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# Complement to the Wigner-Kirkwood Expansion

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We extend the region of applicability of phase-space techniques, for the study of quantum systems, by developing an expansion for the Wigner distribution function and correlation functions, in powers of an interaction potential. These results are not restricted to the near-classical regime (expansion in powers of $\hbar$), in contrast to the Wigner-Kirkwood expansion. The relation to other perturbation methods (Lindstedt-Poincaré, Green's function) is explored.

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Quantum distribution functions, first introduced by Wigner,[1] provide a means of studying quantum mechanical systems while still employing a phase-space framework. In particular, for a canonical ensemble, the Wigner-Kirkwood (WK) expansion[1-3] provides a method for obtaining quantum corrections expressed in powers of $\hbar$ (near-classical regime). Here we investigate the possibility of the use of distribution function techniques to obtain results *not* restricted to the near-classical regime, in contrast to the WK approach. We find that it is possible to go beyond the WK expansion in one respect, by developing instead an expansion in powers of an interaction potential, for the distribution function and—even more significantly—for the correlation function. However, since the WK method does not assume a weak interaction potential (although it must be smooth), our results should be viewed as a complement of the WK method in that *we have extended the region of applicability of phase-space techniques for the study of quantum systems.*

A wealth of information regarding the equilibrium and dynamic properties of a system may be derived from correlation functions of the form

$$C_{AA}(t)=\tfrac{1}{2}\langle \hat{A}(t)\hat{A}(0)+\hat{A}(0)\hat{A}(t)\rangle, \tag{1}$$

where $\hat{A}(t)=e^{i\hat{H}t/\hbar}\hat{A}e^{i\hat{H}t/\hbar}$ is a Heisenberg operator and $\langle \hat{O}\rangle=\mathrm{Tr}(\hat{\rho}\hat{O})$, $\hat{\rho}$ being the density operator for a canonical ensemble at inverse temperature $\beta$:

$$\hat{\rho}=e^{-\beta\hat{H}}/\mathrm{Tr}(e^{-\beta\hat{H}}) \tag{2}$$

($\hat{H}$ is the Hamiltonian). In condensed-matter physics $C_{AA}(t)$ is commonly obtained from the temperature Green's function[4]

$$G(\sigma)=\langle T[\hat{A}(\sigma)\hat{A}(0)]\rangle \tag{3}$$

[where $\hat{A}(\sigma)=e^{\sigma H}\hat{A}e^{\sigma H}$ and $T$ is the time-ordering operator] via analytic continuation. An alternative method for the computation of correlation functions makes use of the Wigner distribution function (WDF).[1,3] This approach has been used to find the quantum corrections (i.e., the near-classical limit) to transport properties,[5-7] but does not appear to have been widely applied otherwise. In particular, the important problem of developing a perturbation theory for the WDF is largely unexplored. The purpose of this work is to present new results concerning the evaluation of correlation functions by use of the WDF. An important feature of our discussion is the avoidance of the WK expansion,[8] so that the validity of our results is not restricted to the near-classical regime.

First, we examine how the WDF may be used to determine time correlation functions for a canonical ensemble. The formal expression of Eq. (1) in phase-space language was given some time ago by Hynes *et al.*,[5] who showed that

$$C_{AA}(t) = \int dq \int dp\, [P_w(q,p;\beta)\cos(\tfrac{1}{2}\hbar\Lambda)A_w(0)]A_w(t), \tag{4}$$

where $q$ and $p$ denote classical coordinate and momentum (all integrations extend from $-\infty$ to $+\infty$ unless otherwise specified),

$$P_w(q,p,\beta)=(\pi\hbar)^{-1}\int dy\langle q-y\,|\hat{\rho}\,|\,q+y\rangle e^{2ipy/\hbar} \tag{5}$$

is the normalized WDF, and

$$\Lambda\equiv\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q}-\frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}, \tag{6}$$

the arrows indicating the direction of operation. [In Eq. (4) $\Lambda$ operates only on the quantities within brackets.] By $O_w$ we denote the phase-space equivalent of the operator $\hat{O}$,

$$O_w(q,p)=2\int dy\,\langle q-y\,|\,\hat{O}\,|\,q+y\rangle e^{2ipy/\hbar}, \tag{7}$$

so that

$$\int dq\int dp\,O_w(q,p)P_w(q,p)=\mathrm{Tr}(\hat{\rho}\hat{O}). \tag{8}$$

In addition, we note from Eqs. (5) and (7) that $P_w$ is $(2\pi\hbar)^{-1}$ times the phase-space function corresponding to the density operator. If $\hat{O}=\hat{O}(\hat{q})$, then $O_w=O(q)$, and similarly for $\hat{O}(\hat{p})$.

The time dependence of $A_w(t)\equiv[\hat{A}(t)]_w$ is governed by[1,3,8]

$$\frac{\partial A_w}{\partial t}=iLA_w(t)=\left[\frac{p}{m}\frac{\partial}{\partial q}-\frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right]V(q)\right]A_w, \tag{9}$$

so that, formally,

$$A_w(t)=e^{iLt}A_w. \tag{10}$$

In the second term of Eq. (9), the $\partial/\partial q$ is understood to operate only on the potential, $V(q)$.

In all but the simplest cases (free particle, harmonic oscillator), $H$ is such that neither $A_w(t)$ nor $P_w(q,p;\beta)$ may be evaluated exactly. We shall be interested in the case

$$\hat{H}=\hat{H}_0+\lambda\hat{H}'=\hat{p}^2/2m+V_0(\hat{q})+\lambda\hat{H}'(\hat{q}), \tag{11}$$

where $P_w^{(0)}(q,p;\beta)$, the WDF corresponding to $\hat{H}_0$, is known exactly. We shall develop an expansion for the correlation function in the coupling $\lambda$.

We shall avoid making an additional expansion in powers of $\hbar$. Thus the validity of our results will *not* be restricted to the nearly classical regime. For simplicity we consider the correlation

$$\begin{aligned}C(t)&=\tfrac{1}{2}\langle\hat{q}(t)\hat{q}(0)+\hat{q}(0)\hat{q}(t)\rangle\\&=\int dq\int dp\,P_w(q,p;\beta)q(0)q(t)\\&=\int dq\int dp\,P_w(q,p,\beta)qe^{iLt}q.\end{aligned} \tag{12}$$

For the Hamiltonian, Eq. (11), the Liouvillian may be written

$$iL=\frac{p}{m}\frac{\partial}{\partial q}-\frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\frac{\partial}{\partial q}\frac{\partial}{\partial p}\right][V_0(q)+\lambda H'(q)]=iL_0+i\lambda L'. \tag{13}$$

Since $L_0$ and $L'$ do not commute, the expansion of $e^{iLt}$ in powers of $\lambda$ is not straightforward. We therefore turn our attention to the Laplace transform

$$J(s)=\int_0^\infty dt\,e^{-st}C(t)=\int_0^\infty dt\int dq\,dp\,P_w(q,p;\beta)qe^{iLt-st}q=\langle q(s-iL)^{-1}q\rangle, \tag{14}$$

where the angular brackets now denote a phase-space average with respect to the WDF. The perturbation expansion of $(s-iL)^{-1}$ is furnished by the "resolvent expansion" of kinetic theory.[9] Then, using $P_n(q,p;\beta)$ to denote the WDF correct to $n$th order in the coupling $\lambda$, and $\langle\ \rangle_n$ to denote a phase-space average with respect to $P_n$, we find after some algebra that

$$\begin{aligned}J(s)=\langle q(s-iL_0)^{-1}q\rangle_n\Bigg[1&+\lambda\frac{\langle q(s-iL_0)^{-1}iL'(s-iL_0)^{-1}q\rangle_{n-1}}{\langle q(s-iL_0)^{-1}q\rangle_{n-1}}+\cdots\\&+\lambda^n\frac{\langle q(s-iL_0)^{-1}iL'\ \ldots\ (s-iL_0)^{-1}q\rangle_0}{\langle q(s-iL_0)^{-1}q\rangle_0}\Bigg]+O(\lambda^{n+1}),\end{aligned} \tag{15}$$

which is our formal expansion for the Laplace transform of the correlation function. We turn now to the evaluation of $P_n$.

For the following discussion it proves convenient to work with an unnormalized WDF,

$$\Omega_w(q,p;\beta)\equiv(e^{-\beta\hat{H}})_w. \tag{16}$$

Then

$$P_w(q,p;\beta)=\Omega_w(q,p;\beta)/\int\int dq\,dp\,\Omega_w(q,p)\equiv\Omega_w(q,p;\beta)/2\pi\hbar Z(\beta), \tag{17}$$

where $Z(\beta)$ is the partition function and $\Omega_w$ satisfies the Wigner phase-space equivalent of the Bloch equation.

Our problem is to evaluate $\Omega_w(q,p;\beta)=\{\exp[-\beta(\hat{H}_0+\lambda\hat{H}')]\}_w$, where $\Omega_w^{(0)}$, the WDF corresponding to $\hat{H}_0$, is known. Since $\hat{H}_0$ and $\hat{H}'$ do not commute, the exponential cannot readily be expanded in powers of $\lambda$. We may, however, use as our starting point an expression familiar from the temperature Green's-function formalism,[4]

$$e^{-\beta\hat{H}}=e^{-\beta\hat{H}_0}U(\beta,0), \tag{18}$$

where

$$U(\beta,0)=1-\lambda\int_0^\beta \tilde{H}'(\sigma)\,d\sigma+\frac{\lambda^2}{2!}\int_0^\beta d\sigma_1\int_0^\beta d\sigma_2\,T[\tilde{H}'(\sigma_1)\tilde{H}'(\sigma_2)]+\ldots$$
$$+\frac{(-\lambda)^n}{n!}\int_0^\beta d\sigma_1\cdots\int_0^\beta d\sigma_n\,T[\tilde{H}'(\sigma_1)\cdots\tilde{H}'(\sigma_n)]+\ldots, \tag{19}$$

where

$$\tilde{H}(\sigma)=e^{\sigma\hat{H}_0}\hat{H}'e^{-\sigma\hat{H}_0} \tag{20}$$

is the perturbation in the "interaction picture," and where $T$ is the time-ordering operator.

We may now use Eqs. (18) and (19) and the well-known rule for the Wigner translation of an operator product to write

$$\Omega_w(q,p;\beta)=\Omega_w^{(0)}(q,p;\beta)e^{\hbar\Lambda/2i}[U(\beta,0)]_w$$
$$=\Omega_w^{(0)}\left[1-\lambda e^{\hbar\Lambda/2i}\int_0^\beta d\sigma[\tilde{H}'(\sigma)]_w+\ldots\right]. \tag{21}$$

When Eqs. (17) and (21) are used in conjunction with Eq. (15) we have our desired result, viz., the expansion of the Laplace transform of the correlation function in powers of the interaction potential.

As an illustration of our results we consider the one-dimensional anharmonic oscillator, i.e., $V_0(\hat{q})=\frac{1}{2}m\omega_0^2\hat{q}^2$ and

$$H'=\hat{q}^4. \tag{22}$$

Then, after some algebra, Eq. (15) reduces to

$$J(s)=\langle q^2\rangle_1\frac{s}{s^2+\omega_0^2}\left[1-\frac{12\lambda}{(s^2+\omega_0^2)m(m\omega_0^2A)}\right]+O(\lambda^2), \tag{23}$$

where

$$A=(2/\hbar\omega_0)\tanh(\beta\hbar\omega_0/2). \tag{24}$$

Now, in the direct Laplace inversion of this expression, the term $\sim\lambda$ is secular ($\propto t\sin\omega_0 t$). To avoid the appearance of a secular term, we interpret the correction term as leading to a *renormalized frequency* $\omega_R$. That is, we write

$$J(s)=\langle q^2\rangle_1\frac{s}{s^2+\omega_0^2}\,\frac{1}{1+12\lambda/m(m\omega_0^2A)(s^2+\omega_0^2)}+O(\lambda^2)=\langle q^2\rangle_1\frac{s}{s^2+\omega_R^2}+O(\lambda^2), \tag{25}$$

where

$$\omega_R^2=\omega_0^2+12\lambda/m(m\omega_0^2A)+O(\lambda^2). \tag{26}$$

At this stage, some comments are in order. First of all, we stress that, whereas there are an infinite number of functions which reduce to first order to Eq. (23), the choice given in Eq. (25) is *unique* in the sense that it satisfies the demand that it has exactly the same form as the $\lambda=0$ result except that $\omega_0$ is replaced by $\omega_R$.

Secondly, it should be further emphasized that the technique we have outlined is not confined to the example shown. In all cases the secular term (which grows with increasing $t$ no matter how small $\lambda$ is) must be reinterpreted and, of course, this is physically reasonable since one expects that the frequencies associated with a particular motion will be changed when one superimposes an interaction. While we cannot give a general proof that frequency renormalization can always get rid of divergences due to secular terms, we have not been able to find a contrary example.

Thirdly, the question might be asked as to whether it might be possible to modify the expansion in Eq. (15) so as to obtain the above results more directly. The answer is that a modification of Eq. (15) does not simplify the problem in general.

We now return to the specific example considered. From Eq. (26) we see that the first-order frequency is thus

$$\Delta=\omega_R-\omega_0=\frac{6\lambda}{m\omega_0}\left[\frac{\hbar}{2m\omega_0}\coth\frac{\beta\hbar\omega_0}{2}\right]. \tag{27}$$

The choice of absorbing the correction term in Eq. (23) into a renormalized frequency is analogous to the Poincaré-Lindstedt approach[10] in nonlinear mechanics. In the latter method the frequency is chosen so as to avoid a secular term in the motion. The manipulations leading to Eq. (25) are also reminiscent of the introduction of the self-energy in the Green's-function method.[4] A previous calculation[11] using the WK method resulted in the first two terms of an expansion of Eq. (27) in powers of $\hbar^2$. We have repeated the calculation using Green's-function techniques and obtained the same result. However, the latter method involves, as is usual, the full machinery of quantum field theory and the evaluation of connected diagrams in the Wick expansion. By contrast, the phase-space distribution method calculates the same quantum corrections in a "classical-like" derivation.

We turn next to the three-dimensional anharmonic lattice problem which, of course, is considerably more complicated per se no matter what method of approach is used. For this reason, we will omit the details and simply state that we have been able to reproduce the results of Maradudin and Fein[12] (obtained by use of Green's function) by means of the method described above.

In summary, the WDF has been shown to provide an alternative method for the evaluation of correlation functions, one which may in certain instances prove simpler than the Green's-function approach. We have shown how to express the WDF in powers of a perturbing potential, without resorting to an expansion in powers of $\hbar$. Explicit evaluation of the correlation terms may be tedious, but for many applications the full details of the WDF are not required. For example, the first-order frequency shift given by Eq. (26) only required an evaluation of the unperturbed distribution function.

The method we have presented goes beyond the WK method in that an expansion in $\hbar$ is not required. However, the latter method retains its usefulness in situations where an expansion in powers of a perturbing potential is not feasible and where one is in the near-classical regime.

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