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CLASSICAL GREEN'S FUNCTIONS FOR THE IDEAL GAS*

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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

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

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

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

with

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

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

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

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

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:

$$G^2(\alpha,\tau) = \int d\Gamma\ f^o(\alpha)\ \left[p_{iz}{}^2\ e^{ikq_{iz}},\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)}\right]$$

$$= -\int d\Gamma\ \frac{\partial f^o(\alpha)}{\partial\alpha}\left[e^{ikq_{iz}},\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)}\right]$$

$$- \frac{1}{\alpha}\int d\Gamma\ g\left[e^{-\alpha p_{iz}{}^2},\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)}\right]\ e^{ikq_{iz}}$$

$$= -\frac{\partial G^0(\alpha,\tau)}{\partial\alpha} + \frac{G^0(\alpha,\tau)}{\alpha}$$

$$- \frac{1}{\alpha}\int d\Gamma\ g\left[e^{-\alpha p_{iz}{}^2}\ e^{ikq_{iz}},\ e^{i\underset{\sim}{\ell}\cdot\underset{\sim}{q}_j(0)}\right]$$

$$= -\alpha\frac{\partial}{\partial\alpha}\left(\frac{G^0(\alpha,\tau)}{\alpha}\right)\ , \qquad (9)$$

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

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

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

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

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

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

[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,

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

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 $\sigma(\tau) = v_0\tau$. The correlation function is related to the coefficient of $\theta(\tau)$ in Eq. (13):[1]

$$\beta\,\frac{d}{d\tau}\,\langle n(x)\ n(y)\rangle = \frac{1}{mv_0}\ \frac{d}{d\sigma(\tau)}\ f(\underset{\sim}{R},\ \sigma(\tau))\ . \tag{15}$$

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.

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FOOTNOTES AND REFERENCES

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