The Equilibrium Statistical Mechanics of a One-dimensional Self-gravitational System

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Abstract

The configurational integral and the single-particle and pair distributions for a one-dimensional gravitating system are calculated using approximate methods. The Helmholtz free energy and single-particle distributions are in good agreement with the exact analytical results. The pair distribution is new and shows that, in the Vlasov limit, it is approximately the product of two one-particle distributions. The method may be easily extended to more general systems.

1. Introduction

One-dimensional self-gravitating systems are of particular interest because they form a readily accessible laboratory for testing plausible theoretical assumptions. In particular, the validity of the Vlasov approximation can be tested, by examining the single-particle and pair distributions in the equilibrium system.

Rybicki (1971) has made some progress towards assessing the Vlasov approximation by evaluating the single-particle distribution exactly. To evaluate more complicated distributions, and to deal with more general systems, there is some advantage in giving up the attempt at exact evaluation and concentrating on approximate methods. The loss of accuracy may then be balanced by greater generality.

In this paper two approximate methods are used. One is a variational method which depends on the convexity properties of the canonical distribution. The other is a perturbation method analogous to that used by J. A. Barker (see e.g. Barker and Henderson 1976). The two methods are found to give similar, accurate results for the Helmholtz free energy and the single-particle distributions. Both may be easily extended to deal with more complicated problems, and in this paper they are used to evaluate the pair distribution. Mass segregation effects can also be studied.

The simplest approximate method is the variational method and we examine it first. The perturbation method is more complicated, but it has the advantage of allowing an increase in accuracy by simply considering more terms.

2. Partition Function

Following Rybicki (1971) we consider a one-dimensional system which is equivalent to a set of mass sheets, of mass per unit area σ , moving freely through each other. We take the centre of mass as fixed at the origin. This last requirement is not essential; we could take the centre of mass to be moving in an oscillator potential and recover similar results. The partition function Z takes the form

$$Z = \frac{1}{N!} \int \dots \int \delta(\bar{x}) \,\delta(\bar{p}) \exp(-\beta H) \,\mathrm{d}x_1 \dots \mathrm{d}x_N \,\mathrm{d}p_1 \dots \mathrm{d}p_N, \qquad (1)$$

with

$$-\infty < x_i, p_i < \infty, \qquad i = 1, 2, \dots, N,$$

where H is the Hamiltonian

$$H = \sum_{j=1}^{N} p_j^2 / 2\sigma + 2\pi G \sigma^2 \sum_{i < j} |x_i - x_j|$$
(2)

and

$$\bar{x} = N^{-1} \sum_{j=1}^{N} x_j, \qquad \bar{p} = \sum_{j=1}^{N} p_j.$$
 (3)

The integration over the momentum is trivial and Z reduces to

$$N^{-\frac{1}{2}}(2\pi\sigma/\beta)^{(N-1)/2}Q,$$
(4)

where Q is the configurational integral

$$Q = \frac{1}{N!} \int \dots \int \exp(-\beta V) \,\delta(\bar{x}) \,\mathrm{d}x_1 \dots \mathrm{d}x_N \tag{5}$$

and V is the potential term in H.

To evaluate Q we choose an approximate potential U defined by

$$U = b \sum_{j=1}^{N} |x_j|,$$
 (6)

where b is an arbitrary constant. This choice is motivated by the expectation that it is a good approximation to treat the particles as if they move independently in a background potential, and by the requirement that the integrals be simple. We now write equation (5) as

$$Q = \frac{1}{N!} \int \dots \int e^{-\beta U} e^{-\beta (V-U)} \delta(\bar{x}) \, \mathrm{d}x_1 \dots \mathrm{d}x_N.$$
⁽⁷⁾

To evaluate equation (7) it is convenient to use a variational principle. By observing that the tangent to e^{-f} always lies below the function, it is easy to establish, in function space, that

$$e^{-f} \ge e^{-a} + (f-a)(-ae^{-a}),$$
 (8)

where a is any value of f. Choosing $a = \langle f \rangle$, we find

$$\langle e^{-f} \rangle \ge e^{-\langle f \rangle}. \tag{9}$$

This variational principle has been used previously for the partition function (Feynman 1955; see also Barker and Henderson 1976). It proves to be a powerful device for the approximate evaluation of the n-particle distribution functions.

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To apply the result (9) to the evaluation of Q we write

$$\left\langle e^{-\beta(V-U)} \right\rangle = \int \dots \int e^{-\beta U} e^{-\beta(V-U)} \delta(\bar{x}) \, \mathrm{d}x_1 \dots \mathrm{d}x_N \Big/ \int \dots \int e^{-\beta U} \delta(\bar{x}) \, \mathrm{d}x_1 \dots \mathrm{d}x_N, \quad (10)$$

so that we have

$$Q \ge \frac{1}{N!} \int \dots \int e^{-\beta U} \delta(\bar{x}) \, \mathrm{d}x_1 \dots \mathrm{d}x_N \, e^{-\beta \langle V - U \rangle}. \tag{11}$$

The best choice of b in the potential U is then the one which maximizes the right-hand side of equation (11). By introducing the representation

$$\delta \bar{x}) = \int_{-\infty}^{\infty} \exp(2\pi i u \bar{x}) \, du \tag{12}$$

for the delta function, we find

$$\frac{1}{N!}\int \dots \int e^{-\beta U} \delta(\bar{x}) \, \mathrm{d}x_1 \dots \mathrm{d}x_N = \frac{1}{N!} \int_{-\infty}^{\infty} \Phi^N(u) \, \mathrm{d}u \,, \tag{13}$$

where

$$\Phi(u) = 2\beta b / (\beta^2 b^2 + 4\pi^2 u^2 / N^2).$$
(14)

The integral over u can be done analytically but there are some advantages in observing that, since N is very large, the integrand has a very sharp maximum at u = 0. Expanding about this point we find

$$\frac{1}{N!} \int_{-\infty}^{\infty} \Phi^{N}(u) \, \mathrm{d}u \approx \frac{1}{(N-1)!} \left(\frac{2}{\beta b}\right)^{N-1} \frac{1}{(\pi N)^{\frac{1}{2}}}.$$
(15)

The exponent of the remaining term in equation (11) can be written

$$\beta \langle V - U \rangle = \int_{-\infty}^{\infty} G(u) \, \mathrm{d}u \, \Big/ \int_{-\infty}^{\infty} \Phi^{N}(u) \, \mathrm{d}u \,, \tag{16}$$

where

$$G(u) = \frac{1}{2}\beta\lambda N(N-1)\Phi^{N-2}(u) \int_{-\infty}^{\infty} \exp\{-\beta b(|x|+|y|) + 2\pi i u(x+y)/N\} |x-y| \, dx \, dy$$
$$-\beta bN \, \Phi^{N-1}(u) \int_{-\infty}^{\infty} \exp\{-\beta b|x| + 2\pi i u x/N\} |x| \, dx \tag{17}$$

and $\lambda = 2\pi G\sigma^2$.

The expression (17) can be greatly simplified by noting that u can be set equal to zero in the slowly varying functions. Performing the integration we find

$$\beta \langle V - U \rangle \approx 3\lambda N(N-1)/4b - N.$$
 (18)

The variational principle now takes the form

$$Q \ge \frac{1}{(N-1)!} \left(\frac{2}{\beta b}\right)^{N-1} \frac{1}{(\pi N)^{\frac{1}{2}}} \exp\left(N - \frac{3\lambda N(N-1)}{4b}\right).$$
 (19)

The best choice of b is that which maximizes the right-hand side. We find it to be

$$b_0 = \frac{3}{4}\lambda N. \tag{20}$$

Using the Stirling approximation, the best estimate of Q, for the form of U chosen, is given by

$$\ln Q \approx -\ln\{((N-1)!)^2 (\beta \lambda)^{N-1}\} + \frac{1}{2} \ln 2 - \frac{1}{52} N.$$
(21)

The first term on the right-hand side of this expression is the exact result found by Rybicki (1971). The second and third terms are always negligible when N is large, because of the $((N-1)!)^2$ in the first term. Since the Helmholtz free energy is linear in $\ln Q$ the variational method reproduces the thermodynamic functions with a small percentage error. In particular the mean energy given by

$$\langle E \rangle = -\partial (\ln Z)/\partial \beta = 3(N-1)/2\beta$$
 (22)

is exact.

3. Single-particle Distribution Function

We define the single-particle distribution by

$$f(P,X) = N^{-1} \left\langle \sum_{j=1}^{N} \delta(x_j - X) \,\delta(p_j - P) \right\rangle,\tag{23}$$

where the angle brackets denote averages over the canonical ensemble. Since the integrand is symmetric in the variables we can select any one of them, for example j = 1, and write equation (23) as

$$f(P,X) = \langle \delta(x_1 - X) \, \delta(p_1 - P) \rangle. \tag{24}$$

The integration over the momentum is trivial (Rybicki 1971). The remaining integration over the spatial coordinates defines a one-particle distribution function $v_1(X)$ according to

$$v_1(X) = \frac{N \int \dots \int \delta(\bar{x}) \,\delta(x_1 - X) \exp(-\beta V) \,\mathrm{d}x_1 \dots \mathrm{d}x_N}{\int \dots \int \delta(\bar{x}) \exp(-\beta V) \,\mathrm{d}x_1 \dots \mathrm{d}x_N}.$$
(25)

If note is taken of the normalization

$$\int_{-\infty}^{\infty} v_1(X) \, \mathrm{d}X = N,$$

then equation (25) can be written

$$v_1(X) = NA \int \dots \int \delta(\bar{x}) \,\delta(x_1 - X) \exp(-\beta V) \,\mathrm{d}x_1 \dots \mathrm{d}x_N, \qquad (26)$$

where A is a normalization constant to be calculated later. The variational principle

can now be used in the form

$$\int \dots \int \delta(\bar{x}) \,\delta(x_1 - X) \exp(-\beta V) \,dx_1 \dots dx_N$$

$$\geq \int \dots \int \delta(\bar{x}) \,\delta(x_1 - X) \exp(-\beta U) \,dx_1 \dots dx_N \exp(-\beta F), \quad (27)$$

where

$$F = \frac{\int \dots \int (V-U) \,\delta(\bar{x}) \,\delta(x_1 - X) \exp(-\beta U) \,\mathrm{d}x_1 \dots \,\mathrm{d}x_N}{\int \dots \int \delta(\bar{x}) \,\delta(x_1 - X) \exp(-\beta U) \,\mathrm{d}x_1 \dots \,\mathrm{d}x_N}.$$
(28)

The calculation of Q shows that the variational calculation can lead to an error of the form $a(h)^N$ where a and h are constants. In the case of the thermodynamic functions this error is unimportant since they depend linearly on $\ln Q$. In the present case, errors of the same form again do not affect the final results because they are removed by the normalization. The combination of the variational principle with the normalization should lead to an accurate expression for $v_1(X)$, and this is borne out by comparison with the exact results.

By using the asymptotic expansions employed in Section 2 the right-hand side of the inequality (27) can be evaluated easily. We find it becomes

$$\left(\frac{2}{\beta b}\right)^{N-2} \left(\frac{N}{\pi}\right)^{\frac{1}{2}} \exp(-\beta b \mid X \mid)$$

$$\times \exp\left(N-1+\beta b \mid X \mid -\beta\lambda(N-1) \mid X \mid -\frac{3\lambda(N-1)(N-2)}{4b} -\frac{\lambda(N-1)\exp(-\beta b \mid X \mid)}{b}\right).$$
(29)

The condition for the function (29) to be stationary is

$$\frac{N-2}{b} - \frac{3\lambda(N-1)(N-2)}{4b^2} - \frac{\lambda(N-1)\exp(-\beta b |X|)}{b^2} - \frac{\lambda\beta(N-1)|X|\exp(-\beta\beta |X|)}{b} = 0.$$
 (30)

This expansion can be written

$$b = \frac{3}{4}\lambda(N-1)(1+\eta),$$
(31)

with

$$\eta = \frac{4}{3}(N-2)^{-1}\exp(-b\beta |X|)(1+b\beta |X|).$$
(32)

Because N is ≥ 1 , it is a good approximation to set $b = \frac{3}{4}\lambda N$ in η . The value of b defined by equation (31) determines the maximum. Finally, by substituting for b in (29) and normalizing the resulting expression, we find

$$v_1(X) \approx \frac{3}{8} \lambda N^2 \beta \exp\left\{1 - \omega - \frac{4}{3} \exp\left(-\frac{3}{4}\omega\right)\right\},\tag{33}$$

where $\omega = \beta \lambda (N-1) |X|$, and the normalization is accurate to 1.5%.

To compare the result (33) with the Vlasov value it is convenient to scale lengths with the unit

$$L = 2\langle E \rangle / 3\pi N^2 G \sigma^2 = 2(N-1)/N^2 \beta \lambda.$$
(34)

Then, with $X = L\xi$,

$$LN^{-1}v_1(X) = \frac{3}{4}\exp\{1-2|\xi| - \frac{4}{3}\exp(-\frac{3}{2}|\xi|)\}.$$
 (35)

The exact value of $v_1(X)$, in the limit $N \to \infty$ with $\langle E \rangle$ and $N\sigma$ constant, is contained in Rybicki's (1971) analysis. In scaled form

$$LN^{-1}v_1(X) = (2\cosh^2\xi)^{-1}, \qquad (36)$$

which is also the self-consistent field or Debye-Hückel result. In Table 1 the results of the present calculation are compared with the exact result. The agreement is very good.

Table 1. Comparison with the exact result of values of the single-particle
distribution according to two approximations in the Vlasov limitThe quantities F and q are defined in Section 5

Parameters			$LN^{-1}v_1(X)$			
ξ	а	F	Variational	Perturbation	Exact	
0.00	0.50	0.00	0.54	0.50	0.50	
0.25	0.62	0.00	0.49	0.45	0.47	
0 50	0.85	0.11	0.40	0.40	0.39	
0.75	0.66	0.20	0.29	0.29	0.30	
1.00	0.66	0.19	0.20	0.21	0.21	
1.25	0.61	0.13	0.14	0.15	0.14	
1.50	0.59	0.02	0.088	0.10	0.09	
1.75	0.73	0.00	0.056	0.057	0.057	
2.00	0.79	0.00	0.035	0.034	0.035	

4. Pair Distribution Function

We define the spatial pair distribution by

$$v_2(X_1, X_2) = \left\langle \sum_{j=1}^N \sum_{k=1}^N \delta(x_j - X_1) \, \delta(x_k - X_2) \right\rangle \quad (j \neq k), \tag{37}$$

where the average is over the canonical ensemble. Because of the symmetry of the integrand we can write

$$v_{2}(X_{1}, X_{2}) = \frac{N(N-1) \int \dots \int \exp(-\beta V) \,\delta(\bar{x}) \,\delta(x_{1} - X_{1}) \,\delta(x_{2} - X_{2}) \,dx_{1} \dots \,dx_{N}}{\int \dots \int \exp(-\beta V) \,\delta(\bar{x}) \,dx_{1} \dots \,dx_{N}}.$$
 (38)

The variational principle can be used to estimate the integral in this expression. We write

$$v_2(X_1, X_2) = N(N-1)A \int \dots \int \exp(-\beta V) \,\delta(\bar{x}) \,\delta(x_1 - X_1) \,\delta(x_2 - X_2) \,\mathrm{d}x_1 \dots \,\mathrm{d}x_N,$$

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where A is a constant chosen to ensure

$$\int \int v_2(X_1, X_2) \, \mathrm{d}X_1 \, \mathrm{d}X_2 = N(N-1) \, .$$

The variational principle then takes the form

$$\int \dots \int \exp(-\beta V) \,\delta(\bar{x}) \,\delta(x_1 - X_1) \,\delta(x_2 - X_2) \,\mathrm{d}x_1 \dots \,\mathrm{d}x_N$$

$$\geq \int \dots \int \exp(-\beta U) \,\delta(\bar{x}) \,\delta(x_1 - X_1) \,\delta(x_2 - X_2) \,\mathrm{d}x_1 \dots \,\mathrm{d}x_N \exp(-\beta G), \qquad (39)$$

where

$$G = \frac{\int \dots \int \exp(-\beta U) \,\delta(\bar{x}) \,\delta(x_1 - X_1) \,\delta(x_2 - X_2) (V - U) \,dx_1 \dots dx_N}{\int \dots \int \exp(-\beta U) \,\delta(\bar{x}) \,\delta(x_1 - X_1) \,\delta(x_2 - X_2) \,dx_1 \dots dx_N}.$$
 (40)

Evaluating the integrals, we find the right-hand side of the inequality (39) to be

$$\left(\frac{2}{\beta b}\right)^{N-3} \left(\frac{1}{\pi N}\right)^{\frac{1}{2}} \exp(-\beta b |X_1| - \beta b |X_2|) \times \exp\left\{-\beta \lambda |X_1 - X_2| - \frac{3\lambda (N-2)(N-3)}{4b} + \beta b(|X_1| + |X_2|) + N-2 -\beta \lambda (N-2)(|X_1| + |X_2|) - \frac{\lambda (N-2)}{b} \left(\exp(-\beta b |X_1|) + \exp(-\beta b |X_2|)\right)\right\}. (41)$$

The maximum of this expression occurs at

$$b = \frac{3}{4}\lambda(N-2)(1+\varepsilon), \qquad (42)$$

where

$$\varepsilon \approx \frac{4}{3}N^{-1}\left\{(1+\omega_1)\exp(-\omega_1) + (1+\omega_2)\exp(-\omega_2)\right\}, \qquad \omega_i = \beta b |X_i|.$$
(43)

Collecting these results we find, after normalizing, that

$$v_{2}(X_{1}, X_{2}) \approx N(N-1) \left(\frac{3}{8} \lambda N \beta\right)^{2} \\ \times \exp\left\{2 - \beta \lambda (N-2)(|X_{1}| + |X_{2}|) - \beta \lambda |X_{1} - X_{2}| - \frac{4}{3} (\exp(-\beta b |X_{1}| + \exp(-\beta b |X_{2}|)))\right\}.$$
(44)

Notice that the term involving $|X_1 - X_2|$ is always much smaller than the term involving $|X_1| + |X_2|$. Accordingly the pair spatial distribution function can be written very accurately as the product of a function of X_1 and a function of X_2 . In terms of the one-particle distribution calculated in Section 3, we have

$$v_2(X_1, X_2) \approx v_1(X_1) v_1(X_2),$$
(45)

which is the Vlasov approximation.

5. Perturbation Method

The perturbation method of Barker and Henderson (1976) involves the following simple idea. Choose a reference potential involving an adjustable parameter. Expand about the reference potential, and choose the parameter to minimize the absolute value of the first correction term. This minimization of the first correction term forces the reference potential to mimic the true potential. When the first correction term vanishes the method is then similar to a variational method, for the error is second order. It is, however, more flexible. An application to radiative transfer has been given by Monaghan (1970).

Table 2. Values of $v_2(X_1, X_2)/v_1(X_1) v_1(X_2)$ obtained using the nerturbation method

Here $X_i = L\xi_i$								
ξ2	Ratio $v_2(X_1, X_2)/v_1(X_1) v_1(X_2)$							
value	$\xi_1=0$	0.5	1.0	1.5	2.0			
0	1.0							
0.5	1.0	1.0						
$1 \cdot 0$	1.0	0.95	1.0					
1.5	1.0	0.91	0.98	1.0				
2.0	0.94	0.82	0.92	1.0	1.0			

Expanding the configurational integral we find

$$Q = \frac{1}{N!} \int \dots \int \delta(\bar{x}) \exp(-\beta U) \{1 - \beta(V - U) + \dots\} dx_1 \dots dx_N.$$
 (46)

With the same reference potential as before, the first correction term is least, in absolute value, for $b = \frac{3}{4}\lambda(N-1)$ and the approximation to Q is the same as that found in Section 2 (equation 21).

To evaluate $v_1(X)$ there is some analytical convenience in expanding both the numerator and denominator of equation (25) to first order. The resulting $v_1(X)$ is approximately then normalized. If this procedure is followed it will be found that

$$v_1(X) = \frac{1}{2}N\beta b \exp(-\beta b | X|)(1+F),$$
(47)

where b is determined by finding the least absolute value of

$$F = \frac{3}{2}(\lambda/b)(N-1) - 1 + \beta |X| \{b - \lambda(N-1)\} - (\lambda/b)(N-1)\exp(-\beta b |X|).$$
(48)

Defining a by $b = \lambda Na$ and using the length scale L, we find that equation (48) becomes

$$F \approx \frac{3}{2}a^{-1} - 1 + 2|\xi|(a-1) - a^{-1}\exp(-2|\xi|a).$$
(49)

For $\xi = 0$, the value of |F| is a minimum for a = 0.5. For $|\xi| \gtrsim 0$, the function |F| has two zeros, one near a = 0.5 and one with $a \ge 1$. We choose the root continuous with the first one. An alternative criterion would be to compute the next correction term and take the root which minimized the two. For larger $|\xi|$, the function |F| first has only a single minimum, and a is specified uniquely. For

still larger $|\xi|$, the function has two roots. One root lies on the track that gives $a \to 0$ (and therefore $b \to 0$) as $|\xi| \to \infty$. We reject this root because it implies that the particles are distributed at large distances as if the background potential were constant. This result is clearly unphysical because in one dimension the potential increases with distance. Accordingly we take the other root.

The one-particle distribution evaluated in this way is given in Table 1. There is evidently very good agreement between the two methods of approximation and the exact results. The values of F are also listed in Table 1 and they give an alternative estimate of the accuracy.

The same procedure as above may be applied to the pair distribution function. The calculations are straightforward and the details are not given here. The final results are presented in Table 2. They show that, in the perturbation approximation, the pair distribution may differ from the product of two single-particle distributions by up to 18%. However, over most of the domain, the approximation of a pair distribution by the product of two single-particle distributions is accurate.

6. Discussion and Conclusions

Since the two present methods of approximation give accurate results for the Helmholtz free energy and the single-particle distribution, it is reasonable to assume that the pair distribution derived here is a good approximation to the true distribution. The generally good agreement between the two different methods of approximation lends further weight to this view.

Taken together, the results of this paper show that the Vlasov approximation, of treating the particles as moving independently in a background potential, is quite accurate in the equilibrium state. It is an open question whether the approximation is good when the system is far from equilibrium.

The present analysis can be improved in two ways. The approximations can be made more accurate by including a more complicated potential in the variational method and by taking more terms in the perturbation method. The latter is easier because the integrals remain trivial. The analysis can also be improved by allowing the masses to be different. Mass segregation effects, of known importance in three dimensions, can then be analysed.

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