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## CLASSICAL GREEN'S FUNCTIONS FOR THE IDEAL GAS\*

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March 31, 1970

## ABSTRACT

We use the equation-of-motion technique to establish a chain of equations for retarded, double-time Green's functions of an ideal gas. Termination of this chain allows reproduction of the usual results obtained by other methods.

Bogolyubov and Sadovnikov<sup>1</sup> have introduced double-time retarded and advanced Green's functions into the statistical mechanics of classical systems. This development is of course closely related to the earlier work of Kubo.<sup>2</sup> In their paper, Bogolyubov and Sadovnikov established a hierarchy of classical Green's functions by varying the single time distribution functions of the Bogolyubov-Born-Green-Kirkwood-Yvon hierarchy with respect to an infinitesimal external field. For a Coulomb plasma, the simplest decoupling of this system allowed them to obtain the usual Debye form for the correlation function. The method was used by Sadovnikov in a number of papers.<sup>3-5</sup> Herzog<sup>6</sup> rederived the Bogolyubov-Sadovnikov Green's function hierarchy using the double-time theory of Rostoker.

This letter investigates the problem of evaluating the Green's function related to the density correlation of an ideal gas. In contradistinction to the Bogolyubov-Sadovnikov approach,<sup>1</sup> we establish

a hierarchy by the equation-of-motion technique common to the development of hierarchies for quantum systems.<sup>7,8</sup> We thereupon introduce a device which allows decoupling of the hierarchy.

To begin, we consider the ideal gas, which has a Hamiltonian given by

$$H = \sum_{i=1}^N \frac{p_i^2}{2m}. \quad (1)$$

The number density is given by

$$n(\underline{r}, t) = V^{-1} \sum_{i=1}^N \sum_{\underline{k}} e^{i\underline{k} \cdot (\underline{q}_i(t) - \underline{r})}. \quad (2)$$

The retarded Green's function we wish to calculate is

$$\langle\langle n(x); n(y) \rangle\rangle = V^{-2} \sum_{\underline{k}, \underline{l}} \sum_{i, j=1}^N G_{ijkl}^0(\tau) e^{-i(\underline{k} \cdot \underline{r} + \underline{l} \cdot \underline{r}')}, \quad (3)$$

where  $V$  is the volume of the system,  $x = (\underline{r}, t)$ ,  $y = (\underline{r}', t')$ , and

$$\begin{aligned} G_{ijkl}^0(\tau) &= \theta(\tau) \langle [ e^{i\underline{k} \cdot \underline{q}_i(\tau)}, e^{i\underline{l} \cdot \underline{q}_j(0)} ] \rangle \\ &= \langle\langle e^{i\underline{k} \cdot \underline{q}_i(\tau)}; e^{i\underline{l} \cdot \underline{q}_j(0)} \rangle\rangle. \end{aligned} \quad (4)$$

Here  $\theta(\tau)$  is the unit step function,  $\langle \dots \rangle$  indicates a statistical average, and  $[ \dots ]$  Poisson brackets. We also have  $\tau = t - t'$ . In what follows we will have occasion to use the following Green's functions

$$G_{ijk\ell}^n(\alpha, \tau) = \left\langle \left\langle p_{iz}^n e^{ikq_{iz}}; e^{i\ell \cdot q_j(0)} \right\rangle \right\rangle_{\alpha}, \quad (5)$$

for  $n = 0, 1, 2,$

with  $\underline{k}$  along the  $z$  axis,  $q_{iz} = q_{iz}(\tau)$ ,  $p_{iz} = p_{iz}(\tau)$ , and the function

$$f^0(\alpha) = g e^{-\alpha p_{iz}^2}, \quad (6)$$

with

$$g = Q^{-1} \exp \left[ -\beta \left( H - \frac{p_{iz}^2}{2m} \right) \right] \quad (7)$$

being used to obtain our statistical average in Eq. (5). We will eventually set  $\alpha = \beta/2m$ , and  $Q$  is the appropriate normalization for  $\alpha = \beta/2m$ . If the equation-of-motion technique is used, the first two equations of our hierarchy will be

$$\begin{aligned} \frac{\partial G^0(\alpha, \tau)}{\partial \tau} &= \frac{ik}{m} G^1(\alpha, \tau), \\ \frac{\partial G^1(\alpha, \tau)}{\partial \tau} &= \frac{ik}{m v_0 (2\alpha)^{1/2}} \delta_{ij} \delta_{-\underline{k}\ell} \delta(\tau) + \frac{ik}{m} G^2(\alpha, \tau). \end{aligned} \quad (8)$$

Indices have been suppressed on our Green's functions, and  $v_0^{-2} = m\beta$ . The special construction of  $f^0$  allows termination of the hierarchy:

$$\begin{aligned}
G^2(\alpha, \tau) &= \int d\Gamma r^0(\alpha) \left[ p_{iz}^2 e^{ikq_{iz}}, e^{i\vec{l} \cdot \vec{q}_j(0)} \right] \\
&= - \int d\Gamma \frac{\partial r^0(\alpha)}{\partial \alpha} \left[ e^{ikq_{iz}}, e^{i\vec{l} \cdot \vec{q}_j(0)} \right] \\
&\quad - \frac{1}{\alpha} \int d\Gamma g \left[ e^{-\alpha p_{iz}^2}, e^{i\vec{l} \cdot \vec{q}_j(0)} \right] e^{ikq_{iz}} \\
&= - \frac{\partial G^0(\alpha, \tau)}{\partial \alpha} + \frac{G^0(\alpha, \tau)}{\alpha} \\
&\quad - \frac{1}{\alpha} \int d\Gamma g \left[ e^{-\alpha p_{iz}^2} e^{ikq_{iz}}, e^{i\vec{l} \cdot \vec{q}_j(0)} \right] \\
&= - \alpha \frac{\partial}{\partial \alpha} \left( \frac{G^0(\alpha, \tau)}{\alpha} \right), \tag{9}
\end{aligned}$$

where  $d\Gamma$  is an element of volume in phase space. The last integral gives no contribution, since  $r^0$  vanishes at the boundaries of phase space. Hence, from Eqs. (8) and (9), we see that  $G^0(\alpha, \tau)$  satisfies

$$\frac{\partial^2 G^0(\alpha, \tau)}{\partial \tau^2} - \alpha \left( \frac{k}{m} \right)^2 \frac{\partial}{\partial \alpha} \frac{G^0(\alpha, \tau)}{\alpha} = - \frac{k^2}{m^2 v_0 (2\alpha)^{1/2}} \delta_{ij} \delta_{\vec{k}\vec{l}} \delta(\tau). \tag{10}$$

It may be verified by direct substitution that the solution of Eq. (10) is

$$G^0(\alpha, \tau) = \frac{-k^2 \tau \theta(\tau)}{m^2 v_0 (2\alpha)^{1/2}} \exp \left[ - \frac{1}{4\alpha} \left( \frac{k\tau}{m} \right)^2 \right] \delta_{ij} \delta_{\vec{k}\vec{l}}. \tag{11}$$

Having found  $G^0(\alpha, \tau)$ , we set  $\alpha = \beta/2m$ , and so obtain

$$G_{ijkl}^0(\tau) = - \frac{k^2 \tau \theta(\tau)}{m} \exp \left[ - \frac{1}{2} (k v_0 \tau)^2 \right] \delta_{kj} \delta_{\vec{k}\vec{l}}. \tag{12}$$

[This result may be obtained easily by evaluating Eq. (4) directly with  $q_i(\tau) = q_i(0) + p_i(0)\tau/m$ , the orbit equation.] Inserting the above expression into Eq. (3), we obtain, after changing the remaining sum over  $k$  to an integral,

$$\langle\langle n(x); n(y) \rangle\rangle = \frac{\theta(\tau)}{m v_0} \frac{d}{d\sigma(\tau)} f(\underline{R}, \sigma(\tau)), \quad (13)$$

where  $\underline{R} = \underline{r} - \underline{r}'$ ,

$$f(\underline{R}, \sigma(\tau)) = \frac{n_0}{(2\pi)^{3/2} \sigma(\tau)^3} \exp \left[ -\frac{1}{2} \left( \frac{\underline{R}}{\sigma(\tau)} \right)^2 \right], \quad (14)$$

$n_0$  is the equilibrium density, and  $\sigma(\tau) = v_0\tau$ . The correlation function is related to the coefficient of  $\theta(\tau)$  in Eq. (13):<sup>1</sup>

$$\beta \frac{d}{d\tau} \langle n(x) n(y) \rangle = \frac{1}{m v_0} \frac{d}{d\sigma(\tau)} f(\underline{R}, \sigma(\tau)). \quad (15)$$

Upon integration of Eq. (15), we get the usual expression

$$\langle n(x) n(y) \rangle = n_0^2 + f(\underline{R}, \sigma(\tau)), \quad (16)$$

which result may be obtained by a direct evaluation of the correlation function.

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FOOTNOTES AND REFERENCES

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