Generalized Langevin Equation of Mori and Kubo

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The generalized Langevin equation of Mori and Kubo is derived from the theory of stochastic processes. This equation is valid for a very large and very diverse class of processes, including cases where the intuitive "physical" interpretation of the equation is incorrect.

ANY dynamical variable X of a classical system in equilibrium defines a stationary stochastic process as the state of the system changes with time.[1] Mori[2] and Kubo[3] have shown that this process can be derived from a generalized Langevin equation,

$$\dot{X}(t)=-\int_0^t d\tau\,\gamma(t-\tau)X(\tau)+f(t), \qquad (1)$$

where the "random force" $f(t)$ is uncorrelated with the initial value of X, $\langle X(0)f(t)\rangle=0$.[4]

In fact, Eq. (1) holds for any differentiable stochastic process; an appeal to mechanics is unnecessary.

The proof is not difficult. Let $X(t)$ be a stationary process with mean zero, correlation function $\rho(t)=\langle X(0)X(t)\rangle\equiv\rho(-t)$. We assume that $\rho(t)$ is continuously differentiable for $t\neq 0$ and that

$$\dot{\rho}(0+)\equiv\lim_{t\to 0+}\dot{\rho}(t)=-\dot{\rho}(0-)$$

exists. Then the Volterra equation

$$\rho(0)\Gamma(t)+\int_0^t d\tau\,\dot{\rho}(t-\tau)\Gamma(\tau)=-\dot{\rho}(t) \qquad (2)$$

has a unique solution $\Gamma(t)=-\Gamma(-t)$, continuous everywhere with the possible exception of $t=0$, where $\Gamma(0\pm)=-\dot{\rho}(0\pm)/\rho(0)$. Integrating (2), we find that Γ satisfies

$$\int_0^t d\tau\,\Gamma(t-\tau)\rho(\tau)=\rho(0)-\rho(t). \qquad (3)$$

Define a process $F(t)$ by[5]

$$X(t)-X(0)=-\int_0^t d\tau\,\Gamma(t-\tau)X(\tau)+F(t). \qquad (4)$$

$F(t)$ is uncorrelated with $X(0)$, since $\langle X(0)F(t)\rangle=\rho(t)-\rho(0)+\int_0^t d\tau\,\Gamma(t-\tau)\rho(\tau)=0$.

To get from Eq. (4) to Eq. (1) we need the result that if the process $X(t)$ is differentiable (in the mean square sense[6]), then $\ddot{\rho}(t)$ exists and is continuous for all t.[7] This implies that $\dot{\rho}(0+)=\dot{\rho}(0-)=0$, that $\Gamma(0+)=\Gamma(0-)=0$, and that $\Gamma(t)$ and $F(t)$ are differentiable (in the ordinary and mean-square senses, respectively). Differentiating (4), we get (1) with $\gamma(t)=\dot{\Gamma}(t)$, $f(t)=\dot{F}(t)$.

Notice that (1) implies (4) but not vice versa: Equation (4) is a valid representation even of processes which are not differentiable and therefore do not satisfy a Langevin equation. The most famous example is the velocity of a Brownian particle,[8] for which, interestingly enough, the original Langevin equation was invented.

It is easy to verify from Eq. (4) that

$$\lim_{t'\to 0\pm}\langle F(t')F(t)\rangle/t'=\rho(0)\Gamma(t)-\dot{\rho}(0\pm). \qquad (5)$$

When Eq. (1) is valid (5) becomes

$$\int_0^t dt'\,\langle f(0)f(t')\rangle=\rho(0)\int_0^t dt'\,\gamma(t') \qquad (6a)$$

or

$$\langle f(0)f(t)\rangle=\rho(0)\gamma(t). \qquad (6b)$$

Mori and Kubo call Eq. (6b) the second fluctuation-dissipation theorem, since it relates the "systematic friction" γ to the autocorrelation of the "random force" f.

We think the lesson of all this is that the appealing

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[1] The sample space is the phase space of the system; probabilities are determined according to the canonical distribution. If P is a phase point and P_t its image a time t later, the random variable $X(t)$ assigns to P the value of X at P_t. The stochastic process in question is the set of all $X(t)$, $-\infty<t<+\infty$. Readers unfamiliar with the notions of probability theory, or unconvinced of their relevance to physics, should consult the characteristically lucid discussion by M. Kac, *Probability and Related Topics in Physical Sciences* (Interscience Publishers, Inc., New York, 1959).

[2] H. Mori, Progr. Theoret. Phys. (Kyoto) **33**, 423 (1965).

[3] R. Kubo in *Tokyo Lectures in Theoretical Physics*, edited by R. Kubo (W. A. Benjamin, Inc., New York, 1966), Part I, p. 1. See also R. Kubo, Rept. Progr. Phys. **29**, 255 (1966).

[4] X is assumed to be "centered": $\langle X\rangle=0$.

[5] The existence of the stochastic integral in (4) follows from the continuity of ρ and Γ.

[6] $X(t)$ is mean square differentiable if there is a random variable $\dot{X}(t)$ such that

$$\lim_{h\to 0}\left\langle\left[\frac{X(t+h)-X(t)}{h}-\dot{X}(t)\right]^2\right\rangle=0.$$

[7] J. L. Doob, *Stochastic Processes* (John Wiley & Sons, Inc., New York, 1953).

[8] See especially J. L. Doob, Ann. Math. **43**, 351 (1942).

"physical" form of Eqs. (1) and (4) may on occasion be dangerously misleading. Equations (1) and (4) are very general; they hold not only for Brownian motion and similar processes, but also for processes in which the stochastic variable $X(t)$ takes only values in a discrete set. In the latter case the continuous change with time of $X(t)$ given by the "friction" term has no real relation to the dynamics of the process.

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Test-Particle Theory for Quantum Plasmas*

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The analysis of a classical plasma in terms of dressed test particles is well known. In this paper, the theory is extended to inhomogeneous quantum plasmas with Coulomb interactions between particles. The Wigner one- and two-particle distribution functions are expressed in terms of a test-particle response function for the plasma. These relations are derived from the operator form of the equations of motion for a quantum plasma. The results for homogeneous systems and for classical systems are obtained as special cases of the general result. A superposition theorem for fluctuations is also given.

I. INTRODUCTION

IT has been shown by Rostoker[1,2] and others[3-5] that a classical plasma can be treated as a collection of noninteracting, dressed particles. The "dressing" or shielding of a particle is obtained by considering the response of the plasma to a single "test charge." In this paper, it is shown that quantum plasmas can also be analyzed in terms of test particles. The connection between a quantum plasma and an appropriate test-particle problem has been suggested in several recent publications.[6-8] If such a relationship exists, then it should be possible to derive these results from the basic equations describing the plasma. Dawson[5] has given such a derivation for a classical plasma and a similar approach is presented here. This treatment is also closely related to that of Wyld and Fried.[9] The result we obtain is a relation between the Wigner two-particle distribution function and the response of a quantum plasma to a single test particle. We include only the Coulomb interaction between particles and assume no magnetic field.[10] A stationary external field, derivable from a scalar potential, is the source of the system inhomogeneity.

In Sec. II, we derive the Heisenberg equation of motion for the quantum mechanical operator whose expectation value is the one-particle distribution function for the system. We linearize this equation of motion with respect to the electric potential in Sec. III and show that the one-particle distribution is a superposition of contributions from independent test particles. The relation between the two-particle correlation function and the test-particle-response function for an inhomogeneous quantum plasma is derived in Sec. IV. It is also shown that this relation reduces to more familiar results for homogeneous and classical systems. A superposition theorem for fluctuations is given in Sec. V.

II. BASIC EQUATIONS

We consider an inhomogeneous system of N electrons moving in a potential $U(\mathbf{x})$ which might represent the lattice of positive ions in a metal or the nucleus in an atom. It is assumed that the only interaction between electrons is the Coulomb potential $\mathcal{V}(\mathbf{x})=e^2/|\mathbf{x}|$. The Hamiltonian for this system is

$$H=\sum_{i=1}^{N}\mathbf{p}_i^2/2m+\sum_{i=1}^{N}U(\mathbf{x}_i)+\tfrac{1}{2}\sum_{\substack{i=1\\ i\neq j}}^{N}\sum_{j=1}^{N}\mathcal{V}(\mathbf{x}_i-\mathbf{x}_j). \quad (1)$$

The microscopic one-particle distribution function for the electrons is

$$f(\mathbf{x},\mathbf{p},t)=\sum_{i=1}^{N}\delta[\mathbf{x}-\mathbf{x}_i(t)]\delta[\mathbf{p}-\mathbf{p}_i(t)], \quad (2)$$

where $\mathbf{x}_i(t)$ and $\mathbf{p}_i(t)$ are the position and momentum of

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[3] W. R. Chappell, J. Math. Phys. **8**, 298 (1967).
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[6] S. Ichimaru, Phys. Rev. **140**, B226 (1965).
[7] N. Rostoker, Proc. Appl. Math. **18**, 270 (1967).
[8] M. E. Rensink, dissertation, University of California, Los Angeles, 1967 (unpublished).
[9] H. W. Wyld, Jr., and B. D. Fried, Ann. Phys. (N. Y.) **23**, 374 (1963).
[10] Electromagnetic radiation in the system could be treated if an appropriate linearization with respect to the electromagnetic field were employed. See, for example, W. R. Chappell, Phys. Rev. **152**, 113 (1966).