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The Boundary Value Problem in Fermion Systems

H. Seibold[1] and C. Toepffer[1]

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The half-space boundary value problem for fermions near zero temperature in plane geometry is solved for diffuse boundary scattering by numerically constructing the spatial propagator in terms of the eigenfunctions of a generalized eigenvalue problem for the linearized Uehling–Uhlenbeck collision integral. The slip length is calculated for several interparticle scattering laws and compared with a relaxation time ansatz result and the experimental values for normal fluid ^{3}He. It is shown that the nonsingular part of the collision operator is relatively compact to the singular part.

KEY WORDS: Boundary value problems; normal phase Fermi fluids; liquid helium-3; Fermion systems; slip flows; Uehling–Uhlenbeck equation.

1. INTRODUCTION

The linearized Uehling–Uhlenbeck (UU) collision integral $\hat{L}$, which applies to normal Fermi liquids, has the remarkable property that its spectral decomposition in the nearly degenerate regime can be constructed in an exact, closed form,[1] which allows the solution of the corresponding initial value problem, i.e., the relaxation of a given space-homogeneous perturbation. It seems reasonable to attempt a similar approach for the simplest boundary value problem, i.e., the calculation of the stationary velocity of flow near a boundary surface in planar geometry, which involves constructing the spectral decomposition of $v_z^{-1}\hat{L}$ (v_z denoting the quasiparticle velocity perpendicular to the wall).

Experiments on normal liquid ^{3}He (relaxation of Poiseuille flow through capillaries,[2] damping of torsional oscillators[3,4] and of vibrating wires[5] as well as attenuation of first sound[6] have shown that a thermo-

[1] Institut für Theoretische Physik, Universität Erlangen-Nürnberg, D-8520 Erlangen, West Germany.

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hydrodynamic description is not sufficient. In order to study deviations thereof, we solve the linearized UU equation[1,7] for some scattering laws assuming purely diffuse reflection at the wall. We explicitly calculate the so-called slip length, i.e., the distance from the wall where the fluid velocity extrapolates to zero. The results are compared with a simpler previous model calculation[8] and the experimental data.[2,4]

In Section 2 we start with linearizing the quasiparticle distribution about a local equilibrium f^{lin} with a velocity proportional to the distance z from the wall. This results in a linearized collision equation with an inhomogeneity. The solution at $z = 0$ is expanded in terms of eigenfunctions of $v_z^{-1}\hat{L}$ and three additional functions, according to a method developed by Case[9] and Cercignani.[10,11] The slip length is expressed in terms of one of the expansion coefficients. The boundary conditions at the wall and far away are formulated in Section 3. In Section 4 we take a closer look at the linearized UU collision operator, which leads us to a Fourier transform with respect to the reduced quasiparticle energy; just as in the works of Sykes and Brooker[12] and Vogel *et al.*[1] Furthermore, we make a first comparison with the relaxation time ansatz of Einzel *et al.*[8] In Section 5 we calculate the transformed eigenfunctions numerically, which we use to evaluate the slip length in Section 6. For that purpose we discretize and cut off the transform of the expansion mentioned above in a suitable manner and project it in the half-space $v_z > 0$ (because of the boundary condition at the wall) on the remaining basis functions, which are the restrictions to the same half-space of the eigenfunctions of $-v_z^{-1}\hat{L}$ belonging to non-negative eigenvalues. The resulting system of linear equations for the expansion coefficients is solved numerically to yield the slip length.

Some calculations concerning the angular part of the collision integral $\hat{L}$ follow in Appendix A, as well as a proof for the relative compactness of the regular part of $\hat{L}$ with respect to the singular part in Appendix B.

2. THE SLIP LENGTH IN TERMS OF A SPECTRAL DECOMPOSITION

We consider a stationary, planar shear flow of a degenerate normal Fermi liquid along a planar, solid, diffusely reflecting wall. This situation corresponds to the Kramers problem in classical transport theory,[11] i.e., a limiting case of plane Couette flow with one of the two plates being removed to infinity. The surface normal defines the z direction, the wall being at $z = 0$, and the flow shall be directed along the x axis.

Under these circumstances, the fluid velocity increases asymptotically linearly with an—as we shall see—exponential deviation near the wall. The so-called slip length ζ is then defined as the distance behind the wall where the bulk velocity extrapolates to zero (Fig. 1)

$$\bar{v}_{\infty}(z) = a(z + \zeta) \tag{1}$$

with $a = \text{const}$. In order to calculate $\bar{v}_{\infty}(z)$ and ζ, respectively, we expand the distribution function $f(z, \mathbf{p})$ for the quasiparticles about a local equilibrium $f^{\text{lin}}(z, \mathbf{p})$ with velocity $\bar{v}^{\text{lin}} = az$:

$$f(z, \mathbf{p}) = f^{\text{lin}}(z, \mathbf{p}) + h(z, \mathbf{p})\, f^{\text{lin}}(z, \mathbf{p})(1 - f^{\text{lin}}(z, \mathbf{p})) \tag{2}$$

with

$$f^{\text{lin}}(z, \mathbf{p}) = f^0(E - \bar{\mathbf{v}}^{\text{lin}}\mathbf{p}) = f^0(E - azp_x) \tag{3}$$

f^0 is the Fermi distribution

$$f^0(E) = \left[1 + \exp\left(\frac{E-\mu}{k_B T}\right)\right]^{-1} = (1 + e^u)^{-1} \tag{4}$$

and $u = (E - \mu)/(k_B T)$.

The equation to be fulfilled by f is the linearized Uehling–Uhlenbeck equation

$$v_z \frac{\partial f}{\partial z} = \hat{L} f \tag{5}$$

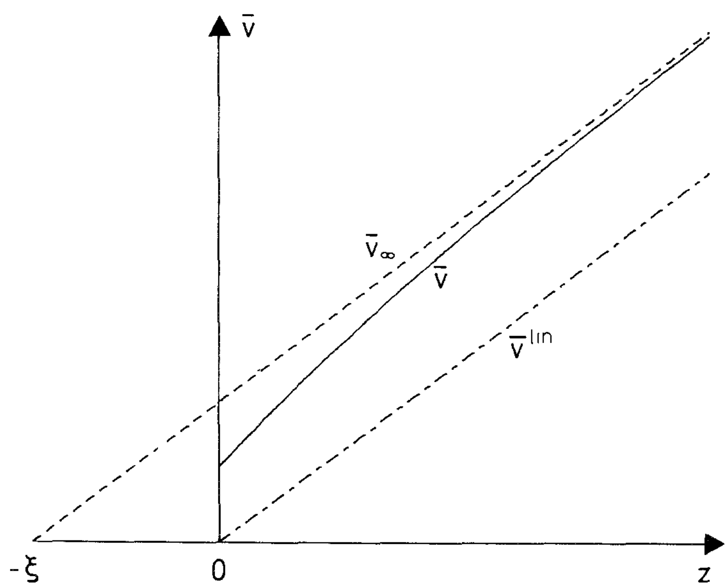

Fig. 1. Schematic profile of the mean velocity $\bar{v}$.

where the linearized collision operator $\hat{L}$ is given by[1,7]

$$\begin{aligned}\hat{L}f &\approx f^{\mathrm{lin}}(1-f^{\mathrm{lin}})\,\hat{L}h \\ &= \frac{2g}{m^{*2}(2\pi\hbar)^3}\int d^9p_{2,3,4}\,\delta(\mathbf{p}+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4)\,\delta(E+E_2-E_3-E_4) \\ &\quad\times\frac{d\bar{\sigma}}{d\Omega}(\mathbf{p}',\mathbf{p}'')\,f^{\mathrm{lin}}f_2^{\mathrm{lin}}(1-f_3^{\mathrm{lin}})(1-f_4^{\mathrm{lin}})(h_3+h_4-h-h_2)\end{aligned} \tag{6}$$

Here g is the spin multiplicity, m^* is the effective mass in the presence of Fermi liquid interactions, $E=p^2/2m^*$ is the energy of the quasiparticles, and $d\bar{\sigma}/d\Omega$ is the spin-averaged effective differential cross section for the quasiparticles depending on the relative momenta $\mathbf{p}'=\frac{1}{2}(\mathbf{p}_2-\mathbf{p})$ and $\mathbf{p}''=\frac{1}{2}(\mathbf{p}_4-\mathbf{p}_3)$ before and after the collision, respectively. (Actually, $d\bar{\sigma}/d\Omega$ depends only on the angle between $\mathbf{p}'$ and $\mathbf{p}''$ and on $|\mathbf{p}'|=|\mathbf{p}''|$.) f_i^{lin} stands for $f^{\mathrm{lin}}(z,\mathbf{p}_i)$, and similarly for h_i.

Expressing the lhs of Eq. (5) in terms of Eqs. (2)–(4) and keeping only terms linear in h, we get a linear inhomogeneous equation for h,

$$\frac{\partial h}{\partial z}-\frac{1}{v_z}\hat{L}h=-\frac{a}{k_B T}p_x=-Bp_x \tag{7}$$

with $B=a/k_B T$. The particular solution vanishing at $z=0$ is given by

$$h_{\mathrm{part}}(z,\mathbf{p})=\int_0^z dz'\,\hat{U}(z-z')(-Bp_x)=-Bzp_x \tag{8}$$

with the propagator

$$\hat{U}(z)=\exp\left(\frac{z}{v_z}\hat{L}\right) \tag{9}$$

Equation (8) results from the fact that p_x is one of the collision invariants of $\hat{L}$, i.e., $\hat{L}p_x=0$. The formal solution of the corresponding homogeneous equation

$$v_z\frac{\partial h}{\partial z}=\hat{L}h \tag{10}$$

is given by

$$h_{\mathrm{hom}}(z,\mathbf{p})=\hat{U}(z)\,h(0,\mathbf{p}) \tag{11}$$

As the collision operator $\hat{L}$ is symmetric with respect to the scalar product

$$\langle a|b\rangle=\int d^3p\,f^0(1-f^0)\,a(\mathbf{p})\,b(\mathbf{p}) \tag{12}$$

it is convenient to expand $h(0, \mathbf{p})$ into eigenfunctions of $v_z^{-1}\hat{L}$:

$$\hat{L}\psi_\kappa = -\kappa v_z \psi_\kappa \qquad (-\infty < \kappa < +\infty) \tag{13}$$

However, as shown by Cercignani,[11] these eigenfunctions do not form a complete system in the corresponding Hilbert space. There are additional solutions of Eq. (10) linear in z, which cannot be written as a superposition of the exponentials $\exp(-\kappa z)\psi_\kappa$ and the collision invariants $\psi_0 = 1$, $\psi_{1,2,3} = p_{x,y,z}$, and $\psi_4 = u$ [cf. Eq. (4)]. These are most conveniently obtained by putting $h = \beta z + \gamma$ in Eq. (10), with $\beta \neq 0$. Comparing coefficients gives $\hat{L}\beta = 0$, i.e., β must be one of the collision invariants ψ_i $(i = 0,..., 4)$, and $\hat{L}\gamma = \beta v_z$. This inhomogeneous equation for γ is only solvable if the inhomogeneity βv_z is orthogonal to the collision invariants, which restricts β further to the possibilities $\beta = \psi_\alpha$ with $\alpha = 1$, 2, or 4.

These additional solutions of Eq. (10) can be written as $\hat{U}\hat{L}^{-1}(v_z\psi_\alpha)$ $(\alpha = 1, 2, 4)$. Cercignani[11] showed that the three functions $\hat{L}^{-1}(v_z\psi_\alpha)$ $(\alpha = 1, 2, 4)$ together with the eigenfunctions of Eq. (13) (including those with $\kappa = 0$, i.e., the collision invariants) form a complete system in our Hilbert space.

Now we can write down the general solution of the inhomogeneous equation (9) as

$$\begin{aligned} h(z, \mathbf{u}) &= h_{\text{part}}(z, \mathbf{u}) + h_{\text{hom}}(z, \mathbf{u}) \\ &= -Bzp_x + \sum_{\alpha = 1,2,4} b_\alpha [z\psi_\alpha + \hat{L}^{-1}(v_z\psi_\alpha)] \\ &\quad + \sum\!\!\!\!\!\!\int d\kappa\, e^{-\kappa z} \sum_n b_{\kappa n}\psi_{\kappa n}(\mathbf{u}) \end{aligned} \tag{14}$$

where $\sum_n$ is due to the anticipated partial degeneracy of the eigenvalues κ, and b_α and $b_{\kappa n}$ are constant coefficients to be determined from the boundary conditions (see next section). The first two terms of the rhs together with the $(\kappa = 0)$ parts of the third one form the asymptotic (i.e., nonrelaxing) part h_∞ of h. Here we have used the symbolic notation $\mathbf{u}$ as an abbreviation for the variables $u, \hat{\mathbf{p}}$. It should be remarked that the integral $\int d^3p$ in Eq. (12) is written in spherical coordinates and is replaced here and in the following by

$$p_F^2 \int_0^\infty dp \int d(\cos\theta)\, d\varphi = p_F m^* k_B T \int_{-\infty}^{\infty} du \int d(\cos\theta)\, d\varphi$$

where the momentum-energy relation has been linearized about the Fermi level and the lower limit of the u integration has been shifted from $-\mu/k_B T \ll -1$ to $-\infty$, which is allowed because of the weight function $f^0(1-f^0) = \frac{1}{4}\operatorname{sech}^2(u/2)$ in Eq. (12); p_F is the Fermi momentum and v_x, v_y, and v_z will be replaced by $v_F \sin\theta\cos\varphi$, $v_F \sin\theta\sin\varphi$, and $v_F\cos\theta$, respectively ($v_F = p_F/m^*$ is the Fermi velocity).

Let c_0 be the sum of the coefficients of $p_x = \psi_1$ (we shall see in the next section that c_0 is actually a constant). Then the slip length ζ is obtained by [cf. ref. 13 and Eqs. (1) and (2)]

$$\begin{aligned} a(z+\zeta) &= \frac{g}{(2\pi\hbar)^3 n} \int d^3p\, v_x f_\infty(z, \mathbf{p}) \\ &= az + \frac{3c_0}{4\pi p_F^3} \int d^3p\, v_x p_x f^0(1-f^0) \end{aligned} \tag{15}$$

where n is the particle density, which has been taken in the low-temperature limit ($n = gk_F^2/6\pi^2$), and it has been used that $\int d^3p\, h_\infty f^{\text{lin}}(1-f^{\text{lin}})$ is equal to $\int d^3p\, h_\infty f^0(1-f^0)$ to first order in h_∞; the integrals over all components of h_∞ other than p_x give zero because of symmetry reasons. The remaining integral on the rhs of Eq. (15) can be easily evaluated to give $\frac{4}{3}\pi p_F^3 k_B T$, so that the slip length ζ is obtained as

$$\zeta = c_0 \left(\frac{a}{k_B T}\right)^{-1} = \frac{c_0}{B} \tag{16}$$

3. THE BOUNDARY CONDITIONS

The boundary conditions that we will use to determine the interesting coefficients in Eq. (14) are: (i) $h(z, \mathbf{u})$ must be finite for $z \to \infty$ and (ii) the fermions (quasiparticles) scattered by the wall must be in thermal equilibrium with the wall, which implies $h(z=0, \mathbf{u}) = 0$ for $v_z > 0$, i.e., for $\theta < \pi/2$. The first condition demands that $h(z, \mathbf{u})$ must not contain any exponentially or linearly increasing parts, so $b_{\kappa n} = 0$ for all $\kappa < 0$ and $b_2 = b_4 = 0$, $b_1 = B = a/k_B T$.

We can get rid of still other parts of h in Eq. (14): First we split up the eigenfunctions of Eq. (13) into symmetric ($\psi^+_{\kappa n}$) and antisymmetric ones ($\psi^-_{\kappa n}$) with respect to reflection at the Fermi surface ($u \to -u$). This is allowed because the linearized collision operator $\hat{L}$ is invariant under this reflection (see, e.g., Sykes and Brooker[12]). Second, as a consequence of the rotational invariance of $\hat{L}$, it does not mix different multipoles.[12] The factor $v_z^{-1} = (v_F\cos\theta)^{-1}$ still leaves the azimuthal part of the multipole expansion invariant. Therefore, we can split up the eigenfunctions $\psi^\pm_{\kappa n}(u, \theta, \varphi)$ of Eq. (13) into new ones,

$$\begin{aligned} \psi^{\pm c}_{\kappa nm}(u, \theta, \varphi) &= \psi^{\pm c}_{\kappa nm}(u, \theta)\cos m\varphi \qquad (m \geq 0) \\ \psi^{\pm s}_{\kappa nm}(u, \theta, \varphi) &= \psi^{\pm s}_{\kappa nm}(u, \theta)\sin m\varphi \qquad (m > 0) \end{aligned} \tag{17}$$

respectively. Now a glance at Eq. (15) [cf. the remarks after Eq. (13)] shows that only eigenfunctions with positive parity $(+)$ and $(\cos\varphi)$ dependence $[m=1, \binom{c}{s}=c]$ contribute to the mean velocity. In a certain analogy to Cercignani,[14] we therefore apply the projection operators $\hat{P}^c_{m=1}=\pi^{-1}\cos\varphi' \int d\varphi \cos\varphi$ and $\hat{P}^+_u=[1+\hat{P}(u\to -u)]$ to Eq. (14), which are fortunately compatible with the boundary conditions, and get from the condition (ii) above the relation

$$0=\left[\frac{a}{k_B T}\hat{L}^{-1}(v_z p_x)+c_0 p_x+\sum_{K>0}\!\!\!\!\!\!\int d\kappa \sum_n b_{\kappa n}\psi_{\kappa n}(u,\theta)\cos\varphi\right]\Theta(v_z) \quad (18)$$

where the indices $m=1$, $(\pm)=+$, and $\binom{c}{s}=c$ have been suppressed, the summation over n contains here only the remaining partial degeneracy for this special case, and Θ stands for the Heaviside step function.

The c_0 obtained from Eq. (18) yields the same slip length ζ as would be obtained by linearizing about a local equilibrium $f^{\text{lin}'}$ with velocity $\bar{v}_\infty(z)=a(z+\zeta)$, and approximating the difference $f^0-f^{\text{lin}'}(z=0)$ in the boundary condition at $z=0$ by the first order part of the Taylor expansion in terms of $\bar{v}_\infty(0)\,p_x$.

In order to determine the coefficients in Eq. (18), we make an assumption, the validity of which has been proved by Cercignani[10] in the classical case for an analytically solvable model collision operator (relaxation time ansatz with momentum conservation): We take the eigenfunctions $[p_x$ and $\psi_{\kappa i}(\mathbf{u})$ belonging to eigenvalues $\kappa\geqslant 0]$ to be a linearly independent complete system in the half-space $v_z>0$, projected on the relevant part by means of $\hat{P}^c_{m=1}$ and $\hat{P}^+_u$.

With this assumption, Eq. (18) represents an expansion of $\hat{L}^{-1}(v_z p_x)$ in terms of eigenfunctions of $v_z^{-1}\hat{L}$ in the half-space $v_z>0$. Whereas Cercignani,[10] however, could give a new scalar product, with respect to which these eigenfunctions become orthogonal in the half-space $v_z>0$ (because of the special structure of his model operator), we have no hope to find such a product for our problem, as in general it is also impossible to orthogonalize a given basis of a finite-dimensional space just by introducing a diagonal matrix into the scalar product. We must therefore take a different approach to calculate the coefficients: We project Eq. (18) on a suitably chosen finite, discrete subset of eigenfunctions; then we only have to solve a system of linear equations to get the coefficients and thereby the slip length ζ. Before doing this, we will first take a closer look at the collision operator and calculate the eigenfunctions numerically, or, to be exact, their Fourier transforms with respect to u.

4. INVESTIGATION OF THE COLLISION OPERATOR

Taking out the $(-h)$ term on the rhs of Eq. (6), we can split up the collision integral operator into a multiplicative, i.e., singular, part $-\nu(u)$ (the negative of the so-called collision frequency) and a regular rest $\hat{K}$, so we have, according to Vogel *et al.*[1] (cf. Sykes and Brooker[12])

$$\hat{L} = -\nu(u) + \hat{K} = -\omega_{\mathrm{B}}(1 + u^2/\pi^2) + \hat{K} \tag{19}$$

where ω_{B} is a fundamental frequency

$$\omega_{\mathrm{B}} = \frac{g m^* (k_{\mathrm{B}} T)^2}{4\hbar^3} \int_{2\pi} d\tilde{\Omega} \, \frac{1}{\cos(\tilde{\theta}/2)} \frac{d\bar{\sigma}}{d\tilde{\Omega}} \tag{20}$$

[here $\tilde{\theta}$ is the angle between $\mathbf{p}$ and $\mathbf{p}_2$ (which in the degenerate regime is approximately equal to the angle between $\mathbf{p}_3$ and $\mathbf{p}_4$) and $\tilde{\varphi}$ is the angle between the planes of $\mathbf{p}$, $\mathbf{p}_2$ and $\mathbf{p}_3$, $\mathbf{p}_4$] and the action of $\hat{K}$ depends on the u parity and multipolarity of the operand:

$$\hat{K}(\psi_{lm}^{\pm}(u)\, Y_{lm}(\Omega)) = \lambda_l^{\pm} Y_{lm}(\Omega) \frac{\omega_{\mathrm{B}}}{\pi^2} 2 \cosh \frac{u}{2}$$
$$\times \int_{-\infty}^{\infty} dv \, \frac{u - v}{\sinh[(u-v)/2]} \, \psi_{lm}^{\pm}(v) \frac{1}{2} \operatorname{sech} \frac{v}{2} \tag{21}$$

with the parameters $\lambda_l^{\pm}$ given by

$$\lambda_l^{\pm} = \left(\frac{4\pi}{2l+1}\right)^{1/2} \left\{ \int d\tilde{\Omega} \, \frac{1}{\cos(\tilde{\theta}/2)} \right.$$
$$\times \left[\mp Y_{l0}(\cos\tilde{\theta}) + Y_{l0}\left(\cos^2\frac{\tilde{\theta}}{2} + \sin^2\frac{\tilde{\theta}}{2}\cos\tilde{\varphi}\right) \right.$$
$$\left. \left. + Y_{l0}\left(\cos^2\frac{\tilde{\theta}}{2} - \sin^2\frac{\tilde{\theta}}{2}\cos\tilde{\varphi}\right)\right] \frac{d\bar{\sigma}}{d\tilde{\Omega}} \right\}$$
$$\times \left(\int d\tilde{\Omega} \, \frac{1}{\cos(\tilde{\theta}/2)} \frac{d\bar{\sigma}}{d\tilde{\Omega}} \right)^{-1} \tag{22}$$

For a constant (or averaged) differential cross section, Eq. (22) simplifies to[1]

$$\lambda_l^{\pm} = \frac{1}{2l+1} \left[2 \pm (-)^{l+1} \right] \tag{23}$$

We now restrict ourselves to the relevant case of $(\cos\varphi)$ dependence $[m = 1, \binom{c}{s} = c]$, positive parity $[(\pm) = +]$, and nonnegative eigenvalues

κ. We expand a given eigenfunction $\psi_\kappa(u, \theta, \varphi) = \psi_\kappa(u, \theta) \cos \varphi$ in terms of the normalized real parts of the $Y_{l1}(\Omega)$,

$$Y_{l1}^c(\Omega) = 2^{1/2} \operatorname{Re} Y_{l1}(\Omega) = 2^{1/2} Y_{l1}(\theta, 0) \cos \varphi \qquad (l \geqslant 1) \tag{24}$$

viz.

$$\psi_\kappa(\mathbf{u}) = \sum_{l=1}^{\infty} \psi_{\kappa l}(u)\, Y_{l1}^c(\Omega) \tag{25}$$

Here the Y_{l1}^c form a complete orthonormal system in the subspace with $m = 1$ under consideration. So we have

$$\psi_{\kappa l}(u) = 2^{1/2}\pi \int_{-1}^{1} d(\cos\theta')\, \psi_\kappa(u, \theta')\, Y_{l1}(\theta', 0) \tag{26}$$

and the eigenvalue equation, Eq. (13), gets transformed after interchange of sum and integrals, dividing by $2\omega_{\mathrm{B}} \cosh(u/2) \cos \varphi$, substituting

$$q_\kappa(u, \theta) = \frac{1}{2} \operatorname{sech} \frac{u}{2}\, \psi_\kappa(u, \theta) \tag{27}$$

and introducing dimensionless eigenvalues

$$\bar{\kappa} = \kappa/(\omega_{\mathrm{B}}/v_{\mathrm{F}}) \tag{28}$$

into

$$\begin{aligned} -\bar{\kappa} \cos\theta\, q_\kappa(u, \theta) = & -\left(1 + \frac{u^2}{\pi^2}\right) q_\kappa(u, \theta) \\ & + \frac{1}{2\pi^2} \int_{-\infty}^{\infty} dv\, \frac{u - v}{\sinh[(u-v)/2]} \\ & \times \int_{-1}^{1} d(\cos\theta')\, w(\theta, \theta')\, q_\kappa(v, \theta') \end{aligned} \tag{29}$$

with the abbreviation

$$w(\theta, \theta') = 4\pi \sum_{l=1}^{\infty} \lambda_l^+ Y_{l1}(\theta, 0)\, Y_{l1}(\theta', 0) \tag{30}$$

Finally, (inverse) Fourier transformation with respect to u,

$$\varphi_\kappa(t, \theta) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} du\, e^{iut} q_\kappa(u, \theta) \tag{31}$$

and substitution $\pi t = \xi$ leads us to the integrodifferential eigenvalue equation

$$-\bar{\kappa} \cos\theta \, \varphi_\kappa(\xi, \theta) = \left[-1 + \left(\frac{\partial}{\partial \xi} \right)^2 \right] \varphi_\kappa(\xi, \theta) + \operatorname{sech}^2 \xi \int_{-1}^{1} d(\cos\theta') \, w(\theta, \theta') \, \varphi_\kappa(\xi, \theta') \tag{32}$$

For a constant differential cross section [cf. Eq. (22)], the kernel $w(\theta, \theta')$ can be expressed as follows (see Appendix A):

$$w(\theta, \theta') = 2f(\theta, \theta') + f(\pi - \theta, \theta')$$

with

$$f(\theta, \theta') = \frac{1}{16} (\sin\theta \sin\theta')^{-1/2} (-t)^{-3/2} \, {}_2F_1\left(\frac{3}{2}, \frac{3}{2}; 3; t \right) \tag{33}$$

where

$$t = -\frac{2 \sin\theta \sin\theta'}{1 - \cos(\theta - \theta')} \in \,]-\infty, 0]$$

This kernel $w(\theta, \theta')$ has a logarithmic singularity for $\theta = \theta'$ and $\theta = \pi - \theta'$ because of

$$f(\theta, \theta') \sim (\pi \sin\theta)^{-1} (-\ln|\theta - \theta'| + \ln \sin\theta + \text{const}) \qquad \text{for} \quad \theta \to \theta' \tag{34}$$

(see Appendix A), which is clearly integrable, however. The factor $(\sin\theta)^{-1}$ does not give trouble because the element of integration is $d(\cos\theta) = -\sin\theta \, d\theta$.

Let us now rewrite Eq. (29) in the form

$$-\bar{\kappa}(\cos\theta) \, q_\kappa = [-v'(u) + \hat{K}'] \, q_\kappa \tag{35}$$

with $v'(u) = v(u)/\omega_B$ and $\hat{K}'$ denoting the double integral operator on the rhs of Eq. (29). As shown in Appendix B, $\hat{K}'$ is relatively compact with respect to $-v'$. This implies that also the operator $\hat{K}'(\cos\theta)^{-1}$ is relatively compact with respect to $-v'/\cos\theta$, because $\hat{K}'(\cos\theta)^{-1}(-v/\cos\theta)^{-1} = -\hat{K}'v'^{-1}$ and the latter operator is compact (see above and Reed and Simon[15]). According to an extension of Weyl's theorem,[15] the continuous spectrum (more precisely, the set of limit points of the spectrum) of Eq. (35) is the same as that of the equation $-\bar{\kappa}(\cos\theta) \, q_\kappa = -v'(u) \, q_\kappa$, viz. $]-\infty, -1] \cup [1, \infty[$. This is particularly useful here, as we had to treat the continuum by discretization.

We can now make a first comparison with the improved relaxation time ansatz of Einzel *et al.*[8] We obtain their collision operator from Eq. (29) by making the following simplifications: (i) The v integration $\int dv\,(u-v)/\sinh[(u-v)/2]$ is replaced by a multiplicative constant chosen to guarantee momentum conservation, (ii) the l summation in $w(\theta, \theta')$ [see Eq. (30)] is cut off after $l=2$ (note: $\lambda_1^+ = 1$ for an arbitrary interaction[12]), (iii) the collision frequency $v(u)=\omega_B(1+u^2/\pi^2)$ is replaced by the inverse of an averaged relaxation time $\tau=(1-\lambda_2^+)\,\tau_\eta$, τ_η being the viscous relaxation time (see, e.g., ref. 12), and (iv) the u dependence of the distribution function and of the eigenfunctions is dropped.

5. THE TRANSFORMED EIGENSOLUTIONS

5.1. The Discrete Spectrum

For simplicity we consider first the discrete part of the spectrum, i.e., those eigenvalues $\bar{\kappa}$ with $0 \leqslant \bar{\kappa} < 1$ (negative eigenvalues have been disposed of above). Any physically reasonable solution of Eq. (32) will be finite for $\xi \to \infty$ (in order to guarantee Fourier transformability), so the second term on the rhs of Eq. (32) will vanish in that limit and a solution of the equation for $0 < \bar{\kappa} < 1$ will be asymptotically given by

$$\varphi_\kappa(\xi, \theta) \sim c_\kappa(\theta) \exp[\Omega_\kappa(\theta)\,|\xi|] + d_\kappa(\theta) \exp[-\Omega_\kappa(\theta)\,|\xi|] \tag{36}$$

with

$$\Omega_\kappa(\theta) = (1-\bar{\kappa}\cos\theta)^{1/2}$$

[We regard eigenfunctions of Eq. (13) with positive u parity only, which leads to transformed eigenfunctions symmetric in ξ.] Again we must require Fourier transformability; so the preexponential factor $c_\kappa(\theta)$ must vanish identically. This gives the criterion for the allowed initial conditions at $\xi = 0$, which can only be fulfilled for certain discrete eigenvalues (see below).

For the purpose of a numerical calculation we proceed as follows. We discretize the integral in Eq. (32) by dividing the interval $[0, \pi]$ into N_θ intervals I_j of the same size π/N_θ centered at $\theta_j = (j-1/2)\pi/N_\theta$ $(j = 1,\dots, N_\theta)$ and assuming that $\varphi_\kappa(\xi, \theta)$ is approximately constant on each interval I_j for any ξ with modulus smaller than a cutoff value ξ_{co}; for $|\xi| \geqslant \xi_{co}$ we take $\operatorname{sech}^2\xi$ to be zero and use the asymptotic form of the eigenfunctions [see Eq. (36)]. In our calculations we used $\xi_{co} = 4.5$ with

$\operatorname{sech}^2 \xi_{co} = 5 \times 10^{-4}$. Putting $\varphi_\kappa^j(\xi) = \varphi_\kappa(\xi, \theta)$ for $\theta \in I_j$ we get a second-order system of coupled linear differential equations,

$$\frac{d^2}{d\xi^2} \varphi_\kappa^j(\xi) = (1 - \bar{\kappa} \cos \theta_j)\, \varphi_\kappa^j(\xi) - \operatorname{sech}^2 \xi \sum_{i=1}^{N_\theta} \varphi_\kappa^i(\xi) \int_{I_i} d\theta \sin \theta\, w(\theta_j, \theta) \tag{37}$$

The symmetry of $\varphi_\kappa^j(\xi)$ mentioned above requires $[(d/d\xi)\, \varphi_\kappa^j](0) = 0$. Leaving aside the condition of Fourier transformability for the moment, we would have N_θ linearly independent initial conditions at $\xi = 0$, for which we can take the canonical basis $\mathbf{e}^{(1)}, \ldots, \mathbf{e}^{(N_\theta)}$ of $\mathbb{R}^{N_\theta}$ with $e_i^{(j)} = \delta_{ij}$. Denoting the corresponding solutions by $\varphi_i^{(j)} = \varphi_\kappa^{(j)i}$ (suppressing the index κ for a while), we get a matrix c_{ij} of preexponential factors:

$$\varphi_i^{(j)}(\xi) \sim c_{ij} \exp(\Omega_i\, |\xi|) + d_{ij} \exp(-\Omega_i\, |\xi|) \tag{38}$$

with $\Omega_i = \Omega_\kappa(\theta_i)$ [see Eq. (36)]. For an arbitrary initial condition, $\varphi_i(0) = a_i$ $(i = 1, \ldots, N_\theta)$, the solution is given by $\varphi_i = \sum_j a_j \varphi_i^{(j)}$, the corresponding preexponential factors $c_i = c_\kappa(\theta_i)$ being

$$c_i = \sum_{j=1}^{N_\theta} c_{ij} a_j \tag{39}$$

Now for an allowed (nontrivial) initial condition, all c_i must vanish, which implies that the determinant of the matrix (c_{ij}) must be zero. This is the case only for certain discrete values of $\bar{\kappa}$. After determining such a discrete eigenvalue up to a certain numerical accuracy, the vector of the corresponding initial conditions $(a_1, \ldots, a_{N_\theta})$ is given as the right-hand singular vector belonging to the smallest singular value of the matrix (c_{ij}) (see ref. 17; also see ref. 18). For $d\bar{\sigma}/d\Omega = \text{const}$ we found two eigenvalues in the range $0 < \bar{\kappa} < 1$ for $N_\theta = 48$ as well as 96, namely 0.979 and 0.998. In order to learn more about the collision operator, we also calculated the corresponding discrete eigenvalues for azimuthal orders other than $m = 1$; the results are shown in Fig. 2. For negative parity and constant differential cross section there seem to be no nontrivial discrete eigenvalues, just as is the case for the eigenvalues of the collision operator $\hat{L}$ itself[1]; the coupling "potentials" $\propto \operatorname{sech}^2 \xi$ appear to be too weak to accommodate negative-parity eigenfunctions. The discrete eigenvalues for positive parity are concentrated immediately below the continuum. Numerically we found that their number increases with N_θ, but remains much smaller than N_θ. In this connection we remark that we could also identify some resonancelike phenomena in the low-lying continuum (i.e., rapid phase changes through

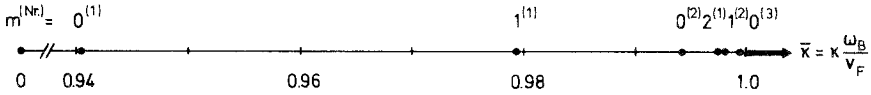

Fig. 2. Nonnegative eigenvalues of $-v_z^{-1}\hat{L}$ for positive parity.

$\pi/2$ in a particular oscillating component φ^i_κ). We will later show that the physical observables like the slip length are not affected by this if N_θ is chosen sufficiently large.

5.2. The Continuum

For eigenvalues $\bar{\kappa} > 1$ the asymptotic form of the eigenfunctions is partly oscillatory and partly exponential, depending on whether θ is smaller or larger than $\theta_\kappa = \arccos(1/\bar{\kappa})$ [cf. Eq. (32)]:

$$\varphi_{\kappa n}(\xi, \theta) \sim \begin{cases} a_{\kappa n}(\theta) \sin[\omega_\kappa(\theta)\,|\xi| + \vartheta_{\kappa n}(\theta)], & \theta < \theta_\kappa \\ c_{\kappa n}(\theta) \exp[\Omega_\kappa(\theta)\,|\xi|] + d_{\kappa n}(\theta) \exp[-\Omega_\kappa(\theta)\,|\xi|], & \theta > \theta_\kappa \end{cases} \tag{40}$$

Here $\omega_\kappa(\theta) = |\Omega_\kappa(\theta)| = (\bar{\kappa}\cos\theta - 1)^{1/2}$ for $\theta < \theta_\kappa$, with Ω_κ as in Eq. (36). The index n denotes again the degeneracy mentioned in connection with Eq. (18). Here the preexponential factor $c_{\kappa n}(\theta)$ must vanish only on the interval $]\theta_\kappa, \pi]$. Therefore we have a certain freedom to choose the initial values at $\xi = 0$; actually—as we shall see—we can choose $\varphi_{\kappa n}(0, \theta)$ for $\theta < \theta_\kappa$; the other initial values are then determined by the vanishing of $c_{\kappa n}(\theta)$ for $\theta > \theta_\kappa$. As a basis for the degenerated eigenfunctions belonging to a given $\bar{\kappa} > 1$, we choose $\varphi_{\kappa n}(\xi, \theta)$ given by the initial condition

$$\varphi_{\kappa n}(0, \theta) = \left\{ \begin{matrix} 1, & n = 1 \\ \sin\left(2\pi \dfrac{n}{2} \dfrac{\theta}{\theta_\kappa}\right), & n > 1 \text{ even} \\ \cos\left(2\pi \dfrac{n-1}{2} \dfrac{\theta}{\theta_\kappa}\right), & n > 1 \text{ odd} \end{matrix} \right\} \quad \text{for} \quad \theta < \theta_\kappa \tag{41}$$

i.e., a Fourier expansion of the initial values in the interval $[0, \theta_\kappa[$.

Numerically we proceed as in the last section. For a given $\bar{\kappa} > 1$ and finite N_θ the number N_{0x} of asymptotically oscillating components is easily found to be

$$N_{0x} = \operatorname{int}(1/2 + N_\theta \theta_\kappa/\pi) \tag{42}$$

where int(r) denotes the greatest integer smaller than r. As initial values we take at first again $\varphi_i^{(j)}(0) = \varphi_\kappa^{(j)i}(0) = \delta_{ij}$. For $N_{0x} < i \leqslant N_\theta$ we get the asymptotic form of Eq. (38) as before, which now defines a $(N_\theta - N_{0x}) \times N_\theta$ matrix (c_{ij}). For an arbitrary initial condition $(a_1,..., a_{N_\theta})$ the preexponential factors $c_i = c_\kappa(\theta_i)$ are again given by Eq. (39), now with the restriction $N_{0x} < i \leqslant N_\theta$. Defining $b_i = \sum_{j=1}^{N_{0x}} c_{ij} a_j$ $(i = N_{0x} + 1,..., N_\theta)$, we can write Eq. (39) in the convenient form

$$\sum_{j=N_{0x}+1}^{N_\theta} c_{ij} a_j = b_i \qquad (i = N_{0x} + 1,..., N_\theta) \tag{43}$$

Aside from singular cases, which are unimportant for the following, we can now arbitrarily choose $a_1,..., a_{N_{0x}}$; the other initial values $a_{N_{0x}+1},..., a_{N_\theta}$ are then uniquely determined by Eq. (43), which guarantees the Fourier transformability. In order to realize Eq. (41) numerically, we naturally put $\varphi^i_{\kappa n}(0) = \varphi_{\kappa n}(0, \theta_i)$ for $i = 1,..., N_{0x}$.

For fixed eigenvalue $\bar{\kappa}$ and initial condition n we calculated the values of $\varphi_{\kappa n}(\xi, \theta)$ on a lattice $\xi = k\,\Delta\xi$ $(k = 0,..., N_\xi;\ N_\xi\,\Delta\xi = \xi_{co})$ and $\theta = \theta_1,..., \theta_{N_\theta}$ (see above). The preexponential factors $d_{\kappa n}(\theta_i)$ [see Eq. (40)] were determined from the function values at ξ_{co} (and analogously for the discrete eigenfunctions). The amplitudes $a_{\kappa n}(\theta_i)$ and phases $\vartheta_{\kappa n}(\theta_i)$ were determined from the asymptotic behavior of the corresponding components.

Here we can compare again with the improved relaxation time ansatz of Einzel *et al.*[8] (cf. Section 4), now with respect to the eigenfunctions. Our continuum eigenfunctions consist of the asymptotic, oscillatory part given by Eq. (40) plus some exponentially decreasing part. Fourier transformation leads, after some elementary manipulations and neglecting multiplicative constants, to

$$\begin{aligned}\psi_{\kappa n}(u, \theta) = \frac{\cosh(u/2)}{u^2 + \pi^2}\, \omega_\kappa(\theta)\, a_{\kappa n}(\theta) \Bigg[&\pi \sin \vartheta_{\kappa n}(\theta)\, \delta(\kappa^{-1} - w) \\ &- \cos \vartheta_{\kappa n}(\theta)\, \mathscr{P} \frac{1}{\kappa^{-1} - w} \Bigg] + \text{background}\end{aligned} \tag{44}$$

where $w = v_z/v(u)$ and "background" comprises all nonsingular terms. The model collision operator of Einzel *et al.*[8] has no nontrivial discrete eigenvalues, $\hat{L}^{-1}(v_z p_x)$ gets replaced by $\tau_\eta v_z p_x$, and the continuum is given by $\kappa \in\,]-\infty, (v_F\tau)^{-1}] \cup [(v_F\tau)^{-1}, \infty[$ (cf. Section 4). The eigenfunctions are of the form $\psi_\kappa(u, \theta, \varphi) = \psi_\kappa(\theta) \cos \varphi$ with

$$\psi_\kappa(\theta) = \sin \theta \left[\lambda_\kappa \delta(\kappa^{-1} - w) + \mu_\kappa \mathscr{P} \frac{1}{\kappa^{-1} - w} \right] \tag{45}$$

where λ_κ and μ_κ are constants depending on κ, and $w = v_z\tau$. Now the difference between the model and the full problem emerges clearly; e.g., the background terms have been dropped and the θ dependence of the phases $\vartheta_{\kappa n}(\theta)$ and all u dependence have been neglected.

6. CALCULATION OF THE SLIP LENGTH

In the last section, we have calculated only the Fourier-transformed eigenfunctions of $v_z^{-1}\hat{L}$. But of course this is sufficient to determine the slip length [or the whole mean velocity $\bar{v}(z)$, if necessary] because we can apply the same transformation to the boundary condition at $z = 0$, Eq. (18). Before doing this, we remark that $v_z p_x \propto \operatorname{Re} Y_{21}(\Omega)$ and $\hat{L}$ is invariant with respect to projections on multipole components and independent of the azimuthal order m [cf. Eq. (21)], so

$$\hat{L}^{-1}(v_z p_x) = v_z p_x \hat{L}^{-1}(Y_{20}(\Omega))/Y_{20}(\Omega) = v_z p_x \psi_c(u)/\omega_{\mathrm{B}} \tag{46}$$

where ψ_c is a function of u only; the index c stands for "collective shear mode,"[8] as $\hat{L}^{-1}(v_z p_x)$ is the only nonrelaxing term that is responsible for the momentum current density. We denote the result of $\psi_c(u)$ under the transformation of Eqs. (27) and (31) by $\varphi_c(\xi)$:

$$\varphi_c(\xi) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} du\, e^{iu\xi/\pi} \psi_c(u) \frac{1}{2} \operatorname{sech} \frac{u}{2} \tag{47}$$

$\varphi_c(\xi)$ is easily calculated by expanding $\hat{L}^{-1}(Y_{20}(\Omega))$ in terms of the normalized eigenfunctions $\psi^+_{\omega 20}$ of $\hat{L}$ belonging to $l = 2$, $m = 0$, parity $+$, and eigenvalue $-\bar{\omega}\omega_{\mathrm{B}}$; see Vogel *et al.*[1] Using the overlaps of the eigenfunctions $\psi^+_{\omega 20}$ with Y_{20} and their transforms $\varphi^+_{\omega 20}$ [cf. Eq. (47)] calculated there, we get

$$\begin{aligned}
\varphi_c(\xi) &= -\sum\!\!\!\!\!\!\int \frac{d\bar{\omega}}{\bar{\omega}} \varphi^+_{\omega 2}(\xi) \langle \psi^+_{\omega 20} | Y_{20} \rangle \\
&= -\frac{2^{2s-3/2}}{1-4s^2} \frac{\Gamma(1/2+2s)[\Gamma(1/2+s)]^2}{s[\Gamma(2s)]^2} \operatorname{sech}^{2s} \xi \\
&\quad - \frac{1}{\sqrt{8}} \int_0^\infty \frac{dk}{k^2+1/4} \operatorname{Re}\left[\frac{G}{|G|} \operatorname{sech}^{2ik} \xi \right.\\
&\quad \left. \times {}_2F_1\left(-s+ik, \frac{1}{2}+s+ik; 1+2ik; \operatorname{sech}^2 \xi\right)\right] \\
&\quad \times \operatorname{Re}\left[\frac{G}{|G|} \frac{\Gamma(1/2+ik)}{\Gamma(1+ik)} \right.\\
&\quad \left. \times {}_3F_2\left(-s+ik, \frac{1}{2}+s+ik, \frac{1}{2}+ik; 1+2ik, 1+ik; 1\right)\right]
\end{aligned} \tag{48}$$

with the abbreviations

$$G = \frac{\Gamma(-2ik)}{\Gamma(-s-ik)\,\Gamma(1/2+s-ik)}, \qquad s = \frac{1}{4}\left[-1+(1+8\lambda_2^+)^{1/2}\right]$$

The same result has been obtained by Sykes and Brooker[12] in a different mathematical form.

For $d\bar{\sigma}/d\Omega = \text{const}$ the quantity s has the value 0.1531 [cf. Eq. (23)]. In Fig. 3 we have plotted this special case, comparing $-\varphi_c(\xi)$ with the relaxation time ansatz equivalent $\tau_\eta \omega_B (\pi/2)^{1/2}\,\mathrm{sech}\,\xi$ (see below), where

$$\tau_\eta = \frac{1}{4\omega_B} \sum_{n=0}^{\infty} \frac{(4n+3)}{(n+1)(2n+1)[(n+1)(2n+1)-\lambda_2^+]} = 1.012\omega_B^{-1} \tag{49}$$

(see Sykes and Brooker[12]; cf. Section 4). We see that both curves agree rather well.

The result of p_x under the transformation of Eq. (47) is $(\pi/2)^{1/2}\, p_x\,\mathrm{sech}\,\xi$. Writing $\varphi_0(\xi) = \mathrm{sech}\,\xi$, $\varphi_0(\xi,\theta) = \varphi_0(\xi)\sin\theta$, and $\varphi_c(\xi,\theta) = \varphi_c(\xi)\sin\theta\cos\theta$, we get from Eq. (18) by transformation [see Eq. (47)] and dividing by $a/(k_B T)\, v_F\, p_F\, \omega_B^{-1}\cos\varphi$ a dimensionless expansion of $\varphi_c(\xi,\theta)$ in terms of transformed eigenfunctions of $v_z^{-1}\hat{L}$ in the half-space $v_z > 0$,

$$\varphi_c(\xi,\theta) = A_0\varphi_0(\xi,\theta) + \sum_d A_d\varphi_d(\xi,\theta) + \int_0^1 d(1/\bar{\kappa}) \sum_n A_{\kappa n}\varphi_{\kappa n}(\xi,\theta) \tag{50}$$

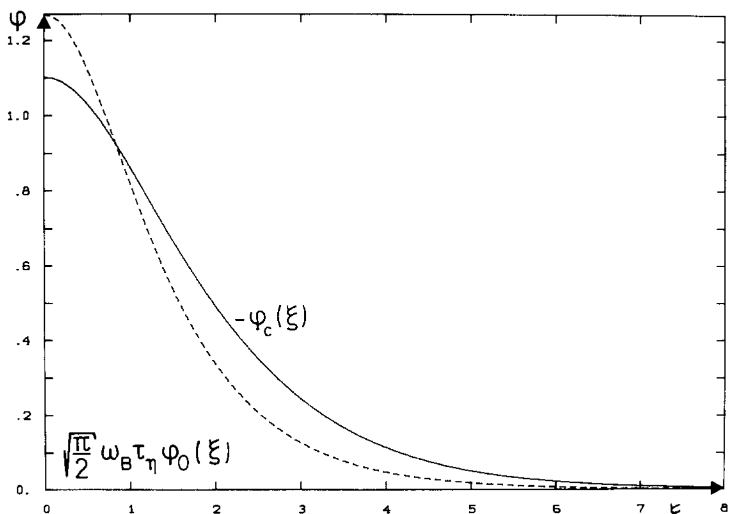

Fig. 3. The radial part $-\varphi_c$ of the transformed collective shear mode $\hat{L}^{-1}(v_z p_x)$ compared to its equivalent in the relaxation time ansatz.

for $\theta < \pi/2$, with

$$A_0 = -\left(\frac{\pi}{2}\right)^{1/2} \frac{\omega_B}{v_F} \frac{k_B T}{a} c_0 = \left(\frac{\pi}{2}\right)^{1/2} \frac{\omega_B}{v_F} \zeta \tag{51}$$

[cf. Eq. (16)] and certain coefficients A_d and $A_{\kappa n}$; the first sum in Eq. (50) is taken over the discrete eigenvalues $0 < \bar{\kappa}_d < 1$.

In order to evaluate Eq. (50) numerically, we restrict the integral over $1/\bar{\kappa}$ to the interval $[1/\bar{\kappa}_{\max}, 1/\bar{\kappa}_{\min}]$ with certain cutoff values $\bar{\kappa}_{\min}$ and $\bar{\kappa}_{\max}$ (see later) and divide this interval into N_κ parts $J_1, \dots, J_{N_\kappa}$ of equal size. We assume that the coefficients $A_{\kappa n}$ are approximately constant on these smaller intervals, $A_{\kappa n} = A_{jn}$ for $1/\bar{\kappa} \in J_j$. Further, we restrict ourselves to a finite number N_d of discrete eigenvalues (for a finite number N_θ of angles this is the case anyway; see Section 5.1) and to a certain number N_{ic} of initial conditions at $\xi = 0$ (see Section 5.2). So we have from Eq. (50)

$$\begin{aligned}\varphi_c(\xi, \theta) = {} & A_0 \varphi_0(\xi, \theta) + \sum_{d=1}^{N_d} A_d \varphi_d(\xi, \theta) \\ & + \sum_{j=1}^{N_\kappa} \sum_{n=1}^{N_{\mathrm{ic}}} A_{jn} \int_{J_j} d(1/\bar{\kappa})\, \varphi_{\kappa n}(\xi, \theta)\end{aligned} \tag{52}$$

for $\theta < \pi/2$. We now define $1/\bar{\kappa}_j$ as the center of J_j and $\varphi_{jn} = \varphi_{\kappa_j n}$ $(j = 1, \dots, N_\kappa)$. Then we get a system of linear equations for the coefficients A_0, A_d, and A_{jn} by projecting Eq. (52) onto φ_0, $\varphi_{d'}$, and $\varphi_{j'n'}$ $(d' = 1, \dots, N_d;\ j' = 1, \dots, N_\kappa;\ n' = 1, \dots, N_{\mathrm{ic}})$, with each function restricted to the half-space $\theta < \pi/2$. For this purpose we use the scalar product (h stands for "half-space")

$$\begin{aligned}\langle \varphi \mid \varphi' \rangle_{\mathrm{h}} &= 2 \int_0^{\pi/2} d\theta \sin\theta \cos\theta \int_0^{\infty} d\xi\, \varphi(\xi, \theta)\, \varphi'(\xi, \theta) \\ &\propto \langle \psi |\, v_z \Theta(v_z)\, | \psi' \rangle\end{aligned} \tag{53}$$

where ψ and ψ' denote the inverse transforms of φ and φ', respectively, in momentum space [cf. Eq. (12)]. Hence we have the system of equations

$$\begin{aligned}\langle \varphi \mid \varphi_c \rangle_{\mathrm{h}} = {} & A_0 \langle \varphi \mid \varphi_0 \rangle_{\mathrm{h}} + \sum_{d=1}^{N_d} A_d \langle \varphi \mid \varphi_d \rangle_{\mathrm{h}} \\ & + \sum_{j=1}^{N_\kappa} \sum_{n=1}^{N_{\mathrm{ic}}} A_{jn} \int_{J_j} d(1/\bar{\kappa})\, \langle \varphi \mid \varphi_{\kappa n} \rangle_{\mathrm{h}}\end{aligned} \tag{54}$$

with φ running over the eigenfunctions mentioned above. Except for $\varphi = \varphi_{jn'}$, the integrals over $1/\bar{\kappa}$ may be approximated by

$$\int_{J_j} d(1/\bar{\kappa})\, \langle \varphi \mid \varphi_{\kappa n} \rangle_{\mathrm{h}} \approx |J_j| \langle \varphi \mid \varphi_{jn} \rangle_{\mathrm{h}} \tag{55}$$

where $|J_j| = \Delta(1/\bar{\kappa}) = (1/\bar{\kappa}_{\min} - 1/\bar{\kappa}_{\max})/N_\kappa$ for each j. We have to treat the case $\varphi = \varphi_{jn'}$ separately because then the integrand has δ and $\mathscr{P}$ singularities (see later).

The ξ integral in Eq. (53) was evaluated by dividing into $\int_0^{\xi_{co}} d\xi$ and $\int_{\xi_{co}}^\infty d\xi$, which gives an inner (int) and an outer (ext) part of $\langle \varphi | \varphi' \rangle_h$:

$$\langle \varphi | \varphi' \rangle_h = \langle \varphi | \varphi' \rangle_h^{\text{int}} + \langle \varphi | \varphi' \rangle_h^{\text{ext}} \tag{56}$$

For the inner part we used the numerically calculated function values and for the outer part the asymptotic form of the eigenfunctions [see Eqs. (36) and (40)] and the approximation $\operatorname{sech} \xi \approx 2e^{-\xi}$. Integrals involving φ_c were cut off at $\xi'_{co} = 10$ (cf. Fig. 3) and the numerical values for φ_c were used throughout.

We calculated the ξ integrals in the outer parts of the overlaps over products of exponential and/or trigonometric functions with well-known formulas, one of which is

$$\begin{aligned}
&\int_{\xi_{co}}^\infty d\xi \sin(\omega\xi + \vartheta) \sin(\omega'\xi + \vartheta') \\
&\quad = \frac{1}{2} \cos(\vartheta - \vartheta') \{\pi\delta(\omega - \omega') - \xi_{co} \operatorname{sinc}[(\omega - \omega')\, \xi_{co}]\} \\
&\quad\quad + \frac{1}{2} \left\{ \frac{1}{\omega + \omega'} \sin[(\omega + \omega')\, \xi_{co} + \vartheta + \vartheta'] \right. \\
&\quad\quad \left. - \sin(\vartheta - \vartheta') \cos[(\omega - \omega')\, \xi_{co}]\, \mathscr{P} \frac{1}{\omega - \omega'} \right\}
\end{aligned} \tag{57}$$

which is valid for $\omega \neq -\omega'$, with $\operatorname{sinc} r = r^{-1} \sin r$. Two of the overlaps can be evaluated analytically:

$$\langle \varphi_0 | \varphi_0 \rangle_h = 1/2 \tag{58}$$

and it can be shown that

$$\langle \varphi_0 | \varphi_c \rangle_h = \frac{4}{15} \int_0^\infty d\xi\, \varphi_c(\xi) \operatorname{sech} \xi = -\frac{4}{15} \left(\frac{\pi}{2}\right)^{1/2} \omega_B \tau_\eta \tag{59}$$

[cf. Eq. (49) and Sykes and Brooker[12]].

With the help of Eq. (57) and the formula

$$\mathscr{P} \int_{-\varepsilon}^{\varepsilon} dy \frac{f(y)}{y} \approx 2\varepsilon \frac{df}{dy}(0) \qquad \text{for} \quad \varepsilon \to 0 \tag{60}$$

we can perform the missing integral in Eq. (54) for the case $\varphi = \varphi_{jn'}$: With the abbreviations $\theta_{(j)} = \theta_{\kappa_j}$ [cf. above and Eq. (40)] and $a_{jn}(\theta) = a_{\kappa_j n}(\theta)$, etc., we get after elementary but somewhat lengthy manipulations

$$\begin{aligned}
&\frac{1}{\Delta(1/\bar{\kappa})} \int_{J_j} d(1/\bar{\kappa}) \langle \varphi_{jn'} \mid \varphi_{\kappa n} \rangle_{\mathrm{h}} \\
&\approx \langle \varphi_{jn'} \mid \varphi_{jn} \rangle_{\mathrm{h}}^{\mathrm{int}} + \int_0^{\theta_{(j)}} d\theta \sin 2\theta \, a_{jn'}(\theta) \\
&\times \Bigg[a_{jn}(\theta) \Bigg(\cos[\vartheta_{jn}(\theta) - \vartheta_{jn'}(\theta)] \left(\frac{\pi \omega_j(\theta)}{\Delta(1/\bar{\kappa}) \, \bar{\kappa}_j^2 \cos\theta} - \frac{\xi_{\mathrm{co}}}{2} \right) \\
&+ \frac{\sin[2\omega_j(\theta)\, \xi_{\mathrm{co}} + \vartheta_{jn}(\theta) + \vartheta_{jn'}(\theta)]}{4\omega_j(\theta)} \\
&+ \sin[\vartheta_{jn}(\theta) - \vartheta_{jn'}(\theta)] \left(\frac{\omega_j(\theta)}{\bar{\kappa}_j \cos(\theta)} - \frac{1}{4\omega_j(\theta)} \right) \Bigg) \\
&- \frac{\omega_j(\theta)}{\cos\theta} \frac{\partial}{\partial \bar{\kappa}} \left\{ a_{\kappa n}(\theta) \sin[\vartheta_{\kappa n}(\theta) - \vartheta_{jn'}(\theta)] \right\} \Bigg|_{\bar{\kappa}_j} \Bigg] \\
&+ \int_{\theta_{(j)}}^{\pi/2} d\theta \sin 2\theta \, d_{jn'}(\theta) \, d_{jn}(\theta) \frac{\exp[-2\Omega_j(\theta)\, \xi_{\mathrm{co}}]}{2\Omega_j(\theta)}
\end{aligned} \tag{61}$$

We replaced the derivative occurring on the rhs by the slope of the corresponding secant

$$\frac{d\alpha}{d\bar{\kappa}}(\bar{\kappa}_j) \approx \frac{\alpha(\bar{\kappa}_{j\mp 1}) - \alpha(\bar{\kappa}_j)}{\bar{\kappa}_{j\mp 1} - \bar{\kappa}_j} \tag{62}$$

which we chose in the direction of increasing $\bar{\kappa}$ (upper sign) unless the number N_{0x} of oscillatory "channels" had jumped [cf. Eq. (42)], because such a discontinuity of N_{0x} involves also a discontinuity of the amplitudes and phases (for a finite number N_θ of angles, at least). Jumps of N_{0x} on both sides were avoided by using a sufficient number N_κ of eigenvalues.

For the parameters N_ξ and N_θ the values 45 and 48, respectively, were sufficient within the accuracy of our numerical calculation: For example, using instead $N_\theta = 96$ changes the slip length typically by 0.02%.

When choosing the cutoff parameters $\bar{\kappa}_{\min}$ and $\bar{\kappa}_{\max}$ [see after Eq. (51)] we had to prevent numerical failure, which occurs when either $\bar{\kappa}_{\max}$ is too high or one of the eigenvalues $\bar{\kappa}_j$ comes too near to the discontinuity points of N_{0x} [see Eq. (42)] from above. The selection of $\bar{\kappa}_{\min}$

together with the number N_{ic} of initial conditions in Fourier space is restricted by the condition

$$N_{\mathrm{ic}} \leqslant N_{0x}(\bar{\kappa}_{\min}) = \mathrm{int}[1/2 + N_\theta \theta_{\kappa_{\min}}/\pi] \tag{63}$$

[cf. Eqs. (40) and (42)]. The possible values of N_{ic} and N_κ are bounded by the capacity of the computer used, assuming a reasonable amount of programming.

A rather good approximation for ζ is achieved by neglecting all basis functions except φ_0 in Eq. (52). The slip length would then be given by

$$\zeta \approx -\left(\frac{2}{\pi}\right)^{1/2} \frac{v_{\mathrm{F}}}{\omega_{\mathrm{B}}} \frac{\langle \varphi_c | \varphi_0 \rangle_{\mathrm{h}}}{\langle \varphi_0 | \varphi_0 \rangle_{\mathrm{h}}} = \frac{8}{15} v_{\mathrm{F}} \tau_\eta = 0.533 v_{\mathrm{F}} \tau_\eta \tag{64}$$

[see Eqs. (51), (58), and (59)], which in the case of $d\bar{\sigma}/d\Omega = \mathrm{const}$ comes to 93% of the true slip length (see Table I). Subsequently, this can be understood because the half-space overlaps of eigenfunctions belonging to different eigenvalues are the negative of the overlaps in the other half-space $v_z < 0$, as the eigenfunctions are orthogonal with respect to the weight function v_z in the entire space. But for $v_z < 0$ all eigenfunctions are exponentially decreasing, so that the overlaps mentioned above turn out to be rather small. Expressing the slip length in terms of φ_0 and φ_1, or of φ_0, φ_1, and φ_2, changes the value of Eq. (64) only negligibly (by less than 0.4%), so that the continuum must be responsible for the missing 7%.

We turn now to the model slip length determined by Einzel *et al.*[8] as

$$\zeta_{\mathrm{model}} = 0.5819 v_{\mathrm{F}} \tau_\eta \tag{65}$$

For a constant differential cross section this becomes

$$\zeta_{\mathrm{model}} = 0.5889 v_{\mathrm{F}} / \omega_{\mathrm{B}} \tag{66}$$

[see Eq. (49)]. In Table I we give our results with three different choices of numerical parameters, as well as the relative deviation from ζ_{model}. We note a small improvement between -1% and -2%.[4]

In order to investigate the slip length for more realistic differential cross sections, we modified our approach by varying λ_2^+, keeping the other parameters λ_l^+ fixed. For this purpose we took the Landau parameters F_0^{s}, F_0^{a}, F_1^{s}, and F_1^{a} determined by Greywall[22] and the consistent value of F_2^{s} by Engel and Ihas[23] and calculated the resulting λ_2^+ as a function in terms of the pressure p (we set F_2^{a} and all higher Landau parameters equal to zero; using the sum rule for F_2^{a} would have given an altogether

Table I. The Slip Length ζ for $d\bar{\sigma}/d\Omega = \text{const}$ and Various Numerical Parameters

N_κ	N_{ic}	$\bar{\kappa}_{min}$	$\bar{\kappa}_{max}$	ζ (v_F/ω_B)	Relative deviation from ζ_{model}, %
67	5	1.046	7.05	0.5799	−1.5
67	3	1.046	7.05	0.5764	−2.1
112	3	1.03	7.5	0.5796	−1.6

unreasonably large value for this parameter). The corresponding singlet and triplet partial wave amplitudes are

$$A_l^{(0)} = A_l^s - 3A_l^a, \qquad A_l^{(1)} = A_l^s + A_l^a \tag{67}$$

with $A_l^g = F_l^g/[1 + F_l^g/(2l+1)]$ ($g = $ s, a; $l = 0, 1, 2$), which result in the singlet and triplet scattering amplitudes

$$A^{(0)}(\tilde{\theta}, \tilde{\varphi}) = A_0^{(0)} + A_1^{(0)} P_1(\cos\tilde{\theta}) + A_2^{(0)}[P_2(\cos\tilde{\theta}) - \tfrac{3}{4}(1-\cos\tilde{\theta})^2 \sin^2\tilde{\varphi}]$$

and

$$A^{(1)}(\tilde{\theta}, \tilde{\varphi}) = [A_0^{(1)} + A_1^{(1)} P_1(\cos\tilde{\theta}) + A_2^{(1)} P_2(\cos\tilde{\theta})] \cos\tilde{\varphi} \tag{68}$$

respectively.[24] From these the spin-averaged transition probability $W(\tilde{\theta}, \tilde{\varphi})$, which is proportional to $d\bar{\sigma}/d\Omega$,[1] is up to a constant factor given by[25]

$$W(\tilde{\theta}, \tilde{\varphi}) \propto [A^{(0)}(\tilde{\theta}, \tilde{\varphi}) + A^{(1)}(\tilde{\theta}, \tilde{\varphi})]^2 + 2[A^{(1)}(\tilde{\theta}, \tilde{\varphi})]^2 \tag{69}$$

Carrying out the $\tilde{\varphi}$ integrations in Eq. (22), we find

$$\lambda_2^+ = A/B \tag{70}$$

where

$$\begin{aligned} A = \int_0^\pi d\tilde{\theta} \sin\frac{\tilde{\theta}}{2} \bigg[& \left(-\frac{1}{2} - \frac{3}{2}\cos^2\tilde{\theta} + 3\cos^4\frac{\tilde{\theta}}{2}\right) \\ & \times \left(\frac{3}{2} h_1^2 + h_0^2 + \frac{3}{8} c^2 h_2^2 - c h_0 h_2\right) \\ & + 3\sin^4\frac{\tilde{\theta}}{2}\left(\frac{9}{8} h_1^2 + \frac{1}{2} h_0^2 + \frac{1}{16} c^2 h_2^2 - \frac{1}{4} c h_0 h_2\right)\bigg] \end{aligned}$$

and

$$B = \int_0^{\pi} d\tilde{\theta} \sin\frac{\tilde{\theta}}{2}\left(\frac{3}{2}h_1^2 + h_0^2 + \frac{3}{8}c^2h_2^2 - \frac{1}{4}ch_0h_2\right) \tag{71}$$

with the abbreviations $c = A_2^{(0)}$, $h_i = A_0^{(i)} + A_1^{(i)}\cos\tilde{\theta} + A_2^{(i)}P_2(\cos\tilde{\theta})$ $(i = 0, 1)$, and $h_2 = \frac{3}{4}(1 - \cos\tilde{\theta})^2$. The remaining $\tilde{\theta}$ integrals were performed numerically for the sake of brevity. The result for λ_2^+ as a function of the pressure p is shown in Fig. 4. Circles mark the values calculated for the parameters $\{F_0^s, F_1^s, F_2^s, F_0^a, F_1^a\}$ of ref. 22 with the help of the interpolation formula for F_2^s given in ref. 23. We see that λ_2^+ varies between 0.31 at zero pressure and 0.71 at melting pressure. In order to span this interval, we additionally calculated the slip length for $\lambda_2^+ = 0.4$, 0.6, and 0.8 ($\lambda_2^+ = 0.2$ corresponds to the constant differential cross section discussed above). The corresponding values for ζ deviated from ζ_{model} by -2.0, -2.3, and -2.5%, respectively [cf. Eqs. (65) and (49)]; these calculations were carried out with the third set of parameters from Table I. The more exact treatment of the boundary value problem presented here yields some improvement in comparison to the model calculation,[8] but is not sufficient to explain the experimental results for the slip length. These differ by -10 to -30%[2] and even by -40%[4] from ζ_{model}. In the first measurement the discrepancies have been explained by finite-size effects,[2,20] but in the second case it seems that the hypothesis of purely diffuse reflection has to be modified in favor of preferred backward scattering[4,19,20] at $z = 0$ (depending on the material and structure of the wall surface, of course).

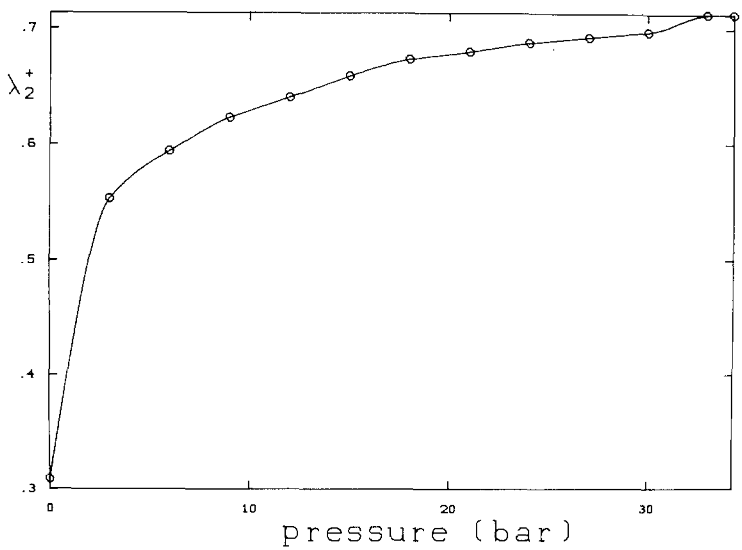

Fig. 4. The interaction parameter λ_2^+ as a function of pressure from data of Greywall[22] and Engel and Ihas.[23]

7. CONCLUSION

We have solved the simplest boundary value problem for fermions, the so-called Kramers problem of a stationary current in a half-space bounded by a diffusely reflecting wall in the nearly degenerate regime, using the framework of the linearized Uehling–Uhlenbeck equation. For this purpose we used a method developed by Case[9] and Cercignani[10,11] involving the spectral decomposition of $v_z^{-1}\hat{L}$, which we carried out using results of Sykes and Brooker[12] and Vogel *et al.*[1]

The original two-dimensional integral equations for the eigenfunctions were changed into integrodifferential equations by a Fourier transformation with respect to the reduced energy. These were solved with suitably chosen initial conditions in Fourier space, in analogy to the traditional coupled-channels approach for the inelastic quantum scattering problem (see, e.g., Rhoades-Brown *et al.*[26]).

The expansion of $\hat{L}^{-1}(v_z p_x)$ in terms of the nonorthogonal system of eigenfunctions belonging to nonnegative eigenvalues in one momentum half-space, which arises from the boundary condition at the wall, was carried out by the aid of discretizations, suitable cutoffs, and projections on the remaining basis functions.

The slip length was evaluated for a constant and also for more realistic differential cross sections and compared with model calculations by Einzel *et al.*[8] Our results are systematically somewhat closer to the experimental values, but there remains a discrepancy between theory and measurement[4,19,21] which may be caused by preferred backward scattering at the boundary.

APPENDIX A

In this appendix we derive Eqs. (33) (Appendix A.1) and (34) (Appendix A.2) for the kernel $w(\theta, \theta')$ of the θ integration within the linearized collision operator $\hat{L}$ in the case of azimuthal order $m = 1$ and constant differential cross section $d\bar{\sigma}/d\Omega$.

A.1. Evaluation of $w(\theta, \theta')$

In order to sum up Eq. (30), we first express the spherical harmonics in terms of associated Legendre functions,

$$Y_{l1}(\theta, 0) = \left[\frac{2l+1}{4\pi l(l+1)}\right]^{1/2} P_l^1(\cos\theta) \tag{A1}$$

Using Eq. (23) for λ_l^+, we get

$$w(\theta, \theta') = \sum_{l=1}^{\infty} [2 - (-)^l] f_l(\theta, \theta') \tag{A2}$$

with the abbreviation

$$f_l(\theta, \theta') = \frac{1}{l(l+1)} P_l^1(\cos\theta) P_l^1(\cos\theta') \tag{A3}$$

We now define

$$f(\theta, \theta') = \sum_{l=1}^{\infty} f_l(\theta, \theta') \tag{A4}$$

and remark that $P_l^1(\cos(\pi - \theta)) = (-)^{l+1} P_l^1(\cos\theta)$. Therefore Eq. (A2) becomes

$$\begin{aligned} w(\theta, \theta') &= \left(3 \sum_{l=1,\mathrm{odd}}^{\infty} + \sum_{l=1,\mathrm{even}}^{\infty}\right) f_l(\theta, \theta') \\ &= \tfrac{3}{2}[f(\theta, \theta') + f(\pi - \theta, \theta')] + \tfrac{1}{2}[f(\theta, \theta') - f(\pi - \theta, \theta')] \\ &= 2f(\theta, \theta') + f(\pi - \theta, \theta') \end{aligned} \tag{A5}$$

We investigate $f(\theta, \theta')$ further by expressing the associated Legendre functions by Gegenbauer polynomials, $P_l^1(\cos\theta) = -\sin\theta\, C_{l-1}^{3/2}(\cos\theta)$. Using $l(l+1) = 2(3)_{l-1}/(l-1)!$, we can write Eq. (A4) in the form

$$f(\theta, \theta') = \frac{1}{2} \sin\theta \sin\theta' \sum_{k=0}^{\infty} \frac{k!}{(3)_k} r^k C_k^{3/2}(\cos\theta)\, C_k^{3/2}(\cos\theta') \bigg|_{r=1} \tag{A6}$$

In this form $f(\theta, \theta')$ can be summed up in the closed form of Eq. (33),[27] if we allow ourselves to extend the domain of validity $r \in]-1, 1[$ given there to $r = 1$. This is permissible according to Abel's theorem if the rhs of Eqs. (A6) or (A4) converges at all. To show this, we use $[l(l+1)]^{-1} = l^{-2} + O(l^{-3})$ and the well-known asymptotic formula for the associated Legendre functions for $\theta, \theta' \neq 0, \pi$

$$P_l^1(\cos\theta) = \left(\frac{2l}{\pi \sin\theta}\right)^{1/2} \cos\left[\left(l + \frac{1}{2}\right)\theta + \frac{\pi}{4}\right] + O(l^{-1/2}) \tag{A7}$$

which gives eight terms in Eq. (A6). Seven of these are at least of the order of l^{-2} and can be summed up without problems. The leading eighth term is, after elementary manipulations, proportional to

$$\begin{aligned} l^{-1}[&\cos(\tfrac{1}{2}\theta_-) \cos(l\theta_-) - \sin(\tfrac{1}{2}\theta_-) \sin(l\theta_-) \\ &+ \cos(\tfrac{1}{2}\theta_+) \sin(l\theta_+) + \sin(\tfrac{1}{2}\theta_+) \cos(l\theta_+)] \end{aligned}$$

with $\theta_{\pm} = \theta \pm \theta'$ and consists itself therefore of four summable terms, provided that $\theta \neq \theta'$. QED

In order to evaluate Eq. (33) numerically, it is convenient to express the hypergeometric function $F(3/2, 3/2; 3; t)$ in terms of complete elliptic integrals, which are available in program libraries. To this end, we apply a well-known linear transformation

$$(-t)^{3/2} F(3/2, 3/2; 3; t) = \tilde{t}^{3/2} F(3/2, 3/2; 3; \tilde{t}) \tag{A8}$$

with

$$\tilde{t} = t/(t-1) = 2 \sin\theta \sin\theta'/[1 - \cos(\theta + \theta')] \in [0, 1]$$

and Gauss' contiguous relations several times to get

$$\begin{aligned} F\left(\frac{3}{2}, \frac{3}{2}; 3; \tilde{t}\right) &= \frac{8}{\tilde{t}^2}\left[(2-\tilde{t})\, F\left(\frac{1}{2}, \frac{1}{2}; 1; \tilde{t}\right) - 2F\left(-\frac{1}{2}, \frac{1}{2}; 1; \tilde{t}\right)\right] \\ &= \frac{16}{\pi \tilde{t}^2}\left[(2-\tilde{t})\, K(\tilde{t}) - 2E(\tilde{t})\right] \end{aligned} \tag{A9}$$

where K and E denote the complete elliptic integrals in the definition of Abramowitz and Stegun.[28]

In Fig. 5 we have plotted level lines of $w(\theta, \theta')$.

A.2. The Asymptotic Behavior of $f(\theta, \theta')$

For $\theta \to \theta'$ the parameter t tends to $-\infty$ [Eq. (33)], and according to Erdélyi *et al.*[29] we have

$$F(3/2, 3/2; 3; t) \sim 8\pi^{-1}(-t)^{-3/2}\,[\ln(-t) + \text{const}] \tag{A10}$$

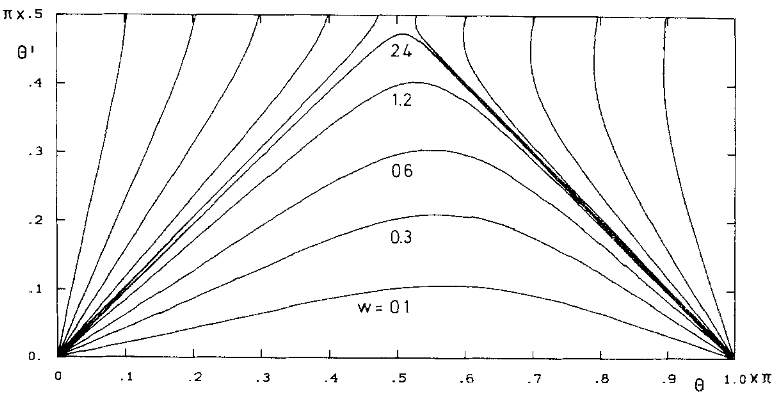

Fig. 5. Level lines of the kernel $w(\theta, \theta')$ of angular integration in the collision operator $\hat{L}$. The figure is to be imagined as reflected at the diagonals $\theta = \theta'$ and $\theta = \pi - \theta'$.

so

$$f(\theta, \theta') \sim (2\pi \sin\theta)^{-1} \{-\ln[1-\cos(\theta-\theta')] + \ln\sin^2\theta + \text{const}\} \tag{A11}$$

[cf. Eq. (33)], which leads to Eq. (34) because of $1-\cos(\theta-\theta') \approx \frac{1}{2}(\theta-\theta')^2$ (being the leading term of the corresponding Taylor expansion).

APPENDIX B

In this appendix we outline the proof for the relative compactness of the operator $\hat{K}'$ with respect to $-v'$. According to Reed and Simon,[15] it suffices to show that $\hat{K}'v'^{-1}$ is square-integrable (and therefore Hilbert–Schmidt and compact). So we have to prove that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} du\, dv \frac{(u-v)^2}{\operatorname{sech}^2[\frac{1}{2}(u-v)]} \frac{1}{(v^2+\pi^2)^2} \times \int_0^{\pi}\int_0^{\pi} d(\cos\theta)\, d(\cos\theta')\, w^2(\theta, \theta') < \infty \tag{B1}$$

[cf. Eq. (29)]. The first double integral is finite, as can be seen by changing from the variable u to $u-v$. The angular integrals are finite as well because $w(\theta, \theta')$ has only very weak (logarithmic) singularities for $\theta = \theta'$ and $\theta = \pi - \theta'$ [cf. Eqs. (33) and (34)] and the intervals of integration are finite. QED

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