A Note On "Irreversibility and Generalized Noise"*

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The response of a dissipative system to a generalized driving force is calculated and an expression for the admittance is obtained. The expression for the conductance is in agreement with the expression obtained by Callen and Welton and a new expression for the out-of-phase component of the admittance is obtained.

IN a recent paper by Callen and Welton[1] a "fluctuation-dissipation" theorem is derived. This theorem relates the spontaneous equilibrium fluctuations in a thermodynamic system to the parameter (the "resistance") which characterizes the irreversible response of the system to a driving force, and constitutes a generalization of the Nyquist electrical noise theorem.[2] The authors consider a system with a Hamiltonian

$$\mathcal{H}=H_0(\cdots q_k\cdots p_k\cdots)+V(t)Q(\cdots q_k\cdots p_k\cdots). \quad (1)$$

Here $H_0(\cdots q_k\cdots p_k)$ is the Hamiltonian of the unperturbed system. The term $V(t)Q(\cdots q_k\cdots p_k\cdots)$ is the interaction between the unperturbed system and an externally applied generalized driving force, $V(t)$. The function $Q(\cdots q_k\cdots p_k\cdots)$ depends only upon the canonical coordinates of the system.

The authors show that a system will be dissipative and linear (and will therefore be describable by an admittance function) if it possesses a dense energy eigenvalue spectrum and if the applied perturbations are small. Under these assumptions the real part of the admittance function, $g(\omega)(=R(\omega)/|Z(\omega)|^2)$ is calculated in terms of the expression for the power dissipated in the presence of a driving force, $V(t)=V_0\sin\omega t$.

Here, a direct calculation will be made of the complex admittance function by explicit consideration of the response of the driven system. The expression for the conductance, $g(\omega)$, obtained by Callen and Welton is thereby corroborated and a new expression for the out-of-phase component of the admittance of dissipative systems is obtained.

Following the notation of reference 1, the average value of $\dot{Q}$ is calculated in the presence of a driving force, $V_0\sin\omega t$. To do this, the expectation of $\dot{Q}$ is calculated for a state Φ_n, which is the perturbed state corresponding to the eigenstate, $\psi_n\exp(iE_nt/\hbar)$, of the unperturbed Hamiltonian. The average value of $\dot{Q}$ for the system is obtained by averaging over all states, weighting each in accordance with the canonical distribution function [here designated by $f(E_n)$].

The perturbed states are written

$$\Phi_n=\psi_n\exp(iE_nt/\hbar)+\sum_m b_{nm}(t)\psi_m\exp(iE_mt/\hbar). \quad (2)$$

Following the procedure of first-order perturbation theory, one obtains for the coefficients

$$2ib_{nm}(t)=V_0\langle E_m|Q|E_n\rangle \times\left\{\left(\frac{\exp[it(E_n-E_m+\hbar\omega)/\hbar]-1}{E_n-E_m+\hbar\omega}\right)-\left(\frac{\exp[it(E_n-E_m-\hbar\omega)/\hbar]-1}{E_n-E_m-\hbar\omega}\right)\right\}. \quad (3)$$

The expectation of $\dot{Q}$ in the state Φ_n is then

$$\begin{aligned}\langle\Phi_n|\dot{Q}|\Phi_n\rangle=&\langle\psi_n\exp(iE_nt/\hbar)|\dot{Q}|\psi_n\exp(iE_nt/\hbar)\rangle\\&+\langle\textstyle\sum_m b_{nm}\psi_m\exp(iE_mt/\hbar)|\dot{Q}|\psi_n\exp(iE_nt/\hbar)\rangle\\&+\langle\psi_n\exp(iE_nt/\hbar)|\dot{Q}|\textstyle\sum_m b_{nm}\psi_m\exp(iE_mt/\hbar)\rangle\\&+(\text{higher order terms}). \quad (4)\end{aligned}$$

Using $\dot{Q}=(i/\hbar)(QH-HQ)$, the first term in the above is seen to be zero and the first-order contribution is

$$\begin{aligned}\langle\Phi_n|\dot{Q}|\Phi_n\rangle=&\left\{\frac{V_0}{2\hbar}\left(\sum_m\frac{\exp(i\omega t)-\exp[i(E_m-E_n)t/\hbar]}{E_n-E_m+\hbar\omega}\right.\right.\\&\left.-\sum_m\frac{\exp(-i\omega t)-\exp[i(E_m-E_n)t/\hbar]}{E_n-E_m-\hbar\omega}\right)\\&\left.\times(E_m-E_n)|\langle E_n|Q|E_m\rangle|^2\right\}\\&+\{\text{complex conjugate}\}. \quad (5)\end{aligned}$$

The final expression for the average value of $\dot{Q}$ for the system is

$$\langle\dot{Q}\rangle=\int\langle\Phi_n|\dot{Q}|\Phi_n\rangle\rho(E_n)f(E_n)dE_n, \quad (6)$$

where $\rho(E_n)$ is the density of states per unit energy and $f(E_n)$ is the statistical weighting factor. Further, the sum over m in Eq. (5) is replaced by an integral over the energy spectrum. The first integral in the resulting expression is then

$$\frac{V_0}{2\hbar}\int\int\rho(E_m)\rho(E_n)f(E_n)(E_m-E_n)|\langle E_n|Q|E_m\rangle|^2\times\left(\frac{\exp(i\omega t)-\exp[i(E_m-E_n)t/(\hbar)]}{E_n-E_m+\hbar\omega}\right)dE_ndE_m.$$

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[1] H. B. Callen and T. A. Welton, Phys. Rev. **83**, 34 (1951).
[2] H. Nyquist, Phys. Rev. **32**, 110 (1928).

For large times the expression in parentheses approaches a δ-function at $E_n=E_m-\hbar\omega$. In addition, there remains the integral over the rest of the energy range, wherein one must take the principle value at the singularity $E_n=E_m-\hbar\omega$. The result is

$$\tfrac{1}{2}i\pi V_0\omega\exp(i\omega t)\int dE_m\rho(E_m)\rho(E_m-\hbar\omega)f(E_m-\hbar\omega)|\langle E_m-\hbar\omega|Q|E_m\rangle|^2$$

$$+\tfrac{1}{2}(V_0/\hbar)\exp(i\omega t)\int\int dE_m dE_n\frac{f(E_n)\rho(E_m)\rho(E_n)(E_m-E_n)|\langle E_n|Q|E_m\rangle|^2}{E_n-E_m+\hbar\omega}.$$

Combining the results of the integrals one finally gets

$$\langle\dot{Q}\rangle=-V_0\sin\omega t\left\{\pi\omega\int\rho(E)f(E)[|\langle E+\hbar\omega|Q|E\rangle|^2\rho(E+\hbar\omega)-|\langle E-\hbar\omega|Q|E\rangle|^2\rho(E-\hbar\omega)]dE\right\}$$

$$+V_0\cos\omega t\left\{2\omega\int\int f(E_n)\rho(E_n)\rho(E_m)(E_n-E_m)|\langle E_n|Q|E_m\rangle|^2/[(E_n-E_m)^2-(\hbar\omega)^2]dE_n dE_m\right\}.$$

The expression multiplying $-V_0\sin\omega t$ is the conductance, in agreement with reference 1 and the term multiplying $V_0\cos\omega t$ is the susceptance.

It may be noted that the negative sign preceding the n-phase response is to be expected, as $\dot{Q}$ will tend to decrease in order to reduce the value of the perturbing energy term $V(t)Q(\cdots q_k\cdots p_k\cdots)$.

The extension of the fluctuation-dissipation theorem to several variables will be given in a subsequent paper by H. B. Callen, M. Barasch, and J. L. Jackson.

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Variational Methods for Periodic Lattices*

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The problem of finding the propagating solutions of the Schrödinger equation in periodic lattices is formulated as a variational principle. This may be used as a starting point to establish the general properties of bands. Furthermore it is shown that by introducing various approximations into the variational principle, the chief existing approximation methods can all be derived from it. Improvements of these methods are suggested. Numerical illustrations are presented and the possibilities of the variational method for more accurate calculations of the energy bands of solids are discussed.

1. INTRODUCTION

IN studying the motion of electrons in a crystal, one adopts as a starting point a picture analogous to the Hartree model for atoms. Thus to a first approximation each electron is considered as moving independently in the potential produced by the nuclei and the charge distribution of all the other electrons. Since the nuclear lattice imposes its regularity also on the electronic charge distribution, this potential has the same periodicity as the lattice.

In general, the wave equation in such a periodic potential cannot be solved exactly. For this reason various approximate methods have been devised which apply especially to this type of potential. The variational method, however, which has been so widely employed for the solution of the Schrödinger equation in other physical situations, has found no extensive application to the case of periodic lattices. To our knowledge, only the work of Slepian,[1] to which we shall come back in Sec. 2, represents a notable exception.

In the present paper a more general approach than that of Slepian will be presented which serves a fourfold purpose:

(1) It may be used as a starting point for a demonstration of the general properties of bands.

(2) It represents the analogon, for periodic potentials, of the variational principles governing bound state and scattering problems.

(3) It unifies the chief approximation methods used up to now for the periodic case. All of these may be shown to be derivable from the variational principle by introducing appropriate restrictions or approximations.

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[1] D. Slepian, thesis, Harvard University (1949).