TECHNIQUE FOR SEPARATION OF CARRIER DENSITIES AND MOBILITIES IN HIGHLY NONDEGENERATE MULTIBAND SEMICONDUCTORS

DISSERTATION

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By

Lonnie M. Rater, B. S.
Denton, Texas

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The developement of the conductivity coefficients is reviewed for both highly degenerate metals, having an energy dependent relaxation time, and semiconductors, obeying Boltzmann statistics and having a relaxation time varying as the energy to the λ power. In each case the energy bands are assumed to be spherical and parabolic. Examination of the Hall conductivity $\sigma_{xy}(H)$ reveals a similarity of form between the metal and semiconductor situations which allows one to determine the number density n and zero-field conductivity mobility μ_0 for a single band semiconductor, by use of the maximum absolute value of $\sigma_{xy}(H)$ and the corresponding magnetic field H_M, as for metals. Constants which relate μ_0 and n to $|\sigma_{xy}(H_M)|$ and H_M are tabled for the following scattering mechanisms: acoustic phonon scattering, $\lambda=-1/2$; neutral impurity scattering, $\lambda=0$; piezoelectric scattering, $\lambda=1/2$; and ionized impurity scattering, $\lambda=3/2$.

A function $S(\lambda;\gamma)$, where γ varies as H^2, which is proportional to $\sigma_{xy}(H)$, is defined. Evaluation of $S(\lambda;\gamma)$ is necessary since least-squares analysis is required in order to determine n and μ_0 for individual bands of a semiconductor

having multiband conduction. By approximating $S(\lambda;\gamma)$ by rational-type functions which are chosen to be best in a Chebyshev sense, a means of computing $\sigma_{xy}(H)$ is developed which does not rely on tables, numerical integration, or otherwise tedious calculation. Thus a means to acquire n and μ_0 rapidly with the aid of a relatively small computer is presented.

These two developements allow for band parameters to be determined even in the absence of magnetic fields sufficiently large as to have saturation of the Hall constant.

Regarding the application of the theory which this work makes convenient to apply, one must consider the nature of real semiconducting materials. They rarely have completely quadratic or spherical energy bands, and over many temperature ranges they do not have power-law dependent relaxation times. These real situations require much more complicated and time consuming calculations, so much that one is usually forced to use simplifications. When applied in a considered manner, the simple model of $\sigma_{xy}(H)$ will provide n and μ_0 adequate for the experimenter's purpose.

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CHAPTER I

INTRODUCTION

Historically the simple theory describing magnetoconductivity and Hall conductivity for spherical, quadratic energy bands with highly degenerate Fermi-Dirac statistics has been invaluable in the analysis of metallic conduction.[1] Although obviously not appropriate for detailed analysis in the usual case where the Fermi surface is decidely nonspherical, the model still provides a simple setting for the definition of various quantities such as density of states effective mass, number density, and mobility. Because this model has been extended to the slightly more sophisticated case of ellipsoidal Fermi surfaces, it has remained useful in the analysis of multiband metals.[2,3]

The primary reason for the utility of this model is that for the case in which relaxation time is dependent only on energy, the integrals defining $\sigma_{xx}(H)$ and $\sigma_{xy}(H)$ can be written in closed form, such that one may directly compare data to theory by graphical or perhaps least-squares techniques. Extension to the case of nonellipsoidal surfaces, such as that given by McClure,[4] are again easy to interpret in terms of a weighted aggregate of spherical surfaces.

It is the purpose of this work to emphasize that a similar situation exists in the case of semiconductors under highly nondegenerate statistics subject to a power law dependence of relaxation time on energy, with bands described by a spherical, quadratic dispersion law. Here the integrals defining $\sigma_{xx}(H)$ and $\sigma_{xy}(H)$ are not reducible to simple closed forms. In fact, historically the dimensionless integrals which appear have only been tabulated to various degrees of accuracy.[5-9]

In this work a study is made of these integrals showing that there is an underlying simplicity of form which lends itself to graphical and curve fitting techniques. A surprising similarity to the metals case is demonstrated, and a simple function approximation to the integrals is obtained which minimizes the maximum error in the sense of Chebyshev.[10] These simple approximating functions may be calculated with the use of a desk calculator, removing the need for the existing tables. A recipe is developed to allow estimation of number density and mobility in the case of multiband conduction.

One must realize that for real semiconductors the energy bands are usually nonspherical and nonparabolic; and the scattering process may often be due to either several scattering mechanisms or to one which does not have a power-law dependence. However, more realsitic models require more computation to realize the conduction parameters. For this reason the experimenter is often forced to use the simpler models discussed in this work. Fortunately the simple models do provide acceptable answers when used with some knowledge of the energy dispersion relationship and scattering mechanisms for the examined conductor. The choice of the order of the approximation used should depend upon the agreement of the model with the actual case examined by the experimenter.

CHAPTER II

ELECTRICAL CONDUCTIVITY

General Statistics

Following the work of Beer[11] consider a conductor described by a single spherical, parabolic energy band, i.e. the energy relative to the band edge is given by

$$\epsilon = (\hbar^2/2m^*)(k_x^2+k_y^2+k_z^2)$$
$$=\hbar^2k^2/2m^* \quad , \qquad (2.1)$$

with m^* the effective mass and $\vec{k}=(k_x,k_y,k_z)$ the wave vector. Furthermore, the relaxation time is dependent only on energy:

$$\tau = \tau(\epsilon) \quad . \qquad (2.2)$$

Defining the reduced energy and reduced Fermi energy, respectively, as $x \equiv \epsilon/k_BT$ and $\eta \equiv \epsilon_F/k_BT$ (where k_B is the Boltzmann constant and T, the absolute temperature), then the Fermi-Dirac distribution function is $f_0=(e^{x-\eta}+1)^{-1}$, and the Fermi-Dirac function of order $\frac{1}{2}$ is

$$F_{\frac{1}{2}}(\eta)=\int_0^\infty x^{\frac{1}{2}} f_0 dx \quad . \qquad (2.3)$$

The number density (also known as carrier concentration) may be written as[12]

$$n=\frac{2}{(2\pi)^3}\int f_0 d^3k$$
$$=(2\pi^2)^{-1}(2m^*k_BT/\hbar^2)^{3/2}F_{\frac{1}{2}}(\eta) \quad . \qquad (2.4)$$

Suppose uniform electric and magnetic fields are applied to the conductor. The current density may be written as

$$\vec{j}=-\frac{2e}{(2\pi)^3}\int\vec{v}f\,d^3k$$
$$=\hat{\sigma}\vec{E} \quad , \tag{2.5}$$

where the charge e is greater than zero for electrons, $\hat{\sigma}$ is the conductivity tensor, and

$$\vec{v}=\hbar^{-1}\nabla_k\epsilon$$
$$=\hbar\vec{k}/m^* \tag{2.6}$$

is the group velocity. In Appendix F Eqs. (2.1), (2.2), and (2.6) together with the assumption of ohmic conduction (which may be obtained by use of sufficently small $\vec{E}$) are employed to solve the Boltzmann equation for the distribution function f.

If the z axis is chosen so that $\vec{H}=(0,0,H)$ then the transverse magnetoconductivity (throughout this work refered to as the magnetoconductivity) is

$$\sigma_{xx}(H)=\frac{e^2}{3\pi^2m^*}\left(\frac{2m^*k_BT}{\hbar^2}\right)^{3/2}\int_0^\infty\tau\left(-\frac{\partial f_0}{\partial x}\right)\frac{x^{3/2}dx}{1+(\omega\tau)^2} \quad , \tag{2.7}$$

the longitudinal magnetoconductivity is

$$\sigma_{zz}(H)=\sigma_{xx}(0) \quad , \tag{2.8}$$

and the Hall conductivity is

$$\sigma_{xy}(H)=-\frac{e^2}{3\pi^2m^*}\left(\frac{2m^*k_BT}{\hbar^2}\right)^{3/2}\int_0^\infty\omega\tau^2\left(-\frac{\partial f_0}{\partial x}\right)\frac{x^{3/2}dx}{1+(\omega\tau)^2} \quad , \tag{2.9}$$

where $\omega=eH/m^*c$ is the cyclotron frequence. By defining the averge of a function G over the Fermi-Dirac distribution as

$$\langle G\rangle \equiv \frac{2}{3}\frac{1}{F_{\frac{1}{2}}(\eta)}\int_0^\infty G(x)x^{3/2}\left(-\frac{\partial f_0}{\partial x}\right)dx \quad , \qquad (2.10)$$

Eqs. (2.7) and (2.9) become, respectively,

$$\sigma_{xx}(H)=\frac{ne^2}{m^*}\langle\tau/(1+\omega^2\tau^2)\rangle \qquad (2.11)$$

and

$$\sigma_{xy}(H)=-\frac{ne^2}{m^*}\langle\omega\tau^2/(1+\omega^2\tau^2)\rangle \quad . \qquad (2.12)$$

If one introduces the common convention of considering e as being the absolute magnitude of the electronic charge and requires that $\omega\geq 0$, then the (zero-field) conductivity mobility μ_0 defined by

$$\sigma_{xx}(0)\equiv ne\mu_0 \qquad (2.13)$$

becomes

$$\mu_0=e\langle\tau\rangle/m^* \qquad (2.14)$$

and is greater than zero for both electrons and holes. Eqs. (2.11) and (2.12) may be rewritten as

$$\sigma_{xx}(H)=ne\mu_0\langle\tau\rangle^{-1}\langle\tau/(1+\omega^2\tau^2)\rangle \qquad (2.15)$$

and

$$\sigma_{xy}(H)=\pm ne\mu_0\langle\tau\rangle^{-1}\langle\omega\tau^2/(1+\omega^2\tau^2)\rangle \quad , \qquad (2.16)$$

where the upper sign is for holes and the lower sign for electrons.

A calculation of $\sigma_{xx}(H)$ and $\sigma_{xy}(H)$ for arbitrary H usually requires numerical integration. However using Eq. (2.13) and the relationship

$$\lim_{H\to\infty} H\sigma_{xy}(H) = \pm nec \qquad (2.17)$$

one may calculate n and μ_0 if the Hall saturation field is available and conduction is due to only one band of carriers; otherwise examination of conductivity data over a range of magnetic field is necessary. The calculation of $\sigma_{xx}(H)$ and $\sigma_{xy}(H)$ for arbitrary H simplifies in two cases: 1) highly degenerate metals ($\epsilon_F >> k_B T$), and 2) nondegenerate semiconductors ($\epsilon_F << 0$), having τ proportional to a power of energy.

Highly Degenerate Metals

Since for a metal

$$-\frac{\partial f_0}{\partial x} \approx \delta(x-\eta) \quad , \qquad (2.18)$$

Eqs. (2.15) and (2.16) become

$$\sigma_{xx}(H) = ne\mu_0/(1+\gamma) \qquad (2.19)$$

and

$$\sigma_{xy}(H) = \pm ne\mu_0 \gamma^{\frac{1}{2}}/(1+\gamma) \quad , \qquad (2.20)$$

where by use of Eq. (2.14)

$$\gamma = \omega^2 \tau^2(\eta)$$
$$= (\mu_0/c)^2 H^2 \quad . \qquad (2.21)$$

Defining the function

$$S(\gamma) \equiv \gamma^{\frac{1}{2}}/(1+\gamma) \qquad (2.22)$$

one observes

$$\gamma^{\frac{1}{2}}\sigma_{xx}(H) = ne\mu_0 S(\gamma) \qquad (2.23)$$

and

$$\sigma_{xy}(H)=\pm\, ne\mu_0 S(\gamma) \quad . \tag{2.24}$$

Noticing the property

$$S(\gamma^{-1})=\gamma^{-\frac{1}{2}}/(1+\gamma^{-1})$$
$$=S(\gamma) \quad , \tag{2.25}$$

one perceives that a plot of $S(\gamma)$ vs $\log(\gamma)$ is even about the point corresponding to $\gamma=1$. Observe $S(\gamma)$ to assume the maximum value of $\frac{1}{2}$ at $\gamma=1$. Since the Hall conductivity is proportional to $S(\gamma)$, then knowledge of $|\sigma_{xy}(H_M)|$, the maximum absolute value of $\sigma_{xy}(H)$, and the corresponding field H_M allows one to calculate, using Eqs. (2.21) and (2.24),

$$\mu_0=c/H_M \tag{2.26}$$

and

$$n=2\,|\sigma_{xy}(H_M)|/(e\mu_0) \quad . \tag{2.27}$$

If M bands contribute to conduction, the Hall conductivity becomes

$$\sigma_{xy}(H)=\sum_{j=1}^{M} \pm n_j e\mu_{0j} S(\gamma_j) \quad , \tag{2.28}$$

where $\gamma_j=(\mu_{0j}H/c)^2$. A least-squares fit of $\sigma_{xy}(H)$ will be required to determine the n_j and μ_{0j}.[13]

Nondegenerate Semiconductors

Often for a semiconductor one may assume both Boltzmann statistics ($\epsilon_F<<0$) and the relaxation time varies as the energy to the λ power,[11] i.e.

$$f_0 \approx e^{\eta - x} \tag{2.29}$$

and

$$\tau(x) = \tau_0 x^{\lambda} \quad . \tag{2.30}$$

From Eq. (2.14) the conductivity mobility is determined as

$$\mu_0 = e\,\tau_0\,\Gamma(\lambda+5/2)/(m^*\,\Gamma(5/2)) \quad ; \tag{2.31}$$

and from Eqs. (2.15) and (2.16) the conductivity coefficients are given by

$$\sigma_{xx}(H) = \frac{ne\mu_0}{\Gamma(\lambda+5/2)} \int_0^\infty \frac{x^{\lambda+3/2} e^{-x} dx}{1+\gamma x^{2\lambda}} \tag{2.32}$$

and

$$\sigma_{xy}(H) = \pm \frac{ne\mu_0}{\Gamma(\lambda+5/2)} \gamma^{\frac{1}{2}} \int_0^\infty \frac{x^{2\lambda+3/2} e^{-x} dx}{1+\gamma x^{2\lambda}} \quad , \tag{2.33}$$

where

$$\gamma = \omega^2 \tau_0^2$$

$$= [H\mu_0\,\Gamma(5/2)/(c\,\Gamma(\lambda+5/2))]^2 \quad . \tag{2.34}$$

Defining the function

$$S(\lambda;\gamma) \equiv \frac{1}{\Gamma(\lambda+5/2)} \gamma^{\frac{1}{2}} \int_0^\infty \frac{x^{3/2} e^{-x} dx}{x^{-2\lambda}+\gamma} \quad , \tag{2.35}$$

then the Hall conductivity is given by

$$\sigma_{xy}(H) = \pm\, ne\mu_0 S(\lambda;\gamma) \quad . \tag{2.36}$$

The $S(\lambda;\gamma)$, for λ corresponding to various common pure power-law scattering mechanisms developed in Nag's book,[14] are shown in Fig. 1 normalized to unity and plotted against the

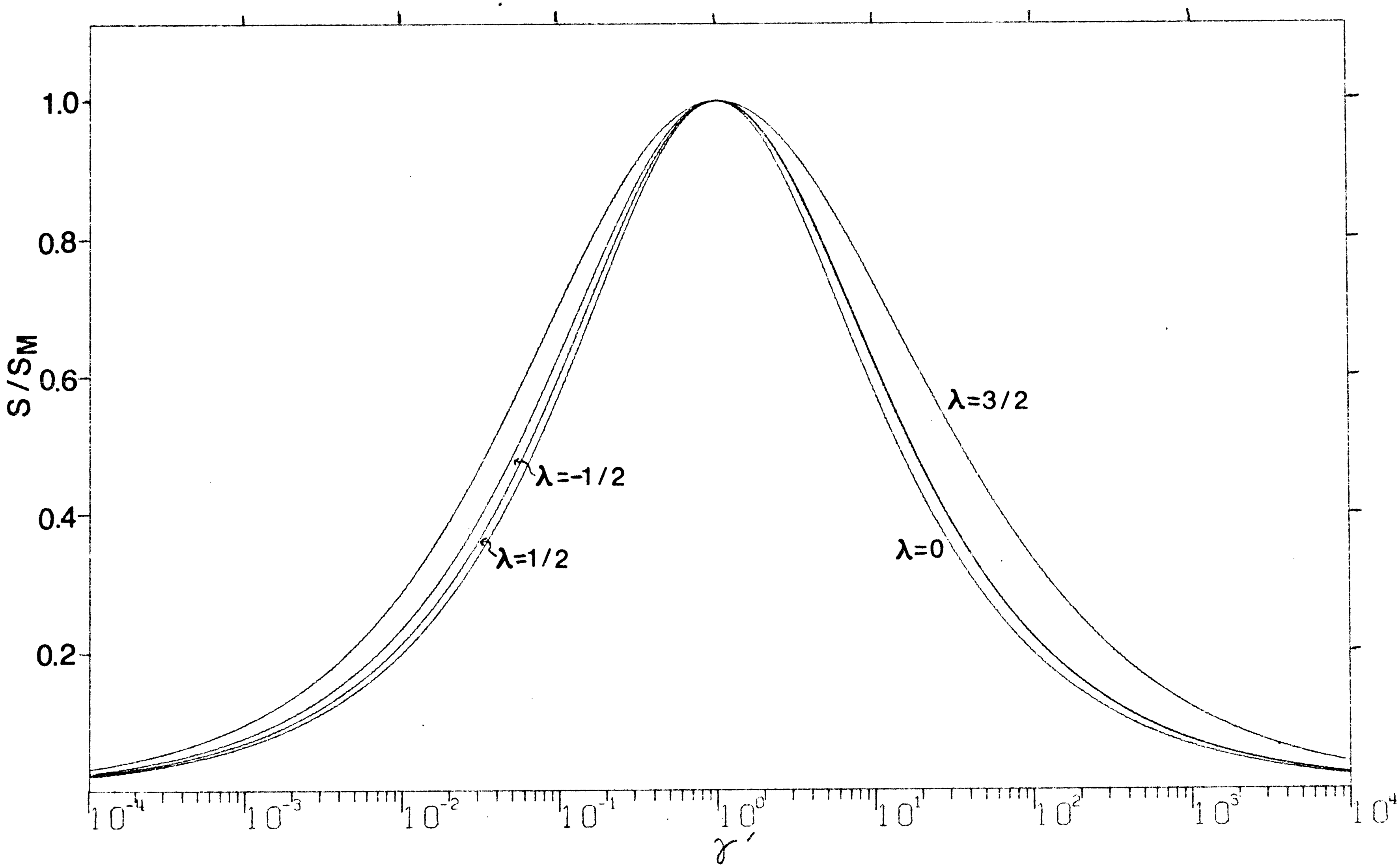

Fig. 1--Several $S(\lambda;\gamma)$ each normalized to unity and plotted <u>vs</u> $\log(\gamma')$ where $\gamma'=\gamma/\gamma_M$

common logarithm of $\gamma'=\gamma/\gamma_M$. These λ and their corresponding scattering mechanisms are: 1) $\lambda=-1/2$, acoustical phonon scattering; 2) $\lambda=0$, neutral impurity scattering; 3) $\lambda=1/2$, piezoelectric scattering; and 4) $\lambda=3/2$, ionized impurity scattering. Early attention was devoted to evaluating the integrals in Eqs. (2.32) and (2.33) for the case of acoustical phonon scattering[15,16] and constructing a table of values.[5] These tables have been extended and improved[6,8,9] and other tables corresponding to $\lambda=3/2$ have been published.[7,9] In Appendix C these integrals are evaluated in terms of commonly tabulated functions. As knowledge of $\sigma_{xy}(H)$ is sufficient to allow for calculation of n and μ_0 in a conductor having spherical, parabolic energy contours, only the $S(\lambda;\gamma)$ are evaluated below. The $S(\lambda;\gamma)$ including their asymptotic expansions, where appropriate, are: for $\lambda=0$,

$$S(0;\gamma)=\gamma^{\frac{1}{2}}/(1+\gamma) = S(\gamma) \quad ; \qquad (2.37)$$

for $\lambda=-1/2$,

$$S(-\tfrac{1}{2};\gamma)=\gamma^{\frac{1}{2}}(\tfrac{1}{2}-\gamma)\pi^{\frac{1}{2}}+\gamma^2 e^{\gamma}\pi[1-\Phi(\gamma^{\frac{1}{2}})]$$
$$=\pi^{\frac{1}{2}}[\tfrac{1}{2}-\gamma-2\gamma^2\sum_{k=0}^{\infty}\frac{(2\gamma)^k}{(2k+1)!!}]\gamma^{\frac{1}{2}}+\pi\gamma^2 e^{\gamma} \qquad (2.38)$$

and

$$S(-\tfrac{1}{2};\gamma)\sim \pi^{\frac{1}{2}}\gamma^{3/2}\sum_{k=2}\frac{(-1)^k(\frac{1}{2})_k}{\gamma^k} \quad , \qquad (2.39)$$

where $\Phi(x)$ is the probability function and $(x)_k=\Gamma(x+k)/\Gamma(x)$;

for $\lambda=1/2$,

$$S(\tfrac{1}{2};\gamma)=\pi^{\frac{1}{2}}[3/4\gamma\ -(2\gamma^2)^{-1}+\gamma^{-3}]\gamma^{\frac{1}{2}}/2\ -\pi\gamma^{-3}e^{1/\gamma}[1-\Phi(\gamma^{-\frac{1}{2}})]/2$$

$$=\pi^{\frac{1}{2}}[3/4\gamma\ -(2\gamma^2)^{-1}+\gamma^{-3}+2\gamma^{-4}\sum_{k=0}^{\infty}\frac{(2/\gamma)^k}{(2k+1)!!}]\gamma^{\frac{1}{2}}/2\ -\pi\gamma^{-3}e^{1/\gamma}/2 \qquad (2.40)$$

and

$$S(\tfrac{1}{2},\gamma)\sim(\pi^{\frac{1}{2}}/2)\gamma^{-5/2}\sum_{k=3}(-1)^{k-1}(\tfrac{1}{2})_k\gamma^k \quad ; \qquad (2.41)$$

and for $\lambda=3/2$,

$$S(3/2;\gamma)=\pi^{\frac{1}{2}}[\frac{3a^3}{4}+2a^6\sum_{k=0}^{\infty}\frac{(2a)^{3k}}{(6k+1)!!}]a^{-3/2}/6\ -$$

$$\pi a^4[e^a-2e^{-a/2}\cos(\frac{a3^{\frac{1}{2}}}{2}+\frac{2\pi}{3})]/6 \qquad (2.42$$

and

$$S(3/2;\gamma)\sim(\pi^{\frac{1}{2}}/6)a^{3/2}\sum_{k=1}\frac{(-1)^k(\frac{1}{2})_{3k+2}}{a^{3k}} \quad , \qquad (2.43)$$

where $a=\gamma^{-1/3}$.

As in the case of a metal, μ_0 and n may be determined for a single band nondegenerate semiconductor having power-law scattering by knowledge of $|\sigma_{xy}(H_M)|$ and H_M. The conductivity mobility is given by

$$\mu_0=\Gamma(\lambda+5/2)c\gamma_M^{\frac{1}{2}}/(H_M\,\Gamma(5/2)) \qquad (2.44)$$

and the number density by

$$n=|\sigma_{xy}(H_M)|/(e\mu_0 S(\lambda;\gamma_M)) \quad , \qquad (2.45)$$

where γ_M corresponds to the maximum value $S(\lambda;\gamma_M)$ of $S(\lambda;\gamma)$. Eqs. (2.44) and (2.45) may be rewritten, respectively, as

$$\mu_0 = C_1/H_M \tag{2.46}$$

and

$$n = C_2\left|\sigma_{xy}(H_M)\right|/\mu_0 \quad . \tag{2.47}$$

Values of C_1 and C_2 for the λ examined in this work are found in Table I which, if H is measured in gauss and $\sigma_{xy}(H)$ in $(\text{ohm-cm})^{-1}$, will allow calculation of μ_0 in cm^2/V-sec and n in carriers per cm^3.

Again, if M bands contribute to conduction then the Hall conductivity may be written as

$$\sigma_{xy}(H) = \sum_{j=1}^{M} \pm n_j e \mu_{0j} S(\lambda_j;\gamma_j) \quad . \tag{2.48}$$

The determination of n_j and μ_{0j} is facilitated by a calculation of $S(\lambda;\gamma)$ which does not rely upon numerical integration or published tables. In Chapter III approximations of $S(\lambda;\gamma)$ are developed which may be calculated quickly and easily with a computer or even a desk calculator. These approximations are of sufficent accuracy to allow precise evaluation of the n_j and μ_{0j} by least-squares analysis, an example of which is provided in Chapter IV.

TABLE I

CONSTANTS USED TO DETERMINE NUMBER DENSITY AND MOBILITY FOR A SINGLE BAND

Scattering Mechanisms	λ	γ_M	S_M	C_1 $(10^8 \frac{G\text{-}cm^2}{V\text{-}sec})$	C_2 $(10^{19}\ C^{-1})$
Acoustic Phonon	-1/2	1.60475	0.467159	0.952944	1.33604
Neutral Impurity	0	1.0	.50	1.0	1.24829
Piezoelectric	1/2	.388434	.478285	.937676	1.30497
Ionized Impurity	3/2	1.97903×10^{-2}	0.404849	0.634953	1.54167

CHAPTER III

APPROXIMATION OF $S(\lambda;\gamma)$

Consideration of the similarity between

$$S(0;\gamma)=\gamma^{\frac{1}{2}}/(1+\gamma) \tag{3.1}$$

and the other $S(\lambda;\gamma)$ displayed in Fig. 1 and the observation that

$$\lim_{\gamma\to 0} S(\lambda;\gamma)\gamma^{-\frac{1}{2}}=\Gamma(2\lambda+5/2)/\Gamma(\lambda+5/2) \tag{3.2}$$

and

$$\lim_{\gamma\to\infty} S(\lambda;\gamma)\gamma^{\frac{1}{2}}=\Gamma(5/2)/\Gamma(\lambda+5/2) \tag{3.3}$$

suggests the $S(\lambda;\gamma)$ may be approximated by

$$S^*(\lambda;\gamma)\equiv\gamma'^{\frac{1}{2}}\sum_{j=1}^{N} a_j\gamma'^{\,j-1}/(1+\sum_{j=1}^{N} b_j\gamma'^{\,j}) \tag{3.4}$$

having order N with a_N and b_N unequal to zero, $\gamma'=\gamma/\gamma_M$, and also the requirement that the denominator and numerator have no common zeros. The a_j and b_j are selected so as to minimize the maximum absolute value of the remainder function

$$R(\gamma)=S^*(\lambda;\gamma)-S(\lambda;\gamma) \tag{3.5}$$

for $0\leq\gamma<\infty$. In other words, by minimizing

$$\delta=\max\left|R(\gamma)\right| \tag{3.6}$$

over the interval $[0,\infty)$, one has found the best approximation of $S(\lambda;\gamma)$ having the form displayed in Eq. (3.4).

Characterization of Best Approximation

The problem of determining the best rational-function approximation of any function f(x) continuous on the closed interval [a,b] is examined by Ralston.[17] If a rational function

$$R_{mn}(x)=P_m(x)/Q_n(x) \quad , \tag{3.7}$$

where $P_m(x)$ is a polynominal of degree m and $Q_n(x)$ is a poly- of degree n, is proposed as an approximation of f(x), then it is the best approximation if and only if

$$r_{mn}=\max_{[a,b]}\left|w(x)[R_{mn}(x)-f(x)]\right| \tag{3.8}$$

is minimized over all P_m and Q_n for any weight function w(x) positive over the open interval (a,b). Ralston[17] proves that if the weighted curve

$$E(x)=w(x)[R_{mn}(x)-f(x)] \tag{3.9}$$

oscillates about zero m+n+2 times with equal amplitude and adjacent extrema have opposite signs, i.e. if there exists $x_1,x_2,...,x_{m+n+2}$ contained in [a,b] such that for i=1,2,..., m+n+2

$$\frac{d}{dx}E(x)\Big|_{x_i}=0 \tag{3.10}$$

and for i=1,2,...,m+n+1

$$x_{i+1}>x_i \tag{3.11}$$

and

$$E(x_{i+1})=-E(x_i) \quad , \tag{3.12}$$

then $R_{mn}(x)$ is the best approximation of f(x) for the chosen w(x). Thus for i=1,2,...,m+n+2 one has

$$r_{mn}=\left|E(x_i)\right| \quad . \tag{3.13}$$

Clearly one can imagine g(x)=w(x)f(x) as the function to be approximated by $w(x)R_{mn}(x)$ and, consequently, apply the above theory to the approximation of $S(\lambda;\gamma)$ by $S^*(\lambda;\gamma)$. From Eqs. (3.2), (3.3), and (3.4) one obtains: 1) for small γ,

$$R(\gamma)\approx\gamma^{\frac{1}{2}}[a_1\gamma_M^{-\frac{1}{2}}-\Gamma(2\lambda+5/2)/\Gamma(\lambda+5/2)] \tag{3.14}$$

and 2) for large γ,

$$R(\gamma)\approx\gamma^{-\frac{1}{2}}[\gamma_M^{\frac{1}{2}}a_N/b_N-\Gamma(5/2)/\Gamma(\lambda+5/2)] \quad . \tag{3.15}$$

Eq. (3.14) implies that if $\gamma<a<<\gamma_M$ then

$$\max_{[0,a]}\left|R(\gamma)\right|\leq\max_{[a,b]}\left|R(\gamma)\right| \quad , \tag{3.16}$$

and Eq. (3.15) implies that if $\gamma>b>>\gamma_M$ then

$$\max_{[b,\infty)}\left|R(\gamma)\right|\leq\max_{[a,b]}\left|R(\gamma)\right| \quad . \tag{3.17}$$

Therefore for the proper [a,b] one has

$$\max_{[a,b]}\left|R(\gamma)\right|=\delta \quad , \tag{3.18}$$

which is the maximum absolute value of $R(\gamma)$ over $[0,\infty)$.

Determination of Best Approximation

Suppose $S^*(\lambda;\gamma)$ is the best approximation of $S(\lambda;\gamma)$ over [a,b] with a and b chosen to satisfy Eqs. (3.16) and (3.17) and, furthermore, suppose there are only 2N+1 γ_i, where $|R(\gamma_i)|=\delta$ for $a\leq\gamma_1<\ldots<\gamma_i<\ldots\ \gamma_{2N+1}\leq b$. Eq. (3.10) implies

$$\frac{d}{d\gamma}R(\gamma)\Big|_{\gamma_i}=0 \quad . \qquad (3.19)$$

If $R(\gamma_1)=-\delta$, then Eq. (3.12) implies

$$R(\gamma_i)=(-1)^i\delta \quad . \qquad (3.20)$$

Rearranging Eq. (3.20) one obtains

$$(a_1+\gamma_i'a_2+\ldots+\gamma_i'^{N-1}a_N)-d(\gamma_i'b_1+\ldots+\gamma_i'^{N}b_N)=d \quad , \qquad (3.21)$$

where $d=[S(\lambda;\gamma_i)+(-1)^i\delta]\gamma_i'^{-\frac{1}{2}}$. After simultaneously solving Eqs. (3.19) and (3.21) for γ_i', $i=1,\ldots,2N+1$; δ; and a_j and b_j, $j=1,\ldots,N$, one may then examine the resulting $R(\gamma)$ to determine if $\max\limits_{[a,b]}|R(\gamma)|=\delta$. Theoretically these equations offer a means of acquiring $S^*(\lambda;\gamma)$; however, as they are nonlinear in nature an iteration procedure, which is similar to a simpler process employed to approximate with polynominals,[18] is adopted to expedite their solution.

An IBM 360/50 computer, using programs detailed in Appendix D, first calculates, for a given λ, $S(\lambda;\gamma)$ at 400 points between $a=10^{-10}\gamma_M$ and $b\approx10^{10}\gamma_M$. For N=1, initial guesses of the zeros of $R(\gamma)$ are provided to the computer. The $R(\gamma)$ is then computed for the 400 stored data points and the extrema are found. Next the N largest maxima, N most negative minima, and the largest remaining extremum are found, which are solutions of Eq. (3.19), and their absolute values are averaged to form δ'. Discarding the γ corresponding to the last data point used to determine δ', the computer utilizes δ', as an estimate of δ, and the other 2N values of to solve Eq. (3.21) for the a_j and b_j. This is now routine since Eq. (3.21) has become a set of 2N linear simultaneous equations. The iterative solution of Eqs. (3.19) and (3.21) is continued until convergence occurs or a counter indicates the program has failed. After determining the $S^*(\lambda;\gamma)$ of order N, the computer is directed to automatically use the $R(\gamma)$ to estimate the $S^*(\lambda;\gamma)$ of order N+1.

In Figs. 2-6 is displayed a series of $R(\gamma)$ for $\lambda=3/2$ and N=6 which converges to the $R(\gamma)$ indicated by the dashed curve. Iteration number six produces a $R(\gamma)$ which is virtually identical to the final fit.

Table II contains the a_j and b_j for the final approximations of the $S(\lambda;\gamma)$ for $\lambda=-1/2$, $\lambda=1/2$, and $\lambda=3/2$. The estimates of the maximum relative error $|(S^*-S)/S_M|_{max}$ are found by fitting $R(\gamma)$ at the three points nearest each extreme value by a parabola. Calculation reveals the approximations are accurate to within the stated error over the extended range $[0,\infty)$. In Figs. 7-23 $R(\gamma)/S_M$ is plotted for each approximation calculated in this work.

The approximation of the $S(\lambda;\gamma)$ is terminated for each λ whenever an $S^*(\lambda;\gamma)$ is found such that $|(S^*-S)/S_M|_{max}$ is less than 10^{-5}. This level of accuracy should by appropriate for their proposed application.

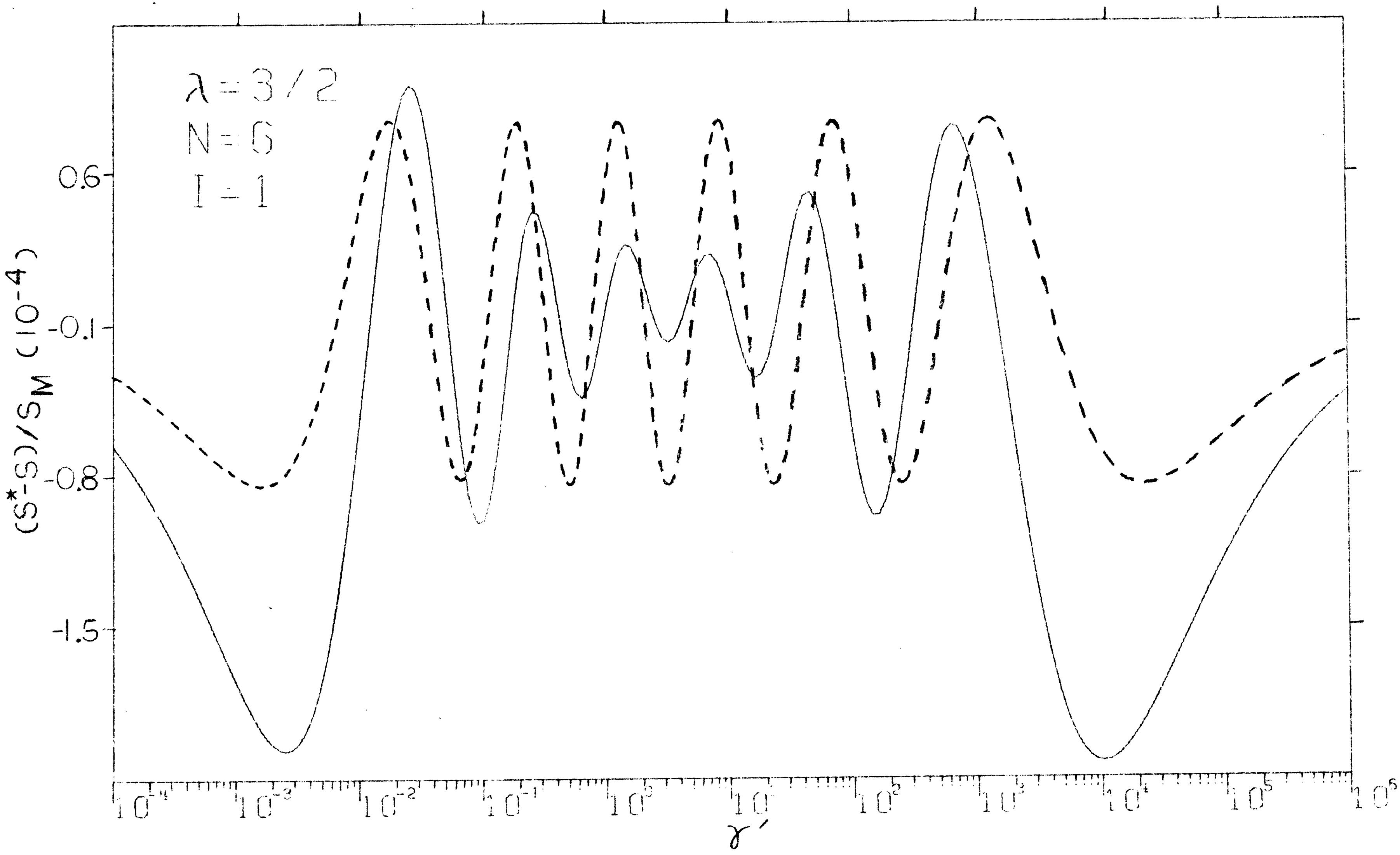

Fig. 2--Error curve of first attempt to determine S*(3/2;γ) of order six

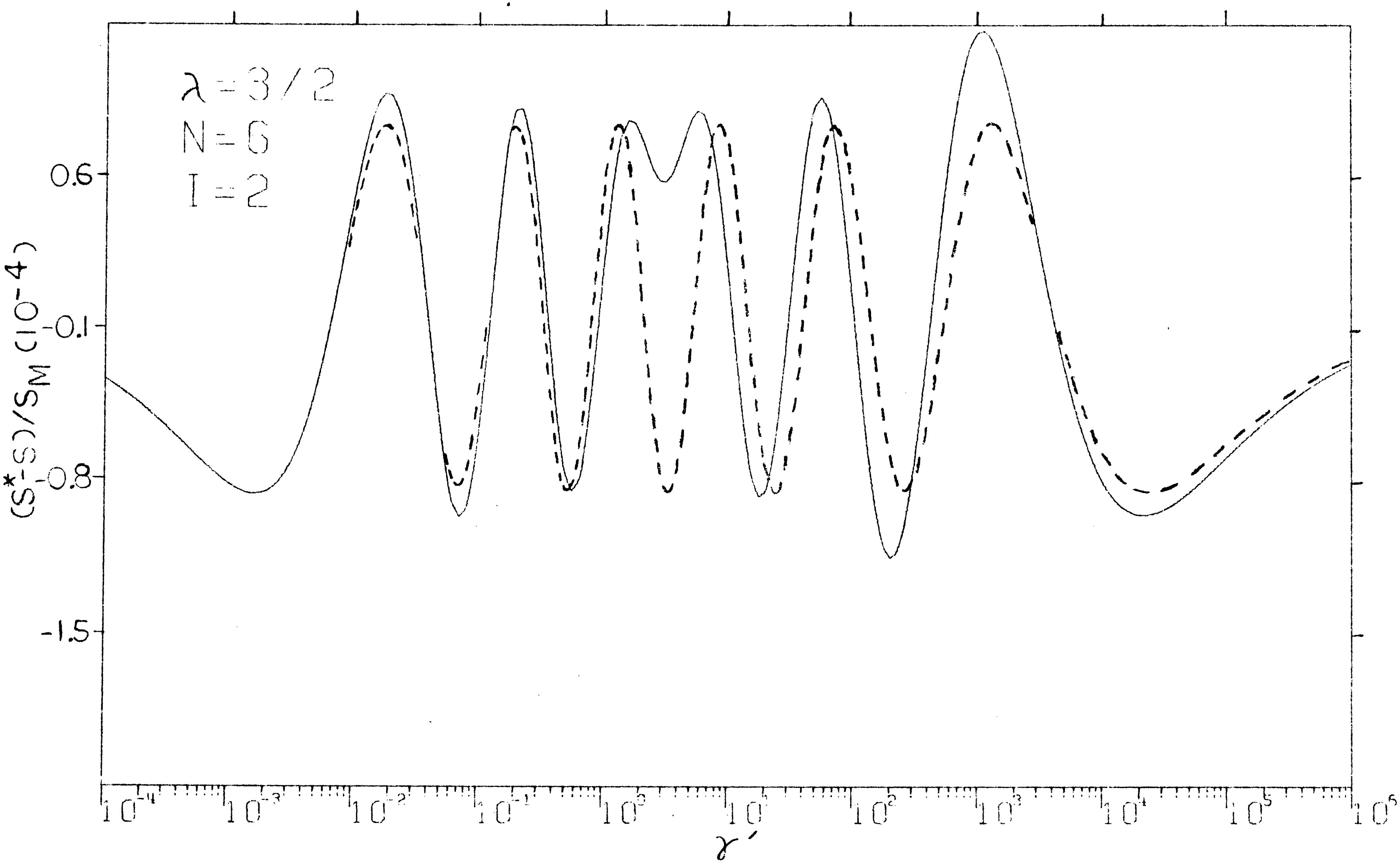

Fig. 3--Error curve of second attempt to determine $S^*(3/2;\gamma)$ of order six

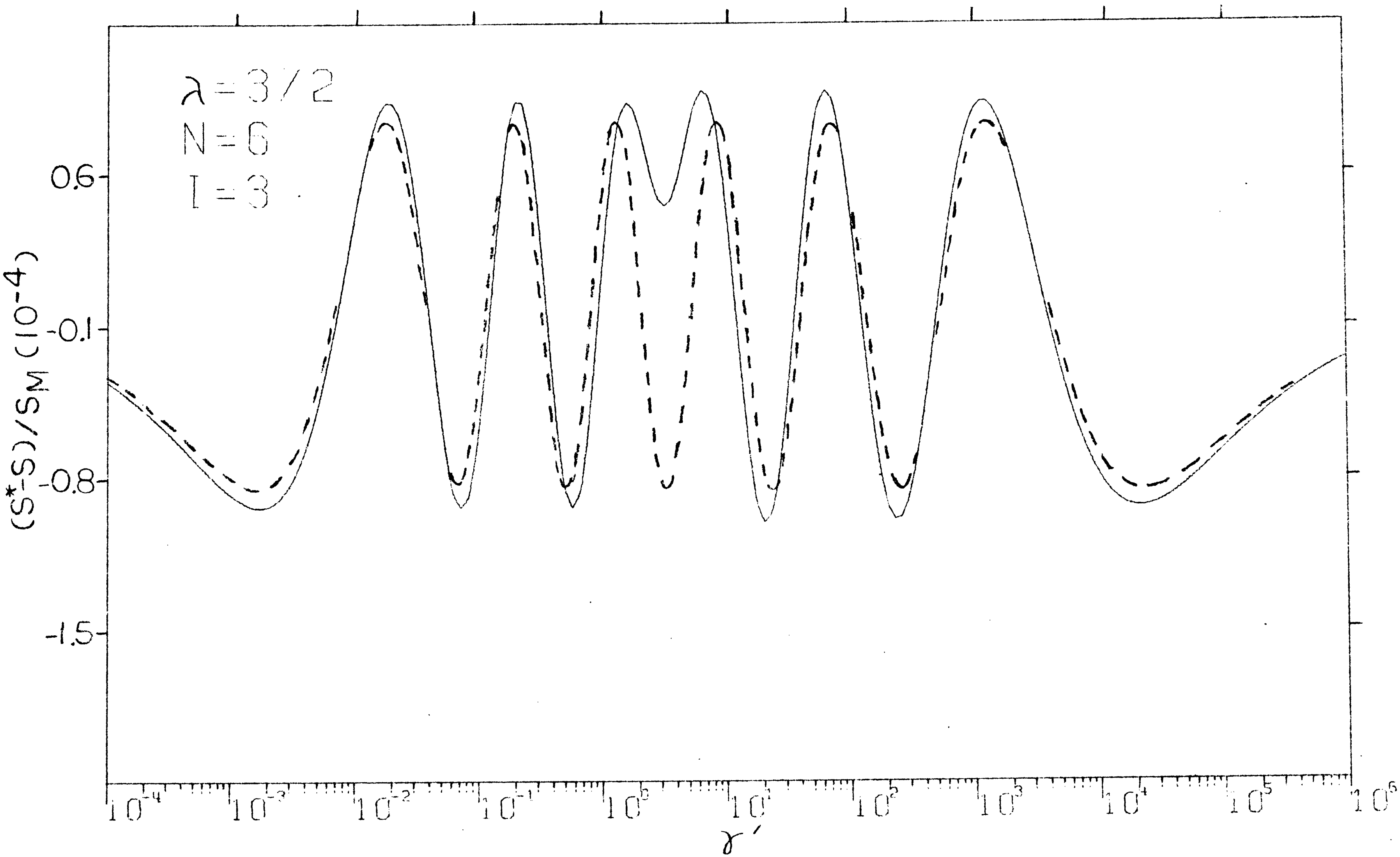

Fig. 4--Error curve of third attempt to determine $S^*(3/2;\gamma)$ of order six

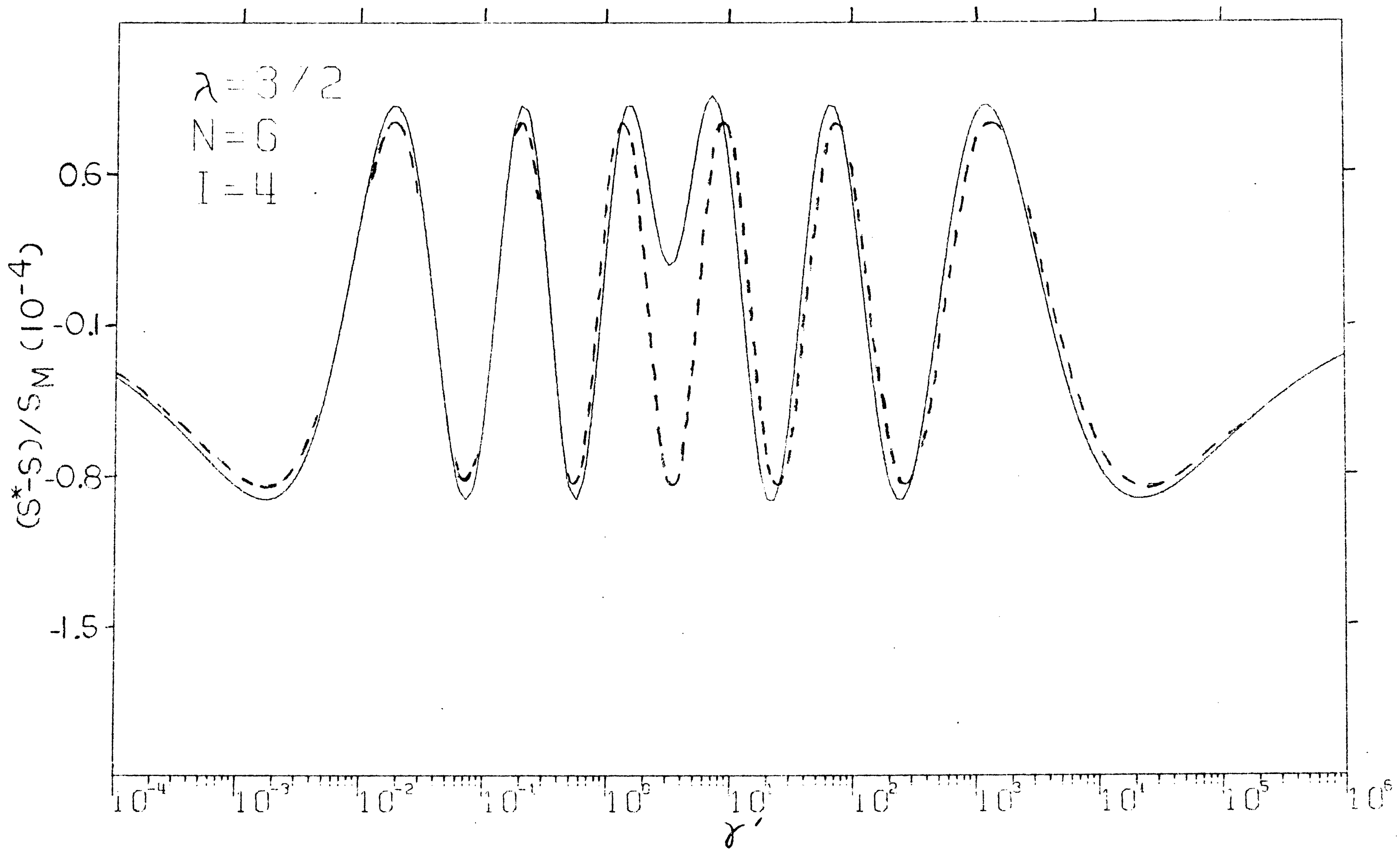

Fig. 5--Error curve of fourth attempt to determine S*(3/2;γ) of order six

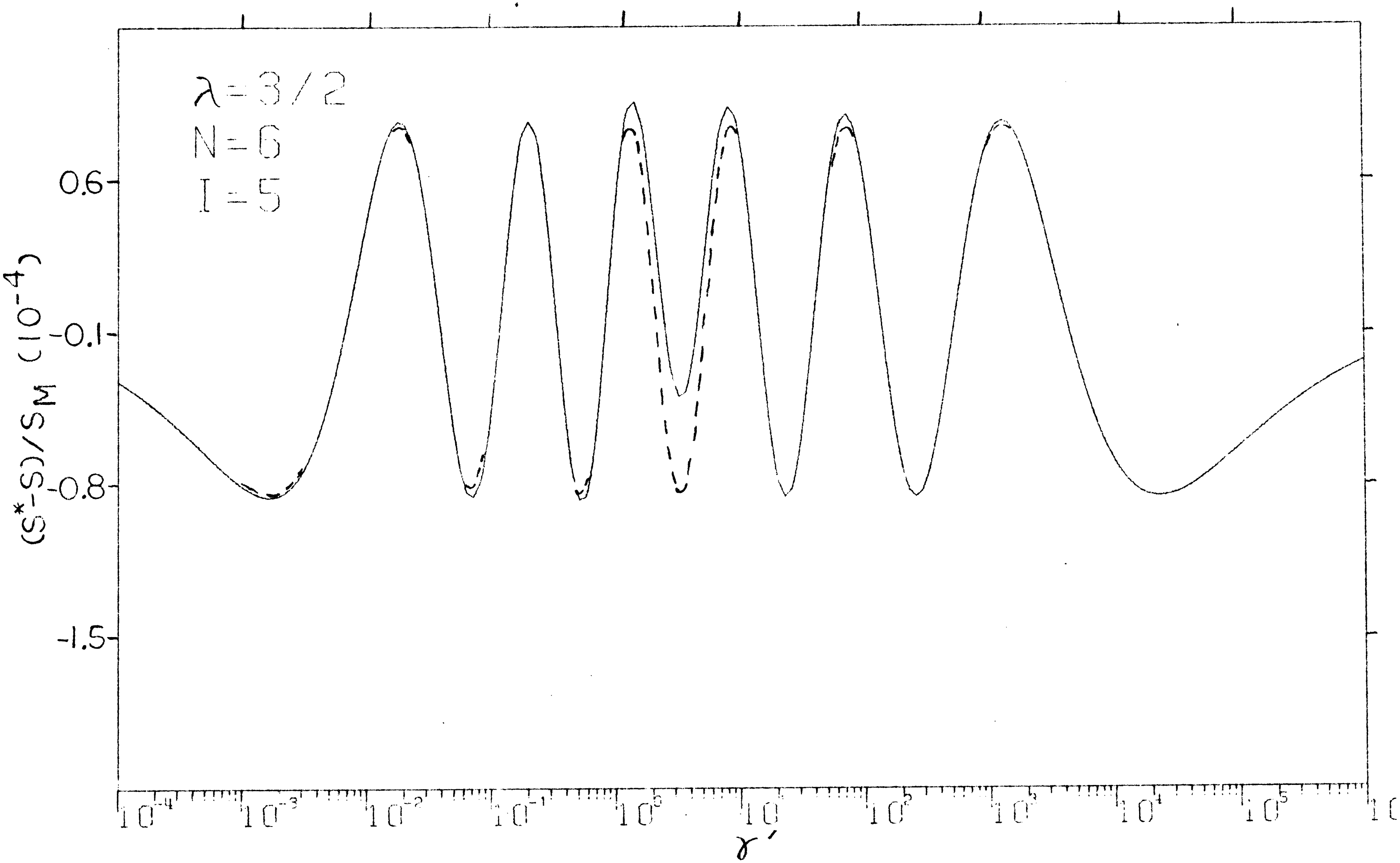

Fig. 6--Error curve of fifth attempt to determine S*(3/2;γ) of order six

TABLE II

COEFFICIENTS OF $S^*(\lambda;\gamma)$

λ	N	$\|(S^*-S)/S_M\|_{max}$	j	a_j	b_j
-1/2	1	0.35×10^{-1}	1	0.986	1.041
	2	$.25 \times 10^{-2}$	1	1.1023	3.6077
			2	1.9005	1.8310
	3	$.27 \times 10^{-3}$	1	1.11879	9.9553
			2	8.4437	16.180
			3	5.6184	5.3623
	4	$.36 \times 10^{-4}$	1	1.121779	25.0571
			2	25.0675	102.1953
			3	67.1806	102.9698
			4	26.4134	25.1771
	5	0.62×10^{-5}	1	1.1224298	59.138480
			2	63.136891	553.54454
			3	479.81762	1317.3871
			4	692.60155	942.89358
			5	190.90399	181.93010

TABLE II--Continued

λ	N	$\lvert (S^*-S)/S_M \rvert_{max}$	j	a_j	b_j
1/2	1	0.23×10^{-1}	1	0.969	0.981
	2	$.11 \times 10^{-2}$	1	1.03066	1.98249
			2	.71880	.67848
	3	$.75 \times 10^{-4}$	1	1.035153	3.002484
			2	1.714556	2.151902
			3	.3518075	.3301353
	4	0.72×10^{-5}	1	1.0355748	4.038167
			2	2.7765076	4.504886
			3	1.4099598	1.5157628
			4	0.12192377	0.11433758
3/2	1	0.12	1	0.856	0.906
	2	$.19 \times 10^{-1}$	1	1.1224	2.8975
			2	.61901	.46468
	3	$.40 \times 10^{-2}$	1	1.1953	5.941
			2	2.871	3.485
			3	.2167	.14694
	4	0.10×10^{-2}	1	1.21676	10.0171
			2	6.9376	13.1971
			3	2.52419	2.23049
			4	0.046038	0.0300750

TABLE II--Continued

λ	N	$\lvert (S^*-S)/S_M \rvert_{max}$	j	a_j	b_j
3/2	5	0.29×10^{-3}	1	1.22359	15.1275
			2	12.6748	35.9592
			3	12.3264	14.6316
			4	1.116166	.845768
			5	.00640489	.00412049
	6	$.86 \times 10^{-4}$	1	1.225900	21.26549
			2	19.91651	80.4167
			3	39.1796	62.3096
			4	9.97617	9.14989
			5	.2876591	.2013202
			6	.000604188	.000386073
	7	$.29 \times 10^{-4}$	1	1.226727	28.41735
			2	28.53870	157.4943
			3	96.47139	202.8298
			4	52.55543	59.32884
			5	4.386376	3.471373
			6	.04690555	.03146105
			7	.00003989812	.00002541464
	8	0.98×10^{-5}	1	1.2270401	36.638433
			2	38.545536	281.41338
			3	201.75930	551.68048
			4	199.74091	278.60135
			5	36.846712	33.692628
			6	1.1595624	.84126769
			7	.0050706179	.0033220921
			8	0.0000018651654	0.0000011862639

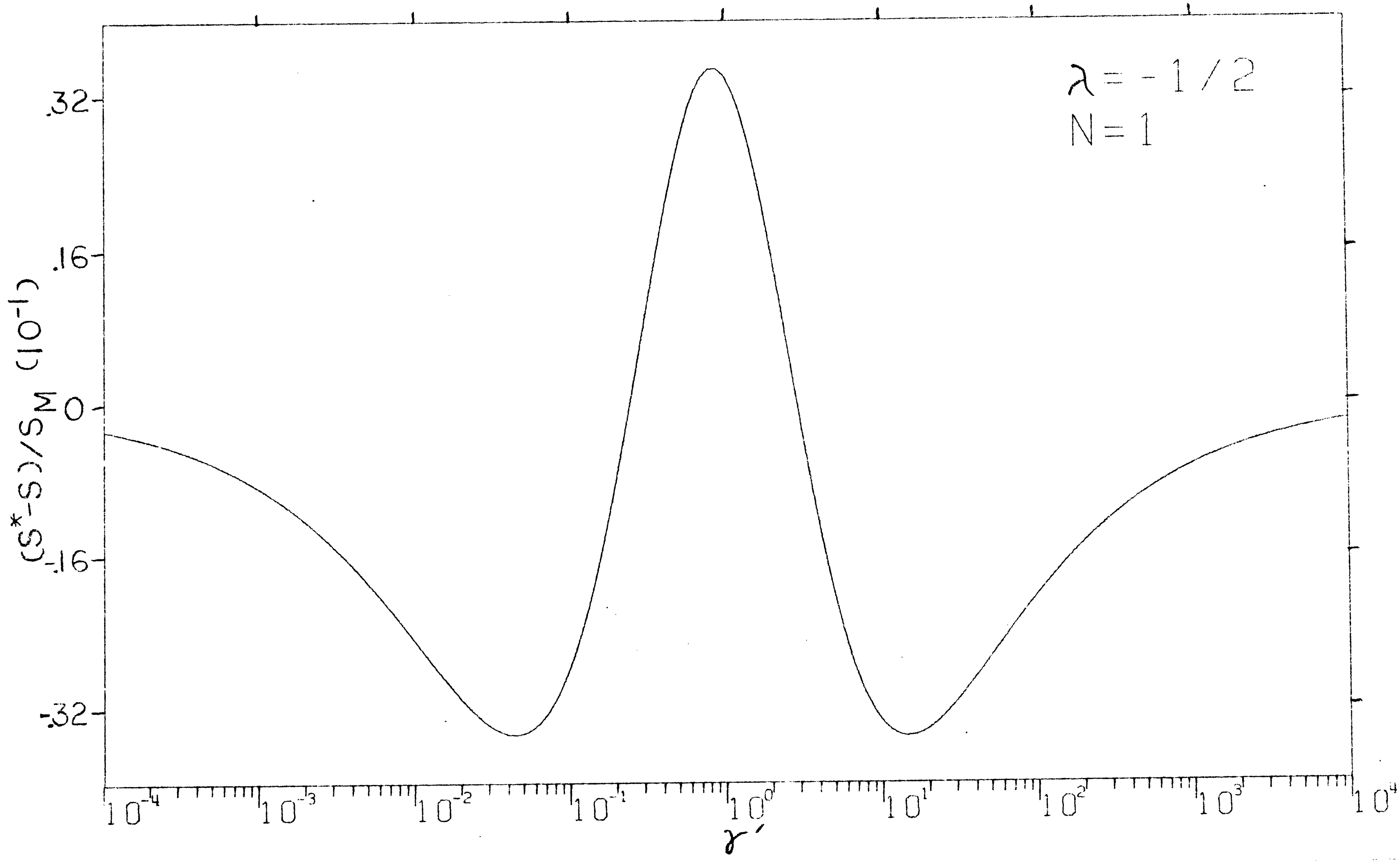

Fig. 7--Error curve for the first order approximation of $S(-1/2;\gamma)$

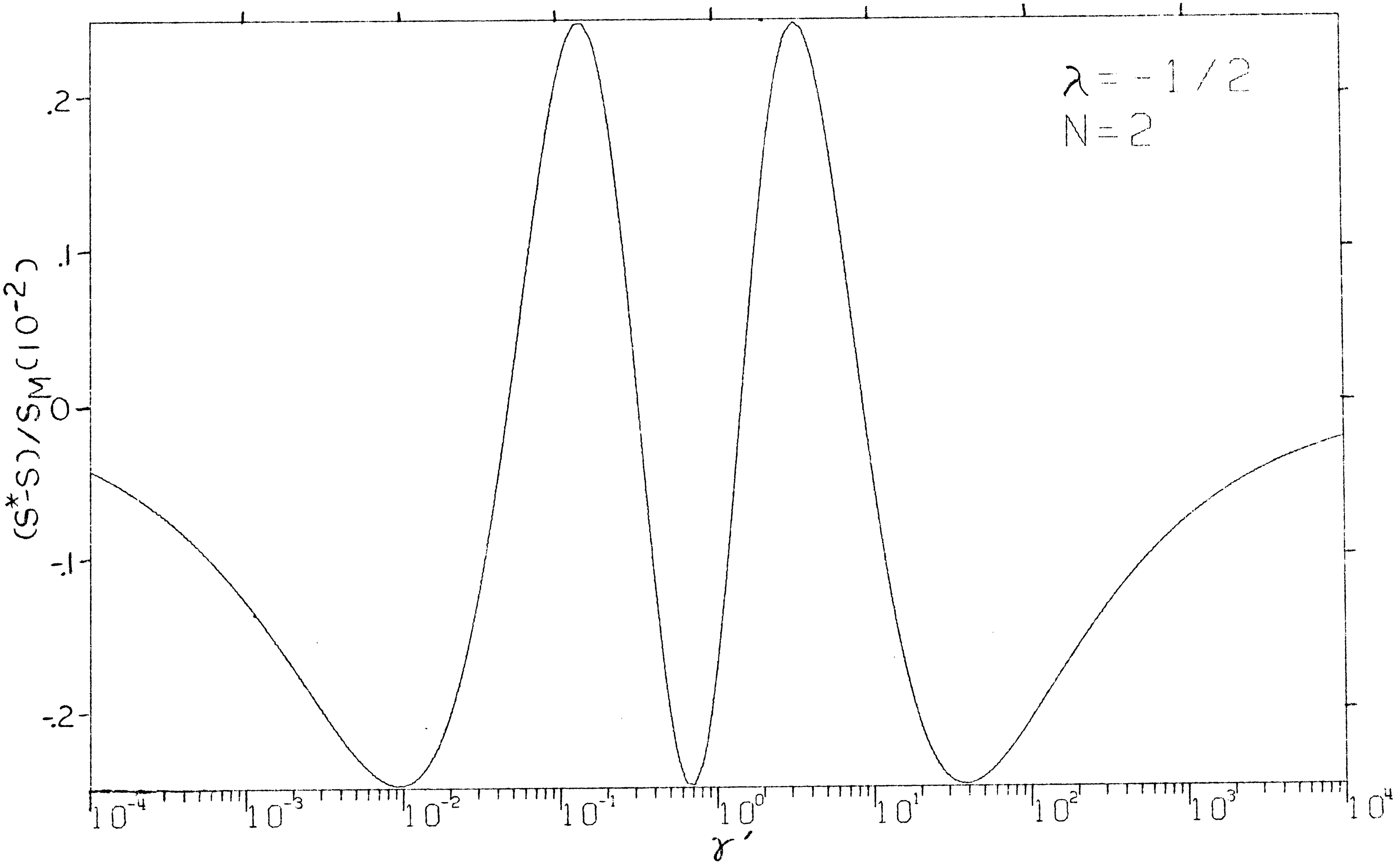

Fig. 8--Error curve for the second order approximation of S(-1/2;γ)

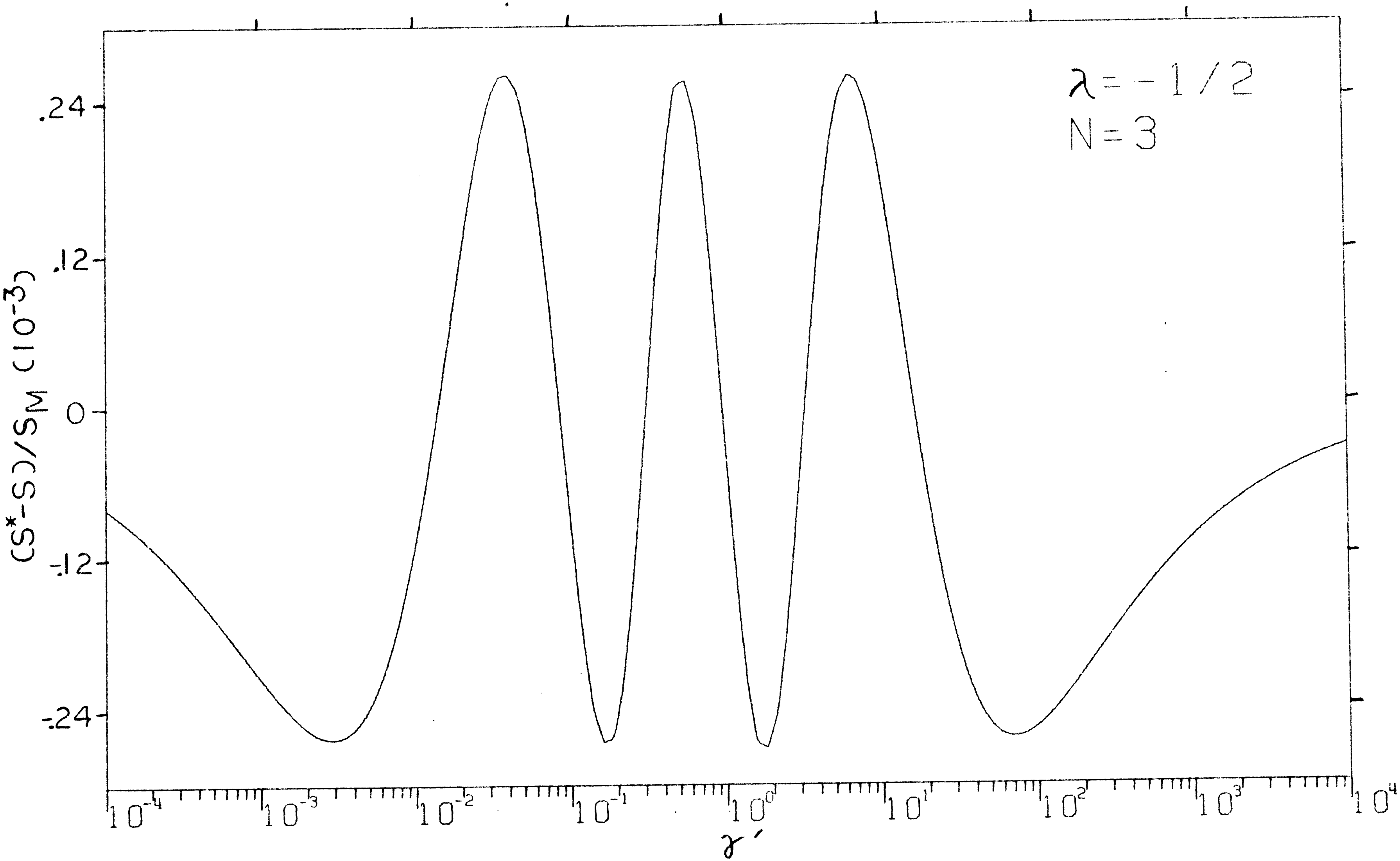

Fig. 9--Error curve for the third order approximation of S(-1/2;γ)

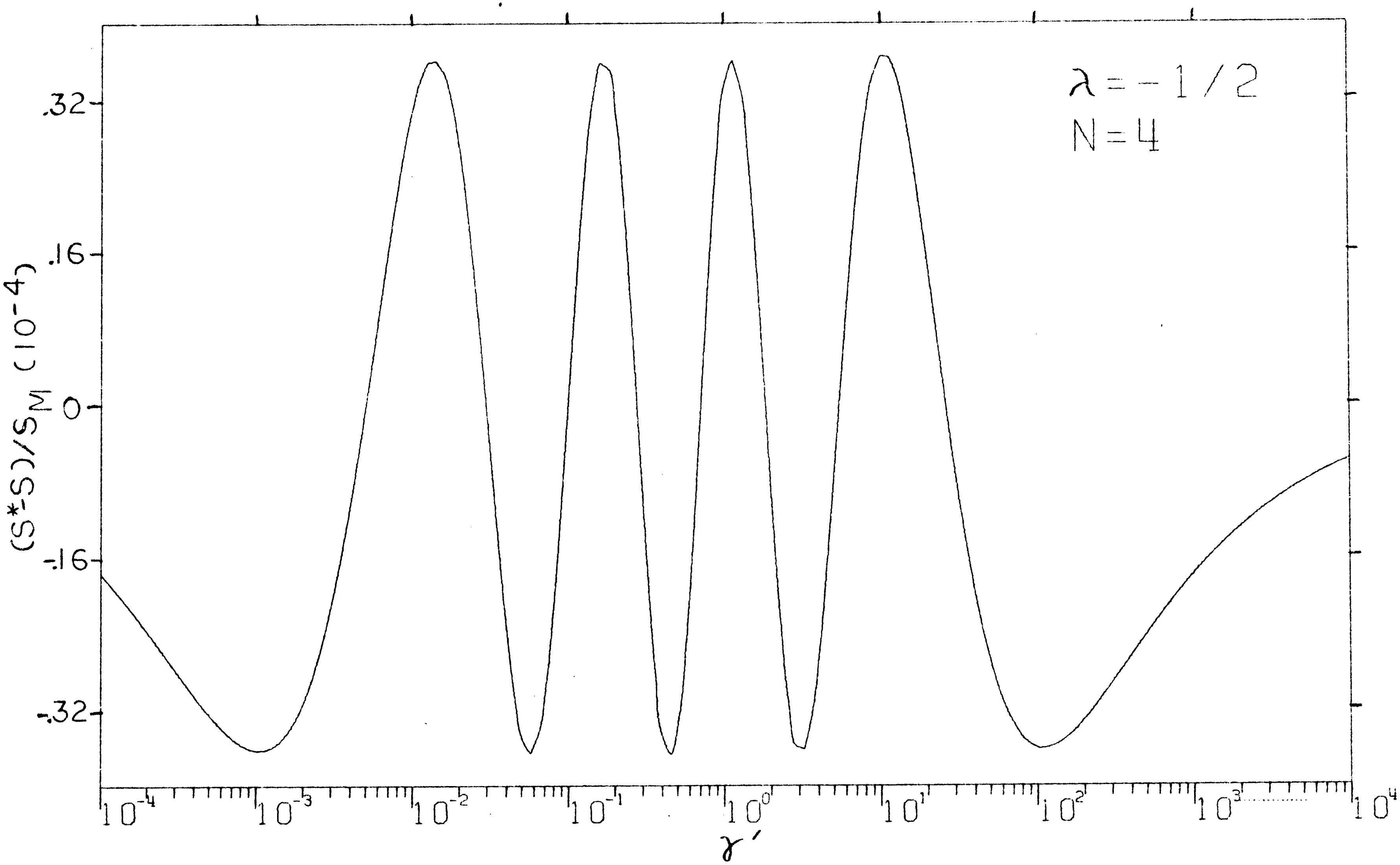

Fig. 10--Error curve for the fourth order approximation of $S(-1/2;\gamma)$

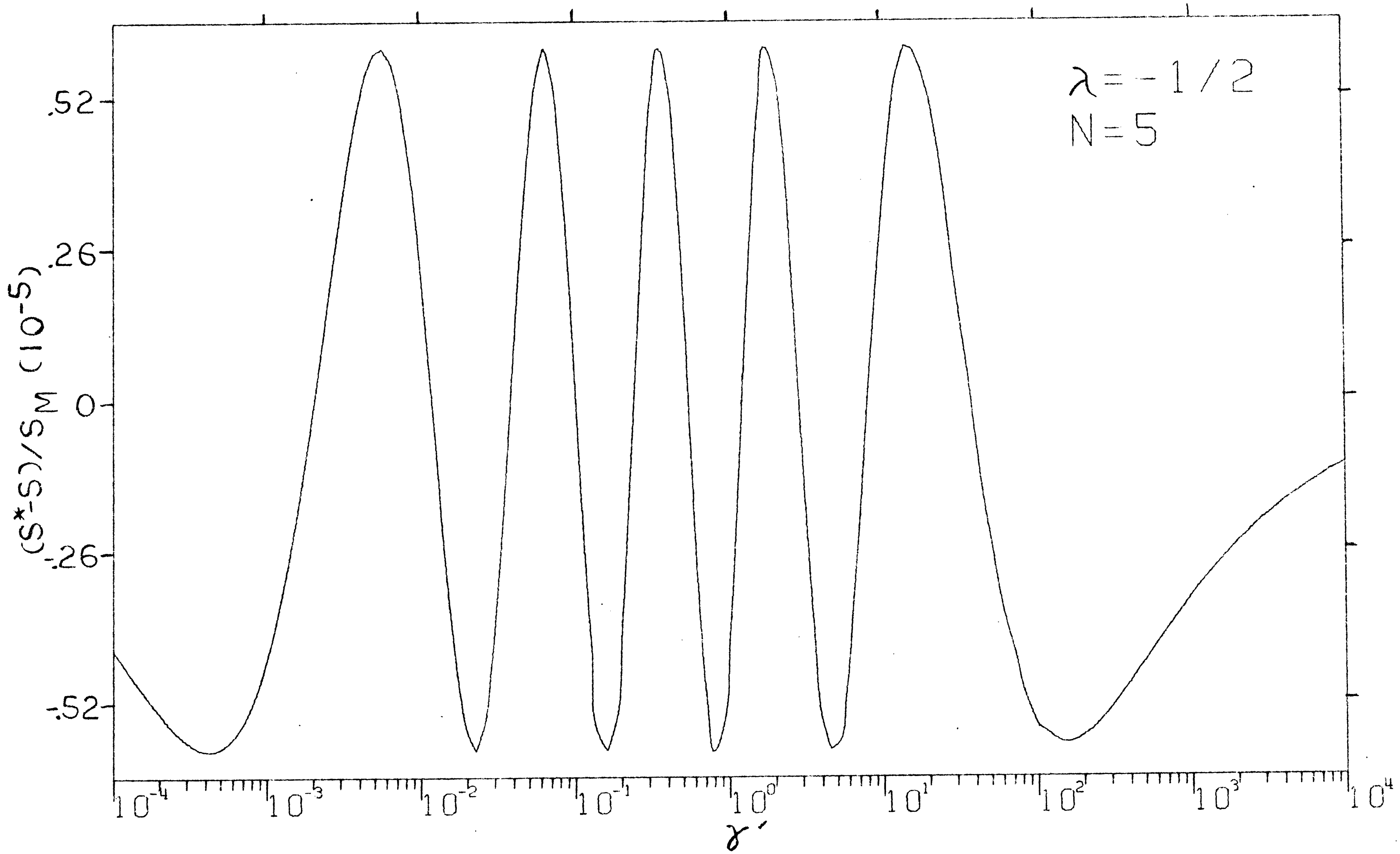

Fig. 11-Error curve for the fifth order approximation of S(-1/2;γ)

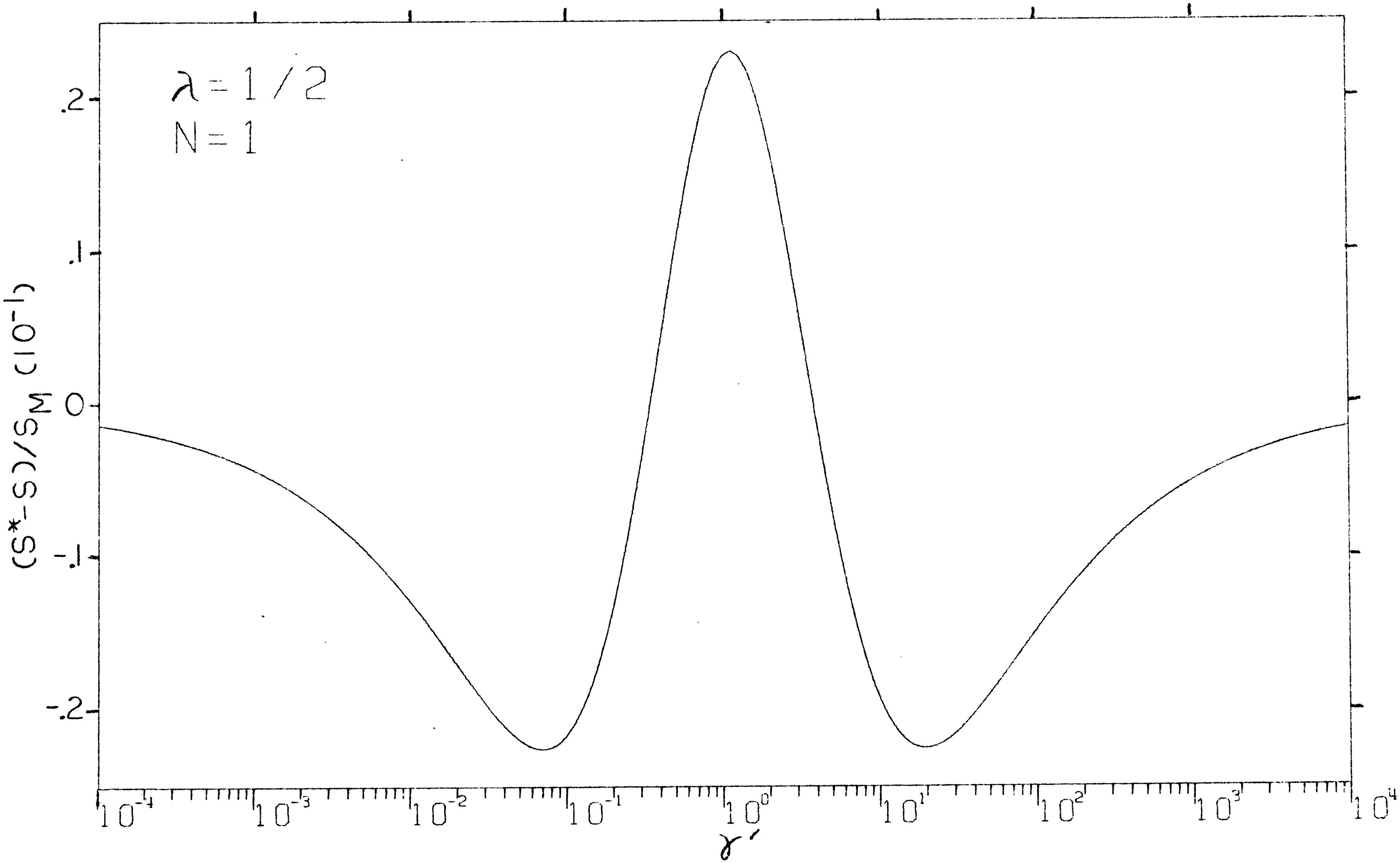

Fig. 12--Error curve for the first order approximation of $S(1/2;\gamma)$

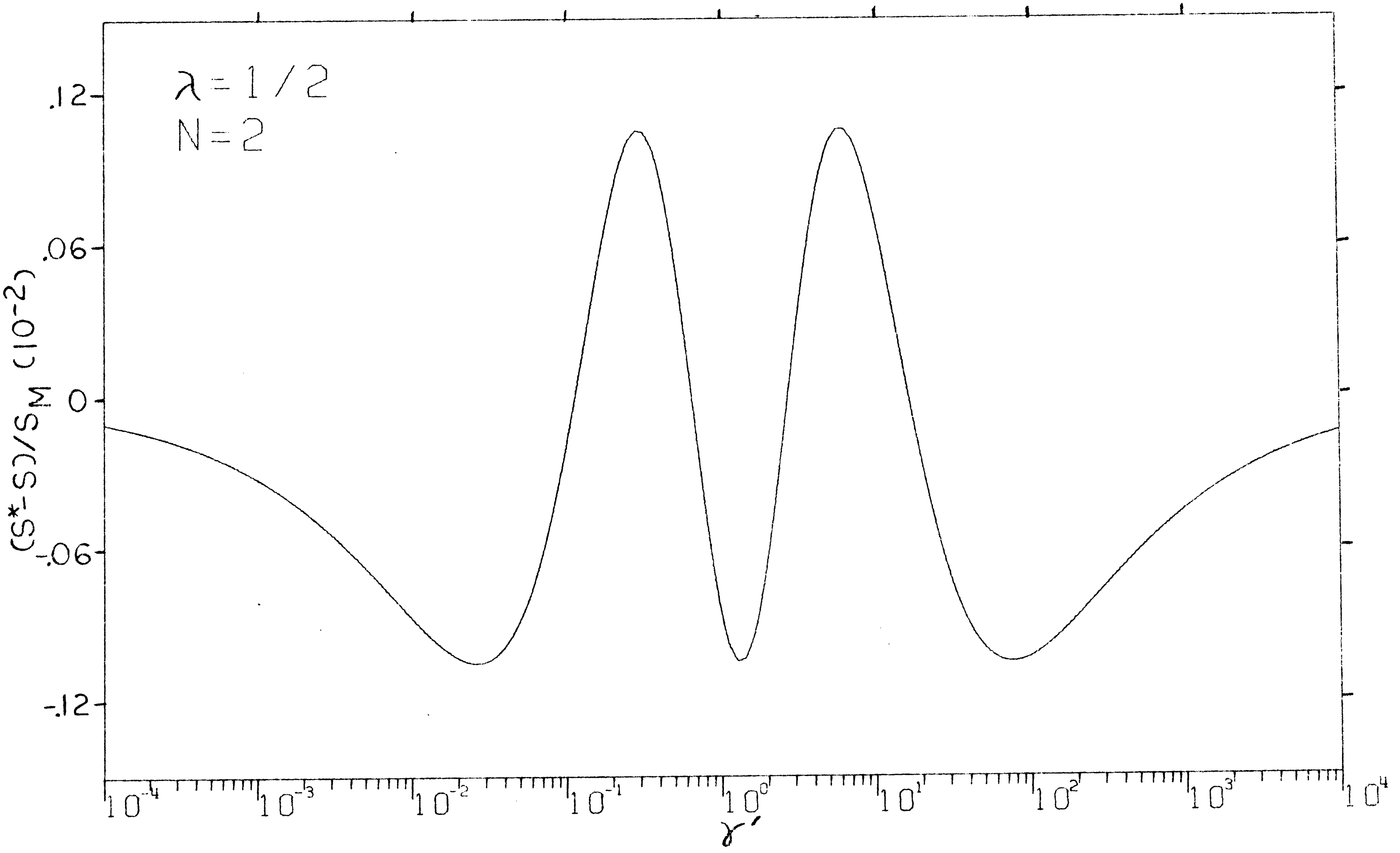

Fig. 13--Error curve for the second order approximation of $S(1/2;\gamma)$

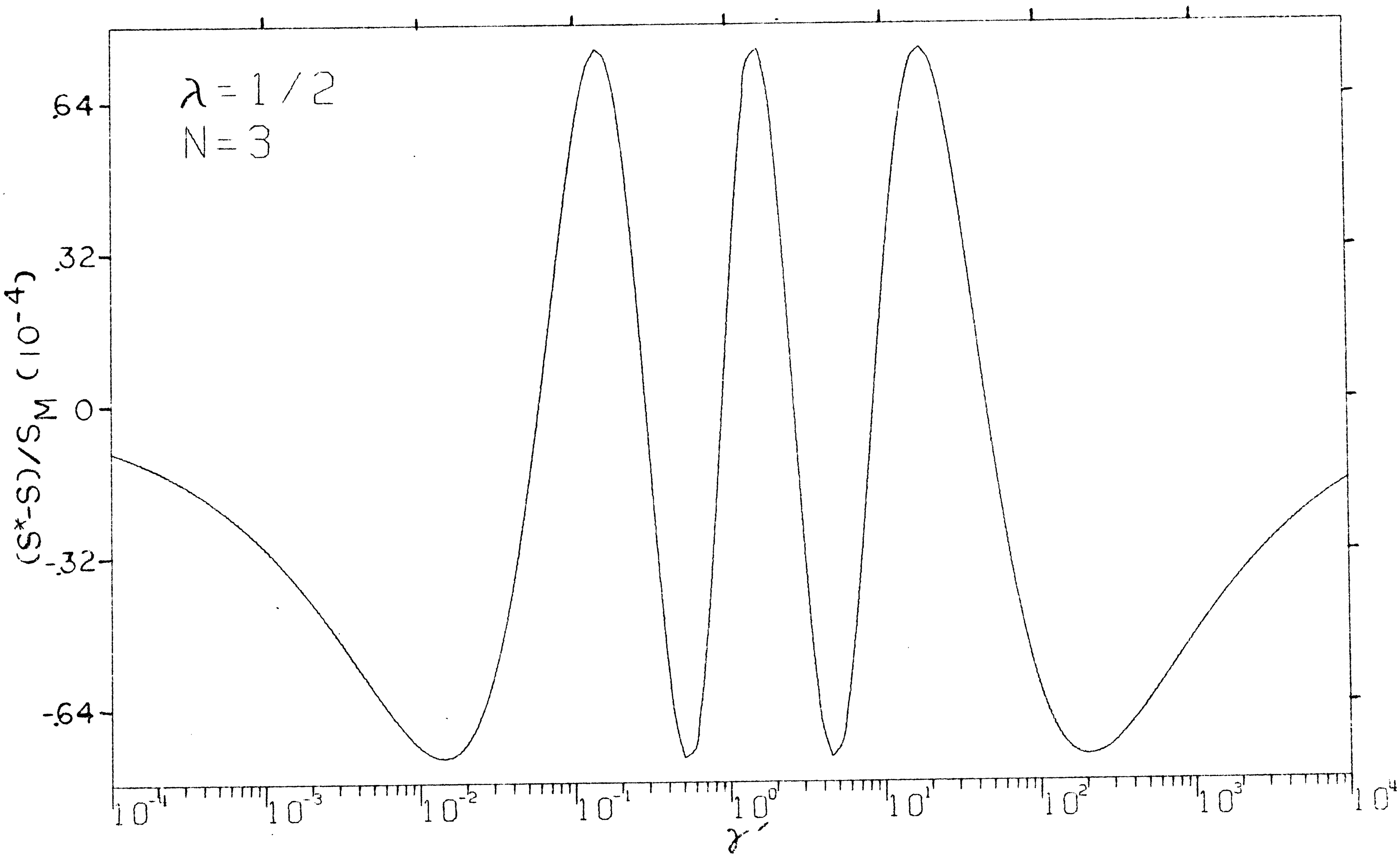

Fig. 14--Error curve for the third order approximation of S(1/2;γ)

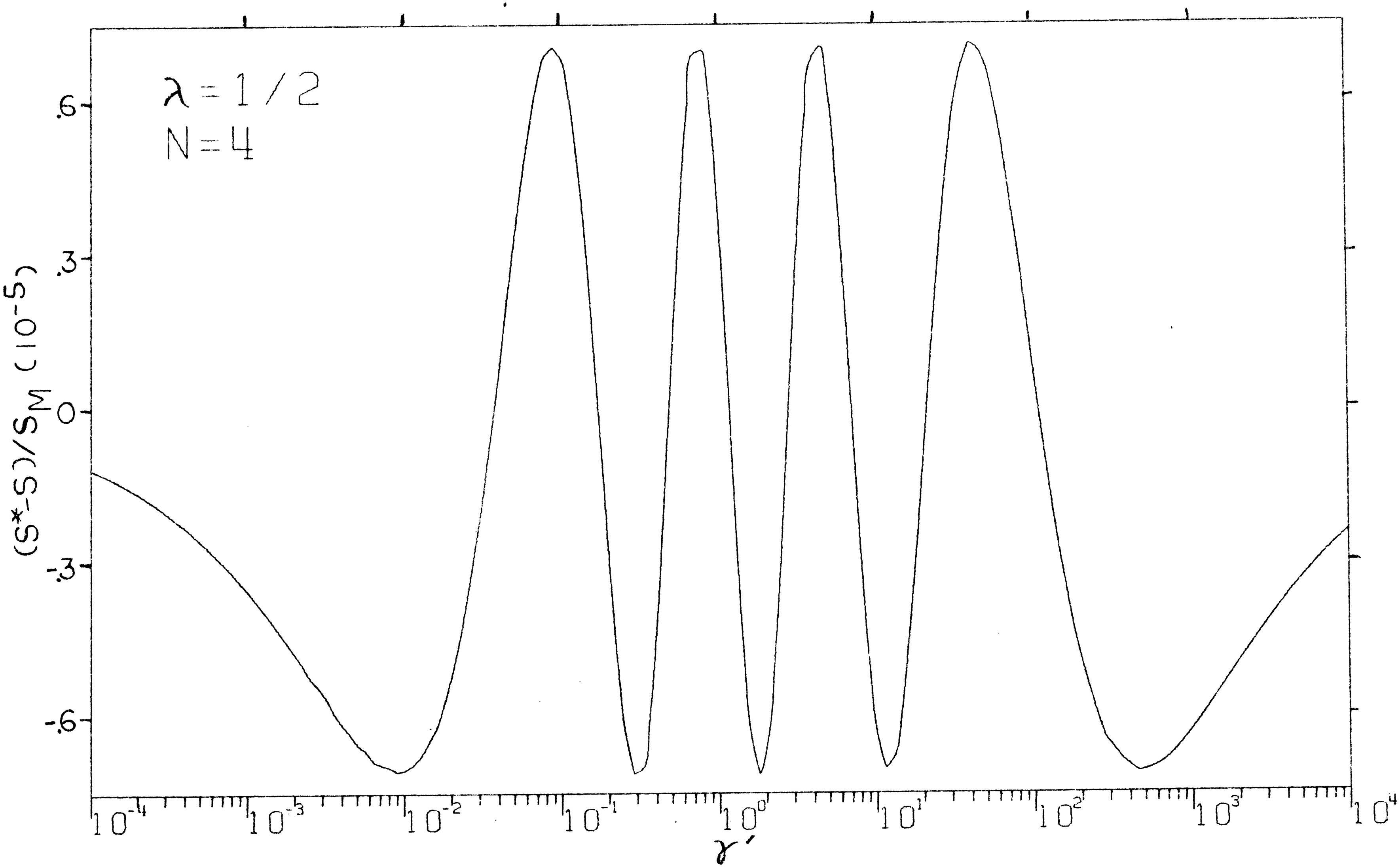

Fig. 15--Error curve for the fourth order approximation of $S(1/2;\gamma)$

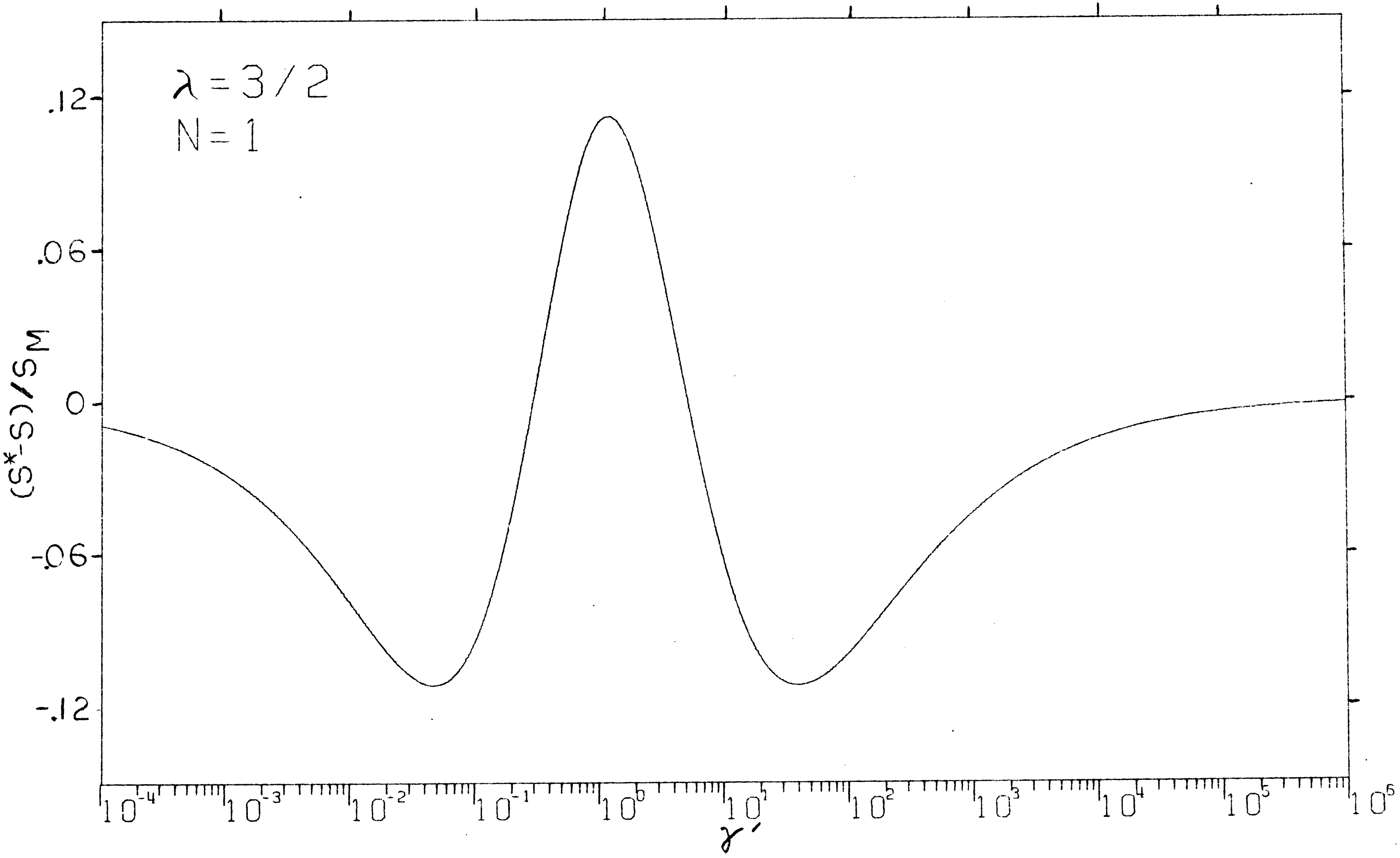

Fig. 16--Error curve for the first order approximation of $S(3/2;\gamma)$

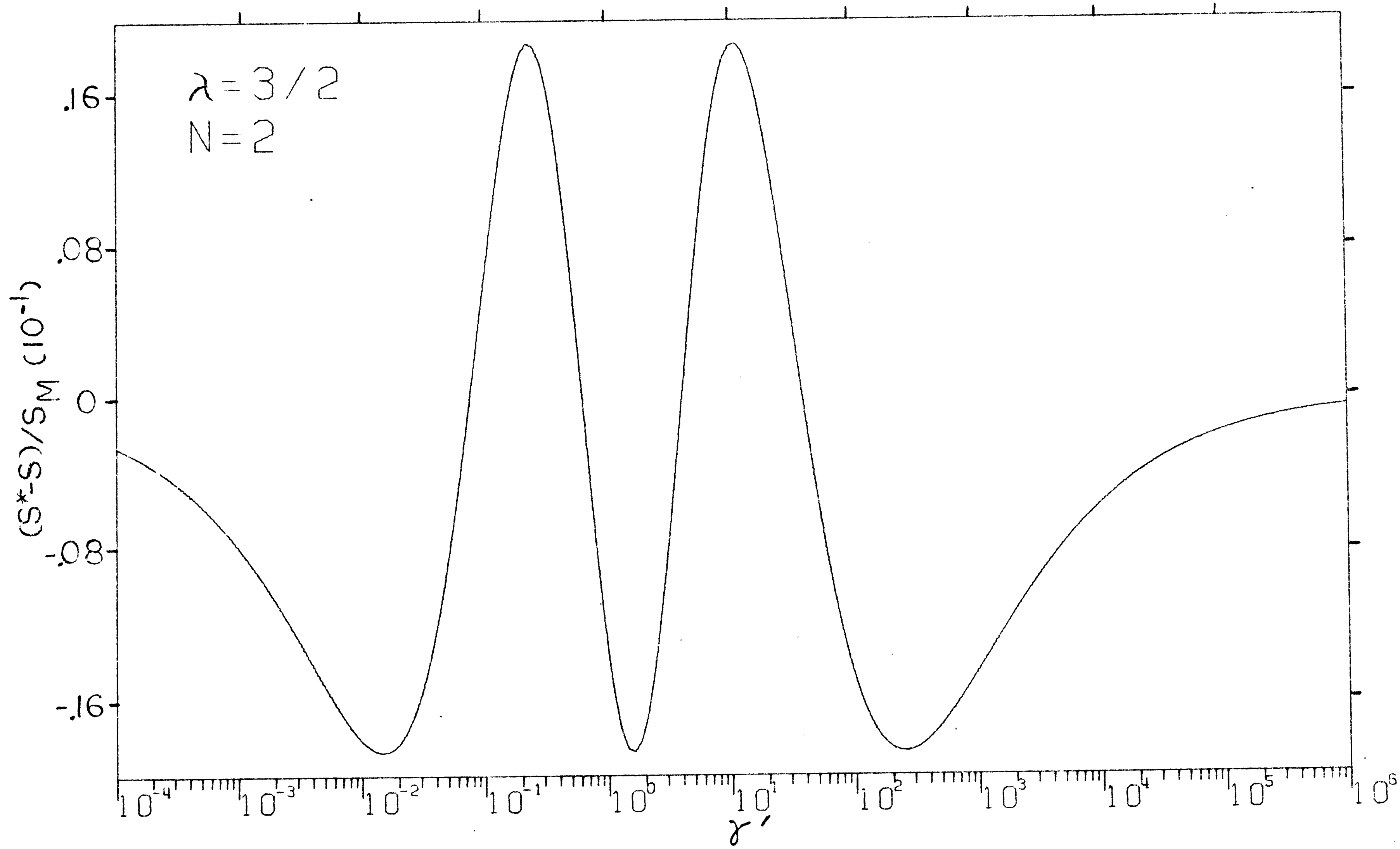

Fig. 17--Error curve for the second order approximation of $S(3/2;\gamma)$

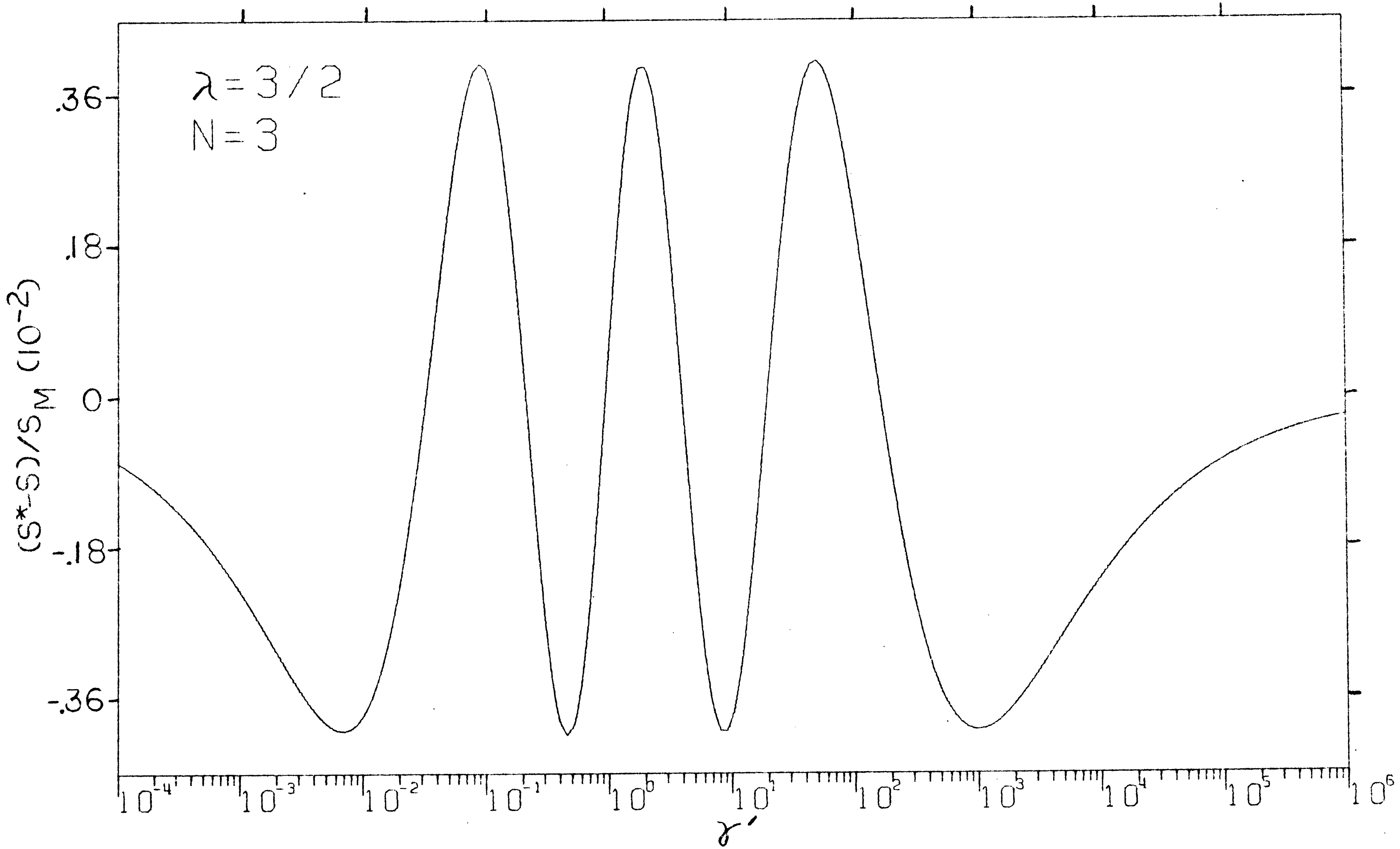

Fig. 18--Error curve for the third order approximation of S(3/2;γ)

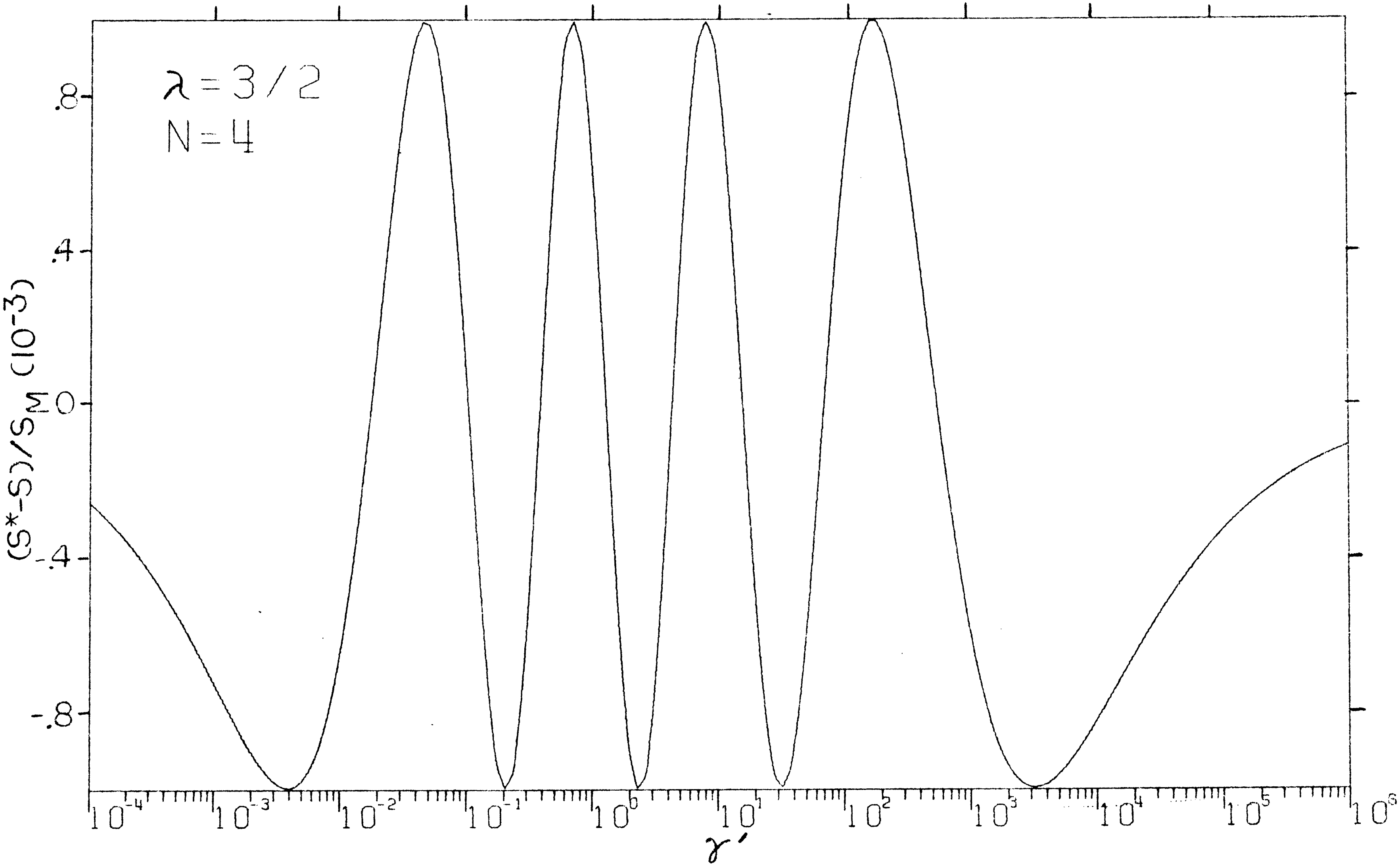

Fig. 19--Error curve for the fourth order approximation of $S(3/2;\gamma)$

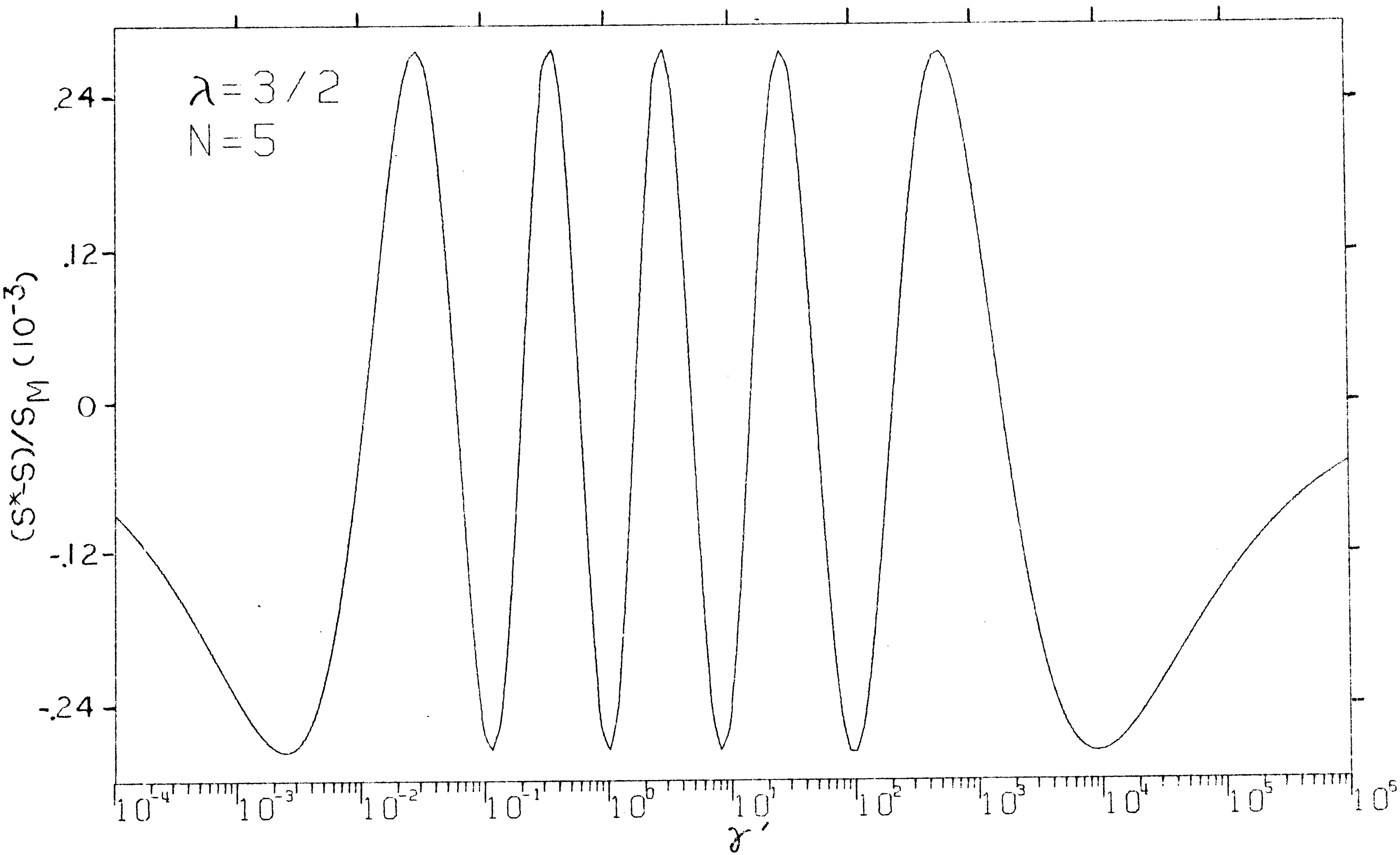

Fig. 20--Error curve for the fifth order approximation of S(3/2;γ)

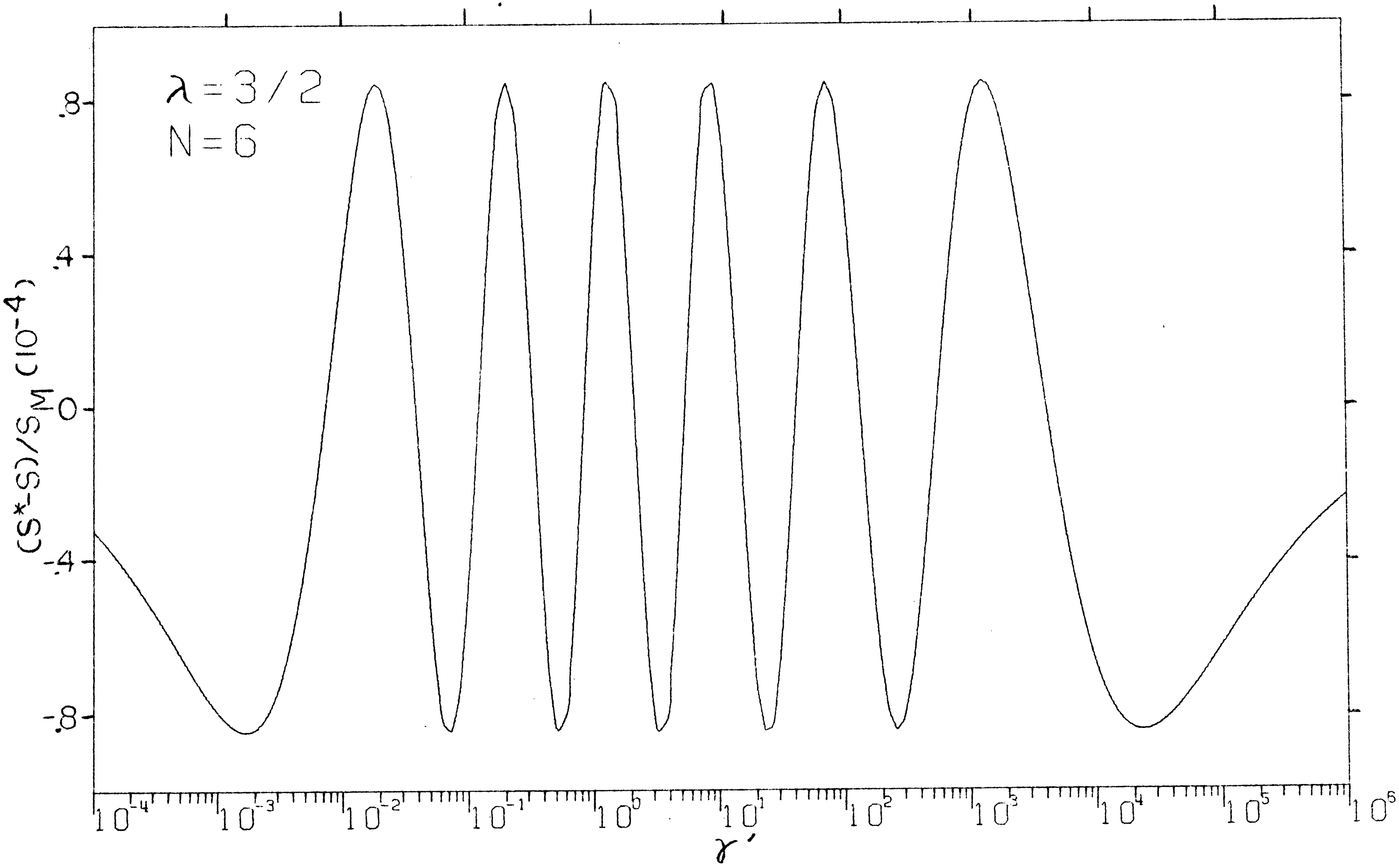

Fig. 21--Error curve for the sixth order approximation of $S(3/2;\gamma)$

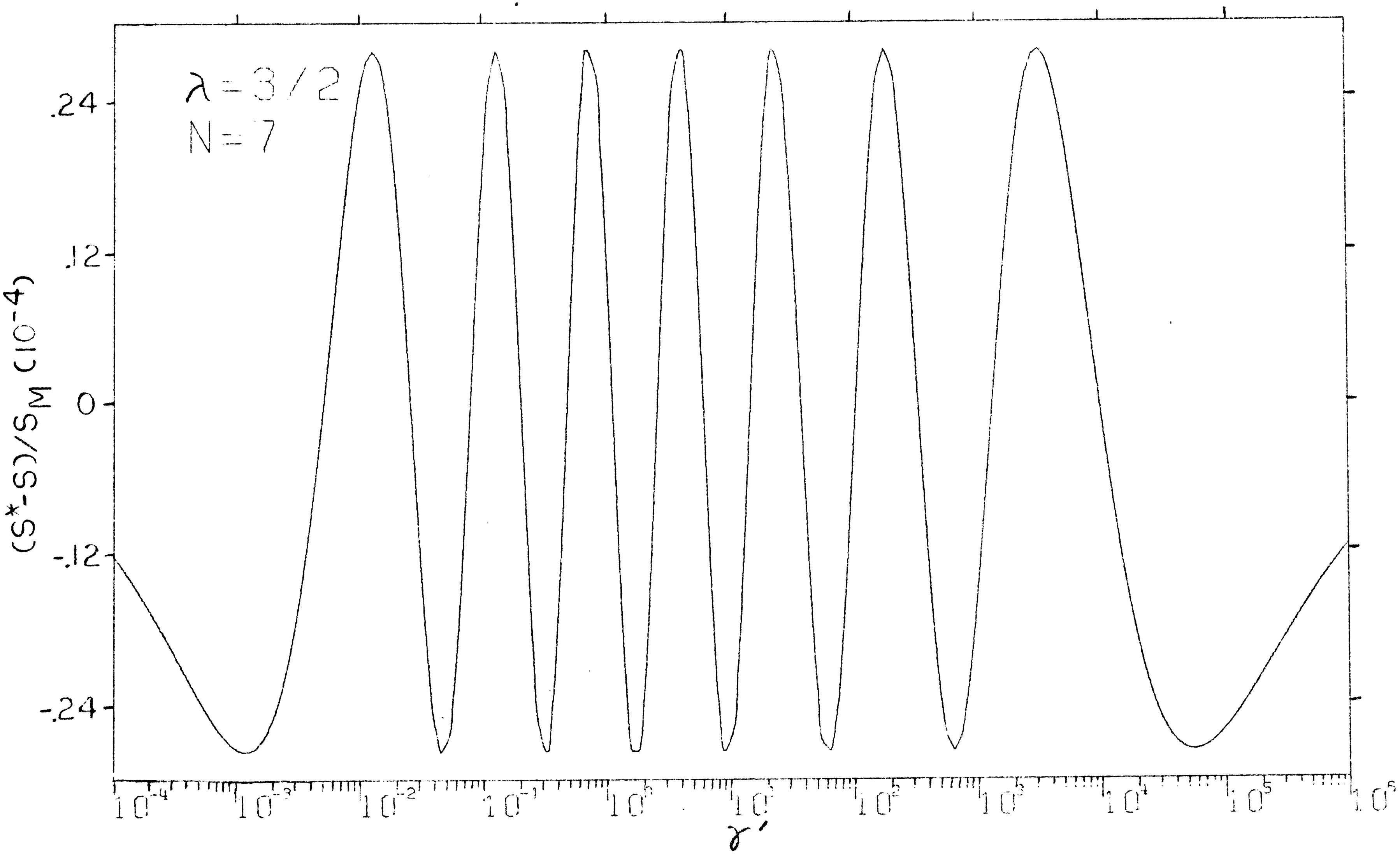

Fig. 22--Error curve for the seventh order approximation of $S(3/2;\gamma)$

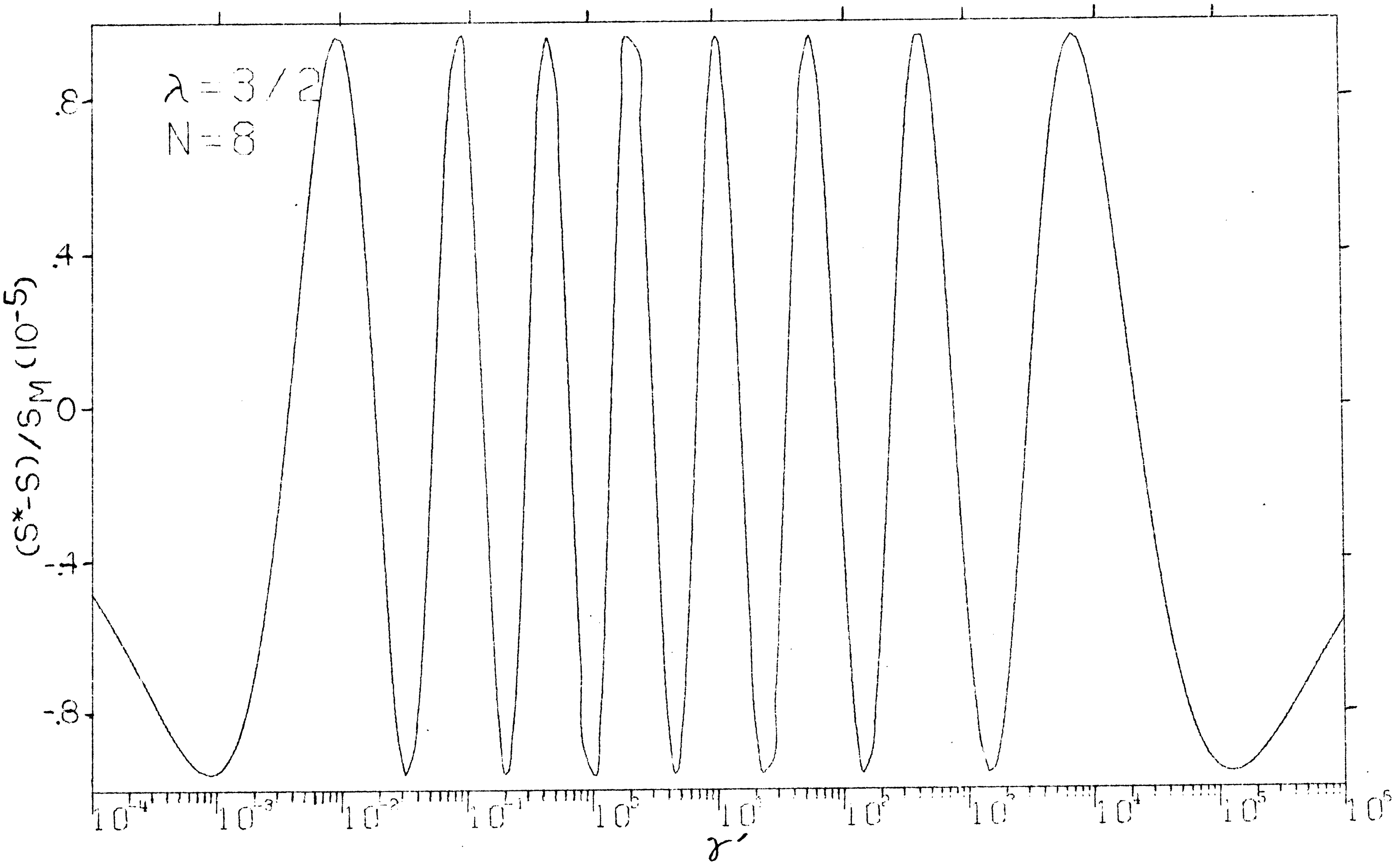

Fig. 23--Error curve for the eighth order approximation of S(3/2;γ)

CHAPTER IV

EXAMPLE APPLICATION OF $S^*(\lambda;\gamma)$

As an example for the use of the approximations of $S(\lambda;\gamma)$, consider an ideal case of conduction by two hole bands having pure acoustical phonon scattering and $\epsilon_F \ll 0$. Using parameters similar to those observed by the author in a sample of p-type InSb at T=77 K, let the heavy hole band have $n=10^{15}$ carriers per cm^3 and $\mu_0=0.953 \times 10^4$ cm^2/V-sec corresponding to H_M=10 kG; and the light holes, $n=10^{13}$ carriers per cm^3 and $\mu_0=0.953 \times 10^5$ cm^2/V-sec corresponding to H_M=1 kG.

Choosing the upper sign for holes in Eq. (2.48), the Hall conductivity becomes

$$\sigma_{xy}(H)=\sum_{j=1}^{2} n_j e\mu_{0j} S(-\tfrac{1}{2};\gamma_j) \quad , \qquad (4.1)$$

where $\gamma_j=(9\pi/16)(H\mu_{0j}/c)^2$. By inserting e in units of coulombs and μ_0 and n as indicated above, the units of $\sigma_{xy}(H)$ are $(\text{ohm-cm})^{-1}$.

Consider least-squares fitting of the imaginary data, indicated in Fig. 24 by squares, with $\sigma_{xy}(H)$ predicted for two hole bands having other power-law scattering mechanisms. Approximation of $S(\lambda;\gamma)$ by

$$S^*(\lambda;\gamma)=\gamma'^{\frac{1}{2}}A_1(\lambda;\gamma)/A_2(\lambda;\gamma) \qquad (4.2)$$

with

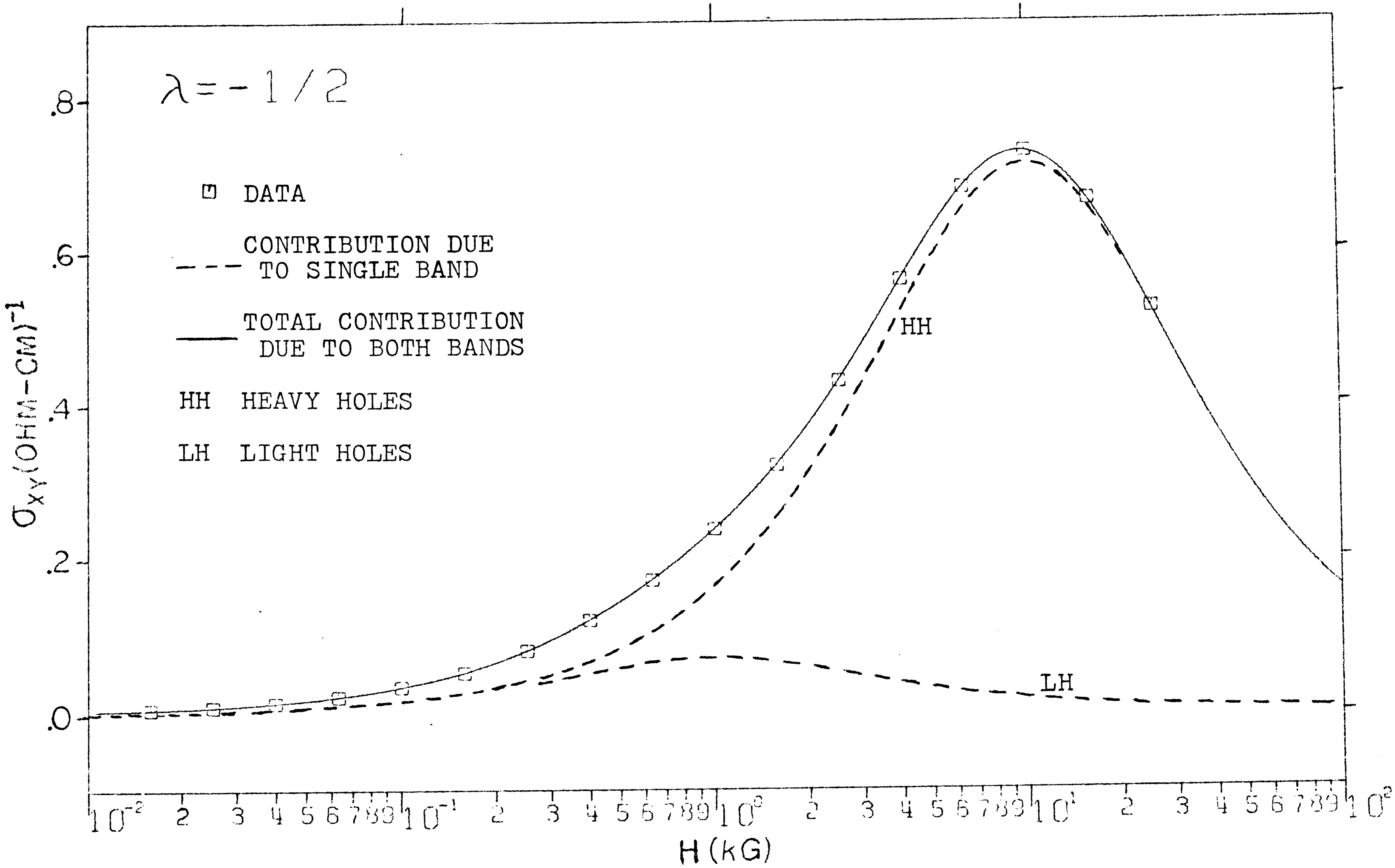

Fig. 24--Example Hall conductivity data due to two hole bands having λ=-1/2. The squares are the data fitted by the curves in the next three figures.

$$A_1(\lambda;\gamma)=\sum_{j=1}^{N} a_j\gamma'^{\,j-1} \quad , \tag{4.3}$$

$$A_2(\lambda;\gamma)=1+\sum_{j=1}^{N} b_j\gamma'^{\,j} \quad , \tag{4.4}$$

and

$$\gamma'=\gamma/\gamma_M$$
$$=H^2/H_M^2 \tag{4.5}$$

(where the a_j and b_j are found in Table II with λ corresponding to: $\lambda=-1/2$, acoustic phonon scattering; $\lambda=1/2$, piezoelectric scattering; and $\lambda=3/2$, ionized inpurity scattering) provides a convenient expression of the proposed Hall conductivity. Thus assume the data can be fitted by

$$\sigma_{xy}(H)=\sum_{j=1}^{2}(p_{2j-1}/p_{2j}^{\frac{1}{2}})S^*(\lambda_i;\gamma_j)$$
$$=\sum_{j=1}^{2}(p_{2j-1}/p_{2j})HA_1(\lambda_i;\gamma_j)/A_2(\lambda_i;\gamma_j) \quad , \tag{4.6}$$

where, in Eq. (4.5), one requires $H_{Mj}^2=p_{2j}$ and $p_1,\ldots,p_4$ are adjustable parameters to be determined by a computer using a program such as the one listed in Appendix E.

Three fits of the data are made and are represented in Figs. 25-27. The λ_i and N chosen are: $\lambda_1=0$ with N=1 ($S(0;\gamma)=S^*(0,\gamma)$ of order N=1); $\lambda_2=1/2$ with N=4; and $\lambda_3=3/2$ with N=6. For a given λ_i, from Eq. (2.46), the conductivity mobility is

$$\mu_{0j}=C_1/p_{2j}^{\frac{1}{2}} \quad , \tag{4.7}$$

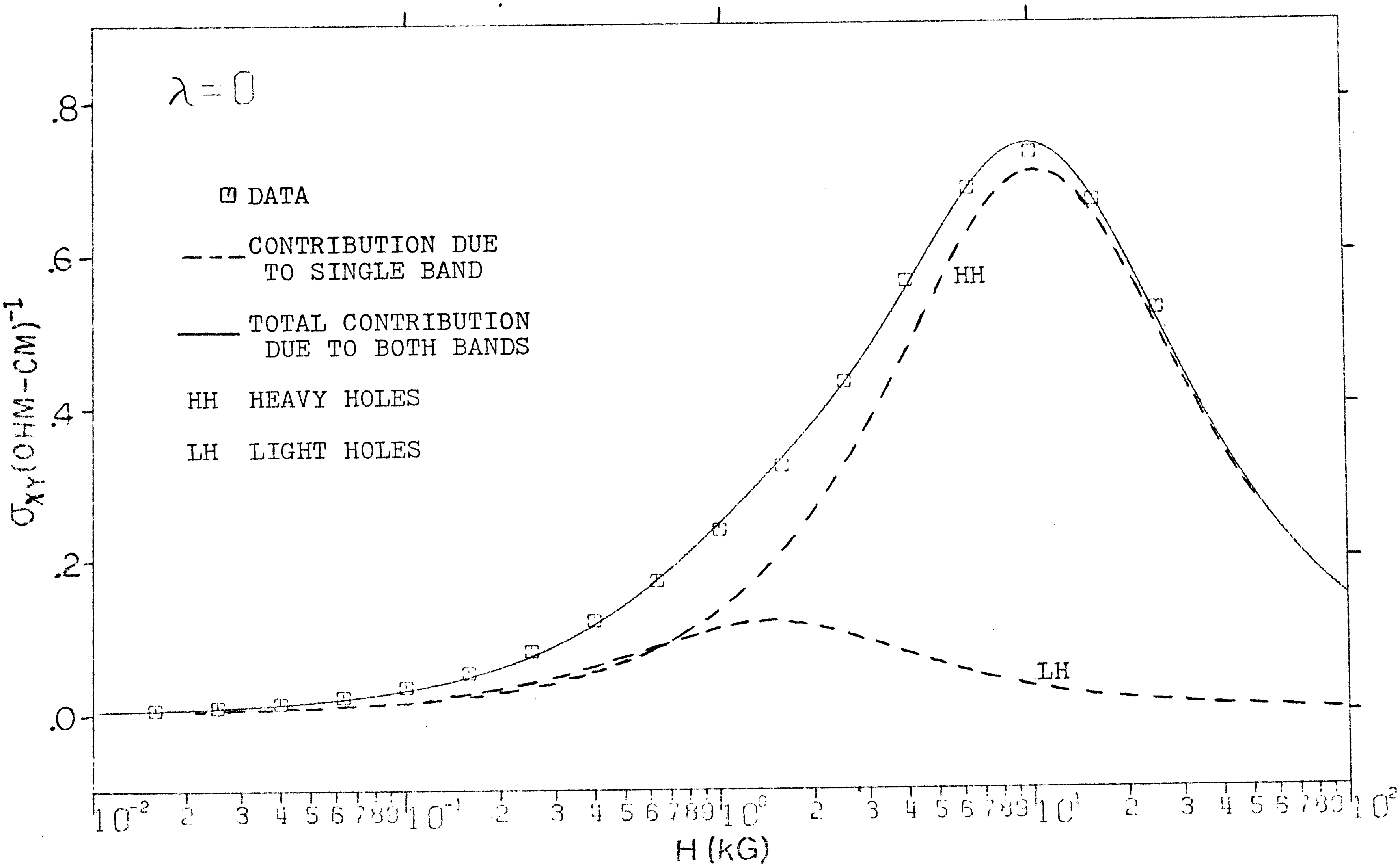

Fig. 25--A least-squares fit of the contribution to the example Hall conductivity data by two hole bands having λ=0.

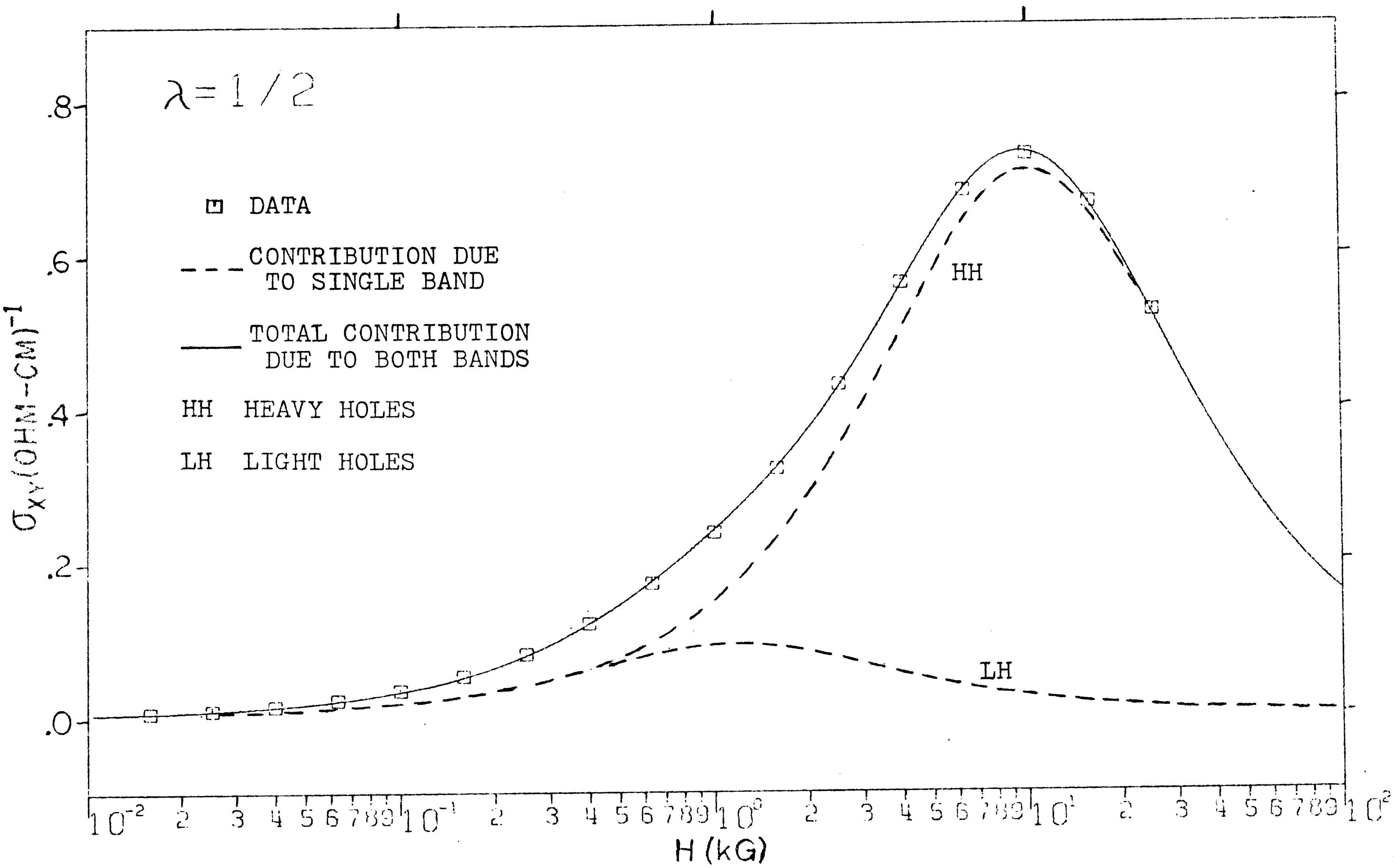

Fig. 26--A least-squares fit of the contribution to the example Hall conductivity data by two hole bands having λ=1/2.

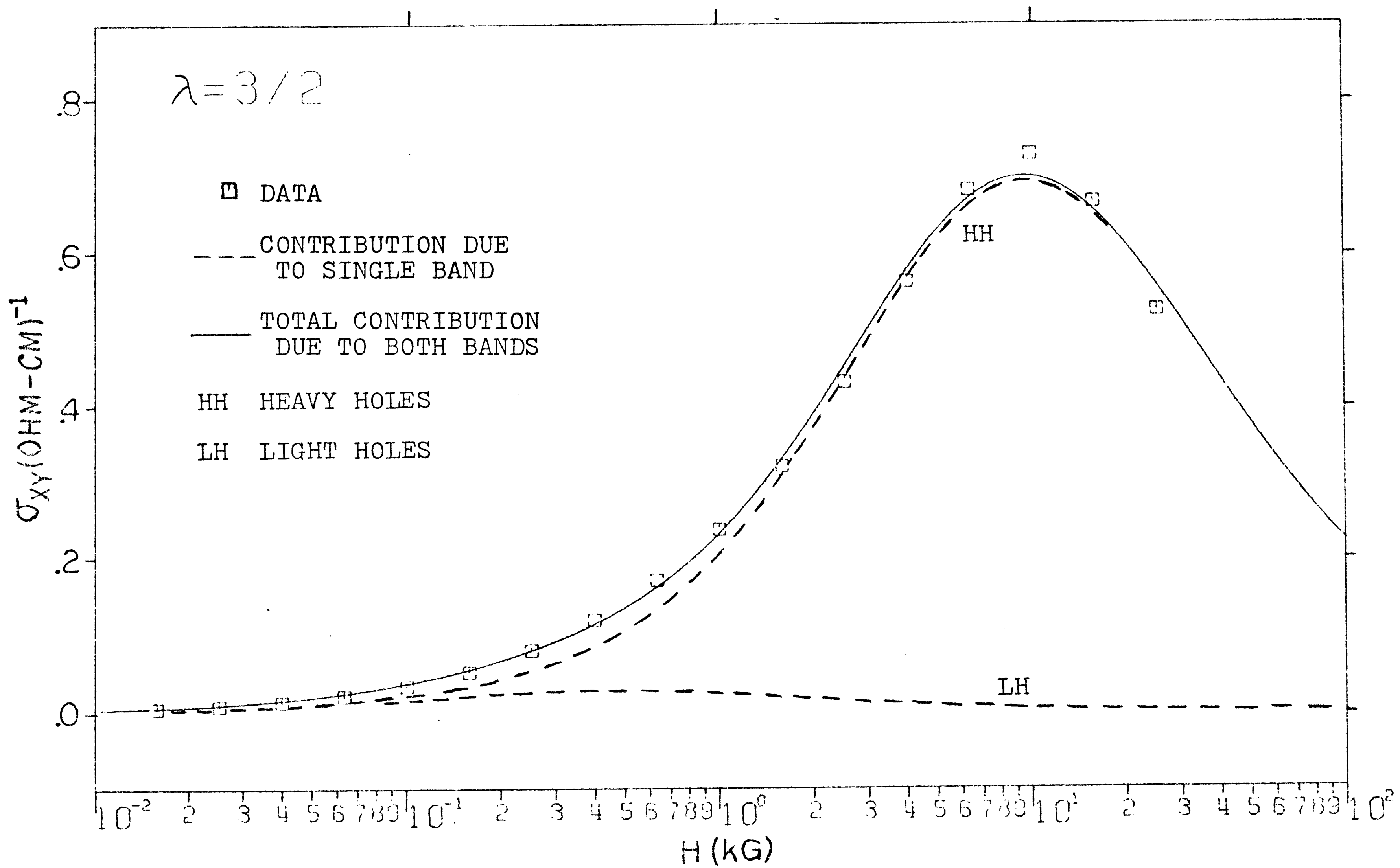

Fig. 27--A least-squares fit of the contribution to the example Hall conductivity data by two hole bands having λ=3/2.

where the C_1 are found in Table I, and the number density, from Eq. (4.1), is

$$n_j = p_{2j-1}/eC_1 \quad . \tag{4.8}$$

These μ_{0j} and n_j are found in Table III.

The standard error of estimate is defined by

$$s_E^2 \equiv (ND-NP)^{-1} \sum_{i=1}^{ND} (y-\hat{y}_i)^2 \quad , \tag{4.9}$$

where ND is the number of data points; NP, the number of parameters; $\hat{y}_i$, the data; and y, the modeled value of the data. Examination of the final fits shown in Figs. 25-27 indicate a correspondence between s_E and the accuracy of the determined constants. Note that although the data is generated using $\lambda=-1/2$ ($s_E=0$), a visually excellent fit is obtained by using the $\lambda=1/2$ model ($s_E=0.252 \times 10^{-2}$ (ohm-cm)$^{-1}$). However it is seen that the light hole band number density so obtained is in error by approximately a factor of 1.5. Such behavior is to be expected since the $S(\lambda;\gamma)$ corresponding to $\lambda=1/2$ and $\lambda=-1/2$ can be made to essentially coincide by translation and scaling (see Fig. 1). Therefore one must be cautious in applying these techniques when the dominant scattering mechanism may be either acoustic phonon or piezoelectric in nature. However, by using this method in conjunction with a study of the temperature dependence of the mobilities, the proper choice should be made.

TABLE III

RESULTS OF EXAMPLE CALCULATION

λ	n_1 (10^{15} cm^{-3})	μ_{01} (10^4 cm^2/V-sec)	n_2 (10^{13} cm^{-3})	μ_{02} (10^5 cm^2/V-sec)	s_E (10^{-2}) $(ohm\text{-}cm)^{-1}$
-1/2	1.000	0.935	1.000	0.935	Identically Zero
0	.916	.964	2.18	.682	0.752
1/2	.992	.932	1.52	.794	.252
3/2	1.63	0.656	0.326	1.38	1.535

CHAPTER V

CONCLUSION

In this dissertation two new means of determining conductivity mobility and number density for nondegenerate semiconductors having spherical, parabolic energy bands and a relaxation time varying as a power of the energy are developed. First, assuming the proper choice of scattering mechanism, then one may for a single band semiconductor determine n and μ_0 from the maximum absolute value of the Hall conductivity. This maximum value occurs at magnetic fields much less than the Hall saturation fields necessary to determine n by use of the high field limit of $H\sigma_{xy}(H)$. Finally, by approximating $S(\lambda;\gamma)$ by a rational type function, one is able to extract information from multiband semiconductors by least-squares analysis of data taken over a wide range of magnetic fields. Clearly this is superior to the use of a low magnetic field expansion[19] of $S(\lambda;\gamma)$ which not only covers a range of field where the per cent accuracy of the measured magnetic field strength and $\sigma_{xy}(H)$ is least, but is itself inadequate.

Consider the other means of determining $S(\lambda;\gamma)$. They are 1) tables, which require either storage of a large number of functional values or entail a loss of accuracy, 2) numerical integration, which requires a relatively large number of calculations, 3) precise expansions, which require the carrying of a larger number of decimal places as γ becomes larger due to the mixture of positive and negative terms, and 4) asymptotic expansions, which are inadequate over much of the range of γ. By replacing these methods of calculating $S(\lambda;\gamma)$ with accurate approximations which may be computed relatively quickly and often require no more decimal places be carried than that commonly used by the BASIC computer language, one has extended the usefulness and convenience of application of a part of semiconductor theory.

For future research, one may create similar approximations of the magnetoconductivity integral. Knowledge of this integral and of $S(\lambda;\gamma)$ allow the constraints for the application of the theory presented in this work to be relaxed to include semiconductors with ellipsoidal energy surfaces.

APPENDIX A

EXPANSION OF FUNCTIONS WITHOUT ESSENTIAL SINGULARITIES

Many functions f(z) may be expanded as a series in terms of the poles in the complex plane.

Mittag-Leffler Expansion Theorem

In particular f(z) may be expanded if the following conditions exist: 1) suppose f(z) has only simple poles located in the finite z plane at $a_1, a_2, \ldots$ arranged in order of increasing absolute magnitude with residues $b_1, b_2, \ldots,$ and 2) there exist circles C_N of radius R_N which do not pass through any poles and on which $|f(z)| < M$, where M is independent of N and $R_N \to \infty$ as $N \to \infty$. The Mittag-Leffler expansion theorem then states that

$$f(z)=f(0)+\sum_{n=1}^{\infty} b_n[(z-a_n)^{-1}+a_n^{-1}] \quad . \tag{A1}$$

A proof of the theorem is provided by Spiegel.[20] Let f(z) have poles at $z=a_n$, n=1,2,... and suppose that $z=\zeta$ is not a pole of f(z). Then the function $f(z)/(z-\zeta)$ has poles at $z=a_n$ where n=1,2,... and at $z=\zeta$. The residue of $f(z)/(z-\zeta)$ at $z=a_n$ is

$$\lim_{z\to a_n} (z-a_n)f(z)/(z-\zeta)=b_n/(a_n-\zeta) \quad , \tag{A2}$$

where b_n is the residue of f(z) at $z=a_n$, and the residue at $z=\xi$ is

$$\lim_{z\to\xi}\ (z-\xi)f(z)/(z-\xi)=f(\xi)\quad . \tag{A3}$$

Then by the residue theorem, one finds

$$\frac{1}{2\pi i}\oint_{C_N} f(z)dz/(z-\xi)=f(\xi)+\sum_n \frac{b_n}{a_n-\xi} \tag{A4}$$

where the last summation is taken over all poles inside circle C_N, centered at the origin, of radius R_N.

Suppose f(z) is analytic at z=0. Then putting $\xi=0$ in Eq. (A4), one has

$$\frac{1}{2\pi i}\oint_{C_N} f(z)dz/z=f(0)+\sum_n \frac{b_n}{a_n}\quad . \tag{A5}$$

Substraction of Eq. (A5) from Eq. (A4) then yields

$$f(\xi)-f(0)+\sum_n b_n[(a_n-\xi)^{-1}-a_n^{-1}]$$

$$=\frac{1}{2\pi i}\oint_{C_N} f(z)\left[\frac{1}{z-\xi}-\frac{1}{z}\right]dz$$

$$=\frac{\xi}{2\pi i}\oint_{C_N}\frac{f(z)dz}{z(z-\xi)}\quad . \tag{A6}$$

Now since $|z-\xi|\geq|z|-|\xi|=R_N-|\xi|$ for z on C_N, one has if $|f(z)|<M$

$$\left|\oint_{C_N}\frac{f(z)dz}{z(z-\xi)}\right|<\frac{M2\,R_N}{R_N(R_N-\xi)}\quad . \tag{A7}$$

As $N\to\infty$ and thus $R_N\to\infty$, the integral on the right side of Eq. (A6) approaches zero. Hence by replacing ξ by z in Eq. (A6), Eq. (A1) results.

Generalized Theorem

This expansion theorem may be easily extended to include functions f(z) having poles of order k. By using Leibnitz's rule for higher derivatives of products,

$$\frac{d^k}{dz^k}[f(z)g(z)] = \sum_{m=0}^{k} \binom{k}{m} \left[\frac{d^{k-m}}{dz^{k-m}} f(z)\right]\left[\frac{d^m}{dz^m} g(z)\right] \quad , \qquad (A8)$$

and

$$\frac{d^k}{dz^k}(z-\zeta)^{-1} = \frac{(-1)^k \, k!}{(z-\zeta)^{k+1}} \qquad (A9)$$

observe that if $f(z)/(z-\zeta)$ has a kth order pole at $z=a_n$ then its residue is

$$\lim_{z \to a_n} \frac{1}{(k-1)!} \frac{d^{k-1}}{dz^{k-1}}\left[\frac{(z-a_n)^k f(z)}{z-\zeta}\right]$$

$$= \frac{1}{(k-1)!} \lim_{z \to a_n} \sum_{m=0}^{k-1} \binom{k-1}{m} \frac{d^{k-1-m}}{dz^{k-1-m}}[(z-a_n)^k f(z)] \frac{d^m}{dz^m}\left(\frac{1}{z-\zeta}\right)$$

$$= \frac{1}{(k-1)!} \sum_{m=0}^{k-1} \binom{k-1}{m} \frac{(-1)^m \, m!}{(a_n-\zeta)^{m+1}} \left\{ \lim_{z \to a_n} \frac{d^{k-1-m}}{dz^{k-1-m}}[(z-a_n)^k f(z)] \right\}_1$$

$$= -\frac{1}{(k-1-m)!} \sum_{m=0}^{k-1} \frac{1}{(\zeta - a_n)^{m+1}} \left\{ \right\}_1 \quad . \qquad (A10)$$

Since the remainder of the proof is identical to that of the previous theorem, the result may now be stated as

$$f(z) = f(0) + \sum_n \sum_{m=0}^{k-1} {}^{n}C^k_m \left[\frac{1}{(z-a_n)^{m+1}} + \frac{(-1)^m}{a_n^{m+1}}\right] \quad , \qquad (A11)$$

where

$$ {}^{n}C^{k}_{m}= \frac{1}{(k-1-m)!} \lim_{z\to a_n} \left\{ \frac{d^{k-1-m}}{dz^{k-1-m}} [(z-a_n)^k f(z)] \right\} . \quad (A12)$$

Expansion of $f(z)=(z^n+a^n)^{-1}$

For a positive integer n and a positive real number a let $g(z)=(z^n+a^n)^{-1}-a^{-n}$. The poles of g(z) are simple and occur at

$$z_k= a \exp[i\pi(1+2k)/n] \quad (A13)$$

for $k=0,1,...,n-1$. At z_k the residue is

$$\lim_{z\to z_k} (z-z_k)g(z)=\lim_{z\to z_k} \frac{(z-z_k)}{z^n+a^n} - \lim_{z\to z_k} \frac{(z-z_k)}{a^n}$$

which by L'Hospital's rule becomes $(nz_k^{n-1})^{-1}$ or

$$-\frac{z_k}{na^n} . \quad (A14)$$

By use of Eq. (A1), g(z) may now be written as

$$g(z)= -\frac{1}{a^n n} \sum_{k=0}^{n-1} z_k \left(\frac{1}{z-z_k} + \frac{1}{z_k}\right)$$

$$= - a^{-n}-(na^n)^{-1} \sum_{k=0}^{n-1} z_k/(z-z_k) . \quad (A15)$$

With the use of Eq. (A13), $f(z)=(z^n+a^n)^{-1}$ becomes

$$f(z)= - (na^{n-1})^{-1} \sum_{k=0}^{n-1} \exp[i\pi(1+2k)/n]/[z-a \exp[i\pi(1+2k)/n]]$$

$$=(na^{n-1})^{-1} \sum_{k=0}^{n-1} \exp[i\pi(1+2k-n)/n]/[z+a \exp[i\pi(1+2k-n)/n]]$$

$$=(na^{n-1})^{-1} \sum_{j=0}^{n-1} \exp[i\pi(n-1-2j)/n]/[z+a \exp[i\pi(n-1-2j)/n]] , \quad (A16)$$

where $j=n-1-k$. If n is even, Eq. (A16) may be compacted to

$$(z^n+a^n)^{-1}=(na^{n-1})^{-1}\sum_{j=0}^{[\frac{n-1}{2}]} u/(z+au) + \text{c.c.} , \qquad \text{(A17a)}$$

where $u=\exp[i\pi(n-1-2j)/n]$ and $[(n-1)/2]$ is the largest integer less than or equal to $(n-1)/2$. If n is odd then f(z) is equal to the right side of Eq. (A17a) plus

$$[na^{n-1}(z+a)]^{-1} . \qquad \text{(A17b)}$$

APPENDIX B

GAMMA FUNCTION AND RELATED FUNCTIONS

Several relationships among known and tabulated functions are necessary in order to evaluate the integrals in Eqs. (2.32) and (2.33). While these relationships appear in the literature, the proofs are included in order to establish an unbroken link between the introduction of the integrals and their evaluation in terms of these well-known functions.

Gamma Function

The gamma function is defined, for $\mathcal{R}(z)>0$, as

$$\Gamma(z) \equiv \int_0^\infty t^{z-1} e^{-t} dt \quad . \tag{B1}$$

Clearly, by integration by parts, one finds the recursion

$$\begin{aligned} \Gamma(z+1) &= \int_0^\infty t^z e^{-t} dt \\ &= -t^z e^{-t} \Big|_0^\infty + z\int_0^\infty t^{z-1} e^{-t} dt \\ &= z\,\Gamma(z) \quad . \end{aligned} \tag{B2}$$

The product

$$\Gamma(z)\,\Gamma(1-z) = \int_0^\infty t^{-z}/(1+t)\,dt \tag{B3}$$

follows from the manipulation

$$\Gamma(z)\,\Gamma(1-z) = \int_0^\infty t^{z-1} e^{-t} dt \int_0^\infty x^{-z} e^{-x} dx$$

$$=2\int_0^\infty u^{2z-1}e^{-u^2}du \; 2\int_0^\infty v^{-2z+1}e^{-v^2}dv$$

$$=4\int_0^\infty\int_0^\infty e^{-(u^2+v^2)}\left(\frac{v}{u}\right)^{-2z+1}du\,dv$$

$$=4\int_0^{\pi/2}\int_0^\infty re^{-r^2}\tan^{-2z+1}(\theta)\,dr\,d\theta$$

$$=-2\int_0^{\pi/2}e^{-r^2}\Big|_0^\infty\tan^{-2z+1}(\theta)\,d\theta$$

$$=2\int_0^{\pi/2}\tan^{-2z+1}(\theta)\,d\theta$$

$$=2\int_0^\infty u^{-2z+1}/(1+u^2)\,du$$

$$=\int_0^\infty t^{-z}dt/(1+t) \quad , \qquad \text{(B4)}$$

where the transformations successively used are: $t=u^2$ and $x=v^2$; $v=r\sin(\theta)$ and $u=r\cos(\theta)$; $u=\tan(\theta)$, which implies $du=(1+u^2)d\theta$; and $t=u^2$. Convergence of the right side of Eq. (B3) occurs only in $0<\mathcal{R}(z)<1$. Since

$$\Gamma(z+n)=z(z+1)\ldots(z+n-1)\,\Gamma(z)$$
$$=(z)_n\,\Gamma(z) \qquad \text{(B5)}$$

follows from Eq. (B2) and thus

$$(1-z-n)_n\,\Gamma(1-z-n)=\Gamma(1-z) \quad , \qquad \text{(B6)}$$

one has

$$\Gamma(z+n)\,\Gamma(1-z-n)=\frac{(z)_n\,\Gamma(z)\,\Gamma(1-z)}{(1-z-n)_n}$$

$$=\frac{(z)_n}{(1-z-n)_n}\int_0^\infty\frac{t^{-z}dt}{1+t} \qquad \text{(B7)}$$

for $0<\Re(z)<1$, which in effect extends the range of convergence of Eq. (B3) to all noninteger z.

Another definition of the gamma function is

$$\Gamma(z) \equiv \lim_{n\to\infty} \frac{1\cdot 2\cdot 3\cdot\ldots n}{z(z+1)(z+2)\ldots(z+n)}\, n^z \quad . \tag{B8}$$

A proof provided by Arfkin[21] follows. Let

$$F(z,n)=\int_0^n \left(1-\frac{t}{n}\right)^n t^{z-1}\,dt \quad , \tag{B9}$$

where $\Re(z)>0$. Since

$$e^{-t}=\lim_{n\to\infty}\left(1-\frac{t}{n}\right)^n \tag{B10}$$

then from Eq. (B1) one acquires

$$\begin{aligned}\lim_{n\to\infty} F(z,n) &= F(z,\infty)\\ &= \Gamma(z) \quad .\end{aligned} \tag{B11}$$

Integrating F(z,n) by parts where u=t/n, one has

$$\begin{aligned}F(z,n)/n^z &= \int_0^1 (1-u)^n u^{z-1}\,du\\ &= \cancel{(1-u)^n \frac{u^z}{z}\Big|_0^1} \to 0 + \frac{n}{2}\int_0^1 (1-u)^{n-1} u^z\,du\\ &\;\vdots\\ &= \frac{n}{z}\,\frac{n-1}{z+1}\cdots\frac{1}{z+n-1}\int_0^1 u^{z+n-1}\,du\\ &= \frac{1\cdot 2\cdots n}{z(z+1)\cdots(z+n-1)}\,\frac{1}{z+n}u^{z+n}\Big|_0^1 \quad ,\end{aligned} \tag{B12}$$

i.e.

$$F(z,n)=\frac{1\cdot 2\cdots n}{z(z+1)\cdots(z+n)}\, n^z \quad . \tag{B13}$$

Thus by use of Eq. (B11) one observes the definitions of $\Gamma(z)$ in Eqs. (B1) and (B8) to be equivalent.

For several z, $\Gamma(z)$ must be evaluated. If z is equal to n, a positive integer, Eqs. (B1) and (B8) imply

$$\Gamma(n)=(n-1)! \quad . \tag{B14}$$

For z equal to one half, first make the substitution $t=u^2$ in Eq. (B1), which provides

$$\Gamma(\tfrac{1}{2})=2\int_0^\infty e^{-u^2}du \quad . \tag{B15}$$

Then by forming the square of $\Gamma(\frac{1}{2})$ one obtains

$$\begin{aligned}\Gamma^2(\tfrac{1}{2})&=4\int_0^\infty\int_0^\infty e^{-(u^2+v^2)}du\,dv\\&=4\int_0^\infty\int_0^{\pi/2} re^{-r^2}d\theta\,dr\\&=4(\pi/2)(-\tfrac{1}{2}e^{-r^2})\Big|_0^\infty\\&=\pi \quad ,\end{aligned} \tag{B16}$$

i.e.

$$\Gamma(\tfrac{1}{2})=\pi^{\frac{1}{2}} \quad . \tag{B17}$$

Incomplete Gamma Function

The incomplete gamma function is defined as

$$\Gamma(\alpha,x)\equiv\int_x^\infty e^{-t}t^{\alpha-1}dt \quad . \tag{B18}$$

Clearly one has

$$\Gamma(\alpha)=\Gamma(\alpha,0) \quad . \tag{B19}$$

A recurrence relation is

$$\begin{aligned}\Gamma(\alpha+1,x)&=\int_x^\infty t^\alpha e^{-t}dt\\&=\alpha\int_x^\infty t^{\alpha-1}e^{-t}dt - t^\alpha e^{-t}\Big|_x^\infty\end{aligned}$$

$$=\alpha\,\Gamma(\alpha,x)+x^{\alpha}e^{-x} \quad , \qquad \text{(B20)}$$

which generalizes to

$$\Gamma(\alpha+n,x)=(\alpha)_n[\,\Gamma(\alpha,x)+x^{\alpha}e^{-x}\sum_{k=1}^{n}\frac{x^{k-1}}{(\alpha)_k}] \qquad \text{(B21)}$$

by use of induction. In order to prove this, assume Eq. (B21) is valid and observe, by utilization of Eq. (B20) that

$$\Gamma(\alpha+n+1,x)=(\alpha+n)\,\Gamma(\alpha+n,x)+x^{\alpha+n}e^{-x}$$

$$=(\alpha)_{n+1}[\,\Gamma(\alpha,x)+x^{\alpha}e^{-x}\sum_{k=1}^{n}\frac{x^{k-1}}{(\alpha)_k}]+x^{\alpha+n}e^{-x}$$

$$=(\alpha)_{n+1}[\,\Gamma(\alpha,x)+x^{\alpha}e^{-x}\sum_{k=1}^{n+1}\frac{x^{k-1}}{(\alpha)_k}] \quad . \qquad \text{(B22)}$$

Hence Eq. (B21) follows.

If $\alpha=-n$ then one acquires from Eq. (B21)

$$\Gamma(-n,x)=\frac{1}{(-n)_n}\,\Gamma(0,x)-x^{-n}e^{-x}\sum_{k=1}^{n}x^{k-1}/(-n)_k$$

$$=\frac{(-1)^n}{n!}\,\Gamma(0,x)-x^{-n}e^{-x}\sum_{k=1}^{n}\frac{(n-k)!}{n!}x^{k-1}(-1)^k$$

$$=\frac{(-1)^n}{n!}\,\Gamma(0,x)+\frac{e^{-x}}{n!}\sum_{j=1}^{n}\frac{(j-1)!}{x^j}(-1)^{n-j} \quad , \qquad \text{(B23)}$$

where $j=n-k+1$. For the case of $\alpha=\frac{1}{2}-n$, first examine

$$(\tfrac{1}{2}-n)_k=(\tfrac{1}{2}-n)(\tfrac{1}{2}-n+1)\cdots(\tfrac{1}{2}-n+k-1)$$

$$=(\frac{1-2n}{2})(\frac{3-2n}{2})\cdots(\frac{2k-2n-1}{2})$$

$$=\frac{(-1)^k}{2^k}(2n-1)(2n-3)\cdots(2n-2k+1)$$

$$= \frac{(-1)^k}{2^k} \frac{(2n-1)!!}{(2n-2k-1)!!} \quad , \tag{B24}$$

which is valid for n=1,2,... , and where $(-1)!! \equiv 1$. From Eq. (B21), one then derives

$$\Gamma(\tfrac{1}{2}-n,x)=\frac{1}{(\frac{1}{2}-n)_n} \Gamma(\tfrac{1}{2},x)-x^{\frac{1}{2}}e^{-x}\sum_{k=1}^{n} x^{k-1}/(\tfrac{1}{2}-n)_k$$

$$=\frac{(-1)^n 2^n}{(2n-1)!!}[\Gamma(\tfrac{1}{2},x)-x^{\frac{1}{2}-n}e^{-x}\sum_{k=1}^{n} x^k(-1)^{k-n}(2n-2k-1)!!]$$

$$=\frac{(-1)^n 2^n}{(2n-1)!!}[\Gamma(\tfrac{1}{2},x)+x^{-\frac{1}{2}}e^{-x}\sum_{j=1}^{n} \frac{(-1)^j(2j-3)!!}{(2x)^{j-1}}] \quad , \tag{B25}$$

where j=n-k+1.

A differential equation of which $\Gamma(\alpha,x)$ is the solution may be created by differentiating Eq. (B18)

$$\frac{d\,\Gamma(\alpha,x)}{dx} = -x^{\alpha-1}e^{-x} \tag{B26}$$

and requiring that $\Gamma(\alpha,0)=\Gamma(\alpha)$. The solution is

$$\Gamma(\alpha,x)=\Gamma(\alpha)-\int_0^x t^{\alpha-1}\sum_{k=0}^{\infty}(-t)^k/k!\ dt$$

$$=\Gamma(\alpha)-\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\int_0^x t^{k+\alpha-1}dt$$

$$=\Gamma(\alpha)-\sum_{k=0}^{\infty}\frac{(-1)^k x^{\alpha+k}}{(\alpha+k)k!} \quad . \tag{B27}$$

Clearly Eq. (B26) may be extended to complex numbers as

$$\frac{d\,\Gamma(\alpha,z)}{dz} = -z^{\alpha-1}e^{-z} \quad , \tag{B28}$$

which together with the same boundary condition provides the solution Eq. (B27) with x replaced by z. Thus $\Gamma(\alpha,z)$ is an analytic continuation of $\Gamma(\alpha,x)$ onto the z plane.

Consider the function

$$f(x)=\frac{e^{-x}}{\Gamma(1-\alpha)}\int_0^\infty e^{-xt}\,\frac{t^{-\alpha}}{1+t}dt \tag{B29}$$

with x>0. One has

$$\begin{aligned}\frac{df}{dx} &=-\frac{e^{-x}}{\Gamma(1-\alpha)}\int_0^\infty e^{-xt}\,\frac{t^{-\alpha}}{1+t}(1+t)\,dt\\ &=-\frac{e^{-x}}{\Gamma(1-\alpha)}\int_0^\infty e^{-u}u^{-\alpha}x^{\alpha}\,\frac{du}{x}\\ &=-\frac{e^{-x}}{\Gamma(1-\alpha)}x^{\alpha-1}\,\Gamma(1-\alpha)\\ &=-e^{-x}x^{\alpha-1}\end{aligned} \tag{B30}$$

which requires the aid of the transformation u=xt. Also by Eq. (B3)

$$\begin{aligned}f(0)&=\frac{1}{\Gamma(1-\alpha)}\int_0^\infty t^{-\alpha}dt/(1+t)\\ &=\frac{1}{\Gamma(1-\alpha)}\,\Gamma(\alpha)\,\Gamma(1-\alpha)\\ &=\Gamma(\alpha)\end{aligned} \tag{B31}$$

results, which together with Eqs. (B30) and (B26) imply

$$\Gamma(\alpha,x)=\frac{e^{-x}}{\Gamma(1-\alpha)}\int_0^\infty e^{-xt}\,\frac{t^{-\alpha}}{1+t}dt \tag{B32}$$

for x>0.[22]

Psi Function

The psi function is defined as

$$\psi(z)=\frac{d}{dz}\ln[\Gamma(z)]$$

$$= \frac{\Gamma'(z)}{\Gamma(z)} \quad . \tag{B33}$$

From Eq. (B8) one acquires

$$\ln \Gamma(z) = \ln \lim_{n\to\infty} \frac{n!\, n^z}{z(z+1)\cdots(z+n)}$$

$$= \lim_{n\to\infty} \left[\ln(n!) + z\ln(n) - \sum_{k=0}^{n} \ln(z+k)\right] \tag{B34}$$

which implies

$$\Psi(z) = \lim_{n\to\infty} \left[\ln(n) - \sum_{k=0}^{n} (z+k)^{-1}\right]$$

$$= \lim_{n\to\infty} \left[\ln(n) - \sum_{k=1}^{n} k^{-1}\right] - \cancelto{0}{\lim_{n\to\infty} (n+1)^{-1}} - \sum_{k=0}^{\infty} \left[(z+k)^{-1} - (k+1)^{-1}\right]$$

$$= -C - \sum_{k=0}^{\infty} \left[(z+k)^{-1} - (1+k)^{-1}\right] \quad , \tag{B35}$$

where

$$C = \lim_{n\to\infty} \left[\sum_{k=1}^{n} k^{-1} - \ln(n)\right]$$

$$= 0.577215664901\ldots \tag{B36}$$

is Euler's constant. Also, by use of Eq. (B1), one determines

$$\Psi(z) = \frac{1}{\Gamma(z)} \frac{d}{dz} \int_0^\infty t^{z-1} e^{-t} dt$$

$$= \frac{1}{\Gamma(z)} \frac{d}{dz} \int_0^\infty e^{(z-1)\ln(t)} e^{-t} dt$$

$$= \frac{1}{\Gamma(z)} \int_0^\infty \ln(t)\, t^{z-1} e^{-t} dt \quad . \tag{B37}$$

Thus from Eqs. (B37) and (B35) one finds

$$\Psi(1) = \int_0^\infty \ln(t) e^{-t} dt$$

$$= -C \quad . \tag{B38}$$

Since the natural logarithm of x may be defined as

$$\ln(x) \equiv \int_1^x dt/t \quad , \tag{B39}$$

then the relationship

$$-C = \lim_{\substack{R\to\infty \\ \epsilon\to 0_+}} \int_\epsilon^R \ln(t)e^{-t}dt$$

$$= \lim_{\substack{R\to\infty \\ \epsilon\to 0_+}} (-1)\left[\ln(t)e^{-t}\Big|_\epsilon^R - \int_\epsilon^R e^{-t}dt/t\right]$$

$$= \lim_{\substack{R\to\infty \\ \epsilon\to 0_+}} (-1)\left[e^{-R}\ln(R) - e^{-\epsilon}\int_1^\epsilon dt/t - \int_\epsilon^R e^{-t}dt/t\right]$$

$$= \lim_{\epsilon\to 0_+}\left[e^{-\epsilon}\int_1^\epsilon dt/t + \int_\epsilon^1 e^{-t}dt/t + \int_1^\infty e^{-t}dt/t\right]$$

$$= \lim_{\epsilon\to 0_+}\int_\epsilon^1 (e^{-t}-e^{-\epsilon})dt/t + \int_1^\infty e^{-t}dt/t \tag{B40}$$

which becomes

$$-C = \int_0^1 (e^{-t}-1)dt/t + \int_1^\infty e^{-t}dt/t \tag{B41}$$

is valid.[23]

Exponential-Integral Function

The exponential-integral function is defined for $x>0$ as

$$Ei(-x) \equiv -\int_x^\infty e^{-t}dt/t \quad . \tag{B43}$$

From Eq. (B18) one has

$$\Gamma(0,x) = -Ei(-x) \quad . \tag{B43}$$

By use of Eq. (B41), Ei(-x) may be evaluated as

$$Ei(-x) = -\int_1^\infty e^{-t}dt/t - \int_x^1 e^{-t}dt/t$$

$$=C + \int_0^1 (e^{-t}-1)dt/t + \int_1^x e^{-t}dt/t$$

$$=C + \int_0^1 (e^{-t}-1)dt/t + \int_1^x dt/t + \int_1^x (e^{-t}-1)dt/t$$

$$=C + \int_1^x dt/t + \int_0^x (e^{-t}-1)dt/t$$

$$=C + \ln(x) - \sum_{k=1}^{\infty} \int_0^x (-t)^{k-1}dt/k!$$

$$=C + \ln(x) + \sum_{k=1}^{\infty} (-x)^k/(k\,k!) \quad . \tag{B44}$$

Selecting a branch cut along the negative x axis, one may extend Eq. (B44) to the z plane as

$$Ei(-z)=C+\ln(z)+\sum_{k=1}^{\infty} (-z)^k/(k\,k!) \quad . \tag{B45}$$

For large x, Eq. (B44) converges so slowly as to warrant the developement of an asymptotic series which may be used to calculate Ei(-x) to sufficient accuracy. By integration by parts of the right side of Eq. (B42), as indicated by Arfkin,[24] one obtains

$$Ei(-x)=-\frac{e^{-x}}{x}+\int_x^{\infty}\frac{e^{-t}}{t^2}dt$$

$$\vdots$$

$$=-\frac{e^{-x}}{x}\sum_{k=0}^{n-1}\frac{(-1)^k k!}{x^k}+(-1)^{n+1}n!\int_x^{\infty}\frac{e^{-t}dt}{t^{n+1}} \quad . \tag{B46}$$

Thus is found

$$\left| Ei(-x)+\frac{e^{-x}}{x}\sum_{k=0}^{n-1}\frac{(-1)^k k!}{x^k}\right| \le n!\int_x^{\infty}t^{-n-1}dt$$

$$=(n-1)!/x^n \quad . \tag{B47}$$

Hence by a judicious choice of n, for a given x, the error of approximation indicated by Eq. (B47) may be minimized. Extension of the asymptotic series in Eq. (B47) to the z plane may be made with the understanding that the error will vary as $|z|^{-n}$ times a function of the argument of z.

Probability Integral

The probability integral $\Phi(x)$, also known as the error function erf(x), is defined as

$$\Phi(x) \equiv \frac{2}{\pi^{\frac{1}{2}}}\int_0^{\infty} e^{-t^2} dt \quad . \tag{B48}$$

Let $u=t^2$, then from application of Eqs. (B1), (B18), and (B17), Eq. (B48) becomes

$$\Phi(x)=\frac{1}{\pi^{\frac{1}{2}}}\int_0^{x^2} u^{-\frac{1}{2}} e^{-u} du$$

$$=\pi^{-\frac{1}{2}}[\Gamma(\tfrac{1}{2})-\Gamma(\tfrac{1}{2},x^2)]$$

$$=1-\pi^{-\frac{1}{2}}\Gamma(\tfrac{1}{2},x^2) \quad . \tag{B49}$$

Thus one obtains

$$\Gamma(\tfrac{1}{2},x^2)=\pi^{\frac{1}{2}}[1-\Phi(x)] \quad . \tag{B50}$$

By application of Eqs. (B27) and (B49) one derives

$$\Phi(x)=\frac{2}{\pi^{\frac{1}{2}}}\sum_{k=0}^{\infty}\frac{(-1)^k x^{2k+1}}{(2k+1)\,k!} \quad . \tag{B51}$$

Also, by integration by parts of Eq. (B48), one acquires the alternate form

$$\Phi(x)=2\pi^{-\frac{1}{2}}[xe^{-x^2}+2\int_0^x t^2e^{-t^2}dt]$$

$$=2\pi^{-\frac{1}{2}}\left\{xe^{-x^2}+\frac{2}{3}[x^3e^{-x^2}+2\int_0^x t^4e^{-t^2}]\right\}$$

$$\vdots$$

$$=2\pi^{-\frac{1}{2}}e^{-x^2}\sum_{k=0}^{\infty}\frac{2^kx^{2k+1}}{(2k+1)!!} \quad . \qquad \text{(B52)}$$

To make an asymptotic expansion of $\Phi(x)$, first write

$$\Gamma(\tfrac{1}{2},x^2)=\int_{x^2}^{\infty}t^{-\frac{1}{2}}e^{-t}dt$$

$$=e^{-x^2}/x - \tfrac{1}{2}\int_{x^2}^{\infty}t^{-3/2}e^{-t}dt$$

$$\vdots$$

$$=\frac{e^{-x^2}}{x}\sum_{k=0}^{n-1}\frac{(-1)^k(\frac{1}{2})_k}{x^{2k}}+(-1)^n(\tfrac{1}{2})_n\int_{x^2}^{\infty}\frac{e^{-t}dt}{t^{n+\frac{1}{2}}} \quad . \qquad \text{(B53)}$$

Hence observe that

$$\left|\Gamma(\tfrac{1}{2},x^2)-\frac{e^{-x^2}}{x}\sum_{k=0}^{n-1}\frac{(-1)^k(\frac{1}{2})_k}{x^{2k}}\right|\le\frac{(\frac{1}{2})_n}{x^{2n+1}} \quad . \qquad \text{(B54)}$$

Thus from Eq. (B49) one developes

$$\Phi(x)\sim 1-\frac{e^{-x^2}}{\pi^{\frac{1}{2}}x}\sum_{k=0}^{n-1}\frac{(-1)^k(\frac{1}{2})_k}{x^{2k}}+O(\frac{(\frac{1}{2})_n}{x^{2n+1}}) \qquad \text{(B55)}$$

which together with the other expansions of $\Phi(x)$ may be extended to the complex plane by means of analytic continuation.

APPENDIX C

CONDUCTIVITY INTEGRALS

The conductivity integrals in Eqs. (2.32) and (2.33) are proportional to

$$I=\int_0^\infty \frac{t^{\nu-1}e^{-t}dt}{t^s+\gamma} \quad . \tag{C1}$$

If s is an integer then Eq. (A17) may be employed to expand Eq. (C1) in terms of

$$I_\nu=\int_0^\infty \frac{t^{\nu-1}e^{-t}dt}{t+\alpha} \quad , \tag{C2}$$

where α may be a complex number but not a negative real number. In order to evaluate I , suppose α is a positive real number and $\nu>0$. Let $\alpha x=t$, then Eq. (C2) becomes

$$I_\nu=\int_0^\infty \frac{\alpha^{\nu-1}x^{\nu-1}e^{-\alpha x}\alpha dx}{\alpha(x+1)}$$

$$=\alpha^{\nu-1}\int_0^\infty \frac{x^{\nu-1}e^{-\alpha x}dx}{x+1}$$

$$=\alpha^{\nu-1}e^{\alpha}\Gamma(\nu)\left[\frac{e^{-\alpha}}{(\nu)}\int_0^\infty \frac{x^{\nu-1}e^{-\alpha x}dx}{1+x}\right]$$

$$=\alpha^{\nu-1}e^{\alpha}\Gamma(\nu)\,\Gamma(1-\nu,\alpha) \tag{C3}$$

through use of Eq. (B32). Since both the left and right sides of Eq. (C3) are analytic over the indicated region then by analytic continuation the relationship

$$\int_0^\infty \frac{t^{\nu-1}e^{-t}dt}{t+\alpha} = \alpha^{\nu-1}e^{\alpha}\,\Gamma(\nu)\,\Gamma(1-\nu,\alpha) \qquad \text{(C4)}$$

follows for $\alpha=re^{i\theta}$ with $r\geq 0$ and $|\theta| \leq \pi$.[25]

Hall Conductivity

The contribution of a single band of carriers to the Hall conductivity, as indicated in Eq. (2.33), is proprotional to

$$I=\int_0^\infty \frac{x^{3/2}e^{-x}dx}{x^{-2\lambda}+\gamma} \quad . \qquad \text{(C5)}$$

For several λ corresponding to distinct scattering mechanisms the I are expanded below in order of complexity.

$\lambda=0$

In this case one has simply

$$I=\int_0^\infty \frac{x^{3/2}e^{-x}dx}{1+\gamma}$$

$$= \Gamma(5/2)/(1+\gamma) \quad . \qquad \text{(C6)}$$

$\lambda=-1/2$

Here one finds

$$I=\int_0^\infty \frac{x^{3/2}e^{-x}dx}{x+\gamma}$$

$$=\gamma^{3/2}e^{\gamma}\,\Gamma(5/2)\,\Gamma(\tfrac{1}{2}-2,\gamma) \qquad \text{(C7)}$$

by Eq. (C4). Through application of Eqs. (B5), (B17), (B25), and (B50), one obtains

$$I=\gamma^{3/2}e^{\gamma}\,\Gamma(5/2)\frac{(-1)^2 2^2}{(2\cdot 2-1)!!}\Big[\,\Gamma(\tfrac{1}{2},\gamma)+\gamma^{-\frac{1}{2}}e^{-\gamma}\sum_{k=1}^{2}\frac{(-1)^k(2k-3)}{(2\gamma)^{k-1}}\Big]$$

$$=\gamma^{3/2}e^{\gamma}\pi^{\frac{1}{2}}[\pi^{\frac{1}{2}}(1-\Phi(\gamma^{\frac{1}{2}}))+\gamma^{-\frac{1}{2}}e^{-\gamma}(-1+\frac{1}{2\gamma})]$$

$$=\pi^{\frac{1}{2}}(\tfrac{1}{2}-\gamma)+\gamma^{3/2}e^{\gamma}\pi^{\frac{1}{2}}[\pi^{\frac{1}{2}}(1-\Phi(\gamma^{\frac{1}{2}}))] \qquad (C8)$$

which, with the aid of Eq. (B52), becomes

$$I=\pi^{\frac{1}{2}}[\tfrac{1}{2}-\gamma-2\gamma^{2}\sum_{k=0}^{\infty}\frac{(2\gamma)^{k}}{(2k+1)!!}]+\pi e^{\gamma}\gamma^{3/2} \quad . \qquad (C9)$$

For large γ, where an asymptotic expansion is more appropreate, I is expanded with aid of Eq. (B55) as

$$I\sim\pi^{\frac{1}{2}}\gamma\sum_{k=2}\frac{(-1)^{k}(\frac{1}{2})_{k}}{\gamma^{k}} \quad . \qquad (C10)$$

<u>$\lambda=1/2$</u>

As the developement of

$$I=\int_{0}^{\infty}\frac{x^{3/2}e^{-x}dx}{x^{-1}+\gamma} \qquad (C11)$$

requires use of the same equations needed for $\lambda=-1/2$, the derivation is indicated with less detail. Let $a=\gamma^{-1}$, then one acquires

$$I=a\int_{0}^{\infty}\frac{x^{5/2}e^{-x}dx}{x+a}$$

$$=a^{7/2}e^{a}\Gamma(7/2)\Gamma(\tfrac{1}{2}-3,a)$$

$$=a^{7/2}e^{a}\pi^{\frac{1}{2}}(-1)[\pi^{\frac{1}{2}}(1-\Phi(a^{\frac{1}{2}}))+a^{-\frac{1}{2}}e^{-a}(-1+\frac{1}{2a}-\frac{3}{(2a)^{2}})]$$

$$=\pi^{\frac{1}{2}}(\frac{3a}{4}-\frac{a^{2}}{2}+a^{3})-a^{7/2}e^{a}\pi^{\frac{1}{2}}[\pi^{\frac{1}{2}}(1-\Phi(a^{\frac{1}{2}}))]$$

$$=-\pi e^{a}a^{7/2}+\pi^{\frac{1}{2}}[\frac{3a}{4}-\frac{a^{2}}{2}+a^{3}+2a^{4}\sum_{k=0}^{\infty}\frac{(2a)^{k}}{(2k+1)!!}] \quad . \qquad (C12)$$

For large a I is approximated by

$$I \sim \pi^{\frac{1}{2}} a^3 \sum_{k=3} \frac{(-1)^{k-1}(\frac{1}{2})_k}{a^k} \quad . \tag{C13}$$

$\underline{\lambda=3/2}$

Here

$$I=\int_0^\infty \frac{x^{3/2}e^{-x}dx}{x^{-3}+\gamma} \tag{C14}$$

becomes, through use of Eq. (A17), if $a=\gamma^{-1/3}$

$$I=a^3\int_0^\infty \frac{x^{9/2}e^{-x}dx}{x^3+a^3}$$

$$=\frac{a}{3}\left[\int_0^\infty \frac{x^{9/2}e^{-x}dx}{x+a}+(e^{i2\pi/3}\int_0^\infty \frac{x^{9/2}e^{-x}dx}{x+ae^{i2\ /3}}+\text{c.c.})\right]$$

$$=\frac{a}{3}\left[a^{9/2}e^{a}\,\Gamma(\tfrac{11}{2})\,\Gamma(\tfrac{-9}{2},a)\ -\right.$$

$$\left.(e^{i2\pi/3}a^{9/2}e^{a\exp(i2\pi/3)}\Gamma(\tfrac{11}{2})\,\Gamma(\tfrac{-9}{2},ae^{i2\pi/3})+\text{c.c.})\right] \quad . \tag{C15}$$

Considering the recursion

$$\Gamma(-9/2,a)=\Gamma(\tfrac{1}{2}-5,a)$$

$$=-\frac{2^5}{9!!}\left[\pi^{\frac{1}{2}}(1-\Phi(a^{\frac{1}{2}}))+a^{-\frac{1}{2}}e^{-a}\sum_{k=1}^{5}\frac{(-1)^k(2k-3)!!}{(2a)^{k-1}}\right] \tag{C16}$$

then through the tedious developement

$$I=\frac{a}{3}\left\{-a^{9/2}e^{a}\pi+2\pi^{\frac{1}{2}}a^5\sum_{k=0}^{\infty}\frac{(2a)^k}{(2k+1)!!}\ -\right.$$

$$\pi^{\frac{1}{2}}a^4(-1+\frac{1}{2a}-\frac{3}{(2a)^2}+\frac{5\cdot 3}{(2a)^3}-\frac{7\cdot 5\cdot 3}{(2a)^4})-$$

$$[e^{i2\pi/3}(-a^{9/2}e^{a\exp(i2\pi/3)}\pi+e^{i\pi/3}a^5\pi^{\frac{1}{2}}2\sum_{k=0}^{\infty}\frac{(2a)^k}{(2k+1)!!}e^{i2\pi k/3}-$$

$$e^{-i\pi/3}\pi^{\frac{1}{2}}a^4(-1+\frac{1}{2a}e^{-i2\pi/3}-\frac{3}{(2a)^2}e^{i2\pi/3}+\frac{5\cdot3}{(2a)^3}-$$

$$\frac{7\cdot5\cdot3}{(2a)^4}e^{-2\pi/3}))+\text{c.c.}]\}$$

$$=\frac{a}{3}\{-a^{9/2}e^a\pi+2\pi^{\frac{1}{2}}a^5\sum_{k=0}^{\infty}\frac{(2a)^k}{(2k+1)!!}+$$

$$\pi^{\frac{1}{2}}a^4(1-\frac{1}{2a}+\frac{3}{(2a)^2}-\frac{5\cdot3}{(2a)^3}+\frac{7\cdot5\cdot3}{(2a)^4})-$$

$$2[-a^{9/2}e^{a\cos(2\pi/3)}\pi\ \cos(a\sin(2\pi/3)+2\pi/3)+$$

$$2\pi^{\frac{1}{2}}[\cos(\pi)(\sum_{k=0}^{\infty}\frac{(2a)^{3k}}{(6k+1)!!})+\cos(-\pi/3)(2a\sum_{k=0}^{\infty}\frac{(2a)^{3k}}{(6k+3)!!})+$$

$$\cos(\pi/3)((2a)^2\sum_{k=0}^{\infty}\frac{(2a)^{3k}}{(6k+5)!!})]a^5+$$

$$\pi^{\frac{1}{2}}a^4[\cos(\pi/3)(1-\frac{5\cdot3}{(2a)^3})+\cos(-\pi/3)(-\frac{1}{2a}+\frac{7\cdot5\cdot3}{(2a)^4})+$$

$$\cos(\pi)(\frac{3}{(2a)^2})]]\}\quad,$$

the expansion

$$I=-a^{11/2}\pi[e^a-2e^{-a/2}\cos(a3^{\frac{1}{2}}/2+2\pi/3)]+3\pi^{\frac{1}{2}}a^3/4+2\pi^{\frac{1}{2}}a^6\sum_{k=0}^{\infty}\frac{(2a)^{3k}}{(6k+1)!!}\tag{C17}$$

is acquired. For large a one has

$$I\sim\frac{a\pi^{\frac{1}{2}}}{3}[-a^4\sum_{k=5}\frac{(-1)^k(\frac{1}{2})_k}{a^k}+(e^{i\pi/3}\sum_{k=5}\frac{(-1)^k(\frac{1}{2})_k}{a^k}e^{-i2\pi k/3}+\text{c.c.})a^4]$$

$$=\frac{a^5\pi^{\frac{1}{2}}}{3}[-\sum_{k=5}\frac{(-1)^k(\frac{1}{2})_k}{a^k}+(e^{i\pi/3}\sum_{k=2}\frac{(-1)^k(\frac{1}{2})_k}{a^{3k}}-$$

$$e^{-i\pi/3}\frac{1}{a}\sum_{k=2}\frac{(-1)^k(\frac{1}{2})_{3k+1}}{a^{3k}}-\sum_{k=1}\frac{(-1)^k(\frac{1}{2})_{3k+2}}{a^{3k+2}}+c.c.)]$$

or

$$I\sim\pi^{\frac{1}{2}}a^3\sum_{k=1}\frac{(-1)^{k-1}(\frac{1}{2})_{3k+2}}{a^{3k}} \quad . \tag{C18}$$

Magnetoconductivity

The expansion of the integral

$$I=\int_0^\infty\frac{x^{3/2-\lambda}e^{-x}dx}{x^{-2\lambda}+\gamma} \tag{C19}$$

found in Eq. (2.32) is similar to that of the above integrals. These integrals are included for several reasons: 1) magnetoconductivity data offers as much information to the experimenter as does Hall conductivity data and thus presents an alternate means to determine number densities and mobilities, 2) the integrals are closely related to the Hall conductivity integrals and require little additional development, and 3) a future extension to these integrals of approximations similar to those in Chapter III may create a convenient means of studying semiconductors having ellipsoidal energy surfaces.

$\underline{\lambda=0}$

Eq. (C6) is identical to

$$I=\int_0^\infty\frac{x^{3/2}e^{-x}dx}{1+\gamma}$$

$$=\Gamma(5/2)/(1+\gamma) \quad . \tag{C20}$$

$\lambda=-1/2$

By use of Eqs. (C19), (C3), (B8), (B2), (B23), (B43), and (B44), one acquires

$$I=\int_0^\infty \frac{x^2 e^{-x}dx}{x+\gamma}$$

$$=\gamma^2 e^\gamma \,\Gamma(3)\,\Gamma(-2,\gamma)$$

$$=\gamma^2 e^\gamma[(-1)^2\,\Gamma(0,\gamma)+e^{-\gamma}\sum_{k=1}^{2}\frac{(k-1)!}{\gamma^k}(-1)^{2-k}]$$

$$=\gamma^2 e^\gamma[-Ei(-\gamma)+e^{-\gamma}(\frac{1}{\gamma^2}-\frac{1}{\gamma})]$$

$$=-\gamma^2 e^\gamma Ei(-\gamma)+1-\gamma$$

$$=1-\gamma-\gamma^2 e^\gamma[C+\ln(\gamma)+\sum_{k=1}^{\infty}\frac{(-\gamma)^k}{k\cdot k!}] \,, \tag{C21}$$

where C is Euler's constant. For large γ an asymptotic expansion is obtained with aid of Eq. (B46)

$$I \sim \sum_{k=2}\frac{(-1)^k k!}{\gamma^{k-1}} \quad . \tag{C22}$$

$\lambda=1/2$

Let $a=\gamma^{-1}$, then use Eq. (C21) to acquire

$$I=\int_0^\infty \frac{xe^{-x}dx}{x^{-1}+\gamma}$$

$$=a\int_0^\infty \frac{x^2 e^{-x}dx}{x+a}$$

$$=a[1-a-a^2 e^a(C+\ln(a)+\sum_{k=1}^{\infty}\frac{(-a)^k}{k\cdot k!})] \;. \tag{C23}$$

For large a, Eq. (C22) provides

$$I \sim \sum_{k=2} \frac{(-1)^k k!}{a^{k-2}} \quad . \tag{C24}$$

λ=3/2

Let $a=\gamma^{-1/3}$, then develop the lengthy expression

$$I=\int_0^\infty \frac{xe^{-x}dx}{x^{-3}+\gamma}$$

$$=a^3\int_0^\infty \frac{x^3e^{-x}dx}{x^3+a^3}$$

$$=\frac{a}{3}\left[\int_0^\infty \frac{x^3e^{-x}dx}{x+a}+(e^{i2\pi/3}\int_0^\infty \frac{x^3e^{-x}dx}{x+ae^{i2\pi/3}}+c.c.)\right]$$

$$=\frac{a}{3}[a^3e^a\,\Gamma(4)\,\Gamma(-3,a)+$$

$$(e^{i2\pi/3}a^3e^{a\exp(i2\pi/3)}\,\Gamma(4)\,\Gamma(-3,ae^{i2\pi/3})+c.c.)]$$

$$=\frac{a^4}{3}\Big\{e^a[Ei(-a)+e^{-a}\sum_{k=1}^{3}\frac{(k-1)!}{a^k}(-1)^{3-k}]+$$

$$[e^{i2\pi/3}e^{a\exp(i2\pi/3)}\,(Ei(-ae^{i2\pi/3})+$$

$$e^{-a\exp(i2\pi/3)}\,\sum_{k=1}^{3}\frac{(k-1)!}{a^k}(-1)^{3-k}e^{i2\pi/3})+c.c.]\Big\}$$

$$=\frac{a}{3}\Big\{a^3e^a[C+\ln(a)+\sum_{k=1}^{\infty}\frac{(-1)^k}{k\cdot k!}]+a^2-a+2+$$

$$[e^{i2\pi/3}(a^3e^{a\exp(i2\pi/3)}\,(C+\ln(a)+\frac{i2}{3}+\sum_{k=1}^{\infty}\frac{(-a)^k}{k\cdot k!}e^{i2\pi k/3})+$$

$$a^2e^{-i2\pi/3}-ae^{i2\pi/3}+2)+c.c.]\Big\}$$

$$=a^3+\frac{a^4}{3}\Big\{e^a[C+\ln(a)+\sum_{k=1}^{\infty}\frac{(-a)^k}{k\cdot k!}]+$$

$$2e^{-a/2}[(C+\ln(a)+\sum_{k=1}^{\infty}\frac{(-1)^k a^{3k}}{(3k)(3k)!})\cos(\frac{a3^{\frac{1}{2}}}{2}+\frac{2\pi}{3})-$$

$$(\sum_{k=1}^{\infty}\frac{(-1)^k a^{3k-1}}{(3k-1)(3k-1)!})\cos(\frac{a3^{\frac{1}{2}}}{2})+$$

$$(\sum_{k=1}^{\infty}\frac{(-1)^k a^{3k-2}}{(3k-2)(3k-2)!})\cos(\frac{a3^{\frac{1}{2}}}{2}-\frac{2\pi}{3})-\frac{2\pi}{3}\sin(\frac{a3^{\frac{1}{2}}}{2}+\frac{2\pi}{3})]\Big\} \quad .(C25)$$

For large a one may write

$$I\sim\frac{a^4}{3}\Big\{[\sum_{k=4}\frac{(-1)^k(k-1)!}{a^k}]+[e^{i2\pi/3}\sum_{k=4}\frac{(-1)^k(k-1)!}{a^k}e^{-i2\pi k/3}+c.c.]\Big\}$$

$$=\frac{a^4}{3}\Big\{[\sum_{k=4}\frac{(-1)^k(k-1)!}{a^k}]+2[\sum_{k=1}\frac{(-1)^{k-1}(3k)!}{a^{3k+1}}+$$

$$\cos(-2\pi/3)(\sum_{k=1}\frac{(-1)^k(3k+1)!}{a^{3k+2}})+\cos(2\pi/3)(\sum_{k=2}\frac{(-1)^k(3k-1)!}{a^{3k}})]\Big\}$$

or

$$I\sim a^3\sum_{k=1}\frac{(-1)^{k-1}(3k)!}{a^{3k}} \quad . \qquad (C26)$$

APPENDIX D

PROGRAMS TO DETERMINE APPROXIMATIONS OF S

The process of determining approximations of

$$S(\lambda;\gamma) \equiv \frac{1}{\Gamma(5/2+\lambda)} \gamma^{\frac{1}{2}} \int_0^\infty \frac{x^{3/2}e^{-x}dx}{x^{-2\lambda}+\gamma} \qquad \text{(D1)}$$

is described in Chapter III. These approximations were determined with the aid of an IBM 360/50 computer using a program written in FORTRAN IV.

Calculation of S_M

Before initiating the approximation process one must calculate S over an appropriate range of γ including γ_M, corresponding to S_M the maximum value of S. The Newton-Raphson method is employed to determine γ such that $\frac{dS}{d\gamma}=0$.[26]

Main

```
      DOUBLE PRECISION X(125),Y(125),B(10),T
      DIMENSION X1(125),Y1(125)
      DO 2 I=2,10
    2 B(I)=0.D0
      X(1)=1.D0
C     PROGRAM FINDS MAXIMUM VALUE OF S BY ITERATION IN LOOP
C     BELOW.  FIRST DERIVATIVE OF S, Y(1), AT X(1) DIVIDED BY
C     SECOND DERIVATIVE OF S, Y(2), AT X(1).  THIS IS THEN
```

```
C  SUBSTRACTED FROM X(1) TO FORM NEW X(1).  IF DIFFERENCE
C  SMALL THEN ITERATION HALTED.
   10 K=1
      B(1)=DSQRT(X(1))
      CALL DGL32(K,X(1),B,T)
      Y(1)=.5D0*T/B(1)
      Y(2)=-.25D0*T/(B(1)*X(1))
      K=2
      CALL DGL32(K,X(1),B,T)
      Y(1)=Y(1)-T*B(1)
      Y(2)=Y(2)-T/B(1)
      K=3
      CALL DGL32(K,X(1),B,T)
      Y(2)=Y(2)+2.D0*B(1)*T
      T=Y(1)/Y(2)
      WRITE (6,102) X(1),Y(1),Y(2),T
  102 FORMAT(4D20.9)
      X(1)=X(1)-T
      IF(DABS(T).GT.1.D-06)GO TO 10
      K=1
      CALL DGL32(K,X(1),B,T)
      WRITE (6,101) X(1),T
  101 FORMAT (2D20.7)
      B(1)=DLOG10(X(1))-2.04D0
C  S IS CALCULATED FOR A RANGE OF VALUES ABOUT THE MAXIMUM
C  OF S AND PLOTTED.
```

```
      DO 1 I=1,125
      T=B(1)+.04D0*DFLOAT(I)
      X1(I)=T
      X(I)=10.D0**T
      CALL DGL32(K,X(I),B,T)
      Y(I)=T*DSQRT(X(I))
      WRITE (6,101) X(I),Y(I)
    1 Y1(I)=Y(I)
      CALL PPLOT(X1,Y1,1,125,0,6)
      STOP
      END
```

<u>DGL32</u>

This subroutine from the IBM Scientific Subroutine Package[27] uses Laguerre-Gauss quadrature to calculate

$$\int_0^\infty f(x)x^{-\frac{1}{2}}e^{-x}dx=\sum_{i=1}^{32} w_i f(x_i)+(32)!\,\Gamma(32.5)f^{(64)}(\xi)/(64)! \quad , \quad \text{(D2)}$$

where $0\leq\xi<\infty$, x_i is the <u>i</u>th zero of $L_{32}^{-\frac{1}{2}}(x)$, one of the generalized Laguerre polynominals, and

$$w_i=(32)!\,\Gamma(32.5)x_i/[L_{33}^{-\frac{1}{2}}(x_i)]^2 \quad .^{28} \quad \text{(D3)}$$

```
      SUBROUTINE DGL32(K,A,B,Y)
C  SUB. COMPUTES INTEGRAL (EXP(-X)*FNC(X)/SQRT(X)),
C  SUMMED OVER X FROM 0 TO INFINITY
      DOUBLE PRECISION X,Y,FNC,B(10)
      X=.11079926894708D3
```

```
Y=.11071413071714D-47*FNC(K,A,B,X)
X=.97916716426063D2
Y=Y+.33594959802163D-42*FNC(K,A,B,X)
X=.87856119943134D2
Y=Y+.68422760225115D-38*FNC(K,A,B,X)
X=.79339086528823D2
Y=Y+.31147812492595D-34*FNC(K,A,B,X)
X=.71868499359551D2
Y=Y+.50993217982260D-31*FNC(K,A,B,X)
X=.65184426376136D2
Y=Y+.38582071909299D-28*FNC(K,A,B,X)
X=.59129027934392D2
Y=Y+.15723595577852D-25*FNC(K,A,B,X)
X=.53597231826149D2
Y=Y+.38234137666013D-23*FNC(K,A,B,X)
X=.48514583867416D2
Y=Y+.59657255685597D-21*FNC(K,A,B,X)
X=.43825886369904D2
Y=Y+.63045091330076D-19*FNC(K,A,B,X)
X=.39488797123368D2
Y=Y+.47037694213516D-17*FNC(K,A,B,X)
X=.35469961396173D2
Y=Y+.25601867826449D-15*FNC(K,A,B,X)
X=.31742543790617D2
Y=Y+.10437247453182D-13*FNC(K,A,B,X)
X=.28284583194971D2
```

```
Y=Y+.32566814614194D-12*FNC(K,A,B,X)
X=.25077856544198D2
Y=Y+.97183555338954D-11*FNC(K,A,B,X)
X=.22107070382206D2
Y=Y+.15230434500291D-9*FNC(K,A,B,X)
X=.19359271087269D2
Y=Y+.23472334846431D-8*FNC(K,A,B,X)
X=.16823405362954D2
Y=Y+.29302506329522D-7*FNC(K,A,B,X)
X=.14489986690780D2
Y=Y+.29910658734545D-6*FNC(K,A,B,X)
X=.12350838217715D2
Y=Y+.25166805020624D-5*FNC(K,A,B,X)
X=.10398891905553D2
Y=Y+.17576998461701D-4*FNC(K,A,B,X)
X=.86280298574059D1
Y=Y+.10251858271573D-3*FNC(K,A,B,X)
X=.70329577982839D1
Y=Y+.50196739702612D-3*FNC(K,A,B,X)
X=.56091034574962D1
Y=Y+.20726581990152D-2*FNC(K,A,B,X)
X=.43525345293301D1
Y=Y+.72451739570689D-2*FNC(K,A,B,X)
X=.32598922564569D1
Y=Y+.21512081019758D-1*FNC(K,A,B,X)
X=.23283376682104D1
```

```
Y=Y+.544062579O7378D-1*FNC(K,A,B,X)
X=.155550823l4789D1
Y=Y+.11747996392820D0*FNC(K,A,B,X)
X=.939483214500 73D0
Y=Y+.216996698612 37D0*FNC(K,A,B,X)
X=.478756477277 49D0
Y=Y+.343371684698 17D0*FNC(K,A,B,X)
X=.172215724145 40D0
Y=Y+.465989572125 36D0*FNC(K,A,B,X)
X=.191275109684 47D-1
Y=Y+.542754849882 61D0*FNC(K,A,B,X)
RETURN
END
```

FNC

Here the integrand in Eq. (D1) for $\lambda=-\frac{1}{2}$ is calculated along with functions necessary to form the first and second derivatives of $S(-\frac{1}{2};\gamma)$ with respect to γ.

```
  FUNCTION FNC(K,A,B,X)
  DOUBLE PRECISION A,B(10),X,FNC
  GO TO (1,2,3),K
1 FNC=X*X/(X+A)
  RETURN
2 FNC=X*X/(X+A)**2
  RETURN
3 FNC=X*X/(X+A)**3
```

RETURN

END

Calculation of S

Four hundred values of S were calculated and stored on cards by a simple program, not listed here, which used the subroutine DGL32 and FNC. These S correspond to γ equally spaced with twenty points per decade in log space from $\gamma=10^{-10}\gamma_M$ to approximately $\gamma=10^{10}\gamma_M$. As a check, for $\lambda=-\frac{1}{2}$, the S were recalculated at selected points by use of Eqs. (2.38) and (2.39). In the range of γ, for which the asymptotic expression is appropreate, errors of one part in 10^7 or less were found which is negligible for the intended use; however, for small γ the errors became substantially larger than one part in 10^5. Over this latter range of γ the S were recomputed using Eq. (2.38) and a set of corrected cards were punched with errors no larger than one part in 10^7. This procedure was repeated for each λ.

Calculation of S*

Main

This program is used to approximate $S(\lambda;\gamma)$ for several λ. By modifying the initial guesses of the zeros of S*-S, allowance may be made for various λ. As listed the program calculates $S^*(3/2;\gamma)$ to order N=6 before failing; however, by removing the statement labeled 85 and inserting

```
      J=210+N
   85 IZ(I)=J+((60+N)*(IZ(I)-J))/80
```

S*(3/2;γ) is determined to order N=8. Additional information is provided by COMMENT statements.

```
      DOUBLE PRECISION X(400),Y(400),E(400),EM(400),EX,SUM
     1ER,EPI,A(10),B(10),XS(20),YS(20),YH,YH1
      DIMENSION XP(125),YP(125),IZ(400)
      READ(5,102)(Y(I),I=1,400)
  102 FORMAT(5D16.7)
      DO 1 I=1,400
    1 X(I)=10.D0**(.05D0*DFLOAT(I-1)-10.D0)
      DO 11 I=1,125
   11 XP(I)=.05*FLOAT(I)-3.15
      EPI=1.D-7
      KP=0
      NP=2
      NP1=3
      N=1
      N1=2
      ER=0.D0
C  INITIAL GUESSES FOR ZEROS OF YH-Y(I) OF ORDER N=1
      XS(1)=X(191)
      YS(1)=Y(191)
      XS(2)=X(211)
      YS(2)=Y(211)
C  ITERATION LOOP TO CALCULATE A AND B BEGINS HERE
```

```
    4 CALL CONST(NP,XS,YS,A,B)
      DO 5 I=1,400
      YH=A(N)
      IF(N.EQ.1) GO TO 51
      DO 52 J=2,N
   52 YH=YH*X(I)+A(N1-J)
   51 YH=YH*DSQRT(X(I))
      YH1=B(N)
      IF(N.EQ.1) GO TO 53
      DO 54 J=2,N
   54 YH1=YH1*X(I)+B(N1-J)
   53 YH1=YH1*X(I)+1.D0
      YH=YH/YH1
    5 E(I)=YH-Y(I)
      DO 55 I=139,263
      I1=I-138
   55 YP(I1)=E(I)
      KP=KP+1
      IF(KP.GT.50) STOP
C  MAKE PRINTER PLOT OF FIRST FIVE APPROXIMATIONS TO YH-Y(I)
C  OF ORDER N
      IF(KP.GT.5) GO TO 56
      CALL PPLOT(XP,YP,1,125,0,6)
   56 WRITE(6,101)((A(I),B(I)),I=1,N)
  101 FORMAT(2D25.16)
C  PRINT ER, THE AVERAGE OF THE 2*N+1 SELECTED EXTREMA OF
```

```
C  YH-Y(I)  (ER SET EQUAL TO ZERO BEFORE FIRST ITERATION)
      WRITE(6,102) ER
C  LOOP DETERMINES ALL EXTREMA OF E(I)=YH-Y(I)
      J=0
      DO 61 I=1,398
      IF((E(I+1)-E(I))*(E(I+2)-E(I+1)).GT.0.D0) GO TO 61
      J=J+1
      IZ(J)=I+1
   61 CONTINUE
      DO 62 I=1,J
      I1=IZ(I)
   62 EM(I)=E(I1)
C  N LARGEST MAXIMA LOADED INTO EM(1) - EM(N)
      DO 91 K=1,N
      DO 91 I=K,J
      IF(EM(I).LT.EM(K)) GO TO 91
      EX=EM(I)
      EM(I)=EM(K)
      EM(K)=EX
      I1=IZ(I)
      IZ(I)=IZ(K)
      IZ(K)=I1
   91 CONTINUE
C  N LARGEST MINIMA LOADED INTO EM(N+1) - EM(2*N)
      DO 92 K=N1,NP
      DO 92 I=K,J
```

```
      IF(EM(I).GT.EM(K)) GO TO 92
      EX=EM(I)
      EM(I)=EM(K)
      EM(K)=EX
      I1=IZ(I)
      IZ(I)=IZ(K)
      IZ(K)=I1
   92 CONTINUE
C  LARGEST REMAINING EXTREMUM LOADED INTO EM(2N+1)
      K=NP1
      DO 93 I=K,J
      IF(DABS(EM(I)).LT.DABS(EM(K))) GO TO 93
      EX=EM(I)
      EM(I)=EM(K)
      EM(K)=EX
      I1=IZ(I)
      IZ(I)=IZ(K)
      IZ(K)=I1
   93 CONTINUE
      SUM=0.D0
      DO 7 K=1,NP1
    7 SUM=SUM+DABS(EM(K))
      ER=SUM/DFLOAT(NP1)
      DO 8 K=1,NP1
      IF(DABS(DABS(EM(K))-ER).GT.EPI) GO TO 81
    8 CONTINUE
```

```
C  AFTER DETERMINING THE BEST YH OF ORDER N, THE COMPUTER
C  FINDS THE 2*N ZEROS OF YH-Y(I)
      J=0
      EX=E(1)
      DO 82 I=2,399
      IF(EX*E(I).GT.0.D0) GO TO 82
      IF(E(I).EQ.0.D0) GO TO 82
      J=J+1
      IZ(J)=I
   82 EX=E(I)
      I1=IZ(J)-IZ(J-1)
      IZ(J+2)=IZ(J)+I1
      DO 83 I=1,J
      I1=J+2-I
   83 IZ(I1)=IZ(I1-1)
      I1=IZ(3)-IZ(2)
      IZ(1)=IZ(2)-I1
      NP=NP+2
      CALL PPLOT(XP,YP,1,125,0,6)
      IF(NP.GT.14) STOP
      NP1=NP+1
      N=NP/2
      N1=N+1
      ER=0.D0
      KP=0
C  THE ZEROS OF YH-Y(I) OF ORDER N+1 ARE ESTIMATED
```

```
      DO 85 I=1,NP
   85 IZ(I)=211+(3*(IZ(I)-211))/4
      DO 84 K=1,NP
      I=IZ(K)
      XS(K)=X(I)
   84 YS(K)=Y(I)
      GO TO 4
   81 DO 9 K=1,NP
      I=IZ(K)
      XS(K)=X(I)
    9 YS(K)=Y(I)+DSIGN(ER,EM(K))
      GO TO 4
      END
```

CONST

After CONST calculates the coefficients of Eq. (3.21), DPG solves for the a_j and b_j.

```
      SUBROUTINE CONST(NP,X,Y,A,B)
      DOUBLE PRECISION X(20),Y(20),A(10),B(10),C(20,21),T,P(20)
C   NP IS THE NUMBER OF PARAMETERS
C   X,Y ARE NP PAIRS OF DATA POINTS
C   A,B ARE NP CONSTANTS DETERMINED FROM NP LINEAR EQUATIONS
C   CONTAINING THE X,Y
      N=NP/2
      N1=N+1
      NP1=NP+1
```

```
      DO 1 I=1,NP
      T=Y(I)/DSQRT(X(I))
      C(I,1)=1.D0
      C(I,NP1)=T
      C(I,N1)=-T*X(I)
      IF(N.LT.2) GO TO 1
      DO 4 J=2,N
      C(I,J)=X(I)*C(I,J-1)
      NJ=N+J
    4 C(I,NJ)=X(I)*C(I,NJ-1)
    1 CONTINUE
      CALL DPG(NP,C,P)
      DO 2 I=1,N
      A(I)=P(I)
    2 B(I)=P(I+N)
      RETURN
      END
```

<u>DPG</u>

This subroutine solves a set of NP linear equations by means of double pivoting and Gaussian eliminiation. The process is described by Isaacson and Keller.[29]

```
      SUBROUTINE DPG(NP,T,DP)
      DIMENSION KEEP(20)
      DOUBLE PRECISION C(20,21),A,B,DP(20),T(20,21)
      NP1=NP+1
```

```
      DO 2 I=1,NP
      KEEP(I)=I
      DO 2 J=1,NP1
    2 C(I,J)=T(I,J)
      L=NP-1
      DO 3 I=1,L
      A=0.D0
      DO 1 II=I,NP
      DO 1 JJ=I,NP
      IF(DABS(C(II,JJ)).LT.A) GO TO 1
      A=DABS(C(II,JJ))
      III=II
      JJJ=JJ
    1 CONTINUE
      DO 4 K=I,NP1
      B=C(I,K)
      C(I,K)=C(III,K)
    4 C(III,K)=B
      KP=KEEP(I)
      KEEP(I)=KEEP(JJJ)
      KEEP(JJJ)=KP
      DO 5 K=1,NP
      B=C(K,I)
      C(K,I)=C(K,JJJ)
    5 C(K,JJJ)=B
      A=C(I,I)
```

```
      DO 10 II=I,NP1
   10 C(I,II)=C(I,II)/A
      I1=I+1
      DO 3 II=I1,NP
      A=C(II,I)
      DO 3 JJ=I1,NP1
    3 C(II,JJ)=C(II,JJ)-A*C(I,JJ)
      C(NP,NP1)=C(NP,NP1)/C(NP,NP)
      DO 7 I=1,NP
    7 DP(I)=C(I,NP1)
      DO 6 I=2,NP
      II=NP1-I
      JJ=NP-1
      DO 6 J=II,JJ
    6 DP(II)=DP(II)-DP(J+1)*C(II,J+1)
      DO 8 I=1,NP
    8 C(1,I)=DP(I)
      DO 9 I=1,NP
      K=KEEP(I)
    9 DP(K)=C(1,I)
      RETURN
      END
```

APPENDIX E

LEAST-SQUARES DETERMINATION OF PARAMETERS

Theory of Least-Squares

By comparing observed values $\hat{y}_i$ for i=1,2,...,ND of a physically neasurable variable with the theoretically expected values $y=y(\vec{p};x)$, where $\vec{p}=(p_1,\ldots,p_j,\ldots,p_{NP})$ represents adjustable parameters p_j and x is an independent variable, one may extract physically meaningful information in terms of $\vec{p}$. A common method is to minimize the sum of the squares of the deviations

$$s=\sum_{i=1}^{ND}(y-\hat{y}_i)^2 \quad . \tag{E1}$$

In practice this may be accomplished by solving

$$\frac{\partial s}{\partial p_k}=2\sum_{i=1}^{ND}(y-\hat{y}_i)\frac{\partial y}{\partial p_k}$$

$$=0 \tag{E2}$$

for k=1,2,...,NP and by rejecting those solutions which are unphysical or do not provide an absolute minimum s. Through expanding y as a Taylor series

$$y(\vec{p};x)=y(\vec{p}^*;x)+\sum_{j=1}^{NP}\frac{\partial y}{\partial p_j}\bigg|_{\vec{p}^*}(p_j-p_j^*)+\ldots \tag{E3}$$

and supposing $\vec{p}^*$ is near a solution $\vec{p}$ of Eq. (E2) so that quadratic and higher terms may be ignored, one obtains

$$\frac{\partial s}{\partial p_k} = 2\sum_{i=1}^{ND}\left[y(\vec{p}^*;x_i) + \sum_{j=1}^{NP}\frac{\partial y}{\partial p_j}(p_j - p_j^*) - \hat{y}_i\right]\frac{\partial y}{\partial p_k}$$

$$= 0 \qquad \text{(E4)}$$

or, equivalently,

$$\sum_{j=1}^{NP}\Delta p_j \sum_{i=1}^{ND}\frac{\partial y_i}{\partial p_j}\frac{\partial y_i}{\partial p_k} = -\sum_{i=1}^{ND}\Delta y_i \frac{\partial y_i}{\partial p_k} \quad , \qquad \text{(E5)}$$

where $\Delta p = p_j - p_j^*$, $\Delta y_i = y(\vec{p}^*;x_i) - \hat{y}_i$, and $k=1,2,\ldots,NP$. Thus Eq. (E5) is a set of NP linear equations which may be solved by Gaussian elimination with the aid of a digital computer.

Least-Squares Program

The program below, written in FORTRAN IV for an IBM 360/50 computer, extracts parameters by means of iteration. After accepting the data and initialization information, a cycle of solving Eq. (E5) for $\Delta\vec{p}$ and then calculating a new estimate of $\vec{p}$ is begun. This process continues until convergence occurs or the number of iterations exceeds a test, in which case the program terminates.

Several subroutines are used. These are: the major subroutine LSQ, which contains the iteration process; DPG, a program, listed in Appendix D, to solve linear equations; and FNDIR, which calculates y and $\frac{\partial y}{\partial p_k}$. COMMENT statements are included to provide additional information. Since LSQ directs the least-squares calculation, a short program necessary in order to load the initial data into storage is not included.

LSQ

```
      SUBROUTINE LSQ(ND,X,Y,NP,FAC,P,IC,BA,BHW)
      DOUBLE PRECISION CF(20,21),ER,F,P(20),PF(20),SE,DP(20),
     1FAC(20),BA(20),BHW(20),ERP,SQ
      DIMENSION X(100),Y(100)
C  ND -- NUMBER OF DATA POINTS
C  NP -- NUMBER OF PARAMETERS
C  X,Y -- DATA
C  P -- PARAMETERS
C  BA -- CENTER OF ALLOWED RANGE OF P
C  BHW -- HALF-WIDTH OF RANGE OF P
C  FAC -- USED TO VARY STEP SIZE OF P
C  IC -- COUNTER
C  F -- CALCULATED VALUE OF Y
C  PF -- PARTIAL DERIVATIVES OF F WITH RESPECT TO P
C  ER -- DEVIATION, F-Y
C  ERP -- PER CENT DEVIATION, 100*ER/Y
C  SQ -- SUM OF ER*ER
C  SE -- STANDARD ERROR OF ESTIMATE
C  CF -- STORES COEFFICIENTS OF LINEAR EQUATIONS
C  DP -- SOLUTION OF LINEAR EQUATIONS
      NDP=ND-NP
      NP1=NP+1
      IC=0
      KNT=-1
      WRITE(6,103)
```

```
  103 FORMAT(//,10X,'X',19X,'Y',19X,'F',18X,'F-Y',16X,
     C'% DIF',//)
C  ITERATION LOOP BEGINS HERE
 1000 IC=IC+1
      IF(IC.LT.100) GO TO 51
      WRITE(6,100)
  100 FORMAT(' LSQ UNABLE TO FIT FUNCTION TO DATA')
      GO TO 700
   51 SQ=0.D0
      KNT=KNT+1
      IF(KNT.EQ.5) KNT=0
      IFD=1
      DO 11 L=1,ND
      CALL FNDIR(IFD,L,X,NP,P,PF,F)
      ER=F-DBLE(Y(L))
      SQ=SQ+ER*ER
      ERP=ER*1.D+2/DBLE(Y(L))
C  X, Y, F, ER, ERP PRINTED EVERY FIFTH ITERATION
      IF(KNT.NE.0) GO TO 11
      WRITE(6,101)X(L),Y(L),F,ER,ERP
   11 CONTINUE
      SE=DSQRT(SQ/DFLOAT(NDP))
      WRITE(6,101)SQ,SE
      DO 1 I=1,NP
      DO 1 J=1,NP1
    1 CF(I,J)=0.D0
```

```
      SQ=0.D0
      IFD=2
      DO 2 K=1,ND
      CALL FNDIR(IFD,K,X,NP,P,PF,F)
      ER=F-DBLE(Y(K))
      SQ=SQ+ER*ER
      DO 2 I=1,NP
      CF(I,NP1)=CF(I,NP1)-ER*PF(I)
      DO 2 J=1,NP
    2 CF(I,J)=CF(I,J)+PF(J)*PF(I)
      DO 4 I=2,NP
    4 CF(I,J)=CF(J,I)
      SE=DSQRT(SQ/DFLOAT(NDP))
      CALL DPG(NP,CF,DP)
      WRITE(6,908)(P(J),J=1,NP)
      WRITE(6,909)(DP(J),J=1,NP)
  909 FORMAT( 12H DEL. PARM. 6D18.8/(12X,6D18.8) )
C  NEW ESTIMATES OF P MADE, P=P+FAC*DP
      DO 5 I=1,NP
      P(I)=P(I)+DP(I)*FAC(I)
      IF(DABS(P(I)-BA(I))-BHW(I).GT.0.D0) GO TO 800
      GO TO 5
  800 IF(P(I)-BA(I).GE.0.D0) GO TO 801
      P(I)=BA(I)-BHW(I)
      GO TO 5
  801 P(I)=BA(I)+BHW(I)
```

```
    5 CONTINUE
C   CHECK FOR CONVERGENCE
      DO 6 I=1,NP
      IF(DABS(DP(I))/(DABS(P(I))+1.D-8).GE.1.D-6) GO TO 1000
    6 CONTINUE
      WRITE(6,908)(P(J),J=1,NP)
  908 FORMAT(/12H PARAMETERS 6D18.8/(12X,6D18.8) )
      WRITE(6,102)SE
  102 FORMAT(/,' THE STANDARD ERROR OF ESTIMATE IS',D18.8,/)
  700 IFD=1
      WRITE(6,103)
      DO 7 K=1,ND
      CALL FNDIR(IFD,K,X,NP,P,PF,F)
      ER=F-DBLE(Y(K))
      ERP=ER*100.D0/DBLE(Y(K))
    7 WRITE(6,101)X(K),Y(K),F,ER,ERP
  101 FORMAT(5D20.7)
      RETURN
      END
```

FNDIR

This subroutine varies depending upon the functional form of y. Here the program is specifically designed to calculate using the y of the example in Chapter IV. The use of subroutine SP indicates the application of piezoelectric scattering. SP and subroutines for other scattering mechanisms are listed in the next section.

```
      SUBROUTINE FNDIR(IFD,K,X,NP,P,PF,F)
      DOUBLE PRECISION P(20),PF(20),F,XX,G,A(4),Y,F1
      DIMENSION X(100)
      XX=DBLE(X(K)*X(K))
      N=NP/2
      F=0.D0
      DO 1 I=1,N
      I2=2*I
      I21=I2-1
      G=XX/P(I2)
      CALL SP(IFD,G,A,Y)
      F1=DBLE(X(K))*A(1)/(P(I2)*A(2))
      GO TO (1,2),IFD
    2 PF(I21)=F1
      PF(I2)=-P(I21)*(F1+XX*DBLE(X(K))*(A(3)-A(1)*A(4)/A(2))
     C/(A(2)*P(I2)*P(I2)))/P(I2)
    1 F=F+P(I21)*F1
      RETURN
      END
```

<u>SA</u>, <u>SP</u>, <u>SI</u>, <u>and</u> <u>SN</u>

Subroutines needed by FNDIR to calculate Hall conductivity for the scattering mechanisms listed in Table I are listed below. Use SA for $\lambda=-1/2$, SP for $\lambda=1/2$, SI for $\lambda=3/2$, and SN for $\lambda=0$. Coefficients used to create the first three subroutines are found in Table II. SN applies Eq. (2.37).

```
 SUBROUTINE SA(IFD,G,A,Y)
 DOUBLE PRECISION G,A(4),Y
 A(1)=(((190.90399D0*G+692.60155D0)*G+479.81762D0)*G+
C63.136891D0)*G+1.1224298D0
 A(2)=((((181.9301D0*G+942.89358D0)*G+1317.3871D0)*G+
C553.54454D0)*G+59.13848D0)*G+1.D0
 IF(IFD.EQ.1)RETURN
 A(3)=((763.61596D0*G+2077.8047D0)*G+959.63524D0)*G+
C63.136891D0
 A(4)=(((909.6505D0*G+3771.5743D0)*G+3952.1613D0)*G+
C1107.0891D0)*G+59.13848D0
 IF(IFD.EQ.2) RETURN
 Y=DSQRT(G)*A(1)/A(2)
 RETURN
 END

 SUBROUTINE SP(IFD,G,A,Y)
 DOUBLE PRECISION G,A(4),Y
 A(1)=((.12192377D0*G+1.4099598D0)*G+2.7765076D0)*G+
C1.0355748D0
 A(2)=(((.11433758D0*G+1.5157628D0)*G+4.504886D0)*G+
C4.038167D0)*G+1.D0
 IF(IFD.EQ.1)RETURN
 A(3)=(.36577131D0*G+2.8199196D0)*G+2.7765076D0
 A(4)=((.45735032D0*G+4.5472884D0)*G+9.009772D0)*G+
C4.038167D0
```

```
      IF(IFD.EQ.2)RETURN
      Y=DSQRT(G)*A(1)/A(2)
      RETURN
      END

      SUBROUTINE SI(IFD,G,A,Y)
      DOUBLE PRECISION G,A(4),Y
      A(1)=((((.604188D-3*G+.2876591D0)*G+9.97617D0)*G+
     C39.1796D0)*G+19.91651D0)*G+1.2259D0
      A(2)=(((((.386073D-3*G+.2013202D0)*G+9.14989D0)*G+
     C62.3096D0)*G+80.4167D0)*G+21.26549D0)*G+1.D0
      IF(IFD.EQ.1)RETURN
      A(3)=(((3.02094D-3*G+1.150636D0)*G+29.92851D0)*G+
     C78.3592D0)*G+19.91651D0
      A(4)=((((2.316438D-3*G+1.006601D0)*G+36.59956D0)*G+
     C186.9288D0)*G+160.8334D0)*G+21.26549D0
      IF(IFD.EQ.2)RETURN
      Y=DSQRT(G)*A(1)/A(2)
      RETURN
      END

      SUBROUTINE SN(IFD,G,A,Y)
      DOUBLE PRECISION G,A(4),Y
      A(1)=1.D0
      A(2)=G+1.D0
      A(3)=0.D0
      A(4)=1.D0
```

```
IF(IFD.EQ.2)RETURN
Y=DSQRT(G)*A(1)/A(2)
RETURN
END
```

APPENDIX F

SOLUTION OF BOLTZMANN EQUATION

Consider an isotropic, isothermal, conducting medium having an energy dependent relaxation time. Let the conductor have spherical, quadratic energy surfaces, i.e.

$$\epsilon=(\hbar^2/2m^*)\vec{k}^2 \qquad \text{(F1)}$$

with m*, the effective mass, and $\vec{k}$, the wave vector. If uniform electric and magnetic fields are applied then the Boltxmann equation is, according to Wilson,[30]

$$(e/\hbar)(\vec{E}+\vec{v}\times\vec{H}/c)\cdot\vec{\nabla}_k f+(f_0-f)/\tau=0 \quad , \qquad \text{(F2)}$$

where e>0 for electrons, and f and f_0 are, respectively, the distribution function and equilibrium distribution function. The group velocity is

$$\vec{v}=\hbar^{-1}\vec{\nabla}_k\epsilon \quad . \qquad \text{(F3)}$$

Suppose, as Wilson does,[31] the requirement

$$f=f_0-\phi(\vec{k})\frac{\partial f_0}{\partial\epsilon} \qquad \text{(F4)}$$

with ϕ containing only terms linear in elements of $\vec{E}$. Since f_0 is a function of energy alone then

$$\vec{\nabla}_k f_0=(\vec{\nabla}_k\epsilon)\frac{\partial f_0}{\partial\epsilon}$$

$$=\hbar\vec{v}\frac{\partial f_0}{\partial\epsilon} \quad . \qquad \text{(F5)}$$

Now observing

$$\vec{\nabla}_k f=\vec{\nabla}_k f_0-(\vec{\nabla}_k\phi)\frac{\partial f_0}{\partial\epsilon}-\phi\vec{\nabla}_k\frac{\partial f_0}{\partial\epsilon}$$

$$=\frac{\partial f_0}{\partial\epsilon}\hbar\vec{v}-\frac{\partial f_0}{\partial\epsilon}(\vec{\nabla}_k\phi)-\phi\frac{\partial^2 f_0}{\partial\epsilon^2}\hbar\vec{v} \tag{F6}$$

and

$$(\vec{v}\times\vec{H})\cdot\vec{v}=0\quad , \tag{F7}$$

the Boltzmann equation may be linearized as

$$e\vec{v}\cdot\vec{E}-(e/\hbar c)\vec{v}\times\vec{H}\cdot\vec{\nabla}_k\phi+\phi/\tau=0\quad . \tag{F8}$$

As the solution of Eq. (F8) is

$$\phi=-e\tau\vec{v}\cdot\vec{E} \tag{F9}$$

if $\vec{H}=0$, then the solution with $\vec{H}\neq 0$ may be

$$\phi=-e\tau\vec{v}\cdot\vec{F} \tag{F10}$$

where $\vec{F}$ is to be determined. Since

$$\vec{\nabla}_k\cdot\vec{v}=\hbar/m^* \tag{F11}$$

then

$$\vec{\nabla}_k\phi=-e\tau\ \hbar\vec{F}/m^*+\vec{v}(\vec{\nabla}_k\cdot\vec{F})\ -e\vec{v}\cdot\vec{F}\hbar\vec{v}\frac{\partial\tau}{\partial\epsilon}\ . \tag{F12}$$

Substitution of Eq. (F12) in Eq. (F8) and use of Eq. (F7) results in

$$\vec{v}\cdot[\vec{E}+(e\tau/m^*c)\vec{H}\times\vec{F}-\vec{F}]=0, \tag{F13}$$

i.e.

$$\vec{E}+(e\tau/m^*c)\vec{H}\times\vec{F}-\vec{F}=0\quad . \tag{F14}$$

Clearly the solution is of the form

$$\vec{F}=a\vec{E}+b\vec{H}+d\vec{E}\times\vec{H}\quad , \tag{F15}$$

where a, b, and d are scalar functions of $e\tau/m^*c$, $\vec{E}$, and $\vec{H}$.

By use of the identities

$$\vec{H}\times\vec{H}\equiv 0$$

and (F16)

$$\vec{E}\times\vec{H}\equiv -\vec{H}\times\vec{E} \quad ,$$

Eq. (F14) becomes

$$\vec{E}(1-a)+(e\tau a/m^*c+d)\vec{H}\times\vec{E}-b\vec{H}+e\tau d\vec{H}\times(\vec{E}\times\vec{H})/m^*c=0 \quad .\text{(F17)}$$

Since $\vec{H}$, $\vec{H}\times\vec{E}$, and $\vec{H}\times(\vec{E}\times\vec{H})$ are mutually perpendicular and $\vec{E}\cdot(\vec{H}\times\vec{E})=0$, one immediately has

$$d=-e\tau a/m^*c \qquad \text{(F18)}$$

and

$$b=\vec{E}\cdot\vec{H}(1-a)/H^2 \quad . \qquad \text{(F19)}$$

By using the identity

$$\vec{A}\times(\vec{B}\times\vec{C})\equiv(\vec{A}\cdot\vec{C})\vec{B}-(\vec{A}\cdot\vec{B})\vec{C} \quad , \qquad \text{(F20)}$$

Eq. (F17) may be written

$$[\vec{E}-(\vec{E}\cdot\vec{H})\vec{H}/H^2][(1-a)-(e\tau/m^*c)^2H^2a]=0 \quad , \qquad \text{(F21)}$$

which implies

$$a=[1+(e\tau/m^*c)^2H^2]^{-1} \quad . \qquad \text{(F22)}$$

Thus one has the solution, noted by Beer,[32]

$$\vec{F}=[\vec{E}-(e\tau/m^*c)\vec{E}\times\vec{H}+(e\tau/m^*c)^2(\vec{E}\cdot\vec{H})\vec{H}][1+(e\tau/m^*c)^2H^2]^{-1}. \quad \text{(F23)}$$

Eq. (F4) is now

$$f=f_0+e\tau\frac{\partial f_0}{\partial\epsilon}\vec{v}\cdot\vec{F} \quad , \qquad \text{(F24)}$$

where using the permutation tensor ε_{ijn} and Einstein notation, the dot product is

$$\vec{v}\cdot\vec{F}=(\hbar/m^*)[1+(e\tau/m^*c)^2H^2]^{-1}[k_j-(e\tau/m^*c)\varepsilon_{ijn}k_iH_n$$

$$+(e\tau/m^*c)^2k_iH_jH_n]E_j \quad . \qquad \text{(F25)}$$

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