Submitted to Physical Review Letters

UCRL-19746
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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[1] 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.[2] 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.[3-5] Herzel[6] 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,[1] we establish

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

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

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

The number density is given by

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

The retarded Green's function we wish to calculate is

$$\langle\langle n(x);\, n(y)\rangle\rangle = V^{-2} \sum_{\underset{\sim}{k}\underset{\sim}{\ell}} \sum_{i,j=1}^{N} G^{0}_{ij\underset{\sim}{k}\underset{\sim}{\ell}}(\tau)\, e^{-i(\underset{\sim}{k}\cdot\underset{\sim}{r}+\underset{\sim}{\ell}\cdot\underset{\sim}{r}')} , \tag{3}$$

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

$$G^{0}_{ij\underset{\sim}{k}\underset{\sim}{\ell}}(\tau) = \theta(\tau) \left\langle \left[e^{i\underset{\sim}{k}\cdot\underset{\sim}{q}_i(\tau)},\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)} \right] \right\rangle$$

$$\equiv \left\langle\!\!\left\langle e^{i\underset{\sim}{k}\cdot\underset{\sim}{q}_i(\tau)};\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)} \right\rangle\!\!\right\rangle . \tag{4}$$

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

$$G^{n}_{ij\underset{\sim}{k}\underset{\sim}{\ell}}(\alpha,\tau) = \left\langle\left\langle p_{iz}{}^{n}\, e^{ikq_{iz}};\, e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)}\right\rangle\right\rangle_{\alpha} , \tag{5}$$

for $n = 0, 1, 2,$

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

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

with

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

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

$$\frac{\partial G^{0}(\alpha,\tau)}{\partial\tau} = \frac{ik}{m}\, G^{1}(\alpha,\tau) ,$$

$$\frac{\partial G^{1}(\alpha,\tau)}{\partial\tau} = \frac{ik}{m\, v_{o}(2\alpha)^{1/2}}\, \delta_{ij}\, \delta_{-\underset{\sim}{k}\underset{\sim}{\ell}}\, \delta(\tau) + \frac{ik}{m}\, G^{2}(\alpha,\tau). \tag{8}$$

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

$$
\begin{aligned}
G^2(\alpha,\tau) &= \int d\Gamma\, f^o(\alpha) \left[p_{iz}^{\,2}\, e^{ikq_{iz}},\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)} \right] \\
&= -\int d\Gamma\, \frac{\partial f^o(\alpha)}{\partial\alpha} \left[e^{ikq_{iz}},\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)} \right] \\
&\qquad - \frac{1}{\alpha}\int d\Gamma\, g \left[e^{-\alpha p_{iz}^{\,2}},\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)} \right] e^{ikq_{iz}} \\
&= -\frac{\partial G^0(\alpha,\tau)}{\partial\alpha} + \frac{G^0(\alpha,\tau)}{\alpha} \\
&\qquad - \frac{1}{\alpha}\int d\Gamma\, g \left[e^{-\alpha p_{iz}^{\,2}}\, e^{ikq_{iz}},\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)} \right] \\
&= -\alpha \frac{\partial}{\partial\alpha}\left(\frac{G^0(\alpha,\tau)}{\alpha} \right) , \qquad (9)
\end{aligned}
$$

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

$$
\frac{\partial^2 G^0(\alpha,\tau)}{\partial\tau^2} - \alpha\left(\frac{k}{m}\right)^2 \frac{\partial}{\partial\alpha}\frac{G^0(\alpha,\tau)}{\alpha} = -\frac{k^2}{m^2\, v_o (2\alpha)^{1/2}}\, \delta_{ij}\, \delta_{-\underset{\sim}{k}\ell}\, \delta(\tau). \qquad (10)
$$

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

$$
G^0(\alpha,\tau) = \frac{-k^2\, \tau\, \theta(\tau)}{m^2\, v_o (2\alpha)^{1/2}} \exp\left[-\frac{1}{4\alpha}\left(\frac{k\tau}{m}\right)^2 \right] \delta_{ij}\, \delta_{-\underset{\sim}{k}\ell} . \qquad (11)
$$

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

$$
G^0_{ij\underset{\sim}{k}\underset{\sim}{\ell}}(\tau) = -\frac{k^2\, \tau\, \theta(\tau)}{m} \exp\left[-\frac{1}{2}(k\, v_o\, \tau)^2 \right] \delta_{kj}\, \delta_{-\underset{\sim}{k}\ell} . \qquad (12)
$$

[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 $\underset{\sim}{k}$ to an integral,

$$\langle\langle n(x);\, n(y)\rangle\rangle = \frac{\theta(\tau)}{m\, v_o} \frac{d}{d\sigma(\tau)} f(\underset{\sim}{R}, \sigma(\tau)) , \tag{13}$$

where $\underset{\sim}{R} = \underset{\sim}{r} - \underset{\sim}{r}'$,

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

n_0 is the equilibrium density, and $\sigma(\tau) = v_o\tau$. The correlation function is related to the coefficient of $\theta(\tau)$ in Eq. (13):[1]

$$\beta \frac{d}{d\tau} \langle n(x)\, n(y)\rangle = \frac{1}{mv_o} \frac{d}{d\sigma(\tau)} f(\underset{\sim}{R}, \sigma(\tau)) . \tag{15}$$

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

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

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

The author wishes to thank Dr. Charlie Harper and Dr. Charles Ray Smith for helpful suggestions and comments.

FOOTNOTES AND REFERENCES

* This work was supported in part by the U. S. Atomic Energy Commission and in part by the Air Office of Scientific Research, Office of Aerospace Research, U. S. Air Force under grant number AF-AFOSR-68-1616A.

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