Collision Operators as Generators of Markov Processes and Their Spectra

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The Markovian description of diffusion in velocity space involves a semigroup, which because of detailed balance is conveniently interpreted in a weighted L^2 -space. The collision operator C, defined by the corresponding generator, is positive semidefinite in this space. For a jump process and a continuous process we obtain the collision operators of the linear Boltzmann and Fokker-Planck equations, respectively. If in the latter case the friction tensor has a nonvanishing limit as $v \rightarrow \infty$, the spectrum of C is discrete. The Fourier-transformed transport operator $T_{\mathbf{k}} = C + i\mathbf{k}\cdot\mathbf{v}$ is studied as a holomorphic family of sectorial operators. In the stated Fokker-Planck example, the spectrum of $T_{\mathbf{k}}$ remains discrete for arbitrary \mathbf{k} .

KEY WORDS: Brownian motion; Markov processes; collision and transport operators; Fokker–Planck equation.

1. TRANSITION PROBABILITIES IN VELOCITY SPACE

Brownian motion of a classical, structureless, indestructible particle in an infinitely extended uniform and isotropic fluid in thermal equilibrium has been described in many ways. If the position of the particle is ignored, we have a stochastic process v(t) in velocity space \mathbb{R}^3 . The process is stationary if the initial probability distribution is Maxwellian with the temperature of the fluid.

Often the motion is approximated as a strict Markov process.^(1,2) Although the approximation is difficult to justify for anything but diffusion in gases, we accept it here as a model. On the basis of general properties of the

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transition probabilities involved, the corresponding semigroups and generators will be examined (Sections 2 and 3). Reinterpretation of these operators in a Hilbert space will facilitate the investigation of their spectra (Sections 4 and 5).

The Markov process is described by transition probabilities $P_t(\mathbf{v} \to \Gamma)$, which determine the evolution of a probability measure of the particle in \mathbb{R}^3 ,

$$\mu_t(\Gamma) = \int_{\mathbb{R}^3} \mu(d^3 v) P_t(\mathbf{v} \to \Gamma) \tag{1}$$

The following properties of transition probabilities are either implied by the adopted model or represent physically reasonable additional assumptions:

(P1) The Markov assumption entails the semigroup property of P_t ,

$$\int_{\mathbb{R}^3} P_t(\mathbf{v} \to d^3 v') P_\tau(\mathbf{v}' \to \Gamma) = P_{t+\tau}(\mathbf{v} \to \Gamma)$$

(P2) Particle conservation means that $P_t(\mathbf{v} \to \mathbb{R}^3) = 1$.

(P3) In view of isotropy of the fluid, $P_t(\mathbf{v} \to \Gamma)$ is invariant under rotations of velocity space, which means that $P_t(R\mathbf{v} \to R\Gamma) = P_t(\mathbf{v} \to \Gamma)$ for any R in the rotation group.

(P4) As a consequence of microscopic reversibility and of the liquid being in equilibrium, P_t obeys the detailed balance symmetry,⁽³⁾

$$\int_{\Gamma'} f_0(\mathbf{v}') P_t(\mathbf{v}' \to \Gamma) \ d^3v' = \int_{\Gamma} f_0(\mathbf{v}) P_t(\mathbf{v} \to \Gamma') \ d^3v$$

where $f_0(\mathbf{v}) = (2\pi)^{-3/2} \exp(-\frac{1}{2}v^2)$. We write v^2 for mv^2/kT , with *m* denoting the mass of the particle and *T* the temperature of the fluid.

(P5) $P_t(\mathbf{v} \to \Gamma) > 0$ for all t > 0, $\mathbf{v} \in \mathbb{R}^3$, and sets $\Gamma \subset \mathbb{R}^3$ of non-vanishing Lebesgue measure.

The last assumption is not necessary for the subsequent derivations and could be replaced by a weaker "mixing" condition. However, nonpathological models consistently yield transition probabilities which are positive in the stated sense, so that the simplified assumption appears justified.

It follows from (P2) and (P4) that the measure μ_0 having Maxwellian density f_0 represents equilibrium, in the sense that it is invariant under transformation (1). Hence we have a Markov process with invariant measure.⁽⁴⁾ As will be shown in Section 2, (P5) makes sure that this is the only invariant bounded measure.

2. SEMIGROUP IN HILBERT SPACE

Transformation (1) defines the dual semigroup⁽¹⁾ associated with the Markov process,

$$H_t^{\dagger}\mu(\Gamma) \coloneqq \int_{\mathbb{R}^3} \mu(d^3 v) P_t(\mathbf{v} \to \Gamma)$$

 H_t^{\dagger} is an operator acting on the set of signed, bounded Borel measures. Particle conservation (P2) and invariance of the equilibrium measure μ_0 are expressed by $H_t^{\dagger}\mu(\mathbb{R}^3) = \mu(\mathbb{R}^3)$ and $H_t^{\dagger}\mu_0(\Gamma) = \mu_0(\Gamma)$, respectively.

The statement that the Maxwellian μ_0 is (up to a constant factor) the only signed, bounded measure invariant against H_i^{\dagger} is an analogy to theorems of Perron and Jentzsch.⁽⁵⁻⁷⁾ We first show that any invariant signed measure μ is a (nonnegative) measure. Assuming the opposite, we consider the Jordan decomposition,⁽⁶⁾ $\mu = \mu_+ - \mu_-$. It is possible to split velocity space into two disjoint sets, $\mathbb{R}^3 = \Gamma_+ \bigcup \Gamma_-$, $\Gamma_+ \bigcap \Gamma_- = \emptyset$, so that $\mu_+(\Gamma_-) = 0$ and $\mu_-(\Gamma_+) = 0$, but $\mu_+(\Gamma_+) > 0$ and $\mu_-(\Gamma_-) > 0$. Clearly at least one of the two sets, say Γ_+ , must have Lebesgue measure greater than zero. By the invariance of μ we see that for this set

$$\mu_{+}(\Gamma_{+}) = \mu(\Gamma_{+}) = H_{t}^{\dagger}\mu(\Gamma_{+}) = H_{t}^{\dagger}\mu_{+}(\Gamma_{+}) - H_{t}^{\dagger}\mu_{-}(\Gamma_{+})$$
(2)

On the other hand,

$$\begin{aligned} H_t^{\dagger}\mu_+(\Gamma_+) &= \int_{\mathbb{R}^3} \mu_+(d^3v) \, P_t(\mathbf{v} \to \Gamma_+) \\ &\leq \int_{\mathbb{R}^3} \mu_+(d^3v) \, P_t(\mathbf{v} \to \mathbb{R}^3) = \mu_+(\mathbb{R}^3) = \mu_+(\Gamma_+) \end{aligned}$$

Now (P5) implies that $H_t^{\dagger}\mu_-(\Gamma_+) > 0$, so that we have a contradiction to Eq. (2).

Suppose then that μ is a normalized (nonnegative) invariant Borel measure different from μ_0 , so that $\mu(\mathbb{R}^3) = \mu_0(\mathbb{R}^3) = 1$. The difference $\mu - \mu_0$ is an invariant signed measure with nontrivial positive and negative parts, in contradiction to the preceding observation. The proof is complete.

We now restrict H_t^{\dagger} to signed measures having densities of the form $f_0(\mathbf{v})\phi(\mathbf{v})$, where ϕ is a continuous bounded function, $\phi \in C^b(\mathbb{R}^3)$. Then for any $\chi \in C^b(\mathbb{R}^3)$, we have

$$\begin{split} \int_{\mathbb{R}^3} \chi(\mathbf{v}) H_t^{\dagger} \mu(d^3 v) &= \int_{\mathbb{R}^3} \int \chi(\mathbf{v}) f_0(\mathbf{v}') \phi(\mathbf{v}') P_t(\mathbf{v}' \to d^3 v) \ d^3 v' \\ &= \int_{\mathbb{R}^3} \int \chi(\mathbf{v}) f_0(\mathbf{v}) \phi(\mathbf{v}') P_t(\mathbf{v} \to d^3 v') \ d^3 v \end{split}$$

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where in the last step detailed balance (P4) has been invoked. Recalling that the (primary) semigroup H_t belonging to a Markov process is defined by^(1,2)

$$H_t \phi(\mathbf{v}) \coloneqq \int_{\mathbb{R}^3} \phi(\mathbf{v}') P_t(\mathbf{v} \to d^3 v') \tag{3}$$

we conclude that

$$\int_{\mathbb{R}^3} \chi(\mathbf{v}) H_t^{\dagger} \mu(d^3 v) = \int_{\mathbb{R}^3} \chi(\mathbf{v}) f_0(\mathbf{v}) H_t \phi(\mathbf{v}) \ d^3 v \tag{4a}$$

i.e., the measure $H_t^{\dagger}\mu$ has density $f_0(\mathbf{v})H_t\phi(\mathbf{v})$. On the other hand,

$$\int_{\mathbb{R}^3} \chi(\mathbf{v}) H_t^{\dagger} \mu(d^3 v) = \int_{\mathbb{R}^3} \phi(\mathbf{v}) f_0(\mathbf{v}) H_t \chi(\mathbf{v}) \, d^3 v \tag{4b}$$

The symmetry between expressions (4a) and (4b) suggests that we consider H_t as a symmetric operator acting in the weighted complex Hilbert space $L^2(\mathbb{R}^3, f_0)$, where the scalar product is

$$(\phi, \chi) = \int_{\mathbb{R}^3} f_0(\mathbf{v}) \phi(\mathbf{v}) \chi^*(\mathbf{v}) \ d^3 v$$

In this space, then, for all $\phi, \chi \in C^b$,

$$(H_t\phi,\chi) = (\phi, H_t\chi) \tag{5}$$

As a real operator, H_t could as well be studied on the corresponding real Hilbert space. For subsequent purposes (Section 5), however, it will be convenient to have the extension to the complex L^2 -space. The properties of H_t on L^2 are largely known.⁽⁴⁾ The obvious inequality

$$\int_{\mathbb{R}^3} \int f_0(\mathbf{v}) P_t(\mathbf{v} \to d^3 v') |H_t \phi(\mathbf{v}) - \phi(\mathbf{v}')|^2 \, d^3 v \ge 0 \tag{6}$$

reduces to

$$\|H_t\phi\| \leq \|\phi\| \tag{7}$$

i.e., H_t is contractive in L^2 . As $C^b(\mathbb{R}^3)$ is dense in L^2 , H_t extends by continuity to a contractive operator on the whole L^2 -space. Obviously $||H_t|| = 1$, because 1 is an eigenvalue corresponding to $\phi(\mathbf{v}) = 1$.

Inequality (7) guarantees stability of equilibrium. If $H_t\phi(\mathbf{v})$ describes a small deviation from equilibrium

$$f(\mathbf{v}, t) = f_0(\mathbf{v})(1 + H_t\phi), \qquad |\phi(\mathbf{v})| \ll 1$$

one can see that (7) is equivalent to a modified *H*-theorem. The latter states that the free energy belonging to the probability measure of the particle,

$$F(t) = kT \int_{\mathbb{R}^3} f[\ln f + \frac{1}{2}v^2] \, d^3v$$

cannot increase in time.

While stability follows from detailed balance, for deriving the approach to equilibrium we call upon the positivity of P_t , (P5). Obviously, equality in (6) and therefore in (7) can only hold if $H_t\phi = \phi = \text{const.}$

Since H_t is the semigroup associated with a strict Markov process, H_t maps $C^b(\mathbb{R}^3)$ into itself.^(1,2) For $\phi \in C^b(\mathbb{R}^3)$, we have

$$H_t \phi(\mathbf{v}) \to \phi(\mathbf{v}) \quad \text{as} \quad t \to 0 \qquad \text{for all} \quad \mathbf{v} \in \mathbb{R}^3$$
 (8)

and by (P2),

$$\sup_{\mathbf{v}\in\mathbb{R}^3}|H_t\phi(\mathbf{v})| \leq \sup_{\mathbf{v}\in\mathbb{R}^3}|\phi(\mathbf{v})| \tag{9}$$

Relations (8) and (9) imply, in view of Lebesgue's dominated-convergence theorem, that

$$\|H_t \phi - \phi\| \to 0 \quad \text{as} \quad t \to 0 \tag{10}$$

As $C^b(\mathbb{R}^3)$ is dense in L^2 , and as H_t is contractive, one easily checks that (10) holds for all $\phi \in L^2$. Referring to (P1)-(P5), we can summarize:

(H1) The H_t form a strongly continuous contractive semigroup of operators in $L^2(\mathbb{R}^3, f_0)$.

(H2) If 1 denotes the function $\phi(\mathbf{v}) = 1$, we have $H_t \mathbf{1} = 1$.

(H3) H_t commutes with all elements of the rotation group.

(H4) Since by Eqs. (5) and (7) H_t is symmetric and bounded, it is self-adjoint.

(H5) $\phi(\mathbf{v}) = \text{const}$ is the only function invariant against H_t , so that 1 is a simple eigenvalue of this operator.

The last statement follows from (6) and the associated remarks, or from an ergodic theorem.⁽⁴⁾

The generator (-C) of the semigroup $\{H_t\}$ is introduced by

$$-C\phi \coloneqq \lim_{t\downarrow 0} \frac{1}{t} (H_t \phi - \phi)$$

for all $\phi \in L^2$ such that the limit exists. It is known⁽⁹⁾ that such an operator is closed and densely defined. Because of (H4) it is symmetric. Moreover, as $\{H_t\}$ is contractive, C is accretive (or equivalently, -C is dissipative),

$$(C\phi, \phi) \ge 0$$
 for all $\phi \in D(C)$ (11)

By a known theorem,⁽¹⁰⁾ C is also maximal accretive, so that it coincides with its Friedrichs extension. Thus C is self-adjoint.

For $\phi \in D(C)$, $H_t \phi := \Phi(\mathbf{v}, t)$ is a solution of the kinetic equation

$$(\partial/\partial t + C)\Phi(\mathbf{v}, t) = 0 \tag{12}$$

with the initial value $\Phi(\mathbf{v}, 0) = \phi(\mathbf{v})$. In this connection C (or -C) is known as the collision operator.

Let us again summarize:

(C1) The collision operator is accretive, $(C\phi, \phi) \ge 0, \forall \phi \in D(C)$.

(C2) C1 = 0, i.e., the equilibrium function $\phi = 1$ is an eigenfunction corresponding to the eigenvalue $\lambda_0 = 0$.

(C3) C commutes with the rotation group.

(C4) $C = C^{\dagger}$.

(C5) $\lambda_0 = 0$ is a simple eigenvalue of C. Consequently, equality in (11) can only hold for $\phi = \text{const.}$

Simplicity of the zero eigenvalue follows from the identity $(H_t - 1)\phi = -\int_0^t H_t C\phi \, d\tau$. The last expression vanishes if $C\phi = 0$, so that $H_t\phi = \phi$, which by (H5) has the unique solution $\phi = \text{const.}$ To derive the second assertion, we use the Cauchy-Schwartz inequality for $(C\phi, \chi)$, with arbitrary $\chi \in D(C)$ and ϕ such that $(C\phi, \phi) = 0$. The equation $C\phi = 0$ follows.

3. EXAMPLES: BOLTZMANN AND FOKKER-PLANCK EQUATIONS

Markov processes describing diffusion in velocity space are usually assumed to be either jump processes or to be continuous.^(1,2) In the first case, C equals the difference of a multiplicative and an integral operator, so that the Boltzmann equation with finite collision rate is obtained. If for $\mathbf{v} \neq \mathbf{v}'$ the transition probability is absolutely continuous, the collision operator can be specified as^{(11),3}

$$C\phi(\mathbf{v}) = \nu(\mathbf{v})\phi(\mathbf{v}) - \int_{\mathbb{R}^3} K(\mathbf{v} \to \mathbf{v}')\phi(\mathbf{v}') \ d^3v'$$
(13)

The consequences of (C1)-(C5) for the scattering kernel K are straightforward, e.g., $v(v) = \int K(\mathbf{v} \rightarrow \mathbf{v}') d^3v'$ from (C2).

In the other extreme of a continuous Markov process the collision operator is local. If the domain of C includes the functions 1, v and the tensor product $v \otimes v$, the restriction of C to twice continuously differentiable functions is a second-order differential operator.⁽²⁾ We then have a diffusion process, described by the Fokker-Planck equation,^(1,2,12) where

$$C\phi(\mathbf{v}) = -(\nabla - \mathbf{v}) \cdot \boldsymbol{\zeta}(\mathbf{v}) \cdot \nabla \phi(\mathbf{v})$$
(14)

³ It is mainly the linearized Boltzmann operator, pertinent to the single-gas problem, that is analyzed in Ref. 11. However, with little modification, the conclusions also apply to the linear Boltzmann equation describing the diffusion of a foreign particle.

The friction tensor $\zeta(v)$ must be once continuously differentiable. Its components are obtained from products of components of velocity increments by averaging over the transition probability,

$$\begin{aligned} \boldsymbol{\zeta}(\mathbf{v}) &= \lim_{t \downarrow 0} \frac{1}{2t} \int_{\mathbb{R}^3} P_t(\mathbf{v} \to d^3 v') (\mathbf{v}' - \mathbf{v}) \otimes (\mathbf{v}' - \mathbf{v}) \\ &= -\frac{1}{2} \lim_{\mathbf{v}' \to \mathbf{v}} C(\mathbf{v}' - \mathbf{v}) \otimes (\mathbf{v}' - \mathbf{v}) \end{aligned} \tag{15}$$

where C acts upon v'. Another relation is

$$\nabla \cdot \boldsymbol{\zeta}(\mathbf{v}) - \mathbf{v} \cdot \boldsymbol{\zeta}(\mathbf{v}) = \lim_{t \to 0} \frac{1}{t} \int_{\mathbb{R}^3} P_t(\mathbf{v} \to d^3 v') (\mathbf{v}' - \mathbf{v}) = -C\mathbf{v}$$
(16)

We notice that ζ is symmetric and positive semidefinite.

Properties (C2) and (C4) have already been taken into account by specializing the differential operator in (14). Use was made of the fact that in our L^2 -space, the adjoint of ∇ is $-(\nabla - \mathbf{v})$. This also helps to verify (C1),

$$(C\phi,\phi) = (\boldsymbol{\zeta} \cdot \nabla\phi, \cdot \nabla\phi) \ge 0 \tag{17}$$

In view of (C5) and Eq. (15), $\zeta(\mathbf{v})$ is positive definite for all \mathbf{v} , so that C is a positive-semidefinite operator in the whole of \mathbb{R}^3 .

Rotational invariance demands that the friction tensor can only have two different eigenvalues, corresponding to directions parallel and perpendicular to v. The eigenvalues can only depend upon speed v (the magnitude of v). Thus^(13,14)

$$\boldsymbol{\zeta}(\mathbf{v}) = \boldsymbol{\zeta}_{\perp}(v)\mathbf{1} + [\boldsymbol{\zeta}_{\parallel}(v) - \boldsymbol{\zeta}_{\perp}(v)](\mathbf{v} \otimes \mathbf{v})/v^2$$
(18)

where 1 is the unit tensor.

Physical arguments by which the Fokker-Planck equation is derived (admittedly in a nonrigorous way) lead to further restrictions for the tensor $\zeta(\mathbf{v})$. Most often the equation is justified either by assuming weak coupling (interaction potential between the diffusing particle and fluid bounded by $U_{\max} \ll kT$), or by taking the Rayleigh gas (very heavy particle in a light gas). In neither case can the Fokker-Planck equation hold on a time scale involving single collisions, since the corresponding velocity increments do not have a Gaussian distribution. Hence the limits in Eqs. (15) and (16) should not be understood literally in physical applications. Multiple scattering, however, produces approximately Gaussian distributions, and the equation becomes approximately valid. Strict validity is, of course, only reached in the appropriate limits. (One must then be careful with the ordering of various limits.)

In both models individual encounters only cause infinitesimal changes in the velocity of the particle. For not too long times the force acting upon the particle and then the velocity increment appearing in Eq. (15) can therefore be expressed as if the trajectory were a straight line.⁽¹²⁾ That force can be written as the gradient $\nabla_{\mathbf{r}}$ in position space of a random potential,

$$\mathbf{F} = -\nabla_{\mathbf{r}} U(\mathbf{r}, \mathbf{r}_2, ..., \mathbf{r}_N)$$

where $\mathbf{r}_2(t),...,\mathbf{r}_N(t)$ describe the random motion of the fluid molecules. In view of the straight-trajectory approximation, $\mathbf{r}(t) = \mathbf{v}t$, $\nabla_{\mathbf{r}}U$ is proportional to a gradient in velocity space. The velocity increment $\mathbf{v}' - \mathbf{v}$ during a suitable time interval then appears as a gradient in velocity space of a random potential. For a random vector field of this nature the formula of Obuhov and Yaglom⁽¹³⁾ asserts that

$$\zeta_{\parallel}(v) = (d/dv)[v\zeta_{\perp}(v)] \tag{19}$$

An explicit derivation in the present context has been given by Corngold.⁽¹⁴⁾

In the rather unrealistic weak coupling model the transverse velocity change in one collision is proportional to v^{-1} , which leads to $\zeta_{\perp}(v) = O(v^{-1})$ and $\zeta_{\parallel}(v) = O(v^{-3})$ for $v \to \infty$.⁽¹⁴⁾ The same asymptotic dependence is obtained for Coulomb interaction, i.e., for the motion of a heavy ion in a plasma.⁽¹⁵⁾

If for the Rayleigh-gas model the linear Boltzmann equation is used as the starting point, a constant isotropic friction tensor is obtained, expressed by moments of the differential scattering cross section. (However, the velocity of the heavy particle must stay small compared to thermal velocities of the gas molecules; at higher velocities the Fokker–Planck equation is no longer a valid approximation.)

The quoted models do not exhaust all possible applications of the Fokker-Planck equation, so that there is good reason to consider more general friction kernels. An intermediate model arises from considering light fluid molecules with small hard cores surrounded by weak long-range fields. One must then expect a variable $\zeta(v)$, approaching a nonvanishing limit at high (but not too high) velocities. With this in mind, we shall henceforth assume that the following conditions hold

$$\lim_{v \to \infty} \zeta_{\parallel}(v) = \lim_{v \to \infty} \zeta_{\perp}(v) > 0, \qquad \lim_{v \to \infty} \frac{1}{v\zeta_{\parallel}(v)} \frac{d\zeta_{\parallel}}{dv} = 0$$
(20)

though somewhat weaker restrictions would suffice for the subsequent derivations. The weak coupling model and the Coulomb case violate the first of conditions (20), and will therefore be considered as exceptions.

4. SPECTRA OF COLLISION OPERATORS

Eigenvalue problems associated with kinetic equations naturally arise when distributions exponentially approaching equilibrium are sought. If $\Phi(\mathbf{v}, t) = \phi(\mathbf{v})e^{-\lambda t}$ in Eq. (12), then

$$C\phi = \lambda\phi \tag{21}$$

Since C is positive semidefinite, its spectrum is confined to the nonnegative part of the real axis. We also know that $\lambda_0 = 0$ is a simple eigenvalue.

The remaining part of the spectrum may differ from case to case. If the scattering operator K represented by the integral in Eq. (13) is compact (as is the case for the hard-sphere model), then the Boltzmann collision operator has an essential spectrum consisting of the values assumed by the collision rate $\nu(v)$.^(11,16) Usually this is the interval $[\nu_{\min}, \infty)$. There may be further eigenvalues within the gap $(0, \nu_{\min})$, or even an infinite series of them accumulating at the infimum ν_{\min} of the collision rate.^(11,17)

We are going to see that Fokker-Planck collision operators have discrete spectra if condition (20) is fulfilled. For the special case with $\zeta = 1/D$ (where D is the diffusion coefficient) this is well known. After symmetrization, the operator differs only by an additive constant from the Schrödinger operator for the isotropic three-dimensional harmonic oscillator. Hence the eigenfunctions are the same in both cases and the spectra identical, except for the displacement. The spectrum of C consists of equidistant eigenvalues: $\lambda_n = n/D$, n = 0, 1, 2,...

In the same way, the more general operator from Eq. (14) is transformed into a Schrödinger-like form, so that use can be made of established criteria for the discreteness of the spectrum. We substitute $\phi(\mathbf{v}) = [\exp(\frac{1}{4}v^2)]\psi(\mathbf{v})$, which leads to

$$\lambda \psi = [\exp(-\frac{1}{4}v^2)]C[\exp(\frac{1}{4}v^2)]\psi = -(\nabla - \frac{1}{2}\mathbf{v})\cdot\boldsymbol{\zeta}(\mathbf{v})\cdot(\nabla + \frac{1}{2}\mathbf{v})\psi$$
$$= [-\nabla\cdot\boldsymbol{\zeta}(\mathbf{v})\cdot\nabla + V(v)]\psi$$
(22)

$$V(v) = \frac{1}{4}\mathbf{v}\cdot\boldsymbol{\zeta}(\mathbf{v})\cdot\mathbf{v} - \frac{1}{2}\operatorname{Tr}\,\boldsymbol{\zeta}(\mathbf{v}) - \frac{1}{2}(\nabla\cdot\boldsymbol{\zeta}(\mathbf{v}))\cdot\mathbf{v}$$
$$= (\frac{1}{4}v^2 - \frac{3}{2})\boldsymbol{\zeta}_{\parallel}(v) - \frac{1}{2}v\,d\boldsymbol{\zeta}_{\parallel}/dv$$
(23)

Though no use has been made of relation (19), V(v) is determined by $\zeta_{\parallel}(v)$ alone.

The operator appearing in Eq. (22) is a modified representation of C, operating in the space $L^2(\mathbb{R}^3)$ without weight. For the spectrum to be discrete it suffices that $\zeta(\mathbf{v})$ is positive definite, that V(v) and the components of $\zeta(\mathbf{v})$ are locally bounded, while $V \to \infty$ for $v \to \infty$.⁽¹⁸⁾ The latter condition is seen to hold for any $\zeta(\mathbf{v})$ satisfying Eqs. (20).

The exceptional case of weak coupling has been investigated by Mazo and Résibois,⁽¹⁹⁾ who found a continuous spectrum covering the whole interval $(0, \infty)$. The Coulomb case is similar. For both models, approach to equilibrium can be arbitrarily slow, which is not true for models obeying conditions (20).

5. SPECTRA OF FOURIER-TRANSFORMED TRANSPORT OPERATORS

If also the position of the diffusing particle is recorded, we have a Markov process in the phase space $\mathbb{R}^6 = \mathbb{R}^3 \times \mathbb{R}_r^3$. (The position space \mathbb{R}_r^3 is distinguished by a subscript from velocity space \mathbb{R}^3 .)

The process is of a special kind insofar as the variable $\mathbf{r}(t)$ is fully determined by $\mathbf{v}(t)$ through

$$\mathbf{r}(t) = \mathbf{r}(0) + \int_0^t \mathbf{v}(\tau) \, d\tau$$

We expect intuitively that the generator of such a process, restricted to the appropriate set of differentiable functions, should have the form $-(\mathbf{v} \cdot \nabla_{\mathbf{r}} + C)$, where -C is the generator of the process in \mathbb{R}^3 . For jump processes this has been proven by Papanicolau.⁽²⁰⁾ Without attempting a more general proof, we trust that for a probability measure with density $f(\mathbf{r}, \mathbf{v}, t) = f_0(\mathbf{v})\Phi(\mathbf{r}, \mathbf{v}, \mathbf{t})$, with sufficiently smooth Φ , the following kinetic equation is valid:

$$(\partial/\partial t + \mathbf{v} \cdot \nabla_{\mathbf{r}} + C)\Phi = 0 \tag{24}$$

The negative of the generator, $(\mathbf{v} \cdot \nabla_{\mathbf{r}} + C)$, will be called the transport operator.

A slightly generalized interpretation of Eq. (24) also admits measures that are not normalized or may even be unbounded in \mathbb{R}^6 . The excuse is that we may think of a suspension of many particles. However, the suspension must be sufficiently dilute so that the particles do not interact with each other.

We refrain from investigating the spectrum of the transport operator and from specifying appropriate functional spaces. Instead, with the idea of a Fourier-Laplace transformation in the back of our mind, we proceed to look for special solutions of Eq. (24) of the form

$$\Phi(\mathbf{r}, \mathbf{v}, t) = \phi(\mathbf{v}) \exp(i\mathbf{k} \cdot \mathbf{r}) \exp(-\lambda t)$$

This leads to an eigenvalue problem for the Fourier-transformed transport operator $T_{\mathbf{k}} = C + i\mathbf{k} \cdot \mathbf{v}$,

$$(T_{\mathbf{k}} - \lambda)\phi = 0 \tag{25}$$

If **k** is regarded as a fixed parameter, T_k is an operator acting on functions of **v** only, so that it can be analyzed in the same space $L^2(\mathbb{R}^3, f_0)$ as before.

Obviously T_k is not self-adjoint and in general not even normal, so that conclusions about its spectrum are more difficult to reach. To start with, we study T_k on $D(T_k) = C_0^{\infty}(\mathbb{R}^3)$, take its closure (again denoted as T_k), and note the following properties:

(T1) T_k is densely defined and accretive, i.e., $\operatorname{Re}(T_k\phi, \phi) \ge 0$, $\forall \phi \in D(T_k)$.

(T2) Since the left-hand side of inequality (T1) merely involves C, it is again true that equality only holds for $\phi(\mathbf{v}) = \text{const.}$

(T3) Simultaneous rotation of \mathbb{R}^3 and of the vector **k** leaves T_k unaffected. Hence, rotation of **k** does not affect the spectrum of T_k . In particular, an eigenvalue $\lambda(k)$ can only depend upon the magnitude of **k**. If $\phi(\mathbf{v})$ is the corresponding eigenfunction, $\phi(\mathbf{R}\mathbf{v})$ is the eigenfunction of $T_{\mathbf{R}\mathbf{k}}$ corresponding to the unchanged eigenvalue $\lambda(k)$.

A rotation by 180° leads to the complex-conjugate operator $T_{\mathbf{k}}^* = C - i\mathbf{k}\cdot\mathbf{v}$. (One of its extensions equals the adjoint $T_{\mathbf{k}}^{\dagger}$.) Spectral points thereby turn into their complex-conjugate values. Yet by (T3) the spectrum remains the same. Hence it is symmetric with respect to the real axis. In particular, eigenvalues are either real or they occur in complex-conjugate pairs.

More can be said about the spectrum if $T_{\mathbf{k}}$ is form-sectorial,⁽²¹⁾ which means that the values of the corresponding quadratic form are within a sector inside some right-hand half-plane. That is, we suppose that real γ and δ , $0 < \delta < \frac{1}{2}\pi$, can be found such that

$$(T_{\mathbf{k}}\phi,\phi)+\gamma = |(T_{\mathbf{k}}\phi,\phi)+\gamma|e^{i\varphi}, \quad -\delta \leqslant \varphi \leqslant \delta$$
(26)

for any $\phi \in D(T_k)$, $\|\phi\|^2 = 1$. By closing the form and taking the associated operator we arrive at the Friedrichs extension of T_k . Henceforth the symbol T_k will be used to denote this extension. We then compare the forms $(T_k\phi, \chi)$ and $(T_{-k}\phi, \chi) = (\phi, T_k\chi)$. Since T_k is closed and densely defined, we conclude ⁽²¹⁾:

(T4) Switching of **k** produces the adjoint operator, $T_{\mathbf{k}}^{\dagger} = T_{-\mathbf{k}}$.

The spectrum of $T_{\mathbf{k}}$ is thus confined to the half-plane $\operatorname{Re}(\lambda) \ge 0$. Another consequence of (T4) and of the symmetry of the spectrum is that the residual spectrum $\sigma_r(T_{\mathbf{k}})$ is empty. Indeed, if $\lambda \in \sigma_r(T_{\mathbf{k}})$, then λ^* is an eigenvalue of $T_{\mathbf{k}}^{\dagger} = T_{-\mathbf{k}}$. However, since eigenvalues are not affected by the switching of \mathbf{k} , we have a contradiction.

In order to assure the sectorial property of Fourier-transformed transport operators, we observe that any operator of the form T = C + iL, where C is positive semidefinite and L self-adjoint, is sectorial if the form

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 $(L\phi, \phi)$ is relatively bounded with respect to $(C\phi, \phi)$. This means⁽²¹⁾ that $D(L) \supseteq D(C)$ and that nonnegative constants *a* and *b* exist such that

$$|(L\phi,\phi)| \leq a \|\phi\|^2 + b(C\phi,\phi) \tag{27}$$

for all $\phi \in D(C)$. The proof of the assertion is straightforward, and we even obtain values of parameters that fit Eq. (26): tg $\delta = b$, $\gamma = a/b$.

We are left with the task of finding out which particular models meet the required conditions. The Boltzmann operator is easy to understand in this respect. If, as is often the case, the scattering operator K represented by the integral in Eq. (13) is bounded in L^2 , we only have to compare both multiplicative parts of $T_{\mathbf{k}}$. The form $(\mathbf{k} \cdot \mathbf{v}\phi, \phi)$ is seen to be relatively bounded with respect to $(\nu\phi, \phi)$ if

$$\lim_{v\to\infty} \left[\nu(v)/v \right] > 0$$

Hence for bounded K this condition suffices for the Boltzmann $T_{\mathbf{k}}$ to be form-sectorial. The condition is also necessary: if $\lim[\nu(v)/v] = 0$, one can see that $T_{\mathbf{k}}$ is not form-sectorial.

The picture is particularly simple if K is a compact operator. We then have an essential spectrum consisting of the values assumed by the multiplicative operator $[\nu(v) + i\mathbf{k}\cdot\mathbf{v}]$. For typical cases (e.g., the hard-sphere model) these values cover an area bounded by a hyperbola-like curve with the vertex at $\lambda = \nu_{\min} = \nu(0)$. This part of the spectrum remains unaffected by the compact perturbation, which, in general, only introduces eigenvalues (real ones and complex conjugate pairs) outside that area.⁽²²⁾

As for the Fokker-Planck case, we are now going to show that the form $(\mathbf{k} \cdot \mathbf{v}\phi, \phi)$ is relatively bounded with respect to $(C\phi, \phi)$ whenever V(v) from Eq. (23) has the property

$$\lim_{v \to \infty} \left[V(v)/v \right] = \infty \tag{28}$$

For friction tensors meeting condition (20) this property is obviously assured, while weak and Coulomb interactions again represent exceptions.

Since, in view of rotational invariance, the direction of **k** is irrelevant, we keep it fixed and only vary the magnitude k of this vector. Thus, effectively, $T_{\mathbf{k}}$ is a one-parameter family of operators. Choosing **k** as the polar axis, we can write

$$T_{\mathbf{k}} = C + ikv\cos\vartheta, \qquad (T_{\mathbf{k}}\phi,\phi) = (C\phi,\phi) + ik(v(\cos\vartheta)\phi,\phi)$$

Next we notice that, since V(v) is locally bounded, (28) implies that for any N > 0, there are constants A = A(N) and B = B(N) such that V(v) > Nv for v > A and |V(v)| < B for v < A. Moreover, for $\phi \in D(C)$, let $\psi = [\exp(-\frac{1}{4}v^2)]\phi$ as in Section 4. A little analysis then yields the estimate

 $|(v(\cos \vartheta)\phi, \phi)| < (v\phi, \phi)$

$$\begin{split} &= \int_{v < A} v |\psi|^2 \, d^3 v + \int_{v > A} v |\psi|^2 \, d^3 v \\ &\leq A(\phi, \phi) + \frac{1}{N} \int_{v > A} V(v) |\psi|^2 \, d^3 v \\ &\leq A(\phi, \phi) + \frac{1}{N} \int_{\mathbb{R}^3} V(v) |\psi|^2 \, d^3 v + \frac{1}{N} \int_{v < A} |V(v)| \, |\psi|^2 \, d^3 v \\ &\leq (A + B/N)(\phi, \phi) + \frac{1}{N} \int_{\mathbb{R}^3} [-\nabla \cdot \boldsymbol{\zeta} \cdot \nabla + V(v)] |\psi|^2 \, d^3 v \\ &= (A + B/N)(\phi, \phi) + N^{-1} (C\phi, \phi) \end{split}$$

It follows that the form $(v(\cos \vartheta)\phi, \phi)$ is relatively bounded with respect to $(C\phi, \phi)$, with the relative bound equal to zero.

An interesting consequence is that T_k has compact resolvent for all k, or, equivalently, T_k has purely discrete spectrum. To prove that this is so, we again fix the direction of k, and admit complex values of the scalar k in

$$t_k[\phi,\phi] \coloneqq (T_\mathbf{k}\phi,\phi)$$

In view of Theorem 1.33 on p. 320 in Kato,⁽²¹⁾ we know that t_k is closable and that $D(\tilde{t}_k)$ is independent of k. The closure is again a sectorial form, so that the set $\{\tilde{t}_k\}$ is a holomorphic family of forms of type (a) (p. 395 in Kato⁽²¹⁾). Since T_k has been extended in the Friedrichs sense, the set $\{T_k\}$ forms a holomorphic family of operators of type (B). As we already know that $T_0 = C$ has compact resolvent, the assertion follows from the theorem on p. 396 in Kato.⁽²¹⁾

For the special case with $\zeta = 1/D$ the spectrum of T_k is known to differ from that of C merely by a translation along the real axis⁽²³⁾; the eigenvalues are $\lambda_n = n/D + k^2D$. For a more general ζ the picture may become more complicated.

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