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Fokker-Planck equation in the absence of detailed balance

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It is shown that the usual Fokker-Planck (FP) equation is not suitable for describing kinetic effects that are caused by breakdown of detailed balance. For the case of elastic scattering, a modified FP equation is obtained, containing third-order derivatives with respect to the momentum. Its properties are investigated. The problem of describing the photogalvanic effect and the anomalous Hall effect on the basis of the FP equation is considered.

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1. It is customary to suppose that one of the basic principles of kinetics is the principle of detailed balancing (PDB).[1,2] In the simplest case of elastic scattering of particles by immovable centers, the PDB states that

$$W_{\mathbf{kk}'}=W_{\mathbf{k}'\mathbf{k}},\qquad(1)$$

where $W_{\mathbf{kk}'}$ is the differential probability of a transition from a state with momentum $\mathbf{k}'$ to a state $\mathbf{k}$. It is well known that the PDB does not reflect any fundamental symmetry relation in either a quantum or a classical description of scattering.[3-5] The fundamental symmetry relations for $W_{\mathbf{kk}'}$, reflecting the invariance of the equations of motion to space and time reflections (P and T transformations), have the form[3,5]

$$W_{\mathbf{kk}'}=W_{-\mathbf{k},-\mathbf{k}'},\qquad W_{\mathbf{kk}'}=W_{-\mathbf{k}',-\mathbf{k}}.\qquad(2)$$

If one of these relations is violated, the PDB is invalid. In particular, P invariance is absent if the scattering potential is deprived of a center of symmetry (Fig. 1), and T invariance is violated in the presence of a magnetic field (Fig. 2).

Until recently, no kinetic phenomena connected in principle with absence of detailed balance were known; but in recent years, the situation has changed. At present a number of such phenomena are known. These are the anomalous Hall effect,[6] the kinetics of gases with rotational degrees of freedom,[7] and the photogalvanic effect in media without a center of symmetry.[8] Investigation of these effects has been carried out essentially on the basis of the Boltzmann equation

$$\frac{\partial f_{\mathbf{k}}}{\partial t}=\int(W_{\mathbf{kk}'}f_{\mathbf{k}'}-W_{\mathbf{k}'\mathbf{k}}f_{\mathbf{k}})d\mathbf{k}'.\qquad(3)$$

The peculiarities of kinetics in the absence of detailed balance are due to the fact that the balance of arrivals and departures is accomplished not according to the scheme $\mathbf{k}\rightleftarrows\mathbf{k}'$, but by means of the cycles $\mathbf{k}\to\mathbf{k}'\to\mathbf{k}''\to\ldots\to\mathbf{k}$.[1)]

2. In many physical situations,[2,10,11] the basic equation of kinetics is the Fokker–Planck (FP) equation

$$\partial f_{\mathbf{k}}/\partial t+\operatorname{div}\mathbf{j}_{\mathbf{k}}(f_{\mathbf{k}})=0.\qquad(4)$$

The current $\mathbf{j}_{\mathbf{k}}$ is connected locally with the distribution function. We pose the following question: how can ab-

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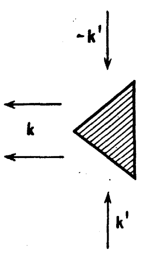

FIG. 1.

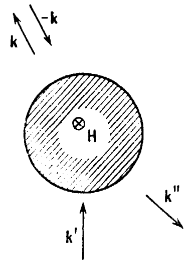

FIG. 2.

sence of detailed balance, i.e., absence of P and T invariance, be taken into account in the FP equation? It has been found that the FP equation used hitherto, with current

$$j_i^0 = A_i^0(\mathbf{k}) f(\mathbf{k}) + D_{ij}^0(\mathbf{k}) \nabla_j f(\mathbf{k}), \quad \nabla_i = \frac{\partial}{\partial k_i}, \tag{5}$$

is in general incorrect for description of kinetic phenomena in the absence of detailed balance. Breakdown of the PDB leads, as we shall show, to a raising of the order of the FP equation; that is, to the appearance of an additional term in the current:

$$\delta j_i = A_i f + {}^1/_2 \nabla_j B_{ijl} \nabla_l f + {}^1/_2 B_{ijl} \nabla_j \nabla_l f; \qquad A_i = B_i - {}^1/_2 \nabla_j \nabla_l B_{ijl}. \tag{6}$$

For derivation of the FP equation, we have used the fact that the ranges of applicability of the Boltzmann equation and of (4) intersect. The FP equation flows directly out of (3) in the case when the scattering occurs with a small change of momentum, $|\mathbf{k}'-\mathbf{k}| \ll k$. In consequence of the rapid character of the change of $W_{\mathbf{kk}'}$, the distribution function $f_{\mathbf{k}'}$ can be expanded as a series near $\mathbf{k}'=\mathbf{k}$, so that finding the form of the current $\mathbf{j_k}$ reduces to calculating the moment of $W_{\mathbf{kk}'}$.

In elastic scattering, the dynamic friction force is absent, $A_i^0 = 0$, while the diffusion tensor D_{ij}^0 is the second moment of the symmetrical part of the scattering probability, $W_{\mathbf{kk}'}^s = W_{\mathbf{k}'\mathbf{k}}^s$. The coefficients B_i and B_{ijl} in (6) are, respectively, the first and third moments of the antisymmetrical part of the probability, $W_{\mathbf{kk}'}^a = W_{\mathbf{k}'\mathbf{k}}^a$. The quantities A_i, D_{ij}^0, and B_{ijl} satisfy a number of relations that follow from conservation of energy and from the unitarity condition[12] for elastic scattering:

$$k_i D_{ij}^0 = 0, \quad k_i B_{ijl} = 0, \quad \nabla_i A_i = 0, \quad k_i A_i + {}^1/_2 \nabla_i B_{ill} = 0. \tag{7}$$

The tensors D_{ij}^0 and B_{ijl} are symmetric in all indices.

The procedure used above is expansion of the current in powers of $\Delta k/k$. Therefore it may be expected that $B_{ijl} \sim \Delta k D_{ij}^0 \sim (\Delta k)^2 A_i$ and that the last terms in (6) will be small. It is found, however, that this is not so. If the mean magnetic field $\bar{H} = 0$, then $B_{ijl} \sim k^2 A_i$. The reason for anomalous smallness of A_i consists in the following: in the first order in the parameter $\Delta k/k$, i.e., in the approximation of straight-line trajectories,[13] the value of $A_i \approx B_i$, and the momentum transferred to the particle during the act of scattering, and averaged over the impact parameter of the trajectory,[2)] has meaning. In the absence of a magnetic field, this quantity is obviously zero. But the second approximation in $\Delta k/k$ gives a detailed-balance contribution to $W_{\mathbf{kk}'}$. Consequently, D_{ij}^0 is a quantity of the second order in the operating force, whereas A_i and B_{ijl} are of the third order (we do not give here explicit expressions for A_i and B_{ijl} in terms of the operating force, because of their complexity).

Despite the smallness of the corrections to the current, their calculation is important in principle, since the symmetry properties of $\mathbf{j}_\mathbf{k}^0$ and of $\delta \mathbf{j_k}$ are different. Under conditions of T invariance, A_i, D_{ij}^0, and B_{ijl} are even functions of the momentum; under conditions of P invariance, odd.

If $\bar{\mathbf{H}} \neq 0$ (scattering by magnetic spots, Fig. 2), then the mean transferred momentum is nonzero even in the first approximation in $\Delta k/k$. In this case, $A_i \gg k^{-2} B_{ijl}$:

$$A_i = \frac{e}{mc} [\mathbf{k}\bar{\mathbf{H}}]_i. \tag{8}$$

Above, we have considered modification of the FP equation for elastic scattering. It is clear that the statements made apply, to a considerable degree, also to the case of inelastic scattering.

3. The FP equation (4) is the equation of continuity in momentum space. It would be natural to identify $\mathbf{j_k}$ with the particle current in this space; that is, with the number of particles that cross unit area perpendicular to $\mathbf{j_k}$ in unit time. Such an interpretation would lead us to the conclusion that particle currents $A_i f$ exist in phase space under conditions of complete thermodynamic equilibrium.

But such an interpretation does not follow, because in our derivation of the FP equation the form of the current $\mathbf{j_k}$ was fixed only to within the curl of an arbitrary function. This ambiguity can be removed by taking into account that according to the Liouville equation, the flow of particles in momentum space is the mean force acting on a particle with momentum $\mathbf{k}$. In thermodynamic equilibrium,

$$\mathbf{j}_\mathbf{k}^T = e \int \left(-\nabla U + \frac{1}{mc} [\mathbf{kH}] \right) \exp\left\{ -T^{-1} \left(\frac{k^2}{2m} + U \right) \right\} d\mathbf{r}. \tag{9}$$

In the absence of a magnetic field $\mathbf{j}_\mathbf{k}^T = 0$, and for scattering by magnetic spots $\mathbf{j}_\mathbf{k}^T$ coincides with (8); the current $\mathbf{j}_\mathbf{k}^T$ is nonzero also when $\bar{H} = 0$, if $\mathbf{H}(\mathbf{r})$ and $U(\mathbf{r})$ are not statistically independent. Thus there is no direct relation between absence of detailed balance and presence of currents in phase under conditions of thermodynamic equilibrium (except for the case when $\bar{\mathbf{H}} \neq 0$).

We consider the right side of the kinetic equations (3)–(4) as an operator acting on $f_\mathbf{k}$. Then the detailed-balancing term corresponds to a Hermitian operator, the nonbalance to an anti-Hermitian. The eigenvalues of such an operator are complex. Therefore the approach to equilibrium in general has an oscillatory character. One can say that the detailed-balancing and nonbalance terms describe processes of diffusion and of drift, respectively, in momentum space. In scattering by magnetic spots, the perturbations $\delta f_{\mathbf{k}}$ drift in the mean magnetic field and slowly spread out. In scattering by a noncentral potential, the situation is the opposite. The perturbations spread out rapidly, while the detailed-nonbalance terms produce a small asymmetric distortion of their shape.

5. We shall discuss briefly the problem of describing, on the basis of (4), transport phenomena produced in **R** space by the absence of detailed balancing. We define the particle current I in coordinate space as $\int \mathbf{k} f_{\mathbf{k}} d\mathbf{k}$. Then we have from (4)

$$\frac{\partial I}{\partial t} = \int j_{\mathbf{k}}\, d\mathbf{k}. \qquad (10)$$

At the initial instant, let there be a currentless perturbation, $\delta f_{\mathbf{k}} = \delta f_{-\mathbf{k}}$. Because of the different parity of the detailed-balance and nonbalance terms in the current $\mathbf{j}_{\mathbf{k}}$, it follows immediately from (10) that the transitional process in the absence of detailed balance will be accompanied by transport of particles. But if there is a source that maintains the symmetric perturbations, $\delta f_{\mathbf{k}} = \delta f_{-\mathbf{k}}$ (for example, a high-frequency field), then the additional terms in the FP equation will produce a constant flow of particles (electric current). Such a photogalvanic effect (and also the anomalous Hall effect[6]) can be immediately described by means of the modified FP equation in terms of the coefficients A_i and B_{ijl}.

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[1)]The idea of cycles goes all the way back to Boltzmann.[9]
[2)]Scattering at small angles may be considered quasiclassical.

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Use of averaging method in problems of high-resolution nuclear magnetic resonance in solids

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The Krylov-Bogolyubov-Mitropol'skiĭ averaging method is used to derive an expression for the average Hamiltonian that describes the evolution of a spin system under the influence of pulse sequences. It is shown that the equation customarily employed for the average Hamiltonian and based on the Magnus expansion is nonsecular in the higher orders of perturbation theory, i.e., the contribution of the latter to the line shape corresponds to satellites at frequencies that are multiples of the fundamental frequency. Some concrete situations are considered where the use of the Magnus expansion leads to incorrect physical results. The limits of applicability of the theory of the average Hamiltonian is investigated.

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New methods of NMR in solids, based on the work of J.S. Waugh and co-workers,[1] have been attracting much attention recently. The idea of the new methods is that a periodic sequence of pulses is applied to a spin system and averages out a definite part of the spin-spin interactions, thus leading to an effective narrowing of the magnetic-resonance lines. It is important to note that by suitably choosing the pulse sequence we can selectively suppress one part of the spin-spin interactions or another, so that the method can provide an increased amount of information.

The response of a spin system to a pulse sequency is usually analyzed mathematically by the average-

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