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Phase-space representations of the Bloch equation

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We discuss the phase-space representation of the Bloch equation and present analytic expressions for two generalized classes of distribution functions. Series solutions to order of $\hbar^2$ are given. We conclude that the Wigner quantum corrections are the simplest among the two general classes of distribution functions.

I. INTRODUCTION

Both analytic and numerical solutions of the Schrödinger equation are often employed to investigate the thermodynamical properties of a system in equilibrium. In order to avoid the direct computation of the energy levels of the system, the so-called phase-space formulation of quantum mechanics has been developed. This work was pioneered by Wigner,¹ who introduced the well-known Wigner distribution function. The main feature of the phase-space formulation of quantum mechanics is to provide a framework for the treatment of quantum-mechanical problems in terms of classical concepts.

In addition to the original distribution of Wigner, other distribution functions have been considered by various authors. Common choices are the normal² and the antinormal³ distribution functions, and also the standard and antistandard (Kirkwood)⁴ distribution functions.⁵ They have been widely used in many subfields of quantum physics, particularly in statistical mechanics and quantum optics.⁶

We wish to consider the question of what the optimum distribution function is to use. As we have emphasized already,⁷⁻⁹ one criterion for deciding on an optimum choice is the simplicity of the associated time dependence which is, of course, of paramount interest when one is dealing with nonequilibrium situations.

In the present paper we would like to discuss another criterion, that is, the simplicity of the related phase-space correspondence of the Bloch equation¹⁰ which has been extensively used in calculations of quantum corrections to classical distribution functions.¹¹ The corresponding analytic expressions for the case of two kinds of generalized distribution functions, which include all the distribution functions mentioned above as special cases, are presented in Sec. II. The solutions to the phase-space correspondences, to order $\hbar^2$, are given in Sec. III. We discuss our results in Sec. IV.

II. PHASE-SPACE CORRESPONDENCES OF THE BLOCH EQUATION

Consider a canonical ensemble. If $\beta = 1/kT$, where k is the Boltzmann constant and T is the temperature, then the density operator of the ensemble is

$$\hat{\rho} = \frac{1}{Z(\beta)} e^{-\beta \hat{H}} \equiv \frac{1}{Z(\beta)} \hat{\Omega} . \quad (1)$$

where $\hat{H}$ denotes the Hamiltonian and $Z(\beta)$ is the partition function, i.e.,

$$Z(\beta) = \text{Tr}(e^{-\beta \hat{H}}) , \quad (2)$$

all operators being indicated by a caret.

The unnormalized density operator $\hat{\Omega}$ satisfies the equation

$$\frac{\partial \hat{\Omega}}{\partial \beta} = -\hat{H} \hat{\Omega} = -\hat{\Omega} \hat{H} , \quad (3)$$

subject to the initial condition $\hat{\Omega}(\beta=0) = \hat{I}$, where $\hat{I}$ is the identity operator. Equation (3) is referred to as the Bloch equation¹⁰ for the density operator of a canonical ensemble.

The discussion in this section is restricted to the case of a single degree of freedom. The generalization of the results for the case of many degrees of freedom is straightforward, as we will demonstrate it in Sec. III.

The Wigner phase-space correspondence of Eq. (3) has the form^{1,6,12}

$$\frac{\partial \Omega_W}{\partial \beta} = \left[-\frac{p^2}{2m} + \frac{\hbar^2}{8m} \frac{\partial^2}{\partial q^2} - \sum_{\lambda} \frac{1}{\lambda!} \left[\frac{i\hbar}{2} \right]^{\lambda} \frac{\partial^{\lambda} V}{\partial q^{\lambda}} \frac{\partial^{\lambda}}{\partial p^{\lambda}} \right] \Omega_W , \quad (4)$$

where we have assumed that the Hamiltonian is of the form

$$\hat{H} = \hat{p}^2/2m + V(\hat{q}) , \quad (5)$$

and the summation in Eq. (4) is to be extended over all positive even integers, as well as zero.

A generalized distribution function,¹³ $\Omega_g(q, p; s)$ say, where s is a parameter, was introduced by Cahill and Glauber. When s assumes the values -1 , 0 , and $+1$, Ω_g becomes the antinormal, the Wigner, and the normal distribution functions, respectively.

It has been shown that^{7,14,15} the generalized distribution function $\Omega_g(q, p; s)$ can be written in terms of the Wigner distribution function $\Omega_W(q, p)$ as follows:

$$\Omega_g(q, p, s) = O \Omega_W(q, p) , \quad (6)$$

where

$$O = CD, \quad (7)$$

$$C \equiv \exp \left[-\frac{s}{2} q_0^2 \frac{\partial^2}{\partial q^2} \right], \quad (8)$$

$$D \equiv \exp \left[-\frac{s}{2} p_0^2 \frac{\partial^2}{\partial p^2} \right] \quad (9)$$

are the operators defined in phase space and the constants q_0, p_0 are given by

$$q_0 = (\hbar/2m\omega)^{1/2} \quad (10)$$

and

$$p_0 = (m\hbar\omega/2)^{1/2} = m\omega q_0. \quad (11)$$

A new generalized distribution function, $\Omega_G(q, p; b)$ say, was introduced by one of us in a recent paper,¹⁶ viz.

$$\Omega_G(q, p; b) = A \Omega_W(q, p), \quad (12)$$

where

$$A = \exp \left[\frac{i\hbar b}{2} \frac{\partial}{\partial q} \frac{\partial}{\partial p} \right], \quad (13)$$

and b is a parameter. Also, the antistandard, the Wigner, and the standard distribution functions correspond to the cases where $b = -1, 0$, and $+1$, respectively.

Equations (6) and (12) are the basic results relating different kinds of distribution functions to the Wigner one. We will use them and Eq. (4) to obtain the corresponding equations for $\Omega_g(q, p; s)$ and $\Omega_G(q, p; b)$. We now turn to a determination of the equations which Ω_g and Ω_G satisfy, which will then be compared to the analogous equation [Eq. (4)] obeyed by Ω_W .

Substituting the inverse of Eq. (6) into Eq. (4) and then operating with O on both sides of the resulting equation, and making use of Eqs. (6)–(9), we obtain

$$\begin{aligned} \frac{\partial \Omega_g}{\partial \beta} = & \left[-\frac{1}{2m} D p^2 D^{-1} + \frac{\hbar^2}{8m} \frac{\partial^2}{\partial q^2} \right. \\ & \left. - \sum_{\lambda} \left[\frac{1}{\lambda} \left[\frac{i\hbar}{2} \right]^{\lambda} C \frac{\partial \lambda^V}{\partial q^{\lambda}} C^{-1} \frac{\partial^{\lambda}}{\partial p^{\lambda}} \right] \right] \Omega_g. \end{aligned} \quad (14)$$

To get a more explicit form, we will make use of an operator identity, which was proved in our previous paper,⁷ viz.

$$\begin{aligned} D f(p) D^{-1} \\ = \sum_{\mu=0}^{\infty} \frac{\partial^{\mu} f(p)}{\partial p^{\mu}} \sum_{k=0}^{[\frac{1}{2}\mu]} \frac{(-s)^{\mu-k} p_0^{2(\mu-k)}}{2^k k! (\mu-2k)!} \frac{\partial^{\mu-2k}}{\partial p^{\mu-2k}}, \end{aligned} \quad (15)$$

where $[\frac{1}{2}\mu]$ is the maximum integer within $\mu/2$, and $f(p)$ is an arbitrary function containing derivatives of arbitrary order. In the case where $f(p) = p^2$, only the $\mu=0, 1$, and 2 terms contribute, so that

$$D p^2 D^{-1} = p^2 - s p_0^2 \left[2p \frac{\partial}{\partial p} + 1 \right] + s^2 p_0^4 \frac{\partial^2}{\partial p^2}. \quad (16)$$

If we replace p by q and D by C and choose $f(q) = V^{(\lambda)}(q)$, we can get the expression for $C V^{(\lambda)}(q) C^{-1}$. Substituting it and Eq. (16) into Eq. (14) we obtain the equation for the generalized distribution function $\Omega_g(q, p; s)$:

$$\begin{aligned} \frac{\partial \Omega_g}{\partial \beta} = & \left[-\frac{1}{2m} \left[p^2 - s p_0^2 \left[2p \frac{\partial}{\partial p} + 1 \right] \right. \right. \\ & \left. \left. + s^2 p_0^4 \frac{\partial^2}{\partial p^2} - \frac{\hbar^2}{4} \frac{\partial^2}{\partial q^2} \right] \right. \\ & \left. - \sum_{\lambda} \sum_{\mu=0}^{\infty} \sum_{k=0}^{[\frac{1}{2}\mu]} \frac{(-s)^{\mu-k} (i\hbar)^{\lambda} p_0^{2(\mu-k)}}{2^{\lambda+k} \lambda! k! (\mu-2k)!} \right. \\ & \left. \times \frac{\partial^{\lambda+\mu} V}{\partial q^{\lambda+\mu}} \frac{\partial^{\lambda}}{\partial p^{\lambda}} \frac{\partial^{\mu-2k}}{\partial q^{\mu-2k}} \right] \Omega_g. \end{aligned} \quad (17)$$

The equation for the other generalized distribution function, $\Omega_G(q, p; b)$, can be obtained in exactly the same way. Corresponding to Eq. (14), Ω_G satisfies the following equation:

$$\begin{aligned} \frac{\partial \Omega_G}{\partial \beta} = & \left[-\frac{1}{2m} A p^2 A^{-1} + \frac{\hbar^2}{8m} \frac{\partial^2}{\partial q^2} \right. \\ & \left. - \sum_{\lambda} \frac{1}{\lambda!} \left[\frac{i\hbar}{2} \right]^{\lambda} A \frac{\partial^{\lambda} V}{\partial q^{\lambda}} A^{-1} \frac{\partial^{\lambda}}{\partial p^{\lambda}} \right] \Omega_G. \end{aligned} \quad (18)$$

We now make use of another useful identity given in our previous work, viz.⁹

$$A f(p) A^{-1} = \sum_{n=0}^{\infty} \frac{f^{(n)}(p')}{n!} \left[p - p' + \frac{i\hbar b}{2} \frac{\partial}{\partial q} \right]^n, \quad (19)$$

where $f(p)$ is an arbitrary function that can be expanded around p' .

Choosing $f(p) = p^2$ and $p' = 0$, then only the $n=2$ term contributes, so that

$$\begin{aligned} A p^2 A^{-1} &= \left[p + \frac{i\hbar b}{2} \frac{\partial}{\partial q} \right]^2 \\ &= p^2 + i\hbar b p \frac{\partial}{\partial q} - \frac{\hbar^2 b^2}{4} \frac{\partial^2}{\partial q^2}. \end{aligned} \quad (20)$$

Also, we have

$$A \frac{\partial^{\lambda} V}{\partial q^{\lambda}} A^{-1} = \sum_{n=0}^{\infty} \frac{V^{(\lambda+n)}(q)}{n!} \left[q - q' + \frac{i\hbar b}{2} \frac{\partial}{\partial p} \right]^n, \quad (21)$$

where the value q' is chosen so that the potential $V(q)$ is infinitely differentiable at this point, but otherwise arbitrary. Combining Eqs. (18), (20), and (21) we finally obtain

$$\frac{\partial \Omega_G}{\partial \beta} = \left[-\frac{1}{2m} \left[p^2 + i\hbar b p \frac{\partial}{\partial q} - \frac{\hbar^2}{4} (b^2 + 1) \frac{\partial^2}{\partial q^2} \right] \right.$$

$$- \sum_{\lambda} \sum_{n=0}^{\infty} \frac{(i\hbar)^{\lambda} V^{(\lambda+n)}(q')}{2^{\lambda} \lambda! n!} \times \left[q - q' + \frac{i\hbar b}{2} \frac{\partial}{\partial p} \right]^n \Omega_G. \quad (22)$$

III. SOLUTIONS TO THE PHASE-SPACE REPRESENTATION OF THE BLOCH EQUATION

By inspection of Eqs. (4), (17), and (22) it is immediately clear that the Wigner phase-space representation of the Bloch equation is the simplest among all the related equations discussed above. However, even the equation for $\Omega_W(q, p)$ can be solved exactly only in a few simple cases, for example, an ensemble of harmonic oscillators.¹⁷ On the other hand, a series solution in powers of $\hbar$ is always obtainable as follows (and we also make a generalization to three dimensions):

$$\Omega(\mathbf{q}, \mathbf{p}) = \Omega_{cl} \sum_{n=0}^{\infty} f_n(\mathbf{q}, \mathbf{p}) \hbar^n, \quad (23)$$

where $\Omega(\mathbf{q}, \mathbf{p})$ stands for an arbitrary quantum distribution function. $\Omega_{cl}(\mathbf{q}, \mathbf{p})$ is the classical distribution function, i.e.,

$$\Omega_{cl}(\mathbf{q}, \mathbf{p}) = \exp(-\beta H), \quad (24)$$

and

$$H(\mathbf{q}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}). \quad (25)$$

When we discuss $\Omega_g(\mathbf{q}, \mathbf{p}; s)$ and $\Omega_G(\mathbf{q}, \mathbf{p}; b)$ we denote the coefficients $f_n(\mathbf{q}, \mathbf{p})$ by $g_n(\mathbf{q}, \mathbf{p}; s)$ and $G_n(\mathbf{q}, \mathbf{p}; b)$, respectively. In particular, $W_n(\mathbf{q}, \mathbf{p}) \equiv g_n(\mathbf{q}, \mathbf{p}; 0) = G_n(\mathbf{q}, \mathbf{p}; 0)$ denotes the coefficients appearing in the expression for $\Omega_W(\mathbf{q}, \mathbf{p})$.

Equation (22) is referred to as the Wigner-Kirkwood expansion.^{1,4,18,19} Since for $\hbar \rightarrow 0$ the quantum-mechanical description approaches the classical one, it follows that

$$f_0(\mathbf{q}, \mathbf{p}) = 1 \quad (26)$$

holds for any distribution function. It has been shown that¹

$$W_{2n+1}(\mathbf{q}, \mathbf{p}) = 0, \quad (27)$$

where $n = 0, 1, \dots$

In general, g_n and G_n can be obtained by solving Eqs. (17) and (22) with the help of Eq. (23). But there is another way to do it, that is, by using the known $W_n(\mathbf{q}, \mathbf{p})$ and the relations between $\Omega_g(\mathbf{q}, \mathbf{p}; s)$, $\Omega_G(\mathbf{q}, \mathbf{p}; b)$, and $\Omega_W(\mathbf{q}, \mathbf{p})$.

We first expand the operators $O \equiv CD$ and A in power series of $\hbar$, i.e.,

$$O = \sum_{l=0}^{\infty} O_l \hbar^l, \quad (28)$$

and

$$A = \sum_{l=0}^{\infty} A_l \hbar^l, \quad (29)$$

where the coefficients are

$$O_l = \frac{(-s)^l}{4^l l!} \left[\frac{1}{m\omega} \nabla_q^2 + m\omega \nabla_p^2 \right]^l, \quad (30)$$

and

$$A_l = \frac{(ib)^l}{2^l l!} (\nabla_q \cdot \nabla_p)^l. \quad (31)$$

Expanding both sides of Eq. (6) in power series of $\hbar$, i.e., using Eqs. (23) and (28), we have

$$\begin{aligned} \Omega_{cl} \sum_{n=0}^{\infty} g_n(\mathbf{q}, \mathbf{p}; s) \hbar^n &= \left[\sum_{j=0}^{\infty} O_j \hbar^j \right] \left[\sum_{k=0}^{\infty} \Omega_{cl} W_k(\mathbf{q}, \mathbf{p}) \hbar^k \right] \\ &= \sum_{n=0}^{\infty} \hbar^n \sum_{l=0}^n O_{n-l} \Omega_{cl} W_l(\mathbf{q}, \mathbf{p}). \end{aligned} \quad (32)$$

Equation equal powers of $\hbar$, it follows that

$$\Omega_{cl} g_n(\mathbf{q}, \mathbf{p}; s) = \sum_{l=0}^n O_{n-l} \Omega_{cl} W_l(\mathbf{q}, \mathbf{p}), \quad (33)$$

which is equivalent to

$$g_n(\mathbf{q}, \mathbf{p}; s) = \sum_{l=0}^n \Omega_{cl}^{-1} O_{n-l} \Omega_{cl} W_l(\mathbf{q}, \mathbf{p}). \quad (34)$$

Using Eq. (27), we can rewrite Eq. (34) as follows:

$$g_n(\mathbf{q}, \mathbf{p}; s) = \sum_{l=0}^{[\frac{1}{2}n]} \Omega_{cl}^{-1} O_{n-2l} \Omega_{cl} W_{2l}(\mathbf{q}, \mathbf{p}). \quad (35)$$

Similarly, we obtain

$$G_n(\mathbf{q}, \mathbf{p}; b) = \sum_{l=0}^{[\frac{1}{2}n]} \Omega_{cl}^{-1} A_{n-2l} \Omega_{cl} W_{2l}(\mathbf{q}, \mathbf{p}). \quad (36)$$

Equations (35) and (36) are the basic results that relate the quantum-correction terms of two generalized distribution functions to those of the Wigner distribution function. They enable us to evaluate g_n and G_n if $W_2, W_4, \dots, W_{[n/2]}$ are known.

Let us now consider g_1 and G_1 . With $n=1$ in Eq. (35) only the $l=0$ term contributes, hence

$$G_1(\mathbf{q}, \mathbf{p}; b) = \Omega_{cl}^{-1} A_1 (\Omega_{cl} W_0). \quad (37)$$

Substituting Eqs. (24), (31), and (26) into Eq. (37) gives

$$\begin{aligned} G_1(\mathbf{q}, \mathbf{p}; b) &= \exp \left[+\beta \left[\frac{\mathbf{p}^2}{2m} + V \right] \right] \left[\frac{ib}{2} \nabla_q \cdot \nabla_p \right] \\ &\quad \times \exp \left[-\beta \left[\frac{\mathbf{p}^2}{2m} + V \right] \right] \\ &= \frac{i\beta^2 b}{2m} \mathbf{p} \cdot \nabla V. \end{aligned} \quad (38)$$

Similarly, we evaluate

$$G_2(\mathbf{q}, \mathbf{p}; b) = W_2(\mathbf{q}, \mathbf{p}) + \left[\frac{-b^2 \beta^2}{8m} \right] \left[\left[\frac{\beta}{m} \right]^2 (\nabla V \cdot \mathbf{p})^2 - \frac{\beta}{m} (\mathbf{p} \cdot \nabla)^2 V - \beta (\nabla V)^2 + \nabla^2 V \right], \quad (39)$$

where

$$W_2(\mathbf{q}, \mathbf{p}) = \frac{1}{24m} \left[\frac{\beta^3}{m} (\mathbf{p} \cdot \nabla)^2 V - 3\beta^2 \nabla^2 V + \beta^3 (\nabla V)^2 \right]. \quad (40)$$

It is easy to verify that $G_1(\mathbf{q}, \mathbf{p}; -1)$ and $G_2(\mathbf{q}, \mathbf{p}; -1)$ agree with the results obtained by Balazs and Jennings¹⁹

$$\begin{aligned} g_2(\mathbf{q}, \mathbf{p}; s) &= W_2(\mathbf{q}, \mathbf{p}) + \exp(\beta H) \frac{s^2}{32} \left[\frac{1}{\delta^2} (\nabla_q^2)^2 + 2\nabla_q^2 \nabla_p^2 + \delta^2 (\nabla_p^2)^2 \right] \exp(-\beta H) \\ &= W_2(\mathbf{q}, \mathbf{p}) + \frac{s^2}{32\delta^2} \{ -\beta \nabla^2 (\nabla^2 V) + 2\beta^2 [\nabla (\nabla^2 V)] \cdot \nabla V + \beta^2 \nabla^2 (\nabla V)^2 + \beta^2 (\nabla^2 V)^2 \\ &\quad - 2\beta^3 [\nabla (\nabla V)^2] \cdot (\nabla V) - 2\beta^3 (\nabla V)^2 (\nabla V) + \beta^4 (\nabla V)^4 \} \\ &\quad + \frac{s^2}{16} \left[\left[\frac{\beta^2 \mathbf{p}}{m} \right]^2 (\nabla V)^2 - \frac{\beta^3 \mathbf{p}^2}{m^2} \nabla^2 V - \frac{3\beta^3}{m} (\nabla V)^2 + \frac{3\beta^2}{m} \nabla^2 V \right] + \frac{s^2 \delta^2}{32} \left[15 \left[\frac{\beta}{m} \right]^2 - 10 \left[\frac{\beta}{m} \right]^3 p^2 + \left[\frac{\beta}{m} \right]^4 \right]. \end{aligned} \quad (43)$$

Again the simplest form for the quantum-correction terms is obtained by taking $s=0$, which corresponds to the Wigner case.

It is easy to verify that [see Eqs. (30) and (35)]

$$g_{2n}(\mathbf{q}, \mathbf{p}; -1) = g_{2n}(\mathbf{q}, \mathbf{p}; +1), \quad (44)$$

and

$$g_{2n+1}(\mathbf{q}, \mathbf{p}; -1) = -g_{2n+1}(\mathbf{q}, \mathbf{p}; +1). \quad (45)$$

Similarly, we have

$$G_n(\mathbf{q}, \mathbf{p}; -s) = (-1)^n G_n(\mathbf{q}, \mathbf{p}; s). \quad (46)$$

IV. DISCUSSION

We have obtained the phase-space representation of the Bloch equation for perhaps all the distribution functions most commonly discussed in the literature. These are all new results with the exception of the result for the Kirkwood (antistandard) distribution, and in the latter case our general results reduce to a result given by Balazs and Jennings. In all cases the result for the Wigner case, Ω_W , is the simplest. In particular, Ω_W contains no $\hbar$ terms.

Needless to say, a correct usage of any of these functions leads to unique answers for physical quantities. In

for the special case of the antistandard (Kirkwood) distribution function [Eqs. (3.8) and (3.9) in Ref. 19]. Also taking $b=0$ in Eqs. (38) and (39), one gets the Wigner corrections W_1 and W_2 .

Next we calculate $g_1(q, p; s)$ and $g_2(q, p; s)$. With

$$\delta = m\omega, \quad (41)$$

we obtain

$$\begin{aligned} g_1(\mathbf{q}, \mathbf{p}; s) &= \exp(\beta H) \left[-\frac{s}{4} \right] \left[\frac{1}{\delta} \nabla_q^2 + \delta \nabla_p^2 \right] \exp(-\beta H) \\ &= \frac{s}{4\delta} [\beta \nabla^2 V - \beta^2 (\nabla V)^2] \\ &\quad + \frac{s\delta}{4} \left[-\left[\frac{\beta \mathbf{p}}{m} \right]^2 + \frac{3\beta}{m} \right], \end{aligned} \quad (42)$$

and

particular, we note that the $\hbar$ term of G_1 is odd in $\mathbf{p}$ and thus gives zero contribution when integrated over momentum space.

On the other hand, it is easily verified that

$$\int \int \Omega_{cl} \left[-\left[\frac{\beta}{m} \right]^2 \mathbf{p}^2 + \frac{3\beta}{m} \right] d^3 q d^3 p = 0, \quad (47)$$

and

$$\int \int \Omega_{cl} [\beta \nabla^2 V - \beta^2 (\nabla V)^2] d^3 q d^3 p = 0. \quad (48)$$

Hence the g_1 term gives zero contribution, too, when integrated over the whole phase space.

The proof of

$$\begin{aligned} \int \int \Omega_{cl} g_2 d^3 q d^3 p &= \int \int \Omega_{cl} G_2 d^3 q d^3 p \\ &= \int \int \Omega_{cl} W_2 d^3 q d^3 p \end{aligned} \quad (49)$$

is lengthy but straightforward. Thus, it follows, as expected, that

$$Z = (2\pi\hbar)^{-3} \int \int \Omega(\mathbf{q}, \mathbf{p}) d^3 q d^3 p \quad (50)$$

is the same no matter what distribution function is used.

Finally, we point out that our considerations so far have been restricted to the case of a potential involving a

function of coordinates only. However, this covers a vast array of problems in many different branches of physics¹² and for such problems we conclude that the optimum phase-space representation is that given by Wigner since the corresponding phase-space representation of the Bloch equation (as well as the time dependence⁷⁻⁹) is the simplest of all possibilities.

Velocity-dependent interactions (corresponding to non-local potentials) have been widely investigated in nuclear physics.²⁰ Recently Srinivas and Prahalad²¹ discussed the Wigner phase-space representation and its $\hbar$ -series solution using a velocity-dependent interaction. They showed that Eq. (27) still holds in general; however, other terms

are much more complicated than the case where the interaction is velocity independent. It is clear that generalizations of their results into other kinds of distribution functions are straightforward. The results are quite complicated and enable us to conclude that the Wigner distribution function is still the simplest one to use even in the case where the interaction is velocity dependent.

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