

## Discrete Relaxation Times in Neutron Thermalization\*

IVAN KUŠČER† AND NOEL CORNGOLD  
*Brookhaven National Laboratory, Upton, New York*  
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On the basis of the Van Hove theory, an analysis is given of those properties of the neutron-scattering law which influence the decay constants (the reciprocal relaxation times) in neutron thermalization. It is shown how the known differences in the long-time behavior of the correlation functions for a gas, a liquid, and a solid are reflected in the different behavior of the differential cross sections at low energies. This behavior ultimately determines the general character of the spectrum of decay constants for a uniform neutron distribution in an infinite medium. For a gaseous moderator, either there is an infinite set of discrete decay constants, strongly accumulating towards the lower limit  $\lambda^* = \min[v\Sigma(v)]$  of the continuous spectrum, or else the spectrum below  $\lambda^*$  is empty altogether. On the other hand, for a solid, the set of discrete decay constants is always finite, or possibly empty. The liquid appears to allow, in principle, all three possibilities, but normally the spectrum is expected to resemble that of a solid. In any case, the existence of the lowest decay constant  $\lambda_0$  (and hence the existence of an infinite set for a gas) is trivial whenever absorption is absent or of the  $1/v$  kind. Only an absorption rate  $v\Sigma_a(v)$  which strongly increased in the small- $v$  region could cause the complete disappearance of the discrete spectrum. In this event any initial neutron distribution slowly evolves towards a singular distribution containing a  $\delta(v)$  term, or some weaker singularity, and the decay rate approaches  $\lambda^*$ .

### I. INTRODUCTION

ONE of the basic problems in neutron-thermalization theory deals with the time evolution of a neutron distribution in an infinite sourceless unchanging medium. Both the medium and the neutron distribution are assumed to be uniform and isotropic.

In the case of a nonabsorbing medium we want to know how, and how fast, thermal equilibrium is approached. A slightly more general problem is posed by considering an absorbing medium, where we have the equation

$$\frac{\partial}{\partial t} N(v, t) = -v\Sigma(v)N(v, t) + \int_0^\infty v'\Sigma_s(v' \rightarrow v)N(v', t)dv'. \quad (1)$$

Herein  $N(v, t)$  is the neutron number density per unit velocity interval, and  $\Sigma(v)$  the macroscopic total cross section (the inverse mean free path of the neutrons), which is the sum of contributions due to scattering and to absorption:

$$\Sigma(v) = \Sigma_s(v) + \Sigma_a(v),$$

$$\Sigma_s(v) = \int_0^\infty \Sigma_s(v \rightarrow v')dv'.$$

The "thermalization kernel"  $\Sigma_s(v \rightarrow v')$  is given by the angular integral of the macroscopic differential scattering cross section (defined here per unit volume in velocity space),

$$\Sigma_s(v \rightarrow v') = \int \Sigma_s(\mathbf{v} \rightarrow \mathbf{v}')v'^2 d\Omega, \quad (2)$$

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† Fulbright-Hays Visiting Scholar. Permanent address: Institute of Physics, University of Ljubljana, Ljubljana, Yugoslavia.

and obeys the detailed balance relation,

$$vM(v)\Sigma_s(v \rightarrow v') = v'M(v')\Sigma_s(v' \rightarrow v),$$

$$M(v) = v^2 \exp(-mv^2/2k_B T).$$

We shall look for solutions of the form

$$N(v, t) = N(v)e^{-\lambda t},$$

with  $N(v)$  satisfying

$$[v\Sigma(v) - \lambda]N(v) = \int_0^\infty v'\Sigma_s(v' \rightarrow v)N(v')dv'. \quad (3)$$

Several recent papers<sup>1-6</sup> have been devoted to this subject, and particularly to the nature of the spectrum of the decay constants  $\lambda$ . Corngold, Michael, and Wollman<sup>1,2</sup> have shown that the values assumed by the function  $v\Sigma(v)$  form the continuous part of the spectrum. As pointed out by Grad<sup>7</sup> in a related context, this is a consequence of a theorem of Weyl and von Neumann.<sup>8</sup> A rigorous investigation of the nature of the spectrum, for the case of a monatomic gaseous moderator, has been carried out by Shizuta.<sup>9</sup>

In view of what has been said, the lower limit of the

<sup>1</sup> N. Corngold and P. Michael, On the Decay Constants in Pulsed Neutron Experiments, 1962 (unpublished).

<sup>2</sup> N. Corngold, P. Michael, and W. Wollman Proceedings of the Conference on Neutron Thermalization, Vol. 4, p. 1103, BNL Rept. 719 (C-32), 1962 (unpublished); Nucl. Sci. & Eng. 15, 13 (1963).

<sup>3</sup> J. U. Koppel, Nucl. Sci. Eng. 16, 101 (1963).

<sup>4</sup> N. Corngold, Nucl. Sci. Eng. 19, 80 (1964); N. Corngold and P. Michael, *ibid.* 19, 91 (1964).

<sup>5</sup> M. J. Ohanian and P. B. Daitch, Nucl. Sci. Eng. 19, 343 (1964).

<sup>6</sup> C. S. Shapiro and N. Corngold, Phys. Rev. 137, A1686 (1965); C. S. Shapiro, Brookhaven National Laboratory Report No. BNL 8433, 1964 (unpublished).

<sup>7</sup> H. Grad, *Proceedings of Third International Symposium on Rarefied Gas Dynamics, 1962* (Academic Press Inc., New York, 1963), Vol. 1, p. 26.

<sup>8</sup> F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Frederick Ungar Publishing Company, New York, 1955).

<sup>9</sup> Y. Shizuta, Progr. Theoret. Phys. (Kyoto) 32, 489 (1964).

continuous spectrum is at

$$\lambda^* = \min[v\Sigma(v)].$$

Usually the collision rate  $v\Sigma(v)$  reaches its minimum value at  $v=0$ , and we shall henceforth assume that this is so, and that  $\lambda^* > 0$ .

It is very plausible that  $\lambda^*$  is a natural upper bound for the decay constant of any non-negative solution of Eq. (3). That is, no neutron distribution can decay faster than the infinitesimal group of neutrons with the smallest possible collision rate.<sup>1,10</sup>

If there is a nonempty discrete spectrum below  $\lambda^*$ , the smallest decay constant  $\lambda_0$  corresponds to the unique non-negative solution  $N_0(v)$ , in view of an extension of the Perron-Jentzsch theorem<sup>11</sup> (see also Sec. III). Any neutron distribution asymptotically approaches this so-called fundamental mode of decay.

For a constant absorption rate (a  $1/v$  absorption law) the existence of this particular mode immediately follows from the detailed balance relation, namely

$$\begin{aligned} N_0(v) &\propto M(v), \\ \lambda_0 &= \lambda^{(a)} \equiv v\Sigma_a(v). \end{aligned}$$

On the other hand, for non- $1/v$  absorption the existence of such a discrete decay mode is not at all trivial. On the contrary, simple artificial models are conceivable where the discrete part of the spectrum is empty altogether (example in Sec. IV).

The results obtained with some realistic kernels also appear quite intriguing. For the proton gas model the existence of an infinite set of discrete decay constants below the bound  $\lambda^*$  has been proved.<sup>2</sup> The computations carried out by Shapiro and Corngold<sup>6</sup> suggest that this is true for the monatomic gas model in general, although the decay constants are strongly bunched towards  $\lambda^*$ . On the other hand, for a model of a solid, the results of those computations indicate that the discrete decay constants are truly finite in number.

The aim of the present paper is to examine the conditions for the existence or nonexistence of the discrete decay constants. It will also be shown which of these conditions we may expect to be fulfilled for real moderators. This should lead to a unified picture for the results previously obtained for special models by analytical or computational means. At the same time we hope for an explanation of the noted different behavior of a gas and a solid in this respect.

## II. PROPERTIES OF THE THERMALIZATION KERNEL

It will be convenient to generalize Eq. (3) by introducing an artificial parameter  $c$ ,

$$c[v\Sigma(v) - \lambda]N(v) = \int_0^\infty v'\Sigma_s(v' \rightarrow v)N(v')dv'. \quad (4)$$

<sup>10</sup> M. Nelkin, *Physica* **29**, 261 (1963).

<sup>11</sup> M. G. Kreĭn and M. A. Rutman, *Uspekhi Matem. Nauk* (N. S.) **3**, 3 (1948). [*Am. Math. Soc. Transl.*, 2nd ed., Ser. 1, Vol. 10, p. 199 (1962). See, in particular, p. 274, proposition ( $\beta'$ ).]

Following an idea of Lehner and Wing,<sup>12</sup> we then look for the eigenvalues of  $c$  for a given  $\lambda \leq \lambda^*$ . The results, when  $\lambda$  is allowed to vary, lead to the desired eigenvalues of  $\lambda$  for  $c=1$ . We are safe in limiting the discussion to real values of  $\lambda$ ; complex  $\lambda$  in Eq. (3) are easily excluded after the thermalization kernel is made symmetric according to detailed balance:

$$\tilde{\Sigma}_s(v, v') = [vM(v)/v'M(v')]^{1/2}\Sigma_s(v \rightarrow v').$$

The form of Eq. (4) is further simplified by introducing

$$\Psi_\lambda(v) = \{[v\Sigma(v) - \lambda]/M(v)\}^{1/2}N(v).$$

The resulting equation

$$c\Psi_\lambda(v) = \int_0^\infty K_\lambda(v, v')\Psi_\lambda(v')dv' \quad (5)$$

contains the kernel

$$K_\lambda(v, v') = \left\{ \frac{vv'}{[v\Sigma(v) - \lambda][v'\Sigma(v') - \lambda]} \right\}^{1/2} \tilde{\Sigma}_s(v, v'). \quad (6)$$

In order to link the problem to the usual theory of integral equations with symmetric kernels, we shall ask for solutions of Eq. (5) which are square integrable in  $(0, \infty)$  and thus belong to the Hilbert space  $L^2(0, \infty)$ . Of course, since the kernel  $K_\lambda$  in general is sufficiently well behaved, the solutions are expected to belong to a much narrower class of functions, which are continuous for  $v > 0$ . The restriction to the  $L^2$  space is meaningful only with respect to the behavior of  $\Psi_\lambda(v)$  at  $v \rightarrow 0$  and  $v \rightarrow \infty$ .

The existence of a nonempty set of such solutions  $\Psi_{\lambda_n}(v)$ , corresponding to a bounded discrete spectrum of eigenvalues  $c_n(\lambda)$ , is guaranteed whenever

$$\int_0^\infty \int_0^\infty K_\lambda^2(v, v')dv dv' < \infty. \quad (7)$$

In order to decide about this condition, we shall have to investigate some of the properties of  $\tilde{\Sigma}_s(v, v')$ . The remainder of this section will be devoted to that task.

For reasons mentioned in the introduction we shall be particularly interested in the behavior of  $K_\lambda(v, v')$  for  $\lambda$  close to  $\lambda^*$ . The factors  $(v\Sigma - \lambda)$  in (6) then enhance the values of the kernel in the near-zero velocity range. Thus we have to know the behavior of  $\tilde{\Sigma}_s(v, v')$  in this range, as well as the behavior of  $v\Sigma(v)$ .

*1. General properties of  $\tilde{\Sigma}_s(v, v')$ .* Several of the general properties of the kernel  $\tilde{\Sigma}_s(v, v')$ , which are of interest here, can be derived from Van Hove's theory of slow-

<sup>12</sup> G. M. Wing, *An Introduction to Transport Theory* (John Wiley & Sons, Inc., New York, 1962).

neutron scattering.<sup>13-17</sup> According to this theory the differential scattering rate, for a macroscopically isotropic medium, is a function of only two variables:

$$v\Sigma_s(\mathbf{v} \rightarrow \mathbf{v}') = (m/4\pi\hbar)\Sigma_b S(\kappa, \omega), \quad (8)$$

where  $\Sigma_b$  is the macroscopic bound-atom scattering cross section, and

$$\kappa = |\boldsymbol{\kappa}| = (m/\hbar) |\mathbf{v} - \mathbf{v}'|, \quad (9)$$

$$\omega = (m/2\hbar)(v^2 - v'^2). \quad (10)$$

$S(\kappa, \omega)$  is expressed by Fourier transforms of certain correlation functions,

$$S(\kappa, \omega) = (2\pi)^{-1} \int_{-\infty}^{\infty} \chi(\kappa, t) e^{-i\omega t} dt \quad (11)$$

$$= (2\pi)^{-1} \int d\mathbf{r} \int_{-\infty}^{\infty} G(\mathbf{r}, t) e^{i(\boldsymbol{\kappa} \cdot \mathbf{r} - \omega t)} dt. \quad (12)$$

For simplicity we shall confine ourselves to the case of a medium consisting of identical atoms, when

$$G(\mathbf{r}, t) = G_s(\mathbf{r}, t) + (\Sigma_{\text{coh}}/\Sigma_b)[G_d(\mathbf{r}, t) - \rho], \quad (13)$$

with  $\Sigma_{\text{coh}}$  being the coherent part of  $\Sigma_b$ , and  $G_s, G_d$  the correlation functions used by Van Hove. If different atoms are present  $G$  is a linear combination of several such functions.<sup>14</sup> We had to subtract from  $G_d(\mathbf{r}, t)$  the limiting value  $G_d(\infty, t) = \rho$  = the number density of the atoms, because for any macroscopic system this term gives rise to a contribution which essentially belongs to the uncollided beam.<sup>13,14</sup>

It is convenient to symmetrize  $S(\kappa, \omega)$  and other relevant functions according to detailed balance. As previously, we shall indicate such symmetrization by a tilde:

$$\tilde{S}(\kappa, \omega) = e^{-\omega\tau} S(\kappa, \omega) = \tilde{S}(\kappa, -\omega),$$

where

$$\tau = \hbar/2kT.$$

The transforms of  $\tilde{S}(\kappa, \omega)$  are

$$\tilde{\chi}(\kappa, t) = \chi(\kappa, t + i\tau),$$

$$\tilde{G}(\mathbf{r}, t) = G(\mathbf{r}, t + i\tau),$$

and they are real.

The incoherent approximation,  $\tilde{G}(\mathbf{r}, t) \approx \tilde{G}_s(\mathbf{r}, t)$ , and in particular the Gaussian approximation,

$$\tilde{G}(\mathbf{r}, t) \approx [4\pi\gamma(t)]^{-3/2} \exp[-r^2/4\gamma(t)], \quad (14)$$

$$\tilde{\chi}(\kappa, t) \approx \exp[-\kappa^2\gamma(t)], \quad (15)$$

<sup>13</sup> L. Van Hove, Phys. Rev. **95**, 249 (1954).

<sup>14</sup> G. H. Vineyard, Phys. Rev. **110**, 999 (1958).

<sup>15</sup> M. Nelkin, *Proceedings of the Symposium on Inelastic Scattering of Neutrons, 1960* (International Atomic Energy Agency, Vienna, 1961), p. 3.

<sup>16</sup> N. Corngold, *Lectures from the Second Neutron Physics Conference, 1962* (University of Michigan Press, Ann Arbor, Michigan, 1964).

<sup>17</sup> V. F. Turčin, Medlennye neitrony (Slow Neutrons), Moscow, 1963 (unpublished).

have been widely used. The latter is exact for the free monatomic gas, where the width function  $\gamma$  is given by

$$\begin{aligned} \gamma(t) &= v_M^2(t^2 + \tau^2), \\ v_M^2 &= k_B T/2M. \end{aligned} \quad (16)$$

For this particular case we have a closed expression for  $\tilde{S}$ ,

$$\tilde{S}(\kappa, \omega) = \frac{1}{2\pi^{1/2}v_M|\kappa|} \exp\left[-(v_M\tau\kappa)^2 - \left(\frac{\omega}{2v_M\kappa}\right)^2\right]. \quad (17)$$

An easy improvement over (14) and (15) can be introduced by Vineyard's convolution approximation,<sup>14</sup> which takes some account of the  $G_d$  contribution to  $G$ , responsible for interference effects. The resulting  $\tilde{\chi}(\kappa, t)$  and  $\tilde{S}(\kappa, \omega)$  are modified by a structure factor,

$$F(\kappa) = 1 + (\Sigma_{\text{coh}}/\Sigma_b)f(\kappa),$$

where  $f(\kappa)$  is the spatial Fourier transform of  $G_d(\mathbf{r}, 0) - \rho = g(\mathbf{r}) - \rho$ . We shall use this kind of approximation only for an estimate of  $\tilde{\chi}(\kappa, t)$  for small  $t$ , and for an asymptotic fit for large  $t$ , where<sup>14,18</sup>

$$\gamma(t) \rightarrow \gamma(\infty) \quad (\text{solid}), \quad (18a)$$

$$\rightarrow D(|t| - \tau_1) \quad (\text{liquid}). \quad (18b)$$

Whereas in the gas case the width function continues to increase like  $t^2$ , corresponding to the free motion of the atoms, the liquid exhibits in the asymptotic limit only a linear increase, which corresponds to the diffusive motion, and is governed by the self-diffusion coefficient  $D$ . In a solid such motion is negligible, and  $\gamma(t)$  tends to a finite limit  $\gamma(\infty)$ .

**2. Small-velocity approximations.** For reasons explained before we want to know how  $\tilde{S}(\kappa, \omega)$  behaves for small  $\kappa$  and  $\omega$ . First we must take care of a singular term which arises from the asymptotic part of  $\tilde{\chi}$ . For a solid we may write

$$\tilde{\chi}(\kappa, t) = F(\kappa) \exp[-\kappa^2\gamma(\infty)] + \tilde{\chi}'(\kappa, t), \quad (19)$$

which results in a decomposition of  $\tilde{S}$  into the elastic and inelastic parts

$$\tilde{S}(\kappa, \omega) = F(\kappa) \exp[-\kappa^2\gamma(\infty)]\delta(\omega) + \tilde{S}'(\kappa, \omega). \quad (20)$$

A similar decomposition can be carried out for a liquid, where we may speak of "quasielastic" and "truly inelastic" scattering:

$$\tilde{\chi}(\kappa, t) = F(\kappa) \exp[-\kappa^2 D(|t| - \tau_1)] + \tilde{\chi}'(\kappa, t), \quad (21)$$

$$\tilde{S}(\kappa, \omega) = F(\kappa) \exp(\kappa^2 D\tau_1) \frac{D\kappa^2}{\pi(D^2\kappa^4 + \omega^2)} + \tilde{S}'(\kappa, \omega). \quad (22)$$

All three cases (17), (20), and (22) agree in

$$\tilde{S}(\kappa, \omega) \rightarrow F(0)\delta(\omega) \quad \text{for } \kappa \rightarrow 0, \quad (23)$$

<sup>18</sup> P. A. Egelstaff and P. Schofield, Nucl. Sci. Eng. **12**, 260 (1962).

which is a consequence of  $\tilde{\chi}(0,t)=F(0)$  being time-independent. The latter can be seen from the definition<sup>15-17</sup> of the correlation function  $\chi$ .

An approximation of  $\tilde{S}'(\kappa,\omega)$  for small  $\kappa$  and  $\omega$  is obtained by expanding  $\tilde{\chi}'(\kappa,t)$  in powers of  $\kappa^2$ , which is certainly permissible. The  $\kappa^0$  term vanishes, in view of what has just been said, so that

$$\tilde{S}'(\kappa,\omega) = \kappa^2 S_1(\omega) + \kappa^4 S_2(\omega) + \dots$$

For a solid, Van Hove's considerations about the asymptotic behavior of the correlation functions lead to the conclusion that  $S_1(0)$  is finite. Assuming that the same is true also for a liquid, we have in both cases

$$\tilde{S}'(\kappa,\omega) \approx \kappa^2 S_1(0), \quad (24)$$

for small  $\kappa$  and  $\omega$ .

An expression for  $\tilde{\Sigma}_s(v,v')$  follows from Eqs. (2) and (8), with the substitution (9):

$$\begin{aligned} \tilde{\Sigma}_s(v,v') &= \frac{\hbar}{2m} \frac{\Sigma_b}{(vv')^{1/2}} \\ &\times \int_{(m/\hbar)|v-v'|}^{(m/\hbar)(v+v')} \tilde{S} \left[ \kappa, \frac{m}{2\hbar}(v^2-v'^2) \right] \kappa d\kappa. \end{aligned} \quad (25)$$

Since  $\tilde{S}$  is a non-negative function, and since it is reasonable to assume that the integrand in (25) does not identically vanish over any interval of  $\kappa$ , it follows that  $\tilde{\Sigma}_s(v,v')$  vanishes only at  $v$  or  $v' \rightarrow \infty$  and, possibly, at  $v$  or  $v' \rightarrow 0$ .

For a monatomic gas Eq. (25) leads to a well-known result,<sup>19</sup> which we need only in the small-velocity approximation,

$$\begin{aligned} \tilde{\Sigma}_s(v,v') &\approx \frac{\Sigma_b}{2\pi^{1/2}v_M} \left( \frac{v'}{v} \right)^{\pm 1/2} \\ &\text{for } v' \leq v \text{ and } v, v' \ll v_M. \end{aligned} \quad (26)$$

In the case of a solid we are going to use only the inelastic part  $\tilde{\Sigma}_s'$  of the kernel, derived from  $\tilde{S}'$  in the way of Eq. (25). For small velocities the approximation (24) leads to

$$\tilde{\Sigma}_s'(v,v') \approx (m/\hbar)^3 \Sigma_b S_1(0) (vv')^{1/2} (v^2+v'^2). \quad (27)$$

For a liquid we obtain

$$\begin{aligned} \tilde{\Sigma}_s(v,v') &= \frac{\eta \Sigma_b F(0)}{4\pi (vv')^{1/2}} \ln \frac{(v+v')^4 + \eta^2 (v^2-v'^2)^2}{(v-v')^4 + \eta^2 (v^2-v'^2)^2} \\ &+ O[(vv')^{1/2}], \end{aligned} \quad (28)$$

where

$$\eta = \hbar/2mD.$$

<sup>19</sup> A. M. Weinberg and E. P. Wigner, *The Physical Theory of Neutron Chain Reactors* (Chicago University Press, Chicago, 1958); E. P. Wigner and J. E. Wilkins, Jr., U. S. Atomic Energy Commission Rept. No. AEC-D-2275, 1944 (unpublished).

The few available data<sup>20-22</sup> indicate that the self-diffusion coefficient of monatomic liquids ordinarily equals a few times  $10^{-5}$  cm<sup>2</sup>/sec, whence it follows that the parameter  $\eta$  introduced here is of the order of 10.

The remarkable differences in the three small-velocity approximations are a direct consequence of the different long-time behavior of the correlation functions, as explained previously in terms of the  $\gamma(t)$ .

The discontinuity in the derivative of  $\tilde{\Sigma}_s(v,v')$  at  $v=v'$  in the gas case, and the logarithmic singularity for the liquid, indicate that neither of these  $\tilde{\Sigma}_s$  can be a degenerate kernel. The same applies to  $\tilde{\Sigma}_s'$  for a solid, where discontinuities are found along some lines in the  $v/v'$  plane, corresponding to certain values of  $\omega$ .<sup>13</sup>

3. *Square-integrability of  $\tilde{\Sigma}_s(v,v')$ .* We are now ready to examine whether the kernel  $\tilde{\Sigma}_s$  is square integrable in the sense of Eq. (7). In the gas case the answer is known to be positive.<sup>4</sup> In general, divergencies might be feared to arise from too slow vanishing of the integrand at  $v$  or  $v' \rightarrow \infty$ , or from singularities either inside the  $v/v'$  plane or at  $v \rightarrow 0$ ,  $v' \rightarrow 0$ .

For large  $|v-v'|$ , that is for large momentum transfers, any medium behaves like a free gas, and there is no doubt about the convergence of the integral in that region. Here  $\tilde{\Sigma}_s$  is found to decrease roughly exponentially. This implies that a strip of constant width along the line  $v=v'$  in the  $v/v'$  plane is excepted, and next we are going to estimate the average of  $\tilde{\Sigma}_s$  across that strip. Equation (25) leads to a double integral of  $\tilde{S}(\kappa,\omega)$ . The integral over  $d\omega$  is estimated to be of the order of  $\tilde{\chi}(\kappa,0) \sim \exp[-\kappa^2\gamma(0)]$ . Since  $\gamma(0) > 0$ , the integral over  $d\omega$  is bounded, and the quoted average is seen to decrease like  $1/v^2$  with  $v \rightarrow \infty$ . For the liquid this suffices to assure the square integrability of  $\tilde{\Sigma}_s$  in the  $(v \rightarrow \infty)$  portion of that strip, since the logarithmic singularity at  $v'=v$  causes no harm. In case of a solid the same can be assured for  $\tilde{\Sigma}_s'$ , which has no such singularity.

We are left with the last possibility that the integral might diverge in the near-zero velocity range. This actually happens with the liquid, as we can see from Eq. (28). Summarizing, we have

$$\int_0^\infty \int_0^\infty \tilde{\Sigma}_s^2(v,v') dv dv' < \infty \quad \text{for gas or solid,} \quad (29a)$$

$$= \infty \quad \text{for liquid,} \quad (29b)$$

where, in case of a solid,  $\tilde{\Sigma}_s$  stands for  $\tilde{\Sigma}_s'$ .

4. *Positive-definiteness of  $\tilde{\Sigma}_s(v,v')$ .* With respect to the problem of eigenvalues of Eq. (5) it would also be useful to know whether  $\tilde{\Sigma}_s(v,v')$  is positive definite. Let us see if we can assure this for the more general kernel  $\tilde{\Sigma}_s(\mathbf{v},\mathbf{v}')$ , i.e., whether

$$O\{\varphi\} = \int d\mathbf{v} \int d\mathbf{v}' \tilde{\Sigma}_s(\mathbf{v},\mathbf{v}') \varphi(\mathbf{v}) \varphi(\mathbf{v}') \geq 0 \quad (30)$$

for arbitrary real  $\varphi(\mathbf{v})$ .

<sup>20</sup> R. E. Hoffman, J. Chem. Phys. **20**, 1567 (1952).

<sup>21</sup> L. D. Hall and S. Rothman, Trans. Am. Inst. Mining, Met., Petrol. Engrs. **206**, 199 (1956).

<sup>22</sup> J. Naghizadeh and S. A. Rice, J. Chem. Phys. **36**, 2710 (1962).

We express  $\tilde{\Sigma}_s(\mathbf{v}, \mathbf{v}')$  in terms of  $\tilde{S}(\kappa, \omega)$ , and the latter function as a transform of  $\tilde{G}(\mathbf{r}, t)$ . After introducing

$$\psi(\mathbf{r}, t) = (2\pi)^{-1} \int v^{-1/2} \varphi(\mathbf{v}) \exp\left[ i \frac{m}{\hbar} (\mathbf{v} \cdot \mathbf{r} - \frac{1}{2} v^2 t) \right] d\mathbf{v} \quad (31)$$

we get

$$Q\{\varphi\} = \frac{m}{2\hbar} \int_{-\infty}^{\infty} d\mathbf{r} \int_{-\infty}^{\infty} dt \tilde{G}(\mathbf{r}, t) |\psi(\mathbf{r}, t)|^2. \quad (32)$$

Thus, non-negativity of  $\tilde{G}(\mathbf{r}, t)$  is a sufficient condition for the positive definiteness of  $\tilde{\Sigma}_s(\mathbf{v}, \mathbf{v}')$ , and hence of  $\tilde{\Sigma}_s(v, v')$ . Let us also observe that, incidentally,  $\psi(\mathbf{r}, t)$  is a solution of the Schrödinger equation for free space, namely that corresponding to an initial wave function in momentum space  $\propto v^{-1/2} \varphi(\mathbf{v})$ .

In the Gaussian approximation, and moreover in any incoherent approximation based upon a classical picture of  $\tilde{G}(\mathbf{r}, t)$ , this function is indeed non-negative. But we cannot hope that this is true in general, because of the oscillatory character of  $\tilde{G}_d(\mathbf{r}, t) - \rho$ , which constitutes a contribution to  $\tilde{G}(\mathbf{r}, t)$ . Still, an occurrence of negative values of  $\tilde{G}(\mathbf{r}, t)$  does not necessarily destroy the definiteness of  $\tilde{\Sigma}_s(\mathbf{v}, \mathbf{v}')$ . Namely,  $\psi(\mathbf{r}, t)$  is not completely arbitrary, because of the extra variable  $t$  introduced by Eq. (31). We may try to produce an example of a negative  $Q$  by choosing  $\psi(\mathbf{r}, 0)$  such that it differs from zero only where  $\tilde{G}(\mathbf{r}, 0)$  is negative. However, according to the mentioned quantum mechanical analogy, such a "wave packet" soon spreads out in space, with  $\int |\psi(\mathbf{r}, t)|^2 d\mathbf{r}$  staying constant. This means that the integral in Eq. (32) involves an averaging over a broad space-time region, and the result might very well be positive. The conclusion is that  $\tilde{\Sigma}_s(\mathbf{v}, \mathbf{v}')$ , and consequently  $\tilde{\Sigma}_s(v, v')$ , are positive definite under much wider conditions than that of  $\tilde{G}(\mathbf{r}, t)$  being non-negative.

5. *Properties of  $\Sigma_s(v)$ .* We now turn to the integrated scattering cross section, for which a convenient expression is obtained from Eq. (25), after inversion of integration order,

$$\Sigma_s(v) = \frac{1}{2} \left( \frac{\hbar}{m} \right)^2 \Sigma_b v^{-2} \int_0^\infty \kappa d\kappa \times \int_{-(\hbar/2m)\kappa^2 - v\kappa}^{-(\hbar/2m)\kappa^2 + v\kappa} S(\kappa, \omega) d\omega. \quad (33)$$

Another useful relation follows then

$$\frac{d}{dv} [v^2 \Sigma_s(v)] = \frac{1}{2} \left( \frac{\hbar}{m} \right)^2 \Sigma_b \times \int_{-\infty}^{\infty} S\left( \kappa, -\frac{\hbar}{2m} \kappa^2 + v\kappa \right) \kappa^2 d\kappa. \quad (34)$$

To make sure that this integral converges we verify from Eqs. (17), (20), (22), and (24) that no singularity arises at  $\kappa \rightarrow 0$ , and we observe that the integrand strongly vanishes as  $\kappa \rightarrow \infty$ .

Since the right-hand side of (34) is even in  $v$ , we

expect, for small  $v$ , an expansion of the form

$$v \Sigma_s(v) = \lambda^{(s)} + b_s v^2 + \dots, \quad (35)$$

and similarly for  $v \Sigma_s'(v)$  in case of a solid. Equation (34) shows that  $\lambda^{(s)}$  is positive and finite. The value of  $b_s$  is obtained through repeated differentiation of this equation. We may mention the known results for the monoatomic gas

$$\lambda^{(s)} = 4\pi^{-1/2} v_M \Sigma_f, \quad (36)$$

$$b_s = \frac{1}{3} \pi^{-1/2} \Sigma_f / v_M, \quad (37)$$

where

$$\Sigma_f = (1 + m/M)^{-2} \Sigma_b.$$

For a liquid the nonanalytic behavior of the integrand in (34) at  $v, \kappa \rightarrow 0$ , as seen from Eq. (22), causes the expansion of  $v \Sigma_s(v)$  to involve also odd powers:

$$v \Sigma_s(v) = \lambda^{(s)} + a_s v + b_s v^2 + \dots \quad (38)$$

After some manipulation Eq. (34) leads to

$$a_s = \frac{\eta^2(\eta^2 - 1)}{(\eta^2 + 1)^2} \Sigma_b F(0). \quad (39)$$

But for the factor  $\eta^2(\eta^2 - 1)/(\eta^2 + 1)^2$ , which for large  $\eta$  is close to unity, this expression is the same as for the elastic part of  $\Sigma_s(v)$  at  $v \rightarrow 0$  for a solid,<sup>13</sup> as we can see from Eqs. (33) and (20).

Since  $\Sigma_s(v) \rightarrow \Sigma_f > 0$  as  $v \rightarrow \infty$ , the scattering rate  $v \Sigma_s(v)$  increases indefinitely with increasing  $v$ . Usually the increase is monotonic, and for all models used in computations so far the absolute minimum of  $v \Sigma_s(v)$  is at  $v=0$ .<sup>23</sup> However, an exception to this rule follows from Eqs. (38) and (39) if  $\eta < 1$ .

Since the absorption rate  $v \Sigma_a(v)$  presumably behaves at  $v \rightarrow 0$  and at  $v \rightarrow \infty$  in a similar way as  $v \Sigma_s(v)$ , their sum,  $v \Sigma(v)$ , has the same general properties as those derived for  $v \Sigma_s(v)$ . In particular, the limits  $\Sigma(\infty)$  and  $[v \Sigma(v)]_{v=0}$  are finite and positive. We continue to maintain the additional restriction that the latter limit coincides with  $\lambda^*$ , the absolute minimum of  $v \Sigma(v)$ . Any case not in accord with this restriction would require a separate investigation, which is hardly justified as no such cases of practical importance are known so far.

In the small-velocity range we are going to use the truncated expansions,

$$v \Sigma(v) \approx \lambda^* + av \quad \text{for a liquid,} \quad (40a)$$

$$\approx \lambda^* + bv^2 \quad \text{for a gas or solid,} \quad (40b)$$

where, in the last case,  $\Sigma(v)$  stands for  $\Sigma_s'(v) + \Sigma_a(v)$ . We shall slightly strengthen the previous restriction by requiring that the (nonnegative) coefficients  $a$  and  $b$ , respectively, do not vanish.

### III. THE EIGENVALUE SPECTRUM

After the above preparation we return to Eq. (5). For the case of a solid an explanation is needed with respect

<sup>23</sup> H. Honeck (private communication).

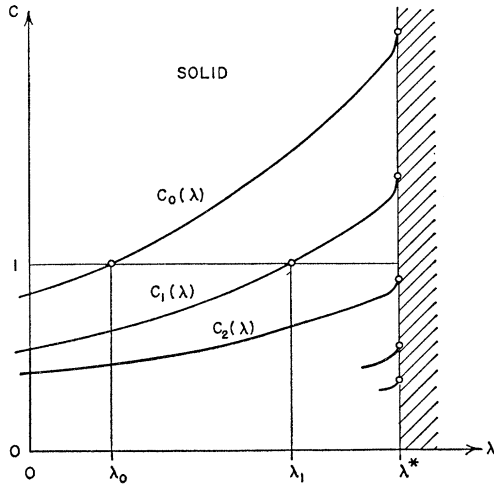


FIG. 1. Qualitative picture of the eigenvalues  $c_n(\lambda)$  for a solid moderator.

to the elastic scattering. Obviously this cannot influence the neutron velocity distribution—the corresponding terms in Eq. (3) cancel. Therefore, we redefine Eq. (4), with  $\Sigma'(v) = \Sigma'_s(v) + \Sigma_a(v)$  and  $\Sigma'_s(v' \rightarrow v)$  substituted for  $\Sigma(v)$  and  $\Sigma_s(v' \rightarrow v)$ , respectively. We shall, however, omit those arrows henceforth.

In view of what has been said about the collision rate  $v\Sigma(v)$ , the kernel  $K_\lambda(v, v')$ , for  $\lambda \leq \lambda^*$ , inherits some of the properties of  $\tilde{\Sigma}_s(v, v')$ . In particular,  $K_\lambda(v, v')$  is positive valued, decreasing to 0 only at  $v$  or  $v' \rightarrow \infty$ , and possibly at  $v$  or  $v' \rightarrow 0$ . Moreover, the kernel is continuous, except, in case of a solid, for jumps across certain slant lines in the  $v/v'$  plane, and except for the logarithmic singularity at  $v' \rightarrow v$  in case of a liquid. Only for  $\lambda = \lambda^*$ , and only for the gas and the liquid, a stronger singularity appears at  $v, v' \rightarrow 0$ . From the behavior of  $\tilde{\Sigma}_s$  for  $v, v' \rightarrow 0$ , we also conclude how the square integrability, as shown by Eqs. (29a) and (29b), is affected by the additional factors in (6), namely

$$\int_0^\infty \int_0^\infty K_\lambda^2(v, v') dv dv' < \infty \quad \text{for } \lambda < \lambda^*, \quad (41)$$

$$\int_0^\infty \int_0^\infty K_{\lambda^*}^2(v, v') dv dv' = \infty \quad \text{for gas or liquid,} \quad (42a)$$

$$< \infty \quad \text{for solid.} \quad (42b)$$

The exception (42a) is due to the mentioned singularity at zero velocities.

We recall that  $\tilde{\Sigma}_s(v, v')$  is nondegenerate, which is then true also for  $K_\lambda(v, v')$ . As the extra factors in (6) may be incorporated into the trial function  $\varphi$  in (30), a positive definite  $\tilde{\Sigma}_s(v, v')$  gives rise to a  $K_\lambda(v, v')$  with the same property. Since many if not all possible  $\tilde{\Sigma}_s(v, v')$  are positive definite we shall adopt this as a general assumption for the  $K_\lambda(v, v')$  under consideration. This assumption is not essential, but will allow us the convenience of

avoiding a discussion of negative eigenvalues of  $c$  in Eq. (5).

An immediate consequence of the symmetry, non-degeneracy, square integrability, and positive definiteness of the kernel is that for any  $\lambda < \lambda^*$ , and also for  $\lambda = \lambda^*$  in case of a solid, there is an infinite set of eigen-solutions  $\Psi_{\lambda n}(v)$ , corresponding to positive eigenvalues  $c_n$ , which are bounded as follows,<sup>8</sup>

$$\int_0^\infty \int_0^\infty K_\lambda^2(v, v') dv dv' > c_0 > c_1 \geq \dots > 0, \quad (43)$$

and which accumulate only at 0. An extension of the Perron-Jentzsch theorem<sup>11</sup> assures that  $c_0$  is simple, that the corresponding solution is non-negative, and that there is no other such solution.

In order to translate these statements into answers to the original problem, we have to see how then  $c_n$  vary with  $\lambda$ . First we prove, by integrating both sides of Eq. (4) over  $v$ , that

$$c_0(0) \leq 1,$$

because of the non-negativeness of the corresponding solution and of the cross sections. The sign of equality applies to a nonabsorbing medium.

For  $\lambda < \lambda^*$  the kernel  $K_\lambda(v, v')$  depends upon  $\lambda$  analytically, and we find that  $(\partial K_\lambda / \partial \lambda)$  too is square integrable in the sense of Eq. (41). This is sufficient for the application of a theorem of Rellich,<sup>8</sup> which guarantees the continuity of  $c_n(\lambda)$ .

A formula well known from perturbation theory<sup>8</sup> equates the derivative of  $c_n(\lambda)$  to the corresponding “diagonal matrix element” of  $\partial K_\lambda / \partial \lambda$ . With the  $\Psi_{\lambda n}(v)$  normalized, with the differentiation of (6) carried out, and through some manipulation, the result simplifies into

$$\frac{dc_n(\lambda)}{d\lambda} = c_n(\lambda) \int_0^\infty \frac{\Psi_{\lambda n}^2(v) dv}{v\Sigma(v) - \lambda}, \quad (44)$$

which is positive. Thus all eigenvalues  $c_n$  increase monotonically with  $\lambda$ . In case of a solid the proof of continuity can be extended up to the limit  $\lambda \rightarrow \lambda^*$ , but the  $dc_n/d\lambda$  are likely to become infinite at that point.

For a solid we now already have a complete qualitative picture of the  $c_n(\lambda)$ , as shown by Fig. 1. On the horizontal line  $c=1$  we read the decay constants  $\lambda_n$ . They are finite in number, as already indicated by Shapiro and Corngold.<sup>6</sup> Their results also show that ordinarily only very few  $\lambda_n$ , or sometimes only the fundamental  $\lambda_0$  do exist. As mentioned in the introduction the existence of the latter decay constant is trivial for any medium with no or only  $1/v$  absorption. [Such absorption merely shifts the curves  $c_n(\lambda)$  to the right.]

By introducing an absorption rate which would increase sufficiently strongly with  $v$ , one could in principle—but not very easily in practice—depress the curves  $c_n(\lambda)$  below the line  $c=1$ , which means, for a solid, that  $c_0(\lambda^*) < 1$ . Then the spectrum of  $\lambda$  below  $\lambda^*$  would be empty.

In the case of a gas for  $\lambda$  close to  $\lambda^*$  only the values of  $K_\lambda(v, v')$  in the near-zero velocity range are significant, and we expect that the limiting behavior of the  $c_n(\lambda)$ , as  $\lambda \rightarrow \lambda^*$ , is not affected by making the kernel equal zero for  $v$  or  $v' > v_1$ , with some fixed  $v_1$ .

We take  $v_1$  small enough so that the approximations (26) and (40b) are valid. After introducing

$$x = [b/(\lambda^* - \lambda)]^{1/2} v, \quad x_1 = [b/(\lambda^* - \lambda)]^{1/2} v_1, \quad (45)$$

$$\Phi(x) = (1 + x^2)^{1/2} \Psi_\lambda(v),$$

the integral equation can be reduced to a second-order differential equation, which happens to be in simple relationship to the hypergeometric equation. The boundary conditions are  $\Phi(0) = 0$  and  $\Phi(x_1) = 0$ . The first one is satisfied by the particular solution [notation as in (24)]

$$\Phi(x) = xF\left(\frac{1}{4}(1 + \nu), \frac{1}{4}(1 - \nu); \frac{3}{2}; -x^2\right), \quad (46)$$

where

$$\nu = (1 - c^*/c)^{1/2}, \quad (47)$$

$$c^* = 2\Sigma_b/bv_M. \quad (48)$$

One of the formulas for the analytic continuation of the hypergeometric function<sup>24</sup> helps us to satisfy also the second boundary condition. If  $x_1$  is sufficiently large, i.e., if  $\lambda$  is sufficiently close to  $\lambda^*$ , we may take only the leading terms of the expansions around infinity, and put the boundary condition into the simpler form

$$\nu \ln x_1 \approx \ln \left\{ \frac{\Gamma^2[\frac{1}{4}(1 + \nu)]\Gamma(1 - \frac{1}{2}\nu)}{\Gamma^2[\frac{1}{4}(1 - \nu)]\Gamma(1 + \frac{1}{2}\nu)} \right\} + 2(n + 1)\pi i. \quad (49)$$

For  $c > 0$  we have either  $0 < \nu < 1$  and  $n + 1 = 0$ , or  $\nu$  is imaginary and  $n$  an integer. The first possibility is excluded by verifying that both sides of Eq. (49) would have opposite signs. Through separate consideration it can also be shown that  $\nu = 0$  is not permissible. We are left with an infinite set of imaginary eigenvalues of  $\nu$ , corresponding to a set  $c_n < c^*$ ,  $n = 0, 1, 2, \dots$ . An expansion in powers of  $\nu$  for small  $|\nu|$ , and Stirling's formula for large  $|\nu|$ , lead to the conclusion that the interval  $(0, c^*)$  is filled by the set  $c_n(\lambda)$  ever more densely as  $x_1 \rightarrow \infty$ , that is, as  $\lambda \rightarrow \lambda^*$ . This result does not depend upon the choice of the cutoff velocity  $v_1$ , so that it no doubt holds also for the original equation (5).

From the picture thus obtained (Fig. 2) we conclude that whenever

$$c^* > 1, \quad (50)$$

there is an infinite set of discrete decay constants  $\lambda_n$  below  $\lambda^*$ , with the only accumulation point  $\lambda^*$ . In the opposite case, when  $c^* < 1$ , there are no such decay constants. Again, through the trivial existence of  $\lambda_0$ , the latter possibility is excluded if the gas exhibits no or only  $1/v$  absorption. Formally this is confirmed by

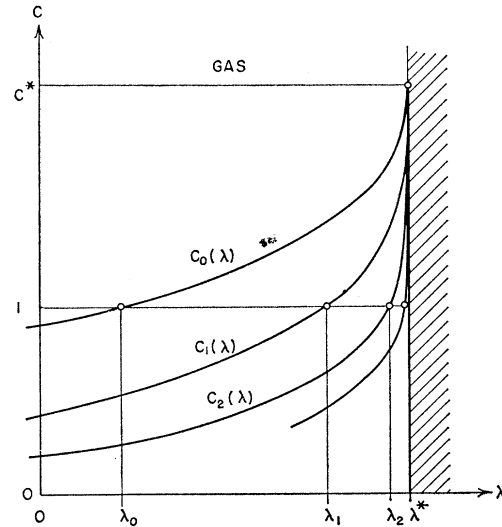


FIG. 2. Qualitative picture of the eigenvalues  $c_n(\lambda)$  for a monatomic gas.

evaluating  $c^*$  with  $b$  from Eq. (37):

$$c^* = 6(\pi)^{1/2}(1 + m/M)^2. \quad (51)$$

The value of this constant ranges from 42.5 to 10.6 for  $1 \leq M < \infty$ . In view of its magnitude the possibility of causing the discrete eigenvalues to disappear, by introducing some non- $1/v$  absorption, does not seem realistic. It would be necessary to increase the value of  $b$  more than 10 times to achieve  $c^* < 1$ . This would require an absorption differing violently from the  $1/v$  law in the small- $v$  range.

The existence of the infinite set of discrete decay constants is no surprise, as it was known earlier<sup>2</sup> that the proton gas model has this property. What matters here is only the behavior in the near-zero velocity range, and this is alike for any free gas. Some correlation between the methods used here and in the proton gas case can be established by observing that the mentioned equation for  $\Phi(x)$  represents an approximation to the Wigner-Wilkins equation,<sup>19</sup> and has actually been obtained in the same way as the latter. The Schrödinger analogy used by Corngold *et al.*<sup>2</sup> leads to the infinite set of eigenvalues only under the condition that the "singular potential" is sufficiently strong.<sup>25</sup> This condition turns out to coincide with (50).

A few more results about the  $\lambda_n$  can be extracted directly from the condition (49). Now  $c = 1$ , and the value of  $\nu$  is given:

$$\nu = i(c^* - 1)^{1/2}. \quad (52)$$

By substituting the definition (45) of  $x_1$  into (49) we see that the higher decay constants  $\lambda_n$  should approach the bound  $\lambda^*$  roughly like a geometrical progression, namely

$$(\lambda^* - \lambda_n)/(\lambda^* - \lambda_{n+1}) \approx e^{4\pi/|\nu|}. \quad (53)$$

<sup>24</sup> Bateman Manuscript Project, edited by A. Erdélyi (McGraw-Hill Book Company, Inc., New York, 1953-1955).

<sup>25</sup> K. M. Case, Phys. Rev. **80**, 797 (1950).

For a nonabsorbing gas, with no or only  $1/\nu$  absorption, where Eq. (51) applies, this ratio varies from 7.0 to 57 for  $1 \leq M < \infty$ . For small  $M$  this crude prediction is quite well verified (to within 25% for the proton gas) by the numerical results of Shapiro and Corngold. On the other hand, for the heavier gases, and for the few eigenvalues computed there, the prediction falls far short, which is understandable: the cutoff is too severe in this case.

In the case of a liquid we apply the substitution  $x = av/(\lambda^* - \lambda)$  and a cutoff  $x_1 = av_1/(\lambda^* - \lambda)$ . For  $\lambda$  close to  $\lambda^*$  Eq. (5) then leads, in an approximate way, to the following equation for the function  $\phi(x) = (1+x)^{-1/2}\Psi_\lambda(\nu)$ :

$$c(1+x)\phi(x) = \int_0^{x_1} L(x'/x)\phi(x')dx'. \tag{54}$$

The kernel

$$L(\xi) = \frac{\eta \Sigma_b F(0)}{4\pi a} \ln \frac{(1+\xi)^4 + \eta^2(1-\xi^2)^2}{(1-\xi)^4 + \eta^2(1-\xi^2)^2}, \tag{55}$$

taken from (28), can be expanded as follows:

$$L(\xi) = \sum_{l=1}^{\infty} A_l \xi^{\pm(2l-1)} \quad \text{for } \xi \leq 1, \tag{56}$$

with all  $A_l \geq 0$ .

Thinking of an expansion around infinity we may try to approximate the solution by  $\phi(x) \propto x^{\nu-1}[1+O(x^{-1})]$ , or by a sum of two complex conjugate such terms if  $\nu$  is complex. Since the integral in (54) acts somehow like a transformation of scale, there is ground to believe that such an approximation is valid for  $x \gg 1$ , where the factor  $(1+x)$  in (54) can be replaced by  $x$ . With this ansatz, and with  $x$  in the range  $1 \ll x \ll x_1$ , the equation shows that the exponent, if  $-1 < \text{Re}(\nu) < 1$ , is related to  $c$  by

$$c \approx \bar{L}(\nu), \tag{57}$$

where  $\bar{L}$  is the Mellin transform of the kernel,

$$\bar{L}(s) = \int_0^{\infty} L(\xi)\xi^{s-1}d\xi.$$

This transform can be expressed in a closed form,<sup>24</sup>

$$\bar{L}(s) = \frac{\eta \Sigma_b F(0)}{2a} \frac{\sin(\pi s/2) - \sin[(\frac{1}{2}\pi - \vartheta)s]}{s \cos(\pi s/2)}, \tag{58}$$

with

$$\vartheta = \arcsin[2\eta/(\eta^2+1)].$$

For  $-1 < s < 1$  the values of  $\bar{L}(s)$  range from the minimum

$$\bar{L}(0) = [\eta \Sigma_b F(0)/2a]\vartheta \tag{59}$$

to infinity. We see that  $\nu$  is imaginary if  $c < \bar{L}(0)$ , whereas  $-1 < \nu < 1$  if  $c > \bar{L}(0)$ . Let us also note that for small  $s$

$$\bar{L}(s) \approx \bar{L}(0)[1 + s^2\vartheta(\frac{1}{4}\pi - \frac{1}{6}\vartheta)]. \tag{60}$$

Information about the possible range of eigenvalues of  $c$  can be gained by applying a finite Mellin transform to Eq. (54). It follows that the function

$$\bar{\phi}(s) = \int_0^{x_1} \phi(x)x^{s-1}dx,$$

for  $-1 < \text{Re}(s) < 1$ , satisfies the equation

$$[c - \bar{L}(s)]\bar{\phi}(s+1) + c\bar{\phi}(s) = -\sum_{l=1}^{\infty} A_l \frac{\bar{\phi}(2l)}{(2l-s-1)x_1^{2l-s-1}}. \tag{61}$$

We recall that the largest eigenvalue  $c_0$  corresponds to a non-negative solution  $\phi_0(x)$ , and hence to a  $\bar{\phi}_0(s)$  positive for  $s > -1$ . This helps to prove that  $c_0 < \bar{L}(0)$ . In fact, if the contrary were true, there should exist a real  $s = \nu$ , causing the first term in (61) to vanish. The remaining terms have contradictory signs.

As a consequence only imaginary  $\nu$  are admissible, so that

$$\phi(x) \approx \frac{1}{2}(e^{i\delta}x^{\nu-1} + e^{-i\delta}x^{-\nu-1}) = x^{-1} \cos(|\nu| \ln x + \delta) \tag{62}$$

for  $1 \ll x \ll x_1$ . If this is to refer to the non-negative solution we have to require that (roughly)  $|\nu| < \pi/\ln x_1$ . Hence in the limit  $x_1 \rightarrow \infty$  (i.e., for  $\lambda \rightarrow \lambda^*$ ) the largest eigenvalue  $c_0(\lambda)$  approaches the limit

$$c^* = \bar{L}(0). \tag{63}$$

If  $a$  has the value (39) this limit is greater than 1, and approaches 1 for large  $\eta$ , when

$$c^* \approx (\eta^2+1)/(\eta^2-1). \tag{64}$$

With (62) the right-hand side of Eq. (61) can be estimated. Setting then  $s = \pm \nu$  we obtain, in a rough way, a condition for the eigenvalues, reading for small  $\nu$  as

$$\cos(2|\nu| \ln x_1 + 2\delta) \approx \text{const}. \tag{65}$$

This looks quite suggestive, and one is tempted to guess that the consecutive eigenvalues of  $c$ , as determined through Eq. (57), correspond to increments of  $2|\nu| \ln x_1$  in steps of  $2\pi$ . In the limit  $x_1 \rightarrow \infty$  the eigenvalues of  $c$  then fill densely the interval  $(0, c^*)$ , as in the gas case.

While it has not been possible to achieve a proof of this conjecture, strong support is obtained from a simplified model. We replace the kernel  $L(x'/x)$  by the first term of the expansion (56). This again leads to a hypergeometric differential equation, and the same technique applies as in the gas case. The solutions indeed behave as we have supposed in the above argument, and the eigenvalues have a similar spacing as predicted by Eq. (65), filling in the limit an interval  $(0, c^*)$ .

Although such an approximation of the kernel on the whole is very poor, especially for large  $\eta$ , it fits asymptotically for both large and small  $x'/x$ , and also preserves the property that the square integrability is lost for  $x_1 = \infty$ . Since the latter property is responsible for the



appearance of the continuum of limiting points, there seems to be sufficient ground for believing that the previous conclusions are correct.

Setting  $c=1$  we can again estimate how fast the discrete decay constants approach the limit  $\lambda^*$ . The above conjecture implies that

$$(\lambda^* - \lambda_n) / (\lambda^* - \lambda_{n+1}) \rightarrow e^{\pi/|\nu|}, \quad (66)$$

where  $\nu$  is the root of  $\bar{L}(\nu)=1$ . If Eq. (64) is valid we find from (60) that  $\nu \approx (4/\pi\eta)^{1/2}$ . With  $\eta=10$  the ratio (66) then equals  $7 \times 10^3$ , so that for any practical purpose the higher  $\lambda_n$  are indistinguishable from the continuum.

The last result again indicates, just as Eqs. (39) and (64) did, an approach to solid-like behavior. This is understandable, because for large  $\eta$  the kernel is strongly peaked, almost resembling a  $\delta$  function. To say it otherwise: for typical liquids the "quasielastic" scattering is almost elastic. Consequently this part of the scattering can be of only of little importance for the decay constants, except for indistinguishable details like those just mentioned.

Another consequence is that, before drawing the final picture, we must take into account also the "truly inelastic" scattering, represented by the terms neglected in (28). If this part of the kernel is non-negative and of comparable magnitude as for a solid, it alone would normally produce one or several discrete limiting points  $c_n(\lambda^*)$  above the value  $c^*$ . The combining of the two parts presumably does not alter the continuum below  $c^*$  (if the Weyl-von Neumann theorem is applicable), whereas the uppermost discrete point  $c_0(\lambda^*)$  can be shifted only upwards, as we may judge from a well-known variational formula.

The picture of the eigenvalues  $c_n(\lambda)$  for a liquid thus, in principle, combines the features of Figs. 1 and 2. However, if  $\eta$  is large the pattern of the decay constants is expected to be practically the same as for a solid (Fig. 1).

#### IV. SINGULAR DECAY MODES AND GENERALIZATIONS OF THE PROBLEM

Although the above criteria for the existence of discrete decay constants appear understandable, the possibility—even if not very realistic—of any empty discrete spectrum is still puzzling. It does not seem clear how a given initial neutron distribution would evolve in such an exceptional case, and whether in any way an exponential decay mode would eventually be approached.

Such questions inevitably involve us with singular solutions of Eq. (3), i.e., solutions  $N(v)$  not square integrable with the weight required by symmetrization; this is to say that  $\int_0^\infty [N^2(v)/M(v)]dv$  diverges. A class of such solutions has been discussed elsewhere,<sup>2,3</sup> and we therefore shall not enter the mathematical details, but rather proceed by a more physical reasoning, and turn our attention to non-negative solutions.

We have seen that the disappearance of the discrete decay constants is caused by non- $1/v$  absorption. Qualitatively, the effect of such absorption is easily understood. If  $v\Sigma_a(v)$  increases with increasing  $v$ , the faster neutrons are depleted sooner than the slow ones, so that an initially Maxwellian neutron gas undergoes "absorption cooling," as we may say. Similarly, in the opposite case of decreasing  $v\Sigma_a(v)$ , one could speak of absorption heating.

Normally, through competition between thermalization and absorption cooling or heating, a certain neutron velocity distribution, which then stays constant in shape, is asymptotically approached. This is the dominant mode. However, an exception is conceivable too. If the absorption cooling effect is extremely strong, the thermalization might be too weak to compete, and the neutron gas cools down so strongly that the neutron distribution slowly approaches a singular one, correspondingly to the decay rate  $\lambda^*$ . Under a restrictive condition, which can be shown to hold for a solid medium, this  $N(v)$  contains a term  $\delta(v)$ , and thus belongs to the known family of singular solutions.<sup>2,3</sup> In other cases, depending upon the properties of the thermalization kernel in the near-zero velocity range, instead of  $\delta(v)$  a weaker peak,  $\propto v^\nu$ , arises, with  $-1 < \nu \leq \frac{1}{2}$ .

It should be possible to base the existence of a singular non-negative solution upon a suitable extension of the Perron-Jentzsch theorem. However, let it be sufficient here to quote one example where the disappearance of the discrete spectrum can be demonstrated, and the singular solution constructed, in a straightforward way. We take the separable kernel,

$$\Sigma_s(v' \rightarrow v) \propto vM(v)\Sigma_s(v)\Sigma_s(v'),$$

and an absorption rate  $v\Sigma_a(v)$  which increases sufficiently strongly with  $v$  in the thermal region. We substitute  $N(v) = \delta(v) + N_1(v)$  and  $\lambda = \lambda^*$  into Eq. (3), and determine  $N_1(v)$  from an inhomogeneous integral equation. The requirement that  $N_1(v)$  be non-negative leads to an inequality involving  $v\Sigma_a(v)$ , which we can verify to coincide with the condition for the disappearance of the regular non-negative solution.

The presence of the  $\delta$  term means that a finite percentage of the neutron gas has cooled down to absolute zero. We may also say, for the time evolution of any regular distribution, that the entropy, reduced to a standard number-density, diverges towards  $-\infty$ . This is contrary to the ordinary case, where the reduced entropy approaches a finite limit, corresponding to the dominant mode  $N_0(v)$ .

The above picture, which lends some understanding for the possible disappearance of discrete decay constants, can be adapted to several more general problems. In some of these the discrete spectrum actually does disappear under quite realistic conditions.

First, we may wish to introduce into Eq. (3) the more general kernel  $\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})$ , and ask for angle-dependent solutions  $N(\mathbf{v})$ . Much of what has been said previously

is likely to remain true also in this context, although there might be some trouble with the square-integrability of the corresponding  $K_\lambda(\mathbf{v}, \mathbf{v}')$ . In view of what has been found for related problems in the kinetic theory of gases<sup>26,27</sup> it may happen that in some cases  $K_\lambda(\mathbf{v}, \mathbf{v}')$  even for  $\lambda < \lambda^*$  is not square integrable, but that some iterated kernel does fulfill this requirement. Such a situation would merely reflect a strong enrichment of the set of the  $c_n(\lambda)$ . Otherwise little would have to be changed in our pictures.

A related problem is that of the diffusion length, where we are assuming a steady neutron distribution of the form

$$N(z, \mathbf{v}) = N(\mathbf{v})e^{-z/L},$$

with  $N(\mathbf{v})$  obeying the equation

$$v[\Sigma(v) - \mu/L]N(\mathbf{v}) = \int v'\Sigma_s(\mathbf{v}' \rightarrow \mathbf{v})N(\mathbf{v}')d\mathbf{v}'.$$

As shown by Corngold<sup>4</sup> a sufficiently strong absorption causes the discrete spectrum of  $L$  to disappear, that is, regular solutions of the quoted form then no longer exist.

A broader problem, which can be looked upon as a combination of the previous two, is that of solutions of the form

$$N(\mathbf{r}, \mathbf{v}, t) = N(\mathbf{v})e^{i\mathbf{B}\cdot\mathbf{r}}e^{-\lambda t}.$$

The finite  $B$  reasonably well simulates the behavior of neutron distributions in systems of finite geometry, as long as the geometry is not too small. It has been shown<sup>4</sup> that the discrete spectrum disappears if  $B$  is sufficiently large. Computational investigations of this problem have been carried out by Shapiro and Corngold,<sup>6</sup> by Travelli and Calame,<sup>28</sup> and by Ghatak and Honeck.<sup>29</sup>

If scattering is isotropic the quoted problem can be reduced to the same form as for  $B=0$ ,<sup>4</sup> and then treated along the lines of Sec. III. The only change to be made consists in the replacement of  $K_\lambda(v, v')$  by

$$K_{\lambda B}(v, v') = B^{-1} \left[ \arctan \frac{Bv}{v\Sigma(v) - \lambda} \arctan \frac{Bv'}{v'\Sigma(v') - \lambda} \right]^{1/2} \bar{\Sigma}_s(v, v').$$

<sup>26</sup> E. Hecke, *Math. Z.* **12**, 277 (1922).

<sup>27</sup> R. Dorfman, *Proc. Natl. Acad. Sci. U. S. A.* **50**, 804 (1963).

<sup>28</sup> A. Travelli and G. P. Calame, *Nucl. Sci. Eng.* **20**, 414 (1964).

<sup>29</sup> A. K. Ghatak and H. C. Honeck, *Nucl. Sci. Eng.* **21**, 227 (1965).

For the gas we notice that  $K_{\lambda^*B}(v, v')$  is still square integrable, as long as  $B > 0$ . Hence the pattern of Fig. 1 applies instead of Fig. 2, and the set of discrete decay constants  $\lambda_n$  is no longer infinite.

The rigorous treatment of the time-dependent problem for finite geometry is significantly more complicated, and can be achieved by methods devised by Lehner and Wing for a one-speed problem. For a separable kernel and for spherical geometry Nelkin<sup>10</sup> has shown that the discrete decay constants no longer exist if the radius is sufficiently small. Recently, a generalization of this work has been reported<sup>30</sup>. The explanation is but little different from that given before. Here the thermalization has to compete not so much with absorption, but rather with the evaporation of neutrons. This produces a well-known effect—that of diffusion cooling. If the radius is too small the diffusion cooling is so strong that again competition is broken and the neutron gas is cooled “indefinitely.”

Even for one-speed theory an example of this kind can be quoted—that of a cylinder of infinite length. As shown by Judge and Daitch<sup>31</sup> (for the case of isotropic scattering) the discrete decay modes disappear if the radius of the cylinder is smaller than 0.737 scattering mean free paths. (The quoted figure has been recomputed to a greater accuracy on the basis of work by Cady and Clark.<sup>32</sup>) The analog to the indefinite diffusion cooling in this case consists in the evolution of the neutron distribution towards one which is progressively more strongly peaked in the axial direction.

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<sup>30</sup> R. J. Bednarz, Summer School on Reactor Physics, Zakopane, 1964 (to be published); S. Albertoni and B. Montagnini, *J. Math. Anal. Appl.* (to be published). Both works will also appear in *Proceedings of the Symposium on Pulsed Neutron Research, 1965* (International Atomic Energy Agency, Vienna, 1965).

<sup>31</sup> F. D. Judge and P. B. Daitch, *Nucl. Sci. Eng.* **20**, 428 (1964).

<sup>32</sup> K. B. Cady and M. Clark, Jr., *Nucl. Sci. Eng.* **18**, 491 (1964).