of V very well.

We now rewrite equation (17), making use of the relations (20) and (26), as

$$Q = (1/N\,!)\exp(\tfrac{1}{2}N\beta\langle\phi\rangle)\,\zeta^N\{1 + (1/2!)\beta^2 E_2 + (1/3!)\beta^3 E_3 + \ldots\}, \tag{27}$$

where $E_3 = \langle(\Delta - \langle\Delta\rangle)^3\rangle$. Unfortunately, $\beta^3 E_3$ and the higher terms are also of order unity, and so the series in equation (27) converges only slowly in general (though, providing the partition function exists, (27) must exist also because the series (16) is uniformly convergent over the entire phase space, and integrating term by term is therefore always allowable).

However, the series term in equation (27) has little effect on the thermodynamics provided that it remains $O(1)$. For example, it only introduces an extra term of relative order N^{-1} into the average total energy $-\partial(\ln Z)/\partial\beta$. For most practical purposes it is therefore acceptable to approximate

$$Q = (1/N\,!)\exp(\tfrac{1}{2}N\beta\langle\phi\rangle)\,\zeta^N. \tag{28}$$

It may be easily demonstrated that this is in agreement with the usual thermodynamic formulae. In particular, the Helmholtz free energy $A = -kT\ln Z$ is identical with that calculated from the thermodynamic formulae for energy and entropy.

4. One-particle Distribution Function

The spatial one-particle distribution function (number density) $\nu_1(\boldsymbol{R})$ is defined, as a function of position $\boldsymbol{R}$, by

$$\nu_1(\boldsymbol{R}) = \left\langle \sum_{j=1}^{N} \delta(\boldsymbol{r}_j - \boldsymbol{R}) \right\rangle, \tag{29}$$

where the angle brackets now denote an averaging with respect to the probability density

$$\exp(-\beta V) \Big/ \int \exp(-\beta V)\, \mathrm{d}\Omega_s .$$

Without loss of generality we may consider only one term in the summation, $j = 1$ say. Hence

$$\nu_1(\boldsymbol{R}) = N\langle\delta(\boldsymbol{r}_1 - \boldsymbol{R})\rangle = (N/N\,!\,Q)\int \exp(-\beta V)\,\delta(\boldsymbol{r}_1 - \boldsymbol{R})\,\mathrm{d}\Omega_s . \tag{30}$$

It is convenient now to define a new average $\langle\ \rangle_1$ by

$$\langle g\rangle_1 \equiv \int \exp(-\beta U)\,\delta(\boldsymbol{r}_1 - \boldsymbol{R})\,g\,\mathrm{d}\Omega_s \Big/ \int \exp(-\beta U)\,\delta(\boldsymbol{r}_1 - \boldsymbol{R})\,\mathrm{d}\Omega_s . \tag{31}$$

* Note that, typically, we have $\beta\phi \sim O(1)$ since it is roughly the ratio of the gravitational to kinetic energies of a single particle.

Equation (30) may be treated in a manner similar to that used for Q in the previous section; thus (defining J)

$$J \equiv \int \exp(-\beta V)\,\delta(\boldsymbol{r}_1-\boldsymbol{R})\,\mathrm{d}\Omega_s$$
$$= \exp(\beta\langle\Delta\rangle_1)\,I\{1+(1/2!)\beta^2(\langle\Delta^2\rangle_1-\langle\Delta\rangle_1^2)+\dots\}, \tag{32}$$

where

$$I = \int \exp(-\beta U)\,\delta(\boldsymbol{r}_1-\boldsymbol{R})\,\mathrm{d}\Omega_s = \zeta^{N-1}\exp\{-\beta\,\phi(\boldsymbol{R})\}. \tag{33}$$

The averages $\langle U\rangle_1$, $\langle V\rangle_1$ etc. may be evaluated as in Section 3. However, because of the delta function $\delta(\boldsymbol{r}_1-\boldsymbol{R})$ and the consequent increase in combinational possibilities, the details are quite complicated. Only the final results are therefore presented:

$$\langle U\rangle_1 = \phi(\boldsymbol{R})+(N-1)\langle\phi\rangle, \tag{34}$$

where

$$\langle\phi\rangle = \zeta^{-1}\int \exp(-\beta\phi)\,\phi\,\mathrm{d}\tau \quad \text{etc.}$$

is as before (see equation 18);

$$\langle V\rangle_1 = \phi(\boldsymbol{R})+\tfrac{1}{2}(N-2)\langle\phi\rangle; \tag{35}$$

$$\langle U^2\rangle_1 = \phi(\boldsymbol{R})^2+2(N-1)\langle\phi\rangle\,\phi(\boldsymbol{R})+(N-1)\langle\phi^2\rangle+(N-1)(N-2)\langle\phi\rangle^2; \tag{36}$$

$$\langle UV\rangle_1 = \phi(\boldsymbol{R})^2+\tfrac{3}{2}(N-2)\langle\phi\rangle\,\phi(\boldsymbol{R})+\chi(\boldsymbol{R})+\tfrac{1}{2}(N-2)(N-3)\langle\phi\rangle^2+(N-2)\langle\phi^2\rangle, \tag{37}$$

where

$$\chi(\boldsymbol{R}) \equiv \{(N-1)/\zeta\}\int F_{r\boldsymbol{R}}\exp(-\beta\phi)\,\phi\,\mathrm{d}\tau; \tag{38}$$

and

$$\langle V^2\rangle_1 = N^{-1}\Lambda(\boldsymbol{R})+\frac{N-2}{N-1}\phi(\boldsymbol{R})^2+\frac{2(N-2)}{N-1}\chi(\boldsymbol{R})+\frac{(N-2)(N-3)}{N-1}\langle\phi\rangle\,\phi(\boldsymbol{R})$$
$$+\frac{N-2}{2N}\langle\Lambda\rangle+\frac{(N-2)(N-3)}{N-1}\langle\phi^2\rangle+\frac{(N-2)(N-3)(N-4)}{4(N-1)}\langle\phi\rangle^2. \tag{39}$$

These results may be combined to give

$$\langle\Delta\rangle_1 = \tfrac{1}{2}N\langle\phi\rangle \tag{40}$$

again, and

$$\beta^2(\langle\Delta^2\rangle_1-\langle\Delta\rangle_1^2) = \beta^2\Big(-\frac{N-3}{N-1}\langle\phi^2\rangle+\frac{N-4}{2(N-1)}\langle\phi\rangle^2+\frac{2}{N-1}\langle\phi\rangle\,\phi(\boldsymbol{R})$$
$$-\frac{1}{N-1}\phi(\boldsymbol{R})^2-\frac{2}{N-1}\chi(\boldsymbol{R})+\frac{1}{N}\Lambda(\boldsymbol{R})+\frac{N-2}{2N}\langle\Lambda\rangle\Big), \tag{41}$$

which is once more $\sim O(1)$.

Note that equation (41) is analogous to the corresponding formula (26) of Section 3, to order unity. In fact

$$\langle \Delta^2\rangle_1 - \langle \Delta\rangle_1^2 = E_2 + \frac{1}{N}\Big(-\langle \Lambda\rangle - \frac{2N}{N-1}\langle\phi\rangle^2 + \frac{3N}{N-1}\langle\phi^2\rangle + \frac{2N}{N-1}\langle\phi\rangle\,\phi(\boldsymbol{R})$$

$$- \frac{N}{N-1}\phi(\boldsymbol{R})^2 - \frac{2N}{N-1}\chi(\boldsymbol{R}) + \Lambda(\boldsymbol{R})\Big)$$

$$= E_2 + N^{-1}a(\boldsymbol{R}) \quad \text{say}, \tag{42}$$

where $\beta^2 a$ is $O(1)$. This near agreement is not surprising since the definitions of the average in the two sections differ solely by the addition of the delta function $\delta(\boldsymbol{r}_1 - \boldsymbol{R})$ in the present case, which reduces the dimensionality of the integral from $3N$ to $3(N-1)$ only.

In the stationary point approximation, the number density is obviously given by (noting equations 28, 30, 32 and 33)

$$\nu_1(\boldsymbol{R}) = (N/\zeta)\exp\{-\beta\,\phi(\boldsymbol{R})\}, \tag{43}$$

in complete agreement with the Emden form (13). If the quadratic correction terms in both J and Q are included, we find instead

$$\nu_1(R) = \frac{N}{\zeta}\exp\{-\beta\,\phi(\boldsymbol{R})\}\left(1 + \frac{\tfrac{1}{2}\beta^2 a}{N(1+\tfrac{1}{2}\beta^2 E_2)}\right)$$

$$= \frac{N}{\zeta}\exp\{-\beta\,\phi(\boldsymbol{R})\}\left(1 + \frac{w(\boldsymbol{R})}{N}\right) \quad \text{say}. \tag{44}$$

Thus we obtain a correction term $O(N^{-1})$. Note also that, since by equations (10) and (38)

$$\langle\chi\rangle = \langle\phi^2\rangle, \tag{45}$$

the correction $a(\boldsymbol{R})$ has an average of zero. Thus, integrating equation (44) over the configuration, we retain exactly the normalization

$$\int \nu_1(\boldsymbol{r})\,\mathrm{d}\tau = N. \tag{46}$$

The important point to note here is that, although the terms in the series in both J and Q are $O(1)$, and converge slowly, the quotient J/Q converges to that order immediately. However, taking both J and Q to third order will produce another term $O(N^{-1})$ in J/Q, and therefore the form of the correction in equation (44) is by no means final. (The convergence should be understood in the sense of the convergence of the sequence $\{S_k\} \equiv \{J_k/Q_k\}$, that is,

$$J/Q = \lim_{k\to\infty} S_k,$$

where the subscript k indicates that the respective series should be taken to the kth order terms.)

However, another difficulty arises. Terms of the form

$$(N^{n-1}/\zeta) \int \exp(-\beta\phi)\, F_{Rr}^{n}\, d\tau, \qquad n \geqslant 3, \tag{47}$$

appear in J, whilst Q contains the double integrals

$$(N^{n-1}/\zeta^2) \iint \exp(-\beta\phi - \beta\phi')\, F_{rr'}^{n}\, d\tau\, d\tau', \qquad n \geqslant 3, \tag{48}$$

in the cubic and later terms. These integrals diverge in the three-dimensional case, for which equation (5a) holds, because the singularities in the integrands are too severe. Thus, in this case, it is meaningless to proceed further than the quadratic terms in the series without somehow modifying the potential at short range. It should be noted, though, that terms of the form (47) and (48) present no difficulties in one or two dimensions. Therefore, in theory, it is possible in these cases to extend the series to any desired degree of approximation.

Table 1. First correction term $w(\xi)$

z is the Emden radius, ρ_c/ρ_b the density contrast and ξ the dimensionless Emden length scale

z	ρ_c/ρ_b	ξ	w	z	ρ_c/ρ_b	ξ	w
0·010	1·000017	0·000	$-8{\cdot}8\times10^{-11}$	5·0	7·722	0·0	0·81
		0·002	$-7{\cdot}1\times10^{-11}$			1·0	0·66
		0·004	$-2{\cdot}6\times10^{-11}$			2·0	0·36
		0·006	$2{\cdot}6\times10^{-11}$			3·0	0·058
		0·008	$4{\cdot}0\times10^{-11}$			4·0	−0·22
		0·010	$14{\cdot}4\times10^{-11}$			5·0	−0·61
1·0	1·172	0·0	−0·0052	8·9931	32·125	0·000	2·4
		0·2	−0·0039			1·799	1·4
		0·4	−0·0006			3·597	0·25
		0·6	0·0028			5·396	−0·30
		0·8	0·0028			7·194	−0·55
		1·0	−0·0124			8·993	−0·90

Returning to equation (44), the correction $w(\boldsymbol{R})$ may be evaluated numerically, though the details of the calculation need not concern us. The results are most conveniently expressed in terms of the dimensionless Emden length scale

$$\xi = (4\pi G m \beta \rho_c)^{\frac{1}{2}} R, \tag{49}$$

where ρ_c is the central density. The Emden radius corresponding to the radius of the boundary R_b shall be denoted by z. It should be noted that the equilibrium isothermal gas spheres form a one-parameter family, that parameter being most conveniently either z or the density contrast ρ_c/ρ_b ($z = 0$ corresponds to $\rho_c/\rho_b = 1$ and $z = 8{\cdot}9931$ to $\rho_c/\rho_b = 32{\cdot}125$, the largest stable configuration). Table 1 gives $w(\xi)$ for various values of z. The very small corrections for $z = 0{\cdot}01$ are expected; for this configuration, gravity is practically absent and therefore, since no position is distinguishable from any other, the Emden density $v_1 = \text{const.}$ is exact.

Conversely, we know from the stability analysis that Q ceases to exist for $z > 8{\cdot}9931$, but since w is well behaved for all z it appears that the instability must manifest itself in the present analysis by the various series diverging. This conclusion seems consistent, in a very crude way, with the apparently monotonic increase in the magnitude of w with increasing z. We might therefore expect that w provides a good estimate of the size of the error for z sufficiently far below the critical value.

5. Two-particle Distribution Function

The two-particle distribution function is defined by

$$\nu_2(\boldsymbol{R},\boldsymbol{R}') = \left\langle \sum_{j=1}^{N}\sum_{i=1}^{N} \delta(\boldsymbol{r}_i-\boldsymbol{R})\,\delta(\boldsymbol{r}_j-\boldsymbol{R}')\right\rangle \qquad (i \neq j), \tag{50}$$

where the average is with respect to $\exp(-\beta V)$ again. Choosing two representative values of i and j, we may rewrite equation (50), as

$$\begin{aligned}\nu_2(\boldsymbol{R},\boldsymbol{R}') &= N(N-1)\langle\delta(\boldsymbol{r}_1-\boldsymbol{R})\,\delta(\boldsymbol{r}_2-\boldsymbol{R}')\rangle \\ &= \frac{N(N-1)}{N!\,Q}\int \exp(-\beta V)\,\delta(\boldsymbol{r}_1-\boldsymbol{R})\,\delta(\boldsymbol{r}_2-\boldsymbol{R}')\,\mathrm{d}\Omega_s .\end{aligned} \tag{51}$$

Defining $\langle\;\rangle_2$ according to

$$\langle g\rangle_2 \equiv \int \exp(-\beta U)\,g\,\delta(\boldsymbol{r}_1-\boldsymbol{R})\,\delta(\boldsymbol{r}_2-\boldsymbol{R}')\,\mathrm{d}\Omega_s \Big/ \int \exp(-\beta U)\,\delta(\boldsymbol{r}_1-\boldsymbol{R})\,\delta(\boldsymbol{r}_2-\boldsymbol{R}')\,\mathrm{d}\Omega_s, \tag{52}$$

and noting that

$$\begin{aligned}L(\boldsymbol{R},\boldsymbol{R}') &\equiv \int \exp(-\beta V)\,\delta(\boldsymbol{r}_1-\boldsymbol{R})\,\delta(\boldsymbol{r}_2-\boldsymbol{R}')\,\mathrm{d}\Omega_s \\ &= \exp(\beta\langle\Delta\rangle_2)\int \exp(-\beta U)\,\delta(\boldsymbol{r}-\boldsymbol{R})\,\delta(\boldsymbol{r}-\boldsymbol{R}')\exp\{\beta(\Delta-\langle\Delta\rangle_2)\}\,\mathrm{d}\Omega_s,\end{aligned} \tag{53}$$

we may expand as before to show that

$$L = \exp(\beta\langle\Delta\rangle_2)\,I\{1+\tfrac{1}{2}\beta^2(\langle\Delta^2\rangle_2-\langle\Delta\rangle_2^2)+\ldots\}, \tag{54}$$

where now

$$I = \int \exp(-\beta U)\,\delta(\boldsymbol{r}_1-\boldsymbol{R})\,\delta(\boldsymbol{r}_2-\boldsymbol{R}')\,\mathrm{d}\Omega_s = \zeta^{N-2}\exp\{-\beta\,\phi(\boldsymbol{R})-\beta\,\phi(\boldsymbol{R}')\}.$$

The relevant averages, although more complicated in form, may be calculated as in Section 4. Firstly, it is seen that

$$\langle\Delta\rangle_2 = -F(|\boldsymbol{R}-\boldsymbol{R}'|)+\frac{1}{N-1}\Big(\phi(\boldsymbol{R})+\phi(\boldsymbol{R}')\Big)+\frac{(N-2)(N+1)}{2(N-1)}\langle\phi\rangle . \tag{55}$$

Thus, in the stationary point approximation, the two-particle distribution function is, by equations (28), (51), (54) and (55),

$$v_2(\boldsymbol{R},\boldsymbol{R}') = \frac{N(N-1)}{\zeta^2}\exp\{-\beta\,\phi(\boldsymbol{R}) - \beta\,\phi(\boldsymbol{R}')\}$$

$$\times\exp\left\{-\beta\,F(|\,\boldsymbol{R}-\boldsymbol{R}'\,|) + \frac{\beta}{N-1}\langle\phi\rangle + \frac{\beta}{N-1}\Big(\phi(\boldsymbol{R})+\phi(\boldsymbol{R}')\Big)\right\}. \tag{56}$$

Noting equation (43), this may be rewritten in terms of the one-particle distribution function as

$$v_2(\boldsymbol{R},\boldsymbol{R}') = \exp\{-\beta\,F(|\,\boldsymbol{R}-\boldsymbol{R}'\,|)\}\,v_1(\boldsymbol{R})\,v_1(\boldsymbol{R}'), \tag{57}$$

except for terms, which depend on $\boldsymbol{R}$ and $\boldsymbol{R}'$ but not on $|\,\boldsymbol{R}-\boldsymbol{R}'\,|$, of relative order N^{-1}.

Equation (57) indicates the required modification to the Vlasov approximation. Although βF is generally $O(N^{-1})$, in two and three dimensions it has a singularity at $\boldsymbol{R} = \boldsymbol{R}'$ which, according to equation (57), enhances the probability of two given particles being extremely close to each other. In one dimension, F has no such singularity; we shall not consider this case further. It remains to be seen to what extent the further terms in the series alter the picture presented by equation (57).

The quadratic term may be calculated. Defining

$$\Lambda_2(\boldsymbol{R},\boldsymbol{R}') = \{N(N-1)/\zeta\}\int\exp(-\beta\phi)\,F_{Rr}\,F_{R'r}\,\mathrm{d}\tau, \tag{58}$$

we may show that, to order N^{-1},

$$\begin{aligned}\langle(\Delta-\langle\Delta\rangle_2)^2\rangle_2 = E_2 - N^{-1}\{&10\langle\phi^2\rangle + 6\langle\phi\rangle^2 + 5\big(\phi(\boldsymbol{R})+\phi(\boldsymbol{R}')\big)^2 + 2\langle\Lambda\rangle \\ &-4\langle\phi\rangle\,\big(\phi(\boldsymbol{R})+\phi(\boldsymbol{R}')\big) + 4\big(\chi(\boldsymbol{R})+\chi(\boldsymbol{R}')\big) \\ &-\big(\Lambda(\boldsymbol{R}) + 2\Lambda_2(\boldsymbol{R},\boldsymbol{R}') + \Lambda(\boldsymbol{R}')\big)\}.\end{aligned} \tag{59}$$

The important point to note here is that $F(|\,\boldsymbol{R}-\boldsymbol{R}'\,|)$ does not appear in this expression. Although it is present in $\langle UV\rangle_2$, $\langle V^2\rangle_2$ and $\langle\Delta\rangle_2^2$, when combined into $\langle(\Delta-\langle\Delta\rangle_2)^2\rangle_2$ it cancels exactly. This is a general property for all terms in the series. To prove this, note that we may write

$$\Delta = g(\boldsymbol{r}_i) - F_{12}, \tag{60}$$

where g contains $\phi(\boldsymbol{r}_1), \ldots, \phi(\boldsymbol{r}_N)$ and all the F's, such as F_{13}, F_{23}, F_{34} etc., but not F_{12}. By the definition (52), it may be seen that, for any function f of the coordinates,

$$\langle f\cdot(F_{12}-F_{RR'})\rangle_2 = 0. \tag{61}$$

Noting that

$$\Delta-\langle\Delta\rangle_2 = (g-\langle g\rangle_2)-(F_{12}-F_{RR'}), \tag{62}$$

we may write, using the binomial expansion,

$$\begin{aligned}\langle(\Delta-\langle\Delta\rangle_2)^m\rangle_2 &= \sum_{k=0}^{m}\tbinom{m}{k}(-1)^{m-k}\langle(g-\langle g\rangle_2)^k(F_{12}-F_{RR'})^{m-k}\rangle_2 \\ &= \langle(g-\langle g\rangle_2)^m\rangle_2,\end{aligned} \tag{63}$$

since, by equation (61), all terms containing $F_{12}-F_{RR'}$ have zero average.

Thus, since we are looking for singular terms which depend on $|\boldsymbol{R}-\boldsymbol{R}'|$, it would appear that no modification of equation (57) is required. However, this is not necessarily true. Consider, for example, the following term which appears in $\langle(\Delta-\langle\Delta\rangle_2)^3\rangle_2$:

$$D(\boldsymbol{R},\boldsymbol{R}') = \int \exp(-\beta\phi)\, F_{Rr}^2 F_{R'r}\, \mathrm{d}\tau\,. \tag{64}$$

For $\boldsymbol{R} \neq \boldsymbol{R}'$ this integral converges; however, in three dimensions, if $\boldsymbol{R} = \boldsymbol{R}'$ then the singularity in the integrand, which is of order 3, is too severe and the integral diverges. Thus, the function $D(\boldsymbol{R},\boldsymbol{R}')$ has a singularity at $\boldsymbol{R} = \boldsymbol{R}'$ (in fact, it behaves as a simple pole).

Note, however, that D, and other terms like it, always converge in two dimensions. Thus, the nature of the singularity suggested in equation (57) is exact in this case.

6. Discussion

It has been verified in Section 3, at least for the system in a heat bath, that the thermodynamics derived from statistical mechanics is equivalent to classical thermodynamics for the spherically symmetric self-gravitating system. This is important in view of the possible objections to the foundations of the classical theory based on the inapplicability of the cycle property (or zeroth law) to systems with long range forces. In addition, the conjecture (13) concerning the form of the one-particle distribution function has been shown to be justified. Thus the hydrostatic (Emden) theory of the equilibrium structure, as well as the global thermodynamics, has been demonstrated to be in accord with the statistical mechanics.

Furthermore, it was found in Section 4 that the deviation of ν_1 from the Emden density is of order N^{-1} (provided that, in three dimensions, the singularities are cut out). A rough approximation to the constant of proportionality multiplying the N^{-1} in this correction term showed that, for $N = 100$ say, the error in adopting the hydrostatic theory is unlikely to be greater than a few per cent, at least for z not too close to the critical value. However, the more important consideration is that the correction is of order N^{-1}, as distinct from $N^{-\frac{1}{2}}$. The particular significance of this result is that, for reasonably large N, the errors in the underlying distribution are small compared with the statistical fluctuations of particle number in a defined region, which typically go as $N^{-\frac{1}{2}}$. Thus, deviations from the Emden density will generally be of little physical significance in the systems which we consider.

A significant advantage of the present method is that any difficulties with singular potentials are not encountered until the cubic correction term, after most of the interesting information has been obtained. Hard core potentials or the like need to be invoked in principle only. This crystallizes, in a mathematical way, the idea that the hydrostatic (continuum) method, in which the physics of close interactions is neglected, provides an adequate description of a large system of particles.

Turning to the two-particle distribution function, we note that the error

$$\nu_2(\boldsymbol{R},\boldsymbol{R}')/\nu_1(\boldsymbol{R})\,\nu_1(\boldsymbol{R}') - 1$$

involved in adopting the Vlasov approximation is generally $O(N^{-1})$, in accordance with analyses based on the Liouville equation (Gilbert 1971).

In three dimensions it can be shown that the condition for the higher terms in the series expansion of v_1 to be small compared with unity is that $|\beta F| \ll 1$. Equation (57) indicates that this is also the condition for the Vlasov approximation to apply. This is not surprising in view of the fact that βF is a measure of the ratio of the gravitational energy of a pair interaction to the average kinetic energy of an individual particle.

However, in two dimensions no short distance cutoff is required to limit the size of the higher terms. Thus, in theory, the Vlasov approximation may break down, according to equation (57), even though the Emden form for v_1 remains valid. In practice, though, this is not important since (57) can be put in the form

$$v_2(\boldsymbol{R}, \boldsymbol{R}') = |\boldsymbol{R} - \boldsymbol{R}'|^{-z\beta\phi_b'/N} v_1(\boldsymbol{R})\, v_2(\boldsymbol{R}'),$$

and thus we see that only unrealistically small separations, of the order of e^{-N}, produce a significant effect.

In one dimension, no difficulties with singularities arise.

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