

Pair Correlation Function for a System with Velocity- Dependent Interactions

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The canonical statistical sum for the Breit–Darwin plasma is investigated by means of a generalized van Kampen cellular method. In particular, the pair correlation function is derived. This function agrees with that previously obtained by Trubnikov from the approximate closure of the BBGKY hierarchy. The method developed in this paper can be used for the description of other systems in which the velocity-dependent forces are pairwise.

KEY WORDS: Statistical sum; pair correlation function; velocity-dependent interactions; Breit–Darwin plasma; functional formulation of statistical mechanics.

1. INTRODUCTION

Two rather important problems are seldom discussed in the numerous papers and books concerning both equilibrium and nonequilibrium statistical mechanics: velocity-dependent interactions (VDI) and many-body forces.

There are many physical problems which require the use of many-body forces, for example, the study of very dense liquids. Also, the VDI become important in a variety of problems involving the motion of “impurities” in a medium. When the concentration of impurities is not too high we may assume

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that the properties of the medium are not dramatically different from those of the pure system. We can then eliminate the medium–impurity interaction by means of a suitable transformation of dynamical variables and, as a result, obtain a system of “impurities” (or “impuritons”) interacting via the VDI. (The interactions usually arise from the back-flow of the medium around the impurities.)

The VDI and many-body forces are intimately associated with the theory of charged particles. If v/c is not too small, we need a better approximation to the equation of motion of the particles than that provided by the Coulomb forces. The elimination of the field variables (to the first order in v/c) leads to a Hamiltonian description of the particle dynamics called the Breit–Darwin description. It was shown by Holstein and Primakoff⁽¹⁾ that in this approximation the Hamiltonian contains not only VDI but also genuine many-body velocity-dependent interactions, the latter being negligible only in systems with few particles.

The Holstein–Primakoff Hamiltonian for the Breit–Darwin plasma can be written as

$$H = T + U + \frac{1}{2} \sum_{A \neq B} \hat{\mathbf{P}}_A \cdot \mathbf{G} \cdot \hat{\mathbf{P}}_B \quad (1)$$

where T and U are the kinetic and Coulomb energies, respectively, and \mathbf{G} is a complicated function of two- and three-particle positions

$$\mathbf{G} = \mathbf{G}^{(2)}(\mathbf{r}_A - \mathbf{r}_B) + \sum_C \mathbf{G}^{(3)}(\mathbf{r}_A, \mathbf{r}_B, \mathbf{r}_C)$$

In (1), $\hat{\mathbf{P}}_A$ are the canonical momenta of the particles.

Since it is not very easy to handle either VDI or many-body forces by means of the methods of conventional statistical mechanics, Trubnikov and Kosachev⁽²⁾ and Trubnikov⁽³⁾ suggest a variant approach, which they call a Lagrangian formulation. By this they mean, for example, that in non-equilibrium problems the Liouville equation is written down directly from the equations of motion rather than from the Hamilton equations.

In the case of equilibrium statistical mechanics the fundamental quantity (canonical statistical sum) can be written as

$$Z = \int \delta \mathbf{r} \delta(mv) \{ \exp[-\beta E(\mathbf{r}, mv)] \} J(\hat{\mathbf{P}}/mv) \quad (2)$$

where \mathbf{r} and mv are the positions and kinematical momenta of the particles and E is the energy of the system expressed in terms of \mathbf{r} and mv . Here $J(\hat{\mathbf{P}}/mv)$ is the Jacobian of the transformation from the canonical momenta $\hat{\mathbf{P}}_A$ to the kinematical mv_A . The symbol $\delta \mathbf{r} \delta(mv)$ denotes integration with respect to all the particles:

$$\int \delta \mathbf{r} \delta(mv) \equiv \frac{1}{N!} \int_{\Omega} \prod_{A=1}^N d^3 r_A \int \prod_{A=1}^N d^3(mv_A)$$

The evaluation of Z in the form (2) is simpler for the reason that the energy E contains no many-body terms and the Jacobian J is velocity independent.

Note that for the systems with VDI for which the matrix \mathbf{G} in the Hamiltonian (1) contains no three-body terms there is no need for the transformation leading to Eq. (2) since the partition function Z is already of the form (2) (with $J = 1$).

The Lagrangian formulation was used in Ref. 2 for derivation of the thermodynamic properties of the Breit–Darwin plasma, for example, the equation of state. A fairly complicated form of BBGKY hierarchy was developed in Ref. 3 and the two-particle equilibrium distribution function was derived from its time-independent version. This function was used in Ref. 4 to investigate the eigenmodes of the Breit–Darwin plasma.

In this paper we propose a simple derivation of the pair correlation function for the Breit–Darwin plasma based on the use of the van Kampen cell method.^(5–7) This method is similar to that previously used by Jackson and Klein⁽⁸⁾ in their theory of the electric field fluctuations in a Coulomb plasma.

2. Q-INTEGRAL APPROXIMATION

We consider a system of N identical particles, “electrons,” each with mass m and charge $-e$ immersed in the neutralizing, positively charged background of infinitely heavy “ions.”

The Lagrangian for such a system, to first order in V/C , can be written as

$$L = \sum_{A=1}^N \frac{1}{2} m \mathbf{v}_A^2 - \frac{1}{2} \sum_{A \neq B} \frac{e^2}{r_{AB}} + \frac{1}{2} \sum_{A \neq B} \frac{e^2}{2c^2} \left\{ \frac{\mathbf{v}_A \cdot \mathbf{v}_B}{r_{AB}} + \frac{\mathbf{v}_A \cdot \mathbf{r}_{AB} \mathbf{v}_B \cdot \mathbf{r}_{AB}}{r_{AB}^3} \right\} \quad (3)$$

The canonical momentum $\hat{\mathbf{P}}_A$ is then equal to

$$\begin{aligned} \hat{\mathbf{P}}_A &= m \mathbf{v}_A + \sum_{B \neq A} \frac{e^2}{2c^2 r_{AB}} (1 + r_{AB}^{-2} \mathbf{r}_{AB} \otimes \mathbf{r}_{AB}) \cdot m \mathbf{v}_B \\ &\equiv m \mathbf{v}_A + \sum_{B \neq A} \mathbf{G}(\mathbf{r}_{AB}) \cdot m \mathbf{v}_B \end{aligned} \quad (4)$$

and the energy E is given by

$$E = \sum_{A=1}^N \frac{1}{2} m \mathbf{v}_A^2 + \frac{1}{2} \sum_{A \neq B} \frac{e^2}{r_{AB}} + \sum_{A \neq B} \frac{1}{2} m \mathbf{v}_A \cdot \mathbf{G}_{AB} \cdot m \mathbf{v}_B \quad (5)$$

In what follows it is more convenient to use the kinematical momenta $\mathbf{P}_A = m \mathbf{v}_A$ instead of the velocities \mathbf{v}_A as the independent variables.

If the transformation (4) is inverted and substituted into (5), we will obtain the Breit–Darwin Hamiltonian in the form derived by Holstein and

Primakoff,⁽¹⁾ i.e., with the many-body VDI. If this is done, any approximate statistical sum (for example, in the Mayer graph expansion form) becomes hopelessly complicated. Therefore we follow Ref. 2 and write the partition function Z as

$$Z = \int \delta\mathbf{r} \delta\mathbf{P} \{ \exp[-\beta E(\mathbf{r}, \mathbf{P})] \} J(\hat{\mathbf{P}}/\mathbf{P}) \quad (6)$$

where E is given by Eq. (5) and J is the Jacobian of the transformation (4).

From Eq. (4) it is obvious that J does not depend on the momenta \mathbf{P} , and its \mathbf{r} dependence is such that it is possible to evaluate J approximately.

It was shown in Ref. 2 that for practical purposes, at least in the ring approximation, the Jacobian J can be approximated by the equilibrium value $\sim \exp(-\Omega/d_c^3)$, where Ω is a volume of the system, and d_c is the characteristic screening length for (transverse) VDI, $d_c = c/\omega_p$, where ω_p is the plasma frequency.

The more detailed considerations of the modifications due to the presence of the Jacobian J are postponed to Appendix A.

Granted that with sufficient accuracy $J(\hat{\mathbf{P}}/\mathbf{P})$ does not enter the integration in (6), we can define the \mathbf{Q} -function as

$$\mathbf{Q} = \int \delta\mathbf{r} \delta\mathbf{P} \exp[-\beta E(\mathbf{r}, \mathbf{P})] = Z/J^{eq} \quad (7)$$

The integral \mathbf{Q} in Eq. (7) can be evaluated by means of the Mayer graph expansion. It should be noted, however, that now the bond functions f_{AB} depend on both the relative distance between particles and the momenta \mathbf{P}_A and \mathbf{P}_B . The Mayer graph expansion for \mathbf{Q} , in the ring approximation (the f_{AB} , as far as their \mathbf{r} dependence is concerned, are as bad as bond functions for the Coulomb gas), leads to the equation of state of the form derived in Ref. 2. Here we propose to use the phase-space generalization of the van Kampen cell method.⁽⁶⁻⁷⁾ It was shown in Ref. 6 that this method allows a relatively simple derivation of the pair correlation function for the Coulomb gas. It turns out that, using a generalized version of the Ornstein-Zernicke-Zwanzig integral transform,^(4,9) we shall be able to derive the pair correlation function for the Breit-Darwin plasma directly from (7) without invoking the apparatus of the BBGKY hierarchy.

3. PHASE-SPACE CELL APPROXIMATION FOR THE \mathbf{Q} INTEGRAL

Let us assume that the $6N$ -dimensional space of variables (\mathbf{r}, \mathbf{P}) is divided into \mathcal{N} cells each of volume Δ . Let us further assume that the cells Δ_α ($\alpha = 1, \dots, \mathcal{N}$) are sufficiently large that it is meaningful to associate with

each of the cells a number of particles f_α which is practically constant inside the cell. The size of a cell Δ should not be too big, however, since then the number of cells \mathcal{N} would decrease and the replacement of the original degrees of freedom (\mathbf{r}, \mathbf{P}) by the set of occupation numbers $\{f_\alpha\}$ would not be legitimate. It should be noted that details of the actual partition of the phase space as well as the actual sizes of the cells are unimportant for the present calculations. However, in some other applications of the cell method they can be quite important.⁽¹⁰⁾

The set of the occupation numbers f_α is obviously subject to the condition $\sum_\alpha f_\alpha = N$.

Associating each of the cells with a vector \mathbf{R}_α (position of the cell) and momentum \mathbf{P}_α , we can approximate the energy E in (5) by

$$E\{f_\alpha\} = \sum_\alpha f_\alpha (\mathbf{P}_\alpha^2/2m) + \frac{1}{2} \sum_{\alpha,\beta} f_\alpha U_{\alpha\beta} f_\beta + \frac{1}{2} \sum_{\alpha,\beta} f_\alpha \mathbf{P}_\alpha \cdot \mathbf{G}_{\alpha\beta} \cdot \mathbf{P}_\beta f_\beta \quad (8)$$

where we use the short-hand notation $U_{\alpha\beta} = U(\mathbf{R}_\alpha - \mathbf{R}_\beta)$, etc.; U is the Coulomb potential and \mathbf{G} is the matrix defined in Eq. (4). The summation in (8) is over all the \mathcal{N} cells, and it is reasonable to replace the distance $|\mathbf{R}_\alpha - \mathbf{R}_\beta|$ for $\alpha = \beta$ by, for example, the characteristic length of the spatial subvolume of the cell Δ . This term, however, as in the van Kampen procedure, is irrelevant for our further considerations and does not affect our results.

The integration $\int \delta\mathbf{r} \delta\mathbf{P}$ in (7) can now be replaced by the summation over all the possible realizations of the occupation numbers f_α consistent with the restriction $\sum_\alpha f_\alpha = N$.

Thus we have

$$\mathbf{Q} = \sum_{f_\alpha} \prod_\alpha \frac{\Delta^{f_\alpha}}{\prod_\alpha f_\alpha!} \exp\left\{-\beta\left(E\{f_\alpha\} - \mu \sum_\alpha f_\alpha\right)\right\} \quad (9)$$

where μ is the Lagrange multiplier associated with the constraint $\sum_\alpha f_\alpha = N$, i.e., the chemical potential, and the origin of the combinatorial factor is obvious.

Using the Stirling approximation for $f!$, we can rewrite the combinatorial factor in a form resembling the entropy of mixing, i.e.,

$$\prod_\alpha (\Delta^{f_\alpha}/f_\alpha!) \cong \exp\left\{-\sum_\alpha [f_\alpha \ln(f_\alpha/\Delta) - f_\alpha]\right\} \quad (10)$$

Then the \mathbf{Q} -function takes the form

$$\mathbf{Q} = \sum_{f_\alpha} \exp(-\beta F\{f_\alpha\}) \quad (11)$$

Here $F\{f_\alpha\}$ can be regarded as a coarse-grained free energy of the system.^(5-7,10)

According to Refs. 5–7, the equilibrium value of the occupation number f_{α}^{eq} is determined by the extremum (minimum) of the function $F\{f_{\alpha}\}$; i.e., $\partial F/\partial f_{\alpha} = 0$; and the quadratic approximation for F in the vicinity of the equilibrium value of f_{α} determines the pair correlation function.

The above scheme is obviously approximate and a rather important question should be answered before going further: What is the approximation involved? For the case of a gas of neutral particles interacting via the velocity-independent forces this question was answered rigorously.⁽¹³⁾

For the case of the Coulomb plasma the situation is much more complicated; nevertheless some conclusions can be achieved here, too. In the limit of the hot, dilute plasma, i.e., when the plasma parameter $\Gamma = \beta e^2 n_0^{1/3} \ll 1$, the quadratic approximation to the \mathbf{Q} -integral (11) is equivalent to the ring approximation in the Mayer graph expansion approach. The smallness of the parameter Γ is crucial for the whole cellular approach to the statistical mechanics of a plasma.⁽⁶⁾

In our case, when the VDI are present the situation remains the same as in the Coulomb case, provided the additional parameter $(d_c^3 n_0)^{-1} = (d/d_c)^3 = r_0/d_c$ is small. Here d is the mean distance between the particles, equal to $n_0^{-1/3}$, $d_c = c/\omega_p$, and r_0 is the classical radius of the electron. This parameter is usually very small indeed; for example, for hot, dilute plasma, where $n_0 = 10^{12} \text{ cm}^{-3}$ and $\omega_p = 5 \times 10^{10} \text{ sec}^{-1}$, $d/d_c \sim 10^{-4}$. For the thermonuclear plasma d/d_c is of the order of 10^{-2} .

If these two conditions $\Gamma \ll 1$ and $d/d_c \ll 1$ are satisfied, then the results obtained from the cellular method are equivalent to those obtained from the ring approximation. To the best of the author's knowledge, the pair correlation function for Breit–Darwin plasma was not derived by this method. The equivalent to our derivation of the correlation function, based on the BBGKY hierarchy, was proposed in Ref. 3.

The easiest way of comparing the ring approximation and the cellular approach is to compute the free energy of the system. If this is done, the results of both methods are indeed the same. The small addition to the free-particle part of the free energy which shows up in the cellular method calculations (see Ref. 6) is essentially an artefact of the lowest-order Stirling approximation in (10) and can be removed by taking into account higher-order terms.

To obtain post-ring approximation corrections to the free energy, correlation function, etc., for the Coulomb plasma is not the easiest thing to do. We are not going to do so for the Breit–Darwin plasma either. We feel, however, that this is not very interesting from the point of view of the velocity-dependent interactions. This is because the VDI corrections to the Coulomb post-ring approximation would be completely negligible, i.e., of higher order in d/d_c . The same refers to the corrections coming from the Jacobian $J(\hat{\mathbf{P}}/\mathbf{P})$ (see Appendix A).

It is a challenging problem to prove, in some detail, that the cellular method applied to the other system with VDI, as the Breit–Darwin plasma, would produce the correct results. We are strongly convinced that this is really the case and we do hope to return to this mathematical question in a separate publication. For the purpose of this paper, however, we feel that this is sufficient to appreciate the fact that the basically simple method proposed in the Ref. 5 can be used for the study of much more complicated systems and produces correct results.

4. EQUILIBRIUM DISTRIBUTION FUNCTION

It is more convenient from now on to use the functional notation, i.e., to replace the occupation numbers f_α by the one-particle distribution function $f(\mathbf{R}_\alpha, \mathbf{P}_\alpha) = f_\alpha/\Delta$, and the summation over cells by integration over continuous variables \mathbf{R}_α and \mathbf{P}_α according to the formula

$$\sum_{\alpha} \rightarrow \Delta^{-1} \int_{\Omega} d^3R \int d^3P$$

With this modification, F is now the functional of $f(\mathbf{R}, \mathbf{P})$ and the sum with respect to f_α should now be understood as a functional integration. The extremum condition $\partial F/\partial f_\alpha = 0$ now assumes the form

$$\delta F/\delta f(\alpha) = 0 \quad (12)$$

where $\alpha = (\mathbf{R}_\alpha, \mathbf{P}_\alpha)$.

Using the explicit form of F , we can write (12) as

$$\begin{aligned} 0 = & -\beta(\mathbf{P}_1^2/2m) - \beta \int d^3R_2 d^3P_2 U(\mathbf{R}_1 - \mathbf{R}_2) f(\mathbf{R}_2, \mathbf{P}_2) \\ & - \beta \int d^3R_2 d^3P_2 \mathbf{P}_1 \cdot \mathbf{G}(\mathbf{R}_1 - \mathbf{R}_2) \cdot \mathbf{P}_2 f(\mathbf{R}_2, \mathbf{P}_2) \\ & - \ln f(\mathbf{R}_1, \mathbf{P}_1) - \mu \end{aligned} \quad (12')$$

The solution of Eq. (12') is the Boltzmann distribution function $f^{\text{eq}} = A \exp(-\beta P^2/2m)$.

To see this, insert $A \exp(-\beta P^2/2m)$ into Eq. (12') and observe that the integral containing \mathbf{G} vanishes, and that the term proportional to $\int d^3R U(R)$ is equal to zero on the assumption of overall neutrality of the system. Since the constant A is obviously determined from the normalization $\int d^3R d^3p f = N$ and is equal to $n_0(2\pi m\beta)^{-3/2}$ ($n_0 = N/\Omega$), then Eq. (12) reduces to the usual relation between the chemical potential and the density n_0 for the ideal gas.

We conclude that the equilibrium distribution function for our system is

the Boltzmann distribution function

$$\begin{aligned} f^{\text{eq}}(\mathbf{R}, \mathbf{P}) &= n_0(2\pi m/\beta)^{-3/2} \exp(-\beta P^2/2m) \\ &\equiv n_0\varphi_B(\mathbf{P}) \end{aligned} \quad (13)$$

Should the full relativistic kinetic energy be used in (3) instead of its nonrelativistic limit, the equilibrium distribution will be the relativistic generalization of the Boltzmann one, i.e., the Jüttner distribution function.

Expanding the functional $F\{f\}$ around its extremum f^{eq} , we obtain

$$F\{f\} = F\{f^{\text{eq}} + \delta f\} = F\{f^{\text{eq}}\} + \frac{1}{2}(\delta f|\hat{\mathcal{F}}|\delta f) + \dots \quad (14)$$

where δf is the deviation of f from its equilibrium value and

$$(\xi|\eta) = \int d^3R d^3P \xi(\mathbf{R}, \mathbf{P})\eta(\mathbf{R}, \mathbf{P})$$

$\hat{\mathcal{F}}$ is the operator corresponding to the second functional derivative of $F\{f\}$. In the next section we will investigate this operator in some detail.

5. PAIR CORRELATION FUNCTION

The \mathbf{Q} -integral (11) can now be written as

$$\mathbf{Q} = [\exp(-\beta F\{f^{\text{eq}}\})] \int D \delta f \exp[-\frac{1}{2}\beta(\delta f|\hat{\mathcal{F}}|\delta f)] \quad (15)$$

where we use the expansion (14) and neglect the higher-order corrections.

Equation (15) indicates that the random variables δf have a Gaussian distribution. Hence, the inverse of the operator $\hat{\mathcal{F}}$ determines the correlation function $\langle \delta f(\mathbf{1}) \delta f(\mathbf{2}) \rangle$. More precisely, the operator $\hat{\mathcal{F}}^{-1}$ is an integral operator, with a kernel equal to $\langle \delta f(\mathbf{1}) \delta f(\mathbf{2}) \rangle$.

The correlation function $\langle \delta f(\mathbf{1}) \delta f(\mathbf{2}) \rangle$ can be identified with the pair correlation function because of its relation with the full two-particle distribution function $f^{(2)}(\mathbf{R}_1, \mathbf{R}_2; \mathbf{P}_1, \mathbf{P}_2)$,

$$\begin{aligned} f^{(2)}(\mathbf{R}_1, \mathbf{R}_2; \mathbf{P}_1, \mathbf{P}_2) &= \langle \delta f(\mathbf{R}_1, \mathbf{P}_1) \delta f(\mathbf{R}_2, \mathbf{P}_2) \rangle \\ &\quad + n_0^2 \varphi_B(\mathbf{P}_1) \varphi_B(\mathbf{P}_2) \\ &\quad - \delta(\mathbf{R}_1 - \mathbf{R}_2) \delta(\mathbf{P}_1 - \mathbf{P}_2) n_0 \varphi_B(\mathbf{P}_1) \end{aligned} \quad (16)$$

The derivation of Eq. (16) is sketched in Appendix B.

Using Eq. (12), we can easily compute the kernel \mathcal{F} of the operator $\hat{\mathcal{F}}$, by simple functional differentiation. We have, then,

$$\begin{aligned} \beta \frac{\delta^2 F}{\delta f(\mathbf{1}) \delta f(\mathbf{2})} \Big|_{f=f^{\text{eq}}} &\equiv \mathcal{F}(\mathbf{R}_{12}; \mathbf{P}_1, \mathbf{P}_2) = \beta \delta(\mathbf{P}_1 - \mathbf{P}_2) U(\mathbf{R}_{12}) \\ &\quad + \beta \mathbf{P}_1 \cdot \mathbf{G}(\mathbf{R}_{12}) \cdot \mathbf{P}_2 \\ &\quad + (f^{\text{eq}})^{-1} \delta(\mathbf{P}_1 - \mathbf{P}_2) \delta(\mathbf{R}_{12}) \end{aligned} \quad (17)$$

In order to find the kernel of the inverse operator \mathcal{F}^{-1} , we shall solve the integral equation

$$\int d^3R_2 d^3P_2 \mathcal{F}(\mathbf{R}_{12}; \mathbf{P}_1, \mathbf{P}_2) \eta(\mathbf{R}_2, \mathbf{P}_2) = \xi(\mathbf{R}_1, \mathbf{P}_1) \quad (18)$$

for the function $\eta(\mathbf{R}, \mathbf{P})$. The solution of Eq. (18) written as $\eta = \int d\mathbf{2} \mathcal{F}^{-1}(\mathbf{1}, \mathbf{2}) \xi(\mathbf{2})$ determines the inverse kernel \mathcal{F}^{-1} .

It is convenient to proceed with solution of (18) after taking its Fourier transform with respect to the space variables and redefining η as $\eta(\mathbf{R}, \mathbf{P}) = n_0 \varphi_B(\mathbf{P}) \chi(\mathbf{R}, \mathbf{P})$. We have then:

$$\begin{aligned} \xi_{\mathbf{k}}(\mathbf{P}_1) &= \chi_{\mathbf{k}}(\mathbf{P}_1) + n_0 \beta U_{\mathbf{k}} \int d^3P_2 \chi_{\mathbf{k}}(\mathbf{P}_2) \varphi_B(\mathbf{P}_2) \\ &+ n_0 \beta \mathbf{P}_1 \cdot \mathbf{G}_{\mathbf{k}} \cdot \int d^3P_2 \varphi_B(\mathbf{P}_2) \chi_{\mathbf{k}}(\mathbf{P}_2) d^3P_2 \end{aligned} \quad (19)$$

We can solve Eq. (19) in two steps. First let us multiply (19) by $\varphi_B(\mathbf{P}_1)$ and then integrate over \mathbf{P}_1 (note that φ_B is normalized to unity). Because the third term on the right-hand side of (19) vanishes, we obtain

$$\int d^3P \varphi_B(\mathbf{P}) \chi_{\mathbf{k}}(\mathbf{P}) = (1 + n_0 \beta U_{\mathbf{k}})^{-1} \int d^3P \varphi_B(\mathbf{P}) \xi_{\mathbf{k}}(\mathbf{P}) \quad (20)$$

Next, let us multiply (19) by $\mathbf{P}_1 \varphi_B(\mathbf{P}_1)$ and again integrate over \mathbf{P}_1 . Since

$$\int d^3P \mathbf{P} \otimes \mathbf{P} \varphi_B(\mathbf{P}) = m \beta^{-1} \mathbf{1}$$

we obtain:

$$\int d^3P P^a \varphi_B(\mathbf{P}) \xi_{\mathbf{k}}(\mathbf{P}) = (\delta^{ab} + n_0 m G_{\mathbf{k}}^{ab}) \int d^3P \varphi_B(\mathbf{P}) P^b \chi_{\mathbf{k}}(\mathbf{P}) \quad (21)$$

Let $\Gamma_{\mathbf{k}}^{ab}$ be the inverse of the matrix $\{\delta^{ab} + n_0 m G_{\mathbf{k}}^{ab}\}$. Then (21) can be re-written as

$$\int d^3P P^a \varphi_B(\mathbf{P}) \chi_{\mathbf{k}}(\mathbf{P}) = \Gamma_{\mathbf{k}}^{ab} \int d^3P P^b \varphi_B(\mathbf{P}) \xi_{\mathbf{k}}(\mathbf{P}) \quad (22)$$

Solving Eq. (19) with respect to χ , we use the integral relations (20) and (22).

In this way we obtain

$$\begin{aligned} \chi_{\mathbf{k}}(\mathbf{P}) &= \xi_{\mathbf{k}}(\mathbf{P}) - n_0 \beta U_{\mathbf{k}} (1 + n_0 \beta U_{\mathbf{k}})^{-1} \int d^3P \varphi_B(\mathbf{P}) \xi_{\mathbf{k}}(\mathbf{P}) \\ &- n_0 \beta \mathbf{P} \cdot \mathbf{G}_{\mathbf{k}} \cdot \Gamma_{\mathbf{k}} \cdot \int d^3P_2 \varphi_B(\mathbf{P}_2) \mathbf{P}_2 \xi_{\mathbf{k}}(\mathbf{P}_2) \end{aligned} \quad (23)$$

We note that the transformation from ξ to χ given by Eqs. (20) and (21) is indeed a generalization of the Ornstein–Zernicke integral transform.^{4,9}

The right-hand side of Eq. (23) multiplied by $n_0\varphi_B(\mathbf{P})$ defines the inverse kernel $\mathcal{F}_{\mathbf{k}}^{-1}(\mathbf{P}_1, \mathbf{P}_2)$

$$\mathcal{F}_{\mathbf{k}}^{-1}(\mathbf{P}_1, \mathbf{P}_2) = n_0\varphi_B(\mathbf{P}_1) \delta(\mathbf{P}_1 - \mathbf{P}_2) + n_0^2\varphi_B(\mathbf{P}_1)\varphi_B(\mathbf{P}_2) \left\{ -\frac{\beta U_{\mathbf{k}}}{1 + n_0\beta U_{\mathbf{k}}} - \beta \mathbf{P}_1 \cdot \mathbf{G}_{\mathbf{k}} \cdot \Gamma_{\mathbf{k}} \cdot \mathbf{P}_2 \right\} \quad (24)$$

Comparing now (24) with (16), we are able to write the two-particle distribution function for our system as

$$f_{\mathbf{k}}^{(2)}(\mathbf{P}_1, \mathbf{P}_2) = n_0^2\varphi_B(\mathbf{P}_1)\varphi_B(\mathbf{P}_2)\{\delta(\mathbf{k}) + g_{\mathbf{k}}(\mathbf{P}_1, \mathbf{P}_2)\} \quad (25)$$

where the pair-correlation function $g_{\mathbf{k}}(\mathbf{P}_1, \mathbf{P}_2)$ is given by

$$g_{\mathbf{k}}(\mathbf{P}_1, \mathbf{P}_2) = -[\beta U_{\mathbf{k}}/(1 + n_0\beta U_{\mathbf{k}})] - \beta \mathbf{P}_1 \cdot \mathbf{G}_{\mathbf{k}} \cdot \Gamma_{\mathbf{k}} \cdot \mathbf{P}_2 \quad (26)$$

The pair correlation function given in (26) consists of two parts. The first part is just the conventional radial pair correlation function for the system with the potential U , and the second is the genuine velocity-dependent correction. Our correlation function $g_{\mathbf{k}}$ can also be written as

$$g_{\mathbf{k}}(\mathbf{P}_1, \mathbf{P}_2) = -\beta U_{\mathbf{k}}^{\text{eff}} - \beta \mathbf{P}_1 \cdot \mathbf{G}_{\mathbf{k}}^{\text{eff}} \cdot \mathbf{P}_2 \quad (26')$$

This allows us to write the $f^{(2)}$ function as $f^{(2)} \sim \exp[-\beta(U^{\text{eff}} + \mathbf{P}_1 \cdot \mathbf{G}^{\text{eff}} \cdot \mathbf{P}_2)]$.

This is the behavior of the two-particle distribution function expected on the basis of general arguments; i.e., the $f^{(2)}$ should be proportional to $\exp(-\beta\bar{U})$, where \bar{U} should be an effective two-particle interaction energy. Effective here means that the bare interaction energy between the particles should be recognizable in terms of \bar{U} only at small relative distances; at large spatial separation \bar{U} should be negligible and the two-particle function $f^{(2)}$ should be just the product of equilibrium distribution functions. This is exactly the case for our function (26), as can be seen from the explicit calculations in the next section.

6. EXPLICIT CALCULATION OF $g_{\mathbf{k}}(\mathbf{P}_1, \mathbf{P}_2)$

Equations (25) and (26) are the solutions of our problem. In order to see that they agree with the BBGKY solution of Trubnikov, we shall compute the various Fourier transforms appearing in them.

The Fourier transform of the $G^{ab}(\mathbf{x})$ matrix from Eq. (4) is

$$\begin{aligned} G_{\mathbf{k}}^{ab} &= \int d^3x (\exp i\mathbf{k} \cdot \mathbf{x}) \frac{e^2}{2m^2c^2} \left(\frac{\delta^{ab}}{|\mathbf{x}|} + \frac{x^a x^b}{|\mathbf{x}|^3} \right) \\ &= (n_0 d_c^2 k^2) \Pi_{\mathbf{k}}^{ab} \end{aligned} \quad (27)$$

where d_c is the characteristic screening length for the VDI (transverse!),

which is incidently the London penetration depth, $d_c = c/\omega_p$, and $\Pi_{\mathbf{k}}^{ab}$ is the projection operator in a direction perpendicular to \mathbf{k} :

$$\Pi_{\mathbf{k}}^{ab} = \delta^{ab} - k^a k^b / k^2$$

The inverse of the matrix $\delta^{ab} + mn_0 G_{\mathbf{k}}^{ab}$ can be computed quite easily and is equal to

$$\Gamma_{\mathbf{k}}^{ab} = (1 + k^2 d_c^2)^{-1} k^2 d_c^2 (\delta^{ab} - k^a k^b / k^2) \quad (28)$$

In this way the effective matrix $\mathbf{G}_{\mathbf{k}}^{\text{eff}}$ is given by

$$\mathbf{G}_{\mathbf{k}}^{\text{eff}} = m^{-1} (1 + k^2 d_c^2)^{-1} \Pi_{\mathbf{k}} \quad (29)$$

and the velocity-dependent part of $g_{\mathbf{k}}$ is

$$-(n_0 \boldsymbol{\beta} / m) (1 + k^2 d_c^2)^{-1} \Pi_{\mathbf{k}}^{ab} P_1^a P_2^b$$

The velocity-independent part is just the Debye–Hückel function; i.e., $1/(1 + k^2 d^2)$, where d is the Debye radius.

The final form of $g_{\mathbf{k}}(\mathbf{P}_1, \mathbf{P}_2)$ is then

$$g_{\mathbf{k}}(\mathbf{P}_1, \mathbf{P}_2) = \frac{1}{1 + k^2 d^2} + \frac{1}{1 + k^2 d_c^2} \frac{\beta}{m} \mathbf{P}_1 \cdot \Pi_{\mathbf{k}} \cdot \mathbf{P}_2 \quad (30)$$

The inverse Fourier transform of (30) is then

$$g(\mathbf{R}_{12}; \mathbf{P}_1, \mathbf{P}_2) = g^{\text{DH}}(\mathbf{R}_{12}) + (\beta e^2 / m^2 c^2 d_c) \mathbf{P}_1 \cdot \mathbf{F}(\mathbf{R}_{12} / d_c) \cdot \mathbf{P}_2 \quad (31)$$

where

$$\mathbf{F}(\mathbf{x}) = 1/|\mathbf{x}|^{-1} (\exp -|\mathbf{x}|) + \nabla \otimes \nabla \{ (1 - \exp -|\mathbf{x}|) / |\mathbf{x}| \}$$

This is the Trubnikov⁽³⁾ form of the pair correlation function. For distances $|\mathbf{x}|$ short compared to d and d_c , the effective energy of interaction between the particles given by (31) is the bare energy of two particles computed from expression (5); for large distances the effective energy of interaction between the particles is negligible.

7. CONCLUSIONS

As was shown above, the simple phase-space cell method allows us to compute the pair correlation function for a Breit–Darwin plasma. Our derivation seems to be much simpler than that in Ref. 3, at least in the opinion of the present author! The above calculations support our use of the correlation function (30) in the Zwanzig equation for the eigenmodes of the Breit–Darwin plasma.⁽⁴⁾ As was mentioned in Ref. 4, the use of the correlation function proposed by Krizan⁽¹¹⁾ leads to divergences in the coefficients in the

kinetic equation. These divergences are due to the long-range oscillations in the space dependence of the Krizan function.

These oscillations apparently result from use of the restricted Darwin–Breit Hamiltonian, i.e., the Hamiltonian in which many-body interactions are omitted. In Ref. 4 the use of the restricted Darwin–Breit Hamiltonian leads to no trouble since the averaged Liouville operator in the Zwanzig variational principle derived from it and that in Trubnikov’s Lagrangian approach coincide.

It is a challenging problem to carry over the calculation of the statistical sum Z directly from the full Hamiltonian⁽¹⁾ since it requires some feeling about how to handle not only velocity-dependent but also many-body forces. The above formalism could be applied to any other physical system with pairwise VDI. One can think about the use of this approach in the theory of solutions, for example, ^3He atoms in ^4He . The interaction between the ^3He atoms due to the back-flow of ^4He is of the form $\mathbf{P}_1\mathbf{P}_2 \cdot \mathbf{f}(r_{12})$. The other possible candidate is the system of quasiparticles in ^4He rotons. Recently Roberts and Donnelly⁽¹²⁾ considered some dynamical problems in ^4He using a dipolelike form of the interaction between the rotons.

These two problems are certainly more interesting than the Breit–Darwin plasma from the point of view of possible practical applications. To now, however, it is only the latter for which the statistical theory has been developed in some detail. It seems to be reasonable, therefore, to use this system as a test of the applicability of a new theoretical technique.

APPENDIX A

The statistical sum (6) contains the Jacobian of the transformation from the generalized momenta $\hat{\mathbf{P}}_A$ to the kinematical momenta $\mathbf{P}_A \equiv m\mathbf{v}_A$. It was assumed in our calculations that this Jacobian is essentially a constant number and, for that reason, it is sufficient to investigate the \mathbf{Q} -integral only.

In this appendix we should like to discuss this approximation in greater detail.

First, let us note that the Jacobian $J(\hat{\mathbf{P}}/\mathbf{P})$ is the determinant of the $3N$ -dimensional matrix

$$\delta^{ab} \delta_{AB} + G_{AB}^{ab}, \quad a = 1, 2, 3, \quad A = 1, \dots, N \quad (\text{A.1})$$

We will denote the $3N$ -dimensional matrix trace by Tr and the trace operation with respect to the tensor indices (a, b) by tr .

We have the following identity valid for all nonsingular matrices:

$$\text{Det } a = \exp(\text{Tr} \log a) \quad (\text{A.2})$$

Equation (A.2) together with the formal expansion $\log(1+a) = -\sum_{n=1}^{\infty} n^{-1}(-1)^n a^n$ allows us to write

$$J(\hat{\mathbf{P}}/\mathbf{P}) = \text{Det}(1 + G) = \exp\left\{-\sum_{n=1}^{\infty} \frac{(-1)^n}{n} \text{Tr } G^n\right\} \equiv \exp \Phi \quad (\text{A.3})$$

We note that the J could be now incorporated into the energy in exponent of (6) in the guise of a potential energy term $V_J = -\beta^{-1}\Phi$, which, however, contains many-body interactions.

Going over to the occupation number representation and then using the functional notation from Sections 3 and 4, we are able to write (A.3) in the form

$$\Phi = -\sum_{n=2}^{\infty} \frac{(-1)^n}{n} \varphi_n \quad (\text{A.4})$$

where

$$\varphi_n = \int d\mathbf{1} \cdots d\mathbf{n} f(\mathbf{1}) \cdots f(\mathbf{n}) \text{tr } \mathbf{G}(\mathbf{1}, \mathbf{2}) \cdots \mathbf{G}(\mathbf{n}, \mathbf{1}) \quad (\text{A.5})$$

The $n = 1$ term is omitted from the cell version of (A.3) on the same basis as the one-cell contributions to the Coulomb energy in Eq. (8), i.e., we replace $\mathbf{G}_{\alpha\alpha}$ by some constant and then $\text{Tr } G$ contributes an additional irrelevant constant to the free energy $F\{f_{\alpha}\}$. Due to the translational invariance of $\mathbf{G}(\mathbf{R}_i - \mathbf{R}_j)$, the structure of the n th integral φ_n is analogous to the ring integrals in the Mayer graph extension.

The Jacobian potential $V_J = -\beta^{-1}\Phi$ contributes terms of the order of r_0/d_c smaller than the other terms in Eq. (12), where r_0 is the classical electron radius, $r_0 = (e^2/mc^2) \sim 10^{-13}$ cm.

To see this, compute the derivative of V_J :

$$\begin{aligned} \frac{\delta V_J}{\delta f(\mathbf{1})} &= -\beta^{-1} \sum_{n=2}^{\infty} (-1)^n \int d\mathbf{2} \cdots d\mathbf{n} f(\mathbf{2}) \cdots f(\mathbf{n}) \\ &\quad \times \text{tr } \mathbf{G}(\mathbf{1}, \mathbf{2}) \cdots \mathbf{G}(\mathbf{n}, \mathbf{1}) \end{aligned} \quad (\text{A.6})$$

The solution of Eq. (12), supplemented by the term (A.6), is again given by the Boltzmann distribution function. Indeed, the integrals on the right-hand side of (A.6) for $f = f^{\text{eq}} = n_0 \varphi_B$ do not depend on \mathbf{R}_1 and can be evaluated by transforming to the Fourier space in \mathbf{R} ,

$$L_n = [\delta \varphi_n / \delta f(\mathbf{1})]_{f=f^{\text{eq}}} = n(n_0)^{n-1} \int d^3k \text{tr}\{\mathbf{G}(\mathbf{k})\}^n$$

Using the Fourier transform of $\mathbf{G}(\mathbf{k})$ given in (27) and noting that the matrix $\mathbf{\Pi}_{\mathbf{k}}$ is idempotent, we obtain $L_n = n_0^{-1} \int d^3k (k^2 d_c^2)^{-n}$ and thus

$$\sum_2^{\infty} \frac{1}{n_0} \int d^3k (-1)^n (k^2 d_c^2)^{-n} = \frac{2\pi^3}{n_0 d_c^3} \sim \frac{r_0}{d_c}$$

This term is negligible in comparison with other terms in Eq. (12), since the classical radius of electron r_0 is always much less than d_c .

As we see, it is quite legitimate to keep the Boltzmann function as an equilibrium distribution function.

In a rather more cumbersome way, it is possible to establish that the corrections to the second derivative of F due to the presence of V_J are also negligible.

The other way of taking into account the Jacobian corrections is via the Mayer graph extension of Z . Using the language of Ref. 2, we have then two kinds of bonds, Mayer bonds $f_{AB} = \exp(-\beta E_{AB}) - 1$ and Jacobian bonds. The ring approximation is equivalent, in the functional formulation, to the following procedure: We write Z as

$$Z = \langle \exp\{-\beta E\} \exp\{-\beta V_J\} \rangle$$

where $\langle \dots \rangle$ denotes functional integration. We compute the equilibrium distribution function taking into account the full functional $E + V_J$. Further we write

$$Z = [\exp(-\beta V_J \{f^{eq}\})][\exp\{-\beta F\{f^{eq}\}\}] \\ \times \langle \exp[-\frac{1}{2}(\delta f | \hat{\mathcal{F}} | \delta f)] \rangle$$

Since the equilibrium distribution function is still of the Boltzmann form, there is no difference between the above formula and the formula in which we use the \mathbf{Q} -integral.

This is exactly the same approximation which was used by Trubnikov and Kosacher in their calculations of the thermodynamic properties of the Breit–Darwin plasma. The pair correlation function which we derive in this paper using the approximation described above is equivalent to that which follows from the approximate closure of the BBGKY hierarchy in Ref. 3.

APPENDIX B

The relation between the two-particle distribution function and the mean value of the product of the two single-particle distribution functions (16) is based upon the following arguments.

Consider the exact one-particle distribution function $\hat{f}(\mathbf{R}, \mathbf{P})$,

$$\hat{f}(\mathbf{R}, \mathbf{P}) = \sum_{A=1}^N \delta(\mathbf{R} - \mathbf{R}_A) \delta(\mathbf{P} - \mathbf{P}_A) \quad (\text{B.1})$$

This function, averaged over the volume Δ_α , gives the microscopic definition of the function $f(\mathbf{R}_\alpha, \mathbf{P}_\alpha)$. The mean value of \hat{f} with respect to the probability

distribution function $\rho(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{P}_1, \dots, \mathbf{P}_N)$ is equal to the one-particle distribution function f^{eq} ,

$$f^{\text{eq}} = n_0 \varphi_B, \quad \text{i.e. } \langle \hat{f} \rangle = f^{\text{eq}}$$

The two-particle distribution function $f^{(2)}$ is defined as

$$\int d^3 R_3 \dots d^3 R_N d^3 P_3 \dots d^3 P_N \rho(\mathbf{R}, \mathbf{R}', \mathbf{R}_3, \dots, \mathbf{R}_N; \mathbf{P}, \mathbf{P}', \mathbf{P}_3, \dots, \mathbf{P}_N) \\ = \left\langle \sum_{A \neq B} \delta(\mathbf{R} - \mathbf{R}_A) \delta(\mathbf{P} - \mathbf{P}_A) \delta(\mathbf{R}' - \mathbf{R}_B) \delta(\mathbf{P}' - \mathbf{P}_B) \right\rangle \quad (\text{B.2})$$

The right-hand side of (B.2) can also be written as

$$\langle \hat{f}(\mathbf{R}, \mathbf{P}) \hat{f}(\mathbf{R}', \mathbf{P}') \rangle - \delta(\mathbf{R} - \mathbf{R}') \delta(\mathbf{P} - \mathbf{P}') \langle \hat{f}(\mathbf{R}, \mathbf{P}) \rangle$$

and therefore

$$f^{(2)}(\mathbf{R}, \mathbf{R}'; \mathbf{P}, \mathbf{P}') = \langle \hat{f}(\mathbf{R}, \mathbf{P}) \hat{f}(\mathbf{R}', \mathbf{P}') \rangle - \delta(\mathbf{R} - \mathbf{R}') \delta(\mathbf{P} - \mathbf{P}') f^{\text{eq}} \quad (\text{B.3})$$

In terms of our coarse-grained function f , (B.3) takes the same form, but now the average denoted by $\langle \dots \rangle$ is taken over the function space with the weight function $\exp(-\beta F\{f\})$.

Assuming $f = f^{\text{eq}} + \delta f$, we can rewrite (B.3) as

$$f^{(2)}(\mathbf{R}_1, \mathbf{R}_2; \mathbf{P}_1, \mathbf{P}_2) = \langle \delta f(\mathbf{R}_1, \mathbf{P}_1) \delta f(\mathbf{R}_2, \mathbf{P}_2) \rangle \\ - \delta(\mathbf{R}_1 - \mathbf{R}_2) \delta(\mathbf{P}_1 - \mathbf{P}_2) n_0 \varphi_B(\mathbf{P}_1) + n_0^2 \varphi_B(\mathbf{P}_1) \varphi_B(\mathbf{P}_2) \quad (\text{B.4})$$

where we use the quadratic (Gaussian) approximation for $F\{f\}$ and hence $\langle \delta f \rangle = 0$.

Note that (B.4) is the formula (16) of the text.

The use of the coarse-grained, one-particle distribution function as a fundamental dynamical variable is analogous to the Vlasov description used in plasma physics.

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