A Discretized Spectral Approximation in Neutron Transport Theory. Some Numerical Considerations

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The half-range weight function, orthogonality integrals, and completeness theorems in the theory of kinetic equations are often not known, or when they are, are too complicated to be of much practical use. This suggests the use of full-range relations to solve half-range problems, and in this paper we investigate the adaptability of such an approach in the theory of one-speed neutron transport by a discretized spectral approximation formulated recently.

KEY WORDS: Neutron transport equation; Fokker-Planck equation; Brownian motion; boundary layer; half- and full-range expansions.

1. INTRODUCTION

The half-space problem in the theory of kinetic equations is an important and fundamental problem in the understanding of a boundary layer near a physical bounding wall. The problem is mathematically difficult for two base reasons. First, the kinetic equations describing the physical process cannot usually be solved exactly in most cases, requiring simplifications and/or approximations. The solution is generally an approximate one (e.g., a truncated series) of an approximate equation. Second, as the exact boundary condition at the wall cannot be satisfied by an approximate solution, the formulation of an appropriate approximate wall condition is needed. This stage is not at all trivial, and can indeed turn out to be as involved as the first. Our main concern in the present numerical adaptation of the discretized spectral approximation will be the investigation of such wall conditions to match the $\Delta \sigma_N$ solution. In general, the difficulty of this exercise

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is increased because the half-range weight function and orthogonality relations are either not known (e.g., Fokker–Planck equation) or are too complicated to be of much practical use (e.g., neutron transport equation). The linear one-speed neutron transport equation occupies, in this context, a special position in the theory of kinetic equations, as it happens to be the only equation whose half-space solutions have been studied fully and extensively by the singular eigenfunction technique.

The main aim of the present paper is to examine, in a systematic manner, the possibility of obtaining approximate, converging solutions of the half-range (HR) problem—which can be solved exactly only if the HR weight function, orthogonality, and completeness relations are fully established—using the full-range (FR) weight function, orthogonality, and completeness relations. These full-range relations are simpler than the corresponding half-range ones and their intelligent use can help obtain needed information on the kinetic boundary layer.

Such an approach was used earlier both in the context of the neutron transport equation and the Brownian motion Fokker–Planck equation. In the former case, the exit distribution at the boundary has been extensively computed by the F_N approximation,⁽¹⁾ while for Brownian motion, Burschka and Titulaer⁽²⁾ used the FR weight function in the HR interval \mathbf{R}_+ to predict the Milne extrapolation length. Marshall and Watson⁽³⁾ recently gave a rather involved exact solution of the boundary layer problem of the Fokker–Plank equation using Weiner–Hopf methods, while Mayya⁽⁴⁾ developed an integral equation for the incident distribution of Brownian particles on a bounding wall—equivalent in neutron transport to the exit distribution from the medium—whose properties he studied asymptotically; see also Titulaer⁽⁵⁾ for a similar approach.

In contrast, our approach to the use of FR properties for HR problems is more direct, and in Schemes 3 and 4 below a complete solution of the HR problem using only FR relations and the HR basis set for representation of all incident and exit distributions is given. Even though the specific example and numerical results given here are for one-speed neutron transport, the methods developed apply to other linear models in the theory of kinetic equations, e.g., the Fokker–Planck equation.

2. THE $\Delta \sigma_N$ APPROXIMATION

A summary of the discretized spectral approximation in neutron transport theory is given here; for details see Sengupta and Venkatesan.⁽⁶⁾ The neutron transport equation

$$\mu \frac{\partial \psi(x,\mu)}{\partial x} + \psi(x,\mu) = \frac{c}{2} \int_{-1}^{1} \psi(x,\mu') \, d\mu' \tag{1}$$

has the exact half-space solution in $x \ge 0$

$$\psi_{ex}(x,\mu) = a(v_0) e^{-x/v_0} \phi(v_0,\mu) + \int_0^1 A(v) e^{-x/v} \phi(v,\mu) dv$$
(2)

which in the $\Delta \sigma_N$ approximation becomes⁽⁶⁾

$$\psi_{\varepsilon}(x,\mu) = a(v_0) e^{-x/v_0} \phi(v_0,\mu) + \sum_{i=1}^{N} a(v_i) e^{-x/v_i} \phi_{\varepsilon}(v_i,\mu)$$
(3)

Here,

$$\phi(v_0, \mu) = \frac{cv_0}{2} \frac{1}{v_0 - \mu}; \qquad \frac{cv_0}{2} \ln \frac{v_0 + 1}{v_0 - 1} = 1$$

and

$$\phi_{\varepsilon}(v_i,\mu) = \frac{cv_i}{2} \frac{v_i - \mu}{(v_i - \mu)^2 + \varepsilon^2} + \frac{\lambda_{\varepsilon}}{\pi_{\varepsilon}} \frac{\varepsilon}{(v_i - \mu)^2 + \varepsilon^2}, \qquad v_i, \mu > 0$$
(4)

is the rational function approximation of the singular eigenfunction

$$\phi(\nu,\mu) = \frac{c\nu}{2} P \frac{1}{\nu-\mu} + \lambda(\nu) \,\delta(\nu-\mu)$$

with

$$\lambda(v) = 1 - \frac{cv}{2} \ln \frac{1+v}{1-v}$$

 $\{v_i\} \in (0, 1)$ is a discretization of the continuous spectrum $v \in (0, 1)$ obtained as the roots of a set of properly constructed orthogonal polynomials that ensures convergence of the sum in Eq. (3) to the integral of Eq. (2). Therefore $\{v_i\}$ are a set of Gaussian nodes in (0, 1). Here $\lambda_{\varepsilon}/\pi_{\varepsilon}$ is to be obtained in conformity with the $\Delta \sigma_N$ approximation. In ref. 6, this was done by requiring that the rational approximation $\phi_{\varepsilon}(v, \mu)$ be normalized to unity just as the distribution $\phi(v, \mu)$ is. Here, however, a different integral constraint on $\phi_{\varepsilon}(v, \mu)$ will be used to ensure better numerical results. ε is the imaginary part of v, i.e., $v \Rightarrow v \pm i\varepsilon$. This is done to avoid the singularity at $\mu = v$, and leads to the rational function approximation of $\phi(v, \mu)$, Eq. (4).⁽⁷⁾ The approximation parameter ε is obtained as in Sengupta and Venkatesan,⁽⁶⁾ i.e., from the transcendental equation

$$\varepsilon = \frac{1}{N^* \pi_{\varepsilon}(v)} \tag{5}$$

which in turn derives from the equality of the step sequence

$$\delta_{N^*}(\nu - \mu) = \begin{cases} N^*, & \nu - \frac{1}{2N^*} \le \mu \le \nu + \frac{1}{2N^*} \\ 0, & \text{otherwise} \end{cases}$$

to the Cauchy equivalent, rational sequence

$$\delta_{\varepsilon}(v-\mu) = \frac{1}{\pi_{\varepsilon}(v)} \frac{\varepsilon}{(v-\mu)^2 + \varepsilon^2}$$

at $\mu = v$. Here

$$N^{*} = \begin{cases} \frac{1}{1 - \nu + 1/(2N)}, & \nu + \frac{1}{2N} > 1\\ \frac{1}{\nu + 1/(2N)}, & \nu - \frac{1}{2N} < 0\\ N, & \text{otherwise} \end{cases}$$
(6)

N is the number of terms of the sum in Eq. (3). This sum is the boundary layer term, or the transient component of the solution of Eq. (1). In Sengupta and Venkatesan,⁽⁶⁾ the discretized spectra $\{v_i\}_{i=1}^{N}$ were obtained as the roots of a set of orthogonal polynomials in (0, 1) with respect to the function

$$W^{(0)}(\mu) = \frac{c}{2\Omega^{(0)}(1-c)} \frac{\mu(\alpha+\mu)}{\nu_0+\mu}, \qquad \alpha = \nu_0(1-c)^{1/2}$$

which is an effective approximation of the HR weight function

$$W(\mu) = \frac{c}{2(1-c)} \frac{\mu}{(v_0 + \mu) X(-\mu)}$$

where $X(\mu)$ is the Case X function, which is related to the Chandrasekhar *H*-function by

$$H(\mu) = \frac{1}{(1-c)^{1/2} (\nu_0 + \mu) X(-\mu)}$$

and hence

$$W(\mu) = \frac{c}{2(1-c)^{1/2}} \, \mu H(\mu)$$

It is interesting to note that as $c \to 0$, $v_0 \to 1$, $X(-\mu) \to (1+\mu)^{-1}$, and both $W(\mu)$ and $W^{(0)}(\mu)$ tend to $c\mu/2(1-c)$. Because of the constant factor c/2(1-c), one has the interesting result that orthogonal polynomials, or moment equations in (0, 1), with respect to either $W(\mu)$ or $W^{(0)}(\mu)$ behave in the limit of vanishing scattering like the corresponding equations with respect to the FR weight function μ in that interval. In Eq. (5), $\pi_{\varepsilon}(\nu)$ is either $\tan^{-1}[(1+\nu)/\varepsilon] + \tan^{-1}[(1-\nu)/\varepsilon]$ if $-1 \le \nu \le 1$, or $\tan^{-1}(\nu/\varepsilon) + \tan^{-1}[(1-\nu)/\varepsilon]$ when $0 \le \nu \le 1$, and is obtained from the required normalizations

$$\int_{-1}^{1} \delta_{\varepsilon}(v-\mu) \, d\mu = 1 \qquad \text{or} \qquad \int_{0}^{1} \delta_{\varepsilon}(v-\mu) \, d\mu = 1$$

according as $-1 \le v \le 1$ or $0 \le v \le 1$, respectively. In this second HR case, $\pi_{\varepsilon}(v) = T_{\varepsilon}(v)$ in the notation of ref. 6, and it is this HR definition that has been used in the calculations of Section 4.

3. NUMERICAL ADAPTATION OF THE $\Delta \sigma_N$ APPROXIMATION

An effective numerical adaptation of the above theory depends upon a reliable determination of the coefficients $\{a(v_i)\}_0^N$ when the HR wall condition

$$\psi_{ex}(0, \mu) = f(\mu), \quad \mu > 0$$

is specified. In ref. 6, this was done by a Nystrom-type collocation method, where μ was also discretized at the zeros of $C_{N+1}(\mu)$ to get N+1 equations in the N+1 unknowns $\{a(v_i)\}_{0}^{N}$. In this paper, we report the results of calculations using three different schemes of generation of Galerkin or moment equations from the boundary condition

$$\psi_{\rm ex}(0,\,\mu) = h^+(\mu) + h^-(\mu) \tag{7}$$

valid at the wall x = 0, where

$$h^{+}(\mu) = \begin{cases} \psi_{ex}(0, \mu), & \mu > 0\\ 0, & \mu < 0 \end{cases}$$
$$h^{-}(\mu) = \begin{cases} 0, & \mu > 0\\ \psi_{ex}(0, \mu), & \mu < 0 \end{cases}$$

In the $\Delta \sigma_N$ approximation, $\psi_{\varepsilon}(0, \mu)$ replaces $\psi_{ex}(0, \mu)$ in Eq. (7) for Schemes 1 and 2 defined below, and $h^+(\mu)$ and $h^-(\mu)$ are given by

$$h^{+}(\mu) = h_{\varepsilon}^{+}(\mu) = a^{+}(\nu_{0}) \phi(\nu_{0}, \mu) + \sum_{i}^{N} a^{+}(\nu_{i}) \phi_{\varepsilon}(\nu_{i}, \mu), \qquad \mu > 0$$
$$h^{-}(\mu) = \frac{c\nu_{i}}{2} \sum_{0}^{N} a^{-}(\nu_{i}) \frac{1}{\nu_{i} - \mu}, \qquad \mu < 0$$

where use has been made of the fact that for $\mu < 0$, $\nu > 0$, $\phi_{\varepsilon}(\nu, \mu) = c\nu/2(\nu - \mu)$, and $h^{-}(\mu)$ is independent of ε . We now examine the following three different types of approximate boundary conditions at x = 0:

- Scheme 1. μ interval: (0, 1) Weight function: $W^{(0)}(\mu)$ Moments with respect to: $\phi(v_j, \mu), j = 0, 1, ..., N$ Boundary condition: $f(\mu) = h_{\varepsilon}^+(\mu)$ Scheme 2. μ interval: (0, 1)
 - Weight function: μ Moments with respect to: $\phi(v_j, \mu), j = 0, 1, ..., N$ Boundary condition: $f(\mu) = h_{\varepsilon}^+(\mu)$
- Scheme 3. μ interval: (-1, 1)Weight function: μ Moments with respect to: $\phi(-v_j, \mu), j = 0, 1, ..., N$ Boundary condition: $\psi_{ex}(0, \mu) = h_{\varepsilon}^+(\mu) + h^-(\mu)$

While in Scheme 1 the weight function is our simple approximation $W^{(0)}$ to the HR function, in Schemes 2 and 3 it is the FR function μ . With respect to Scheme 3, the following is to be noted. Let $\{\{\varphi_i^{\pm}(\mu)\}_{i=1}^{\infty}, \varphi_0(\mu)\}$ be a complete set of functions in $L^2(-a, a)$ such that they are orthogonal in (-a, a) with respect to $w(\mu)$, i.e.,

$$(\varphi_{i}^{+}, \varphi_{j}^{+})_{w} = N_{i}^{+} \delta_{ij}, \qquad (\varphi_{i}^{-}, \varphi_{j}^{-})_{w} = N_{i}^{-} \delta_{ij}$$
$$(\varphi_{i}^{+}, \varphi_{j}^{-})_{w} = 0$$

where $(f, g)_w = \int_{-a}^{a} wfg \, d\mu$. If half of the functions $\{\varphi_0, \{\varphi_i^+\}_1^\infty\}$ are complete in (0, a), i.e., if

$$h^+(\mu) = \sum_{i=0}^{\infty} a_i^+ \varphi_i^+(\mu), \qquad \mu > 0$$

then we can write with respect to the FR weight function and φ_j^- applied to the Scheme 3 boundary condition

$$\sum a_i(\varphi_i^+, \varphi_j^-)_w = (f, \varphi_j^-)_w^+ + \sum a_i^- (\varphi_i^+, \varphi_j^-)_w^-$$
(8)

where

$$(f, g)_w = (f, g)_w^- + (f, g)_w^+$$

and

$$(f, g)_w^- = \int_{-a}^0 wfg \, d\mu, \qquad (f, g)_w^+ = \int_0^a wfg \, d\mu$$

are HR integrals with respect to the FR weight function w. Now, since

$$(\varphi_i^+, \varphi_j^-)_w = 0 = (\varphi_i^+, \varphi_j^-)_w^+ + (\varphi_i^+, \varphi_j^-)_w^-$$

i.e.,

$$(\varphi_i^+, \varphi_j^-)_w^- = -(\varphi_i^+, \varphi_j^-)_w^+$$
(9)

Eq. (8) becomes

$$(f, \varphi_j^-)_w^+ = \sum_{i=0}^N a_i^- (\varphi_i^+, \varphi_j^-)_w^+, \qquad j = 0, 1, ..., N$$
(10)

However, in the $\Delta \sigma_N$ approximation, with

$$\varphi_i^+ = \phi_\varepsilon(v_i, \mu), \qquad \varphi_j^- = \phi(-v_j, \mu)$$

 φ_i^+ and φ_j^- have different forms and Eq. (9) does not apply. In the $\Delta \sigma_N$ approximation, therefore, Scheme 3 is represented by Eq. (8), and not by Eq. (10).

The notion of a different set of expansion coefficients $\{a_i^+\}$ and $\{a_i^-\}$ for μ in the respective positive and negative half-ranges needs some comment. With regard to the Fokker–Planck equation, such a "bimodal ansatz" has often been employed. Harris,⁽⁸⁾ for example, remarks, "experience has shown that those approximations which explicitly incorporates the half-range structure into the character of the solution generally lead to a more accurate description of the boundary layer than other approaches. This is effected by looking for a solution that is discontinuous at v = 0"; see also Titulaer⁽⁹⁾ for similar remarks on the desirability of

treating the positive and negative half-ranges separately. Thus, let us consider

$$h(\mu) = \begin{cases} h^{-}(\mu) = \sum a_{i}^{-} \varphi_{i}^{+}(\mu), & \mu < 0 \end{cases}$$
(11b)

Then, assuming that the HR properties are fully established with a weight $W(\mu)$, Eq. (11a) leads to

$$(f, \varphi_j^+)_W^+ = \sum a_i^+ (\varphi_i^+, \varphi_j^+)_W^+, \quad j = 0, 1, \dots$$
 (12a)

as the unique solution of the HR problem. For Eq. (11b), $\{a_i^-\}$ can be obtained using the FR relations only so as to link the negative HR (-a, 0) to the positive HR (0, a) on which the boundary function is specified. Thus, $\{a_i^-\}$ are obtained from Eq. (10),

$$(f, \varphi_j^-)_w^+ = \sum a_i^- (\varphi_i^+, \varphi_j^-)_w^+, \qquad j = 0, 1,...$$
 (12b)

It is of course true that Eqs. (12a) and (12b) for the coefficients $\{a_i^+\}$ and $\{a_i^-\}$ are two distinct equations whose solutions are not, *a priori*, the same. For the neutron transport equation, Eq. (8) becomes

$$\int_{0}^{1} \mu f(\mu) \, \phi(-\sigma, \, \mu) \, d\mu = a^{-}(v_{0}) \, \mathscr{I}(v_{0}, \, -\sigma) + \int_{0}^{1} A^{-}(v) \, \mathscr{I}(v, \, -\sigma) \, dv,$$

$$\sigma = v_{0} \cup v \in (0, \, 1) \quad (13)$$

for the coefficients a^- , A^- , where

$$\begin{aligned} \mathscr{I}(v_0, -\sigma) &= -\int_{-1}^{0} \mu \phi(v_0, \mu) \, \phi(-\sigma, \mu) \, d\mu \\ &= \int_{0}^{1} \mu \phi(v_0, \mu) \, \phi(-\sigma, \mu) \, d\mu \\ &= \begin{cases} \frac{1}{2} \left(\frac{cv_0}{2}\right)^2 \ln \frac{v_0^2}{v_0^2 - 1}, & \sigma = v_0 \\ \frac{c^2 v_0 v'}{4} \frac{1}{v_0 + v'} \left(v_0 \ln \frac{v_0}{v_0 - 1} - v' \ln \frac{1 + v'}{v'}\right), & \sigma = v' \in (0, 1) \end{cases} \end{aligned}$$

$$\begin{aligned} \mathscr{I}(v, -\sigma) &= -\int_{-1}^{0} \mu \phi(v, \mu) \, \phi(-\sigma, \mu) \, d\mu \\ &= \int_{0}^{1} \mu \phi(v, \mu) \, \phi(-\sigma, \mu) \, d\mu \\ &= \begin{cases} \frac{c^{2}v_{0}v}{4} \frac{1}{v_{0} + v} \left(v_{0} \ln \frac{v_{0}}{v_{0} - 1} - v \ln \frac{1 + v}{v}\right), & \sigma = v_{0} \\ \frac{cvv'}{2(v + v')} \left[1 - \frac{c}{2} \left(v' \ln \frac{1 + v'}{v'} + v \ln \frac{1 + v}{v}\right)\right], & \sigma = v' \in (0, 1) \end{aligned}$$

and $\mathscr{I}(v_0, -v) = \mathscr{I}(v, -v_0)$. Equations (13) are not the same as the usual equations for $a^+(v_0)$ and $A^+(v)$ obtained from the HR orthogonality of $\{\phi(v_0), \phi(v), 0 \le v \le 1\}$ with respect to the HR weight $W(\mu)$. For the $\Delta \sigma_N$ approximation, Eq. (13) becomes

$$\int_{0}^{1} \mu f(\mu) \phi(-\sigma, \mu) d\mu$$

= $a^{-}(v_{0}) \mathscr{I}(v_{0}, -\sigma) + \sum a^{-}(v_{i}) \mathscr{I}_{\varepsilon}(v_{i}, -\sigma), \qquad \sigma = \{v_{0}, \{v_{j}\}_{1}^{N}\}$ (14)

where

$$\begin{aligned} \mathscr{I}_{\varepsilon}(v_{i};\sigma) &= -\int_{-1}^{0} \mu \phi_{\varepsilon}(v_{i},\mu) \phi(-\sigma,\mu) \, d\mu \\ &= \mathscr{I}(v_{i},-\sigma) \\ &\neq \int_{0}^{1} \mu \phi_{\varepsilon}(v_{i},\mu) \, \phi(-\sigma,\mu) \, d\mu \end{aligned}$$

Equation (14) is the working equation for Scheme 3. For the purpose of comparison, the relations

$$\int_{0}^{1} \mu f(\mu) \phi(-\sigma, \mu) d\mu$$

= $a^{-}(v_{0}) \mathscr{I}(v_{0}, -\sigma) + \sum_{i}^{N} a^{-}(v_{i}) \int_{0}^{1} \mu \phi_{\varepsilon}(v_{i}, \mu) \phi(-\sigma, \mu) d\mu, \quad \sigma = \{v_{0}, \{v_{j}\}_{1}^{N}\}$

were also used to obtain the coefficients, but were found to give unsatisfactory results and were not investigated further. We note that the coefficients of Schemes 1 and 2 are ε -dependent, while those of Scheme 3 are not.

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In the μ -weighted integrals of Schemes 2 and 3, $\lambda_{\epsilon}/\pi_{\epsilon}$ in Eq. (4) is obtained by requiring $\phi_{\epsilon}(v_i, \mu)$ to satisfy

$$\int_{-1}^{1} \mu \phi_{\varepsilon}(v_{i}, \mu) \phi(v_{0}, \mu) d\mu = 0$$
(15)

to give

$$\frac{\lambda_{\varepsilon}}{\pi_{\varepsilon}} = \frac{X}{Y} \tag{16}$$

where

$$X = \frac{cv_{i}}{2(v_{0} - v_{i})} \left(v_{0} \ln \frac{v_{0} + 1}{v_{0}} - v_{i} \ln \frac{1 + v_{i}}{v_{i}} \right) - \frac{1}{2} \frac{cv_{i}}{(v_{0} - v_{i})^{2} + \varepsilon^{2}} \times \left[v_{0}(v_{i} - v_{0}) \ln \frac{v_{0}}{v_{0} - 1} + \frac{1}{2} (v_{i}^{2} - v_{0}v_{i} + \varepsilon^{2}) L_{\varepsilon}(v_{i}) + v_{0}\varepsilon T_{\varepsilon}(v_{i}) \right]$$

$$Y = \frac{1}{(v_{0} - v_{i})^{2} + \varepsilon^{2}} \left\{ v_{0}\varepsilon \left[\ln \frac{v_{0}}{v_{0} - 1} + \frac{1}{2} L_{\varepsilon}(v_{i}) \right] - (v_{i}^{2} - v_{0}v_{i} + \varepsilon^{2}) T_{\varepsilon}(v_{i}) \right\}$$
(17a)
$$(17b)$$

and

$$L_{\varepsilon}(v) = \ln \frac{(1-v)^2 + \varepsilon^2}{v^2 + \varepsilon^2}, \qquad T_{\varepsilon}(v) = \tan^{-1} \frac{v}{\varepsilon} + \tan^{-1} \frac{1-v}{\varepsilon}$$

while for Scheme 1, $\lambda_{\varepsilon}/\pi_{\varepsilon}$ was obtained from

$$I_{\varepsilon+}^{(0)}(v_i) = \int_0^1 W^{(0)}(\mu) \,\phi_{\varepsilon}(v_i,\,\mu) \,\phi(v_0,\,\mu) \,d\mu = 0 \tag{18}$$

to give in eq. (16)

$$X = \frac{cv_i}{2} \left[(v_0 + v_i) A_{0+} + (v_0 - v_i) A_{0-} + B_0 L_{\varepsilon}(v_i) + 2\varepsilon C_0 T_{\varepsilon}(v_i) \right]$$
$$Y = 2B_0 T_{\varepsilon}(v_i) - \varepsilon \left[A_{0+} - A_{0-} + C_0 L_{\varepsilon}(v_i) \right]$$

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where

$$A_{0+} = \frac{v_0 - \alpha}{(v_0 + v_i)^2 + \varepsilon^2} \ln \frac{v_0 + 1}{v_0}$$

$$A_{0-} = \frac{v_0 + \alpha}{(v_0 - v_i)^2 + \varepsilon^2} \ln \frac{v_0 - 1}{v_0}$$

$$B_0 = \frac{1}{A_0} \left[(v_i^2 + \varepsilon^2)^2 - v_0^2 (v_i^2 - \varepsilon^2) - \alpha v_i (v_0^2 - v_i^2 - \varepsilon^2) \right]$$

$$C_0 = \frac{1}{A_0} \left[2v_i v_0^2 + \alpha (v_0^2 + v_i^2 + \varepsilon^2) \right]$$

$$A_0 = \left[(v_0 + v_i)^2 + \varepsilon^2 \right] \left[(v_0 - v_i)^2 + \varepsilon^2 \right]$$

The matrix elements for Schemes 1 and 3 are given in ref. 6 and by $\mathscr{I}(v_i, -\sigma)$ above, respectively; those for Scheme 2 are as follows:

$$\begin{split} \int_{0}^{1} \mu \phi^{2}(v_{0}, \mu) \, d\mu \\ &= \left(\frac{cv_{0}}{2}\right)^{2} \left(\frac{1}{v_{0}-1} - \ln \frac{v_{0}}{v_{0}-1}\right) \\ \int_{0}^{1} \mu \phi(v_{0}, \mu) \, \phi_{\varepsilon}(v_{i}, \mu) \, d\mu \\ &= \frac{cv_{0}}{2} \left\{ \left[\frac{cv_{i}}{2} \left(v_{i}-v_{0}\right) + \varepsilon \frac{\lambda_{\varepsilon}}{\pi_{\varepsilon}}\right] v_{0} \ln \frac{v_{0}}{v_{0}-1} \right. \\ &+ \frac{1}{2} \left[\frac{cv_{i}}{2} \left(v_{i}^{2}-v_{0}v_{i}+\varepsilon^{2}\right) + v_{0}\varepsilon \frac{\lambda_{\varepsilon}}{\pi_{\varepsilon}}\right] L_{\varepsilon}(v_{i}) \\ &+ \left[\frac{cv_{i}}{2} v_{0}\varepsilon + \frac{\lambda_{\varepsilon}}{\pi_{\varepsilon}} \left(v_{0}v_{i}-\varepsilon^{2}-v_{i}^{2}\right)\right] T_{\varepsilon}(v_{i}) \right\} \left[(v_{0}-v_{i})^{2} + \varepsilon^{2} \right]^{-1} \\ &\int_{0}^{1} \mu \phi(v_{0}, \mu) \, \phi(v_{j}, \mu) \\ &= \frac{cv_{0}}{2} \frac{v_{j}}{v_{0}-v_{j}} \left[1 - \frac{c}{2} \left(v_{0} \ln \frac{v_{0}}{v_{0}-1} + v_{j} \ln \frac{1+v_{j}}{v_{j}} \right) \right] \end{split}$$

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$$\int_{0}^{1} \mu \phi_{\varepsilon}(v_{i}, \mu) \phi(v_{j}, \mu) d\mu$$

$$= v_{j} \left(\frac{c}{2} \left\{ \left[\frac{cv_{i}}{2} (v_{i} - v_{j}) + \varepsilon \frac{\lambda_{\varepsilon}}{\pi_{\varepsilon}} \right] v_{j} \ln \frac{v_{j}}{1 - v_{j}} + \frac{1}{2} \left[\frac{cv_{i}}{2} (v_{i}^{2} - v_{i}v_{j} + \varepsilon^{2}) + v_{j}\varepsilon \frac{\lambda_{\varepsilon}}{\pi_{\varepsilon}} \right] L_{\varepsilon}(v_{i}) + \left[\frac{cv_{i}}{2} v_{j}\varepsilon + \frac{\lambda_{\varepsilon}}{\pi_{\varepsilon}} (v_{i}v_{j} - v_{i}^{2} - \varepsilon^{2}) \right] T_{\varepsilon}(v_{i}) \right\}$$

$$+ \lambda(v_{j}) \left[\frac{cv_{i}}{2} (v_{i} - v_{j}) + \varepsilon \frac{\lambda_{\varepsilon}}{\pi_{\varepsilon}} \right] \left[(v_{i} - v_{j})^{2} + \varepsilon^{2} \right]^{-1}$$

where

$$\lambda(v_j) = 1 - \frac{cv_j}{2} \ln \frac{1+v_j}{1-v_j}$$

A scheme linking the two sets of coefficients $\{a_i^+\}$ and $\{a_i^-\}$ not been investigated in this paper is, in the notation of the discussions following Scheme 3, as follows:

Scheme 4. μ interval: (-a, a)Weight function: $w(\mu)$ Moments with respect to: $\varphi_j^+(\mu)$ Boundary condition: $\psi_{ex}(0, \mu) = h^+(\mu) + h^-(\mu)$

According to this scheme, one has

$$\sum_{i} a_{i}(\varphi_{i}^{+}, \varphi_{j}^{+})_{w} = (f, \varphi_{j}^{+})_{w}^{+} + \sum_{i} a_{i}^{-}(\varphi_{i}^{+}, \varphi_{j}^{+})_{w}^{-}$$

and hence, using the orthogonality of the basis functions in FR,

$$N_j a_j = (f, \varphi_j^+)_w^+ + \sum_{i=1}^N a_i^- N_{ij}^-, \qquad j = 0, 1, ..., N$$

where

$$N_{ij}^{\pm} = (\varphi_i^+, \varphi_j^+)_w^{\pm} \equiv N_j^{\pm} \qquad \text{for} \quad i = j$$

Obviously,

$$a_j = a_j^+ + a_j^-, \qquad N_{ij} = N_{ij}^+ + N_{ij}^-$$
 (19)

and there follows

$$(f, \varphi_j^+)_w^+ = N_j(a_j^+ + a_j^-) + \sum_i a_i^- N_{ij}^+, \qquad j = 0, 1, ..., N$$

Using $f = \sum a_i^+ \varphi_i^+$, one finally gets the required relation between the two sets of coefficients $\{a_i^+\}$ and $\{a_i^-\}$ on the positive and negative intervals, respectively:

$$a_j^+ N_j^- + a_j^- N_j^+ = \sum_{i \neq j}^N (a_i^+ N_{ij}^+ + a_i^- N_{ij}^-), \qquad j = 0, 1, ..., N$$

For the $\Delta \sigma_N$ approximation, since the boundary layer integral is replaced by a sum, the respective coefficients do not follow relation (19) except for j = 0. In this approximation, therefore, we get the single relation obtained with $\phi(v_0, \mu)$, i.e., the following equation for $a^+(v_0)$:

$$N(v_0)[a^+(v_0) + a^-(v_0)] = \int_0^1 \mu f(\mu) \,\phi(v_0,\mu) \,d\mu - \sum_{i=0}^N a^-(v_i) \,\mathscr{I}(v_i,v_0) \quad (20)$$

where

$$N(v_0) = \left(\frac{cv_0}{2}\right)^2 \int_{-1}^{1} \frac{\mu}{(v_0 - \mu)^2} d\mu = \frac{cv_0}{2} \left(\frac{cv_0^2}{v_0^2 - 1} - 1\right)$$

Use of $a = a^+ + a^-$ reduces Eq. (20) to an equation for $a^+(v_0)$,

$$N(v_0)[a^+(v_0) + a^-(v_0)] = \int_0^1 \mu f(\mu) \,\phi(v_0, \mu) \,d\mu - \sum_{i=0}^N a_i^-(v_i) \,\mathscr{I}(v_i, v_0)$$

where

$$N^{+}(v_{0}) = \left(\frac{cv_{0}}{2}\right)^{2} \int_{0}^{1} \frac{\mu}{(v_{0} - \mu)^{2}} d\mu = \left(\frac{cv_{0}}{2}\right)^{2} \left(\frac{1}{v_{0} - 1} - \ln\frac{v_{0}}{v_{0} - 1}\right)$$

and

$$N^{-}(v_{0}) = \left(\frac{cv_{0}}{2}\right)^{2} \int_{-1}^{0} \frac{\mu}{(v_{0} - \mu)^{2}} d\mu = \left(\frac{cv_{0}}{2}\right)^{2} \left(\frac{1}{v_{0} + 1} - \ln\frac{v_{0} + 1}{v_{0}}\right)$$
$$= -\mathscr{I}(v_{0}, v_{0})$$

While this scheme has not been investigated in this paper, we note its possibility as a natural complement of Scheme 3, and observe that Schemes 3 and 4 together constitures a complete solution of the HR

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problem by FR methods: apply Scheme 3 to obtain the a_i^- , followed by Eq. (20) of Scheme 4 for the a_i^+ . This determines the function $h(\mu)$ for both the half-intervals $\mu \ge 0$, thereby giving the complete solution of the half-range problem.

4. NUMERICAL RESULTS

We consider in this section the following three problems for the halfspace $x \ge 0$.

Problem A:	Equation: $\mu \psi_x + \psi = \frac{1}{2}c \int_{-1}^{1} \psi(x, \mu') d\mu'$ Boundary condition: $\psi(0, \mu) = 0, \mu \ge 0$
	Boundary condition. $\varphi(0, \mu) = 0, \ \mu \ge 0$
	Asymptotic condition: $\psi \to e^{x/v_0}\phi(-v_0, \mu), x \to \infty$
Problem B:	Equation: $\mu \psi_x + \psi = \frac{1}{2} c \int_{-1}^{1} \psi(x, \mu') d\mu' + q$
	Boundary condition: $\psi(0, \mu) = 1 - q, \mu > 0$
	Asymptotic condition: $\psi \rightarrow q/(1-c), x \rightarrow \infty$

By Problems B_0 and B_1 we will denote the special cases q = 0 and q = 1, respectively, of Problem B. Problem A is the standard source-free Milne problem, while Problems B_0 and B_1 have been considered by Grandjean and Siewert⁽¹⁾ by the F_N method, assuming a polynomial form of the exiting flux. We study both problems here by Schemes 1–3 by the following four choices of collocation points: zeros of orthogonal polynomials in (0, 1) with respect to specified weight function (choice 1), zeros of shifted Legendre polynomials (choice 2), equally spaced points (choice 3), and zeros of shifted Chebyshev polynomials (choice 4). It was found, in general, that choices 1 and 2 gave better results than choices 3 and 4 for $N \le 10$ (the range investigated in this paper). We will restrict our further considerations to the first two choices.

Tables I–V show the leakage and extrapolated endpoints for problems A, B_0 , and B_1 by Schemes 1 and 2 and nodes selected according to choices 1 and 2, while Tables VI–VIII display the same results according to Scheme 3. We note the following points of interest.

1. The results of Schemes 1 and 2 are qualitatively similar (Tables I–V). The numerical values do not converge to the exact results for the values of N studied, but should probably display an oscillatory character converging to the exact value for larger N. Though it has not been possible to test this so far because of computational limitations, the results shown appear to be suggestive of this. This trend would also imply that N would take on fairly large values for a properly converging behavior.

These remarks apply not only to a "sum" result such as the leakage, but also to an individual quantity such as the coefficient $a^+(v_0)$, i.e., the

с		<i>N</i> = 2	<i>N</i> = 4	<i>N</i> = 6	<i>N</i> = 8	N = 10	Exact
0.2	S1 C1 C2 S2 C1 C2	0.8229 0.8225 0.8230 0.8227	0.8260 0.8263 0.8261 0.8264	0.8270 0.8272 0.8270 0.8272	0.8275 0.8276 0.8275 0.8276	0.8279 0.8279 0.8279 0.8279	0.8280
0.4	\$1 C1 C2 \$2 C1 C2	0.6514 0.6504 0.6518 0.6511	0.6579 0.6584 0.6581 0.6587	0.6602 0.6605 0.6603 0.6606	0.6614 0.6616 0.6615 0.6617	0.6623 0.6623 0.6623 0.6624	0.6627
0.6	S1 C1 C2 S2 C1 C2	0.5020 0.4994 0.5030 0.5012	0.5115 0.5118 0.5120 0.5124	0.5145 0.5149 0.5149 0.5152	0.5161 0.5162 0.5163 0.5164	0.5169 0.5171 0.5170 0.5172	0.5170
0.8	S1 C1 C2 S2 C1 C2	0.3577 0.3535 0.3597 0.3574	0.3667 0.3669 0.3677 0.3681	0.3695 0.3698 0.3701 0.3704	0.3709 0.3711 0.3712 0.3714	0.3718 0.3719 0.3719 0.3720	0.3713
0.9	S1 C1 C2 S2 C1 C2	0.2663 0.2621 0.2692 0.2673	0.2736 0.2737 0.2748 0.2751	0.2759 0.2762 0.2765 0.2768	0.2771 0.2773 0.2774 0.2775	0.2782 0.2779 0.2778 0.2779	0.2772

Table I. Leakage for Problem A^a

^a S1, S2, Schemes 1, 2; C1, C2, choices 1, 2.

с		N = 2	N = 4	N = 6	N = 8	N = 10	Exact
0.2	S1 S2	3.9241 3.9288	3.9261	3.9254	3.9251	3.9249	{3.9255
0.4	S1 S2	1.8254 1.8364	1.8294	1.8276	1.8266	1.8260	{1.8263
0.6	S1 S2	1.1930 1.2117	1.1979	1.1946	1.1931	1.1922	{1.1925
0.8	S1 S2	0.8899 0.9183	0.8958	0.8910	0.8889	0.8877	{0.8891
0.9	S1 S2	0.7904 0.8263	0.7973	0.7913	0.7887	0.7871	{ 0.7896

Table II. Extrapolation Length for Problem A^a

^a S1, S2, Schemes 1, 2.

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					-		
с		<i>N</i> = 2	N = 4	<i>N</i> = 6	N = 8	N = 10	Exact
0.2	S1 C1 C2 S2 C1 C2	0.1235 0.1211 0.1221 0.1194	0.07646 0.07043 0.07580 0.06981	0.06203 0.05842 0.06160 0.05805	0.05406 0.05208 0.05378 0.05183	0.04852 0.04749 0.04835 0.04730	0.02313
0.4	S1 C1 C2 S2 C1 C2	0.1446 0.1430 0.1417 0.1393	0.09709 0.09205 0.09575 0.09070	0.03805 0.08069 0.07805 0.07988 0.07734	0.07122 0.06997 0.07074 0.06951	0.04730 0.06508 0.06439 0.06478 0.06408	0.05365
0.6	S1 C1 C2 S2 C1 C2	0.1643 0.1690 0.1602 0.1627	0.1215 0.1193 0.1197 0.1174	0.1084 0.1068 0.1073 0.1058	0.1019 0.1010 0.1013 0.1005	0.09825 0.09759 0.09794 0.09730	0.09735
0.8	S1 C1 C2 S2 C1 C2	0.2074 0.2147 0.2022 0.2061	0.1823 0.1813 0.1802 0.1790	0.1751 0.1741 0.1740 0.1731	0.1715 0.1709 0.1710 0.1705	0.1694 0.1691 0.1694 0.1690	0.1710
0.9	\$1 C1 C2 \$2 C1 C2	0.2606 0.2668 0.2551 0.2577	0.2457 0.2454 0.2435 0.2429	0.2413 0.2407 0.2403 0.2398	0.2390 0.2387 0.2387 0.2384	0.2377 0.2375 0.2378 0.2376	0.2390

Table III. Leakage for Problem B₀^a

^a S1, S2, Schemes 1, 2; C1, C2, choices 1, 2.

Table IV. Extrapolation Length for Problems B_0 and $B_1{}^a$

с		<i>N</i> = 2	N = 4	<i>N</i> = 6	N = 8	N = 10	Exact
0.2	S1 S2	5.5812 5.5833	5.5845	5.5836	5.5831	5.5827	{5.5825
0.4	S1 S2	2.1054 2.1213	2.1117	2.1091	2.1075	2.1065	{2.1058
0.6	S1 S2	1.2347 1.2613	1.2419	1.2370	1.2348	1.2334	{1.2337
0.8	S1 S2	0.8791 0.9163	0.8866	0.8803	0.8774	0.8758	{0.8779
0.9	S1 S2	0.7764 0.8204	0.7846	0.7772	0.7739	0.7720	{ 0.7752

^a S1, S2, Schemes 1, 2.

с		N = 2	N = 4	<i>N</i> = 6	N = 8	N = 10	Exact
0.2	S1 C1 C2 S2 C1 C2	0.4706 0.4737 0.4723 0.4758	0.5294 0.5370 0.5303 0.5373	0.5475 0.5520 0.5480 0.5524	0.5575 0.5599 0.5578 0.5602	0.5643 0.5656 0.5646 0.5659	0.5961
0.4	\$1 C1 C2 \$2 C1 C2	0.5923 0.5950 0.5972 0.6011	0.6715 0.6799 0.6734 0.6821	0.6988 0.7032 0.7002 0.7044	0.7146 0.7167 0.7154 0.7175	0.7249 0.7260 0.7254 0.7265	0.7439
0.6	S1 C1 C2 S2 C1 C2	0.8391 0.8276 0.8496 0.8431	0.9463 0.9519 0.9507 0.9566	0.9791 0.9830 0.9817 0.9854	0.9952 0.9975 0.9966 0.9988	1.0074 1.0060 1.0051 1.0067	1.0066
0.8	S1 C1 C2 S2 C1 C2	1.4629 1.4265 1.4890 1.4696	1.5883 1.5934 1.5991 1.6052	1.6244 1.6293 1.6302 1.6344	1.6425 1.6453 1.6449 1.6475	1.6529 1.6546 1.6531 1.6550	1.6453
0.9	S1 C1 C2 S2 C1 C2	2.3936 2.3317 2.4856 2.4229	2.5427 2.5475 2.5646 2.5712	2.5866 2.5929 2.5974 2.6021	2.6097 2.6131 2.6130 2.6158	2.6299 2.6248 2.6217 2.6238	2.6099

Table V. Leakage for Problem B₁

^a S1, S2, Schemes 1, 2; C1, C2, choices 1, 2.

Table VI. Leakage and $a^-(v_0)$ for Problem A by Scheme 3

с		N = 2	N = 4	N = 6	N = 8	N = 10	Exact
0.2	Leakage $a^{-}(v_0)$	0.8293 0.0015	0.8293 0.0239	0.8293 0.2016	0.8293 2.2183	0.8293 30.1805	0.8280
0.4	Leakage $a^{-}(v_0)$	0.6636 -0.0237	0.6636 0.0091	0.6636 0.2092	0.6636 1.9345	0.6636 19.2966	$0.6627 \\ -0.0273$
0.6	Leakage $a^{-}(v_0)$	0.5171 - 0.1075	0.5171 0.0960	0.5171 0.0513	0.5171 0.1586	0.5171 1.2770	0.5170 0.1149
0.8	Leakage $a^{-}(v_0)$	0.3713 -0.2790	0.3713 -0.2785	0.3713 0.2759	0.3713 -0.2692	0.3713 -0.2509	0.3713 0.2827
0.9	Leakage $a^{-}(v_0)$	0.2772 -0.4346	0.2772 - 0.4349	0.2772 0.4349	0.2772 -0.4346	0.2772 - 0.4340	0.2772 - 0.4362

с		<i>N</i> = 2	N = 4	<i>N</i> = 6	N = 8	N = 10	Exact
0.2	Leakage $a^{-}(v_0)$	0.02312 0.00776	0.02314 0.2512	0.02313 - 2.0686	0.02313 -22.2252	0.02313 - 297.3231	0.02313 0.00753
0.4	Leakage $a^{-}(v_0)$	0.05365 0.2304	0.05367 0.05821	$0.05367 \\ -0.9133$	0.05367 9.1082	0.05367 90.6294	0.05367 0.2510
0.6	Leakage $a^{-}(v_0)$	0.09734 0.6171	0.09736 0.5896	0.09736 0.4595	0.09736 0.1540	0.09736 	0.09736 0.6531
0.8	Leakage $a^{-}(v_0)$	0.1709 1.0598	0.1709 1.0627	0.1709 1.0583	0.1709 1.0454	0.1709 1.0105	0.1709 1.0719
0.9	Leakage $a^{-}(v_0)$	0.2390 1.3269	0.2390 1.3287	0.2390 1.3288	0.2390 1.3284	0.2390 1.3275	0.2390 1.3309

Table VII. Leakage and $a^-(v_0)$ for Problem B₀ by Scheme 3

Milne extrapolated length, calculated by Scheme 2. In Scheme 1, λ/π is chosen so as to satisfy Eq. (18) and $a^+(v_0)$ is given simply by

$$a^{+}(v_{0}) = \int_{0}^{1} W^{(0)}(\mu) f(\mu) \phi(v_{0}, \mu) d\mu \Big/ \int_{0}^{1} W^{(0)}(\mu) \phi^{2}(v_{0}, \mu) d\mu$$

and is therefore constant with N. For problems B_0 and B_1 the extrapolated length was calculated as follows:

Problem B_0 : $z_0 = v_0 \ln(2/a^+)$ where the exact value of $a^+(v_0)$, given by

$$a_{\rm ex}^{+}(v_0) = -\frac{2}{cv_0} \frac{1}{X(v_0)}$$

is a positive quantity.

Table VIII. Leakage and for $a^-(v_0)$ for Problem B₁ by Scheme 3

с		N = 2	<i>N</i> = 4	N = 6	N = 8	N = 10	Exact
0.2	Leakage $a^{-}(v_0)$	0.5961 -0.3534	0.5961 	0.5961 8.1578	0.5961 90.2158	0.5961 	0.5961
0.4	Leakage $a^{-}(v_0)$	0.7439 -0.7682	0.7439 	0.7439 6.3825	0.7439 49.1637	0.7439 480.264	0.7439 0.4183
0.6	Leakage $a^{-}(v_0)$	1.0066 	1.0066 	1.0066 2.9791	1.0066 	1.0066 29.7884	1.0066 -1.6328
0.8	Leakage $a^{-}(v_0)$	1.6453 5.5088	1.6453 5.4824	1.6453 5.5298	1.6453 5.6803	1.6453 6.0922	1.6453 5.3594
0.9	Leakage $a^{-}(v_0)$	2.6098 	2.6099 	2.6099 	2.6099 13.3612	2.6099 13.3813	2.6099 13.3091

Problem B₁: $z_0 = v_0 \ln(2/(1-c) |a^+|)$ where the exact $a^+(v_0)$ is negative,

$$a_{\rm ex}^{+}(v_0) = \frac{2}{c(1-c) v_0} \frac{1}{X(v_0)}$$

Thus,

$$(1-c) |a^+(v_0)|_{\mathbf{B}_1} = a^+(v_0)|_{\mathbf{B}_0}$$

and the two extrapolated endpoints of problems B_0 and B_1 are identical.

The above results suggest that the FR relations can be used to get accurate HR results, though this would require inverting fairly large matrices. This coincides with the main conclusions of Burschka and Titulaer⁽²⁾ in the context of the Fokker-Planck equation where the HR weight function is unknown. These authors find that their calculations do not converge even for N = 140, and use empirical extrapolation to arrive at a "converged" Milne extrapolation length.

With regard to the choice of nodes for Schemes 1 and 2, there does not appear to be any particular overall preference shown in Tables I–V.

Scheme 3 gives quite a different picture altogether. Here con-2. vergence for a "sum" quantity such as leakage can be astonishingly rapid, even in spite of the low-c cases in problem A, which remain unexplained. Use of the full integration range (-1, 1) with the FR complete set of eigenfunctions-half as the basis expansion set, and the other half as the moment functions—is probably responsible for this very different behavior as compared to the other two schemes. However, the individual coefficient $a^{-}(v_0)$ calculated by Scheme 3 bears, as expected from the discussions of the previous section, little relation to the Milne extrapolation length. In fact, in Tables VI–VIII, the coefficient a^- is shown, rather than z_0 , to explicitly demonstrate the sign changes that take place especially for low values of c. This leads to the very important conclusion that although Scheme 3 generally produces very satisfactory "sum" results, it fails completely to predict a physically meaningful component of this sum. Remembering that the basis functions of this scheme are simply the discretized versions of the exact nonsingular $\phi(v, \mu)$, v > 0, $\mu < 0$, unlike the situation in Schemes 1 and 2, which require $\phi_{e}(v, \mu)$, it can be concluded that this limitation of the scheme is due to the particular adoption of the FR condition that is used in place of the HR ones. A further criticism that follows from the above is that since this scheme leaves ε undetermined, that is, since it employs explicitly the exiting flux only, it is unsuited for obtaining the flux inside the medium for $\mu > 0$. It is also found that the numerical results of Scheme 3 are insensitive to the choice of nodes to 6-7 significant figures.

It is therefore possible to summarize our findings as follows. Scheme 3, which has essentially been used by Siewert and co-workers in the F_N method, is good for the exit distribution, but fails in the interval $\mu > 0$. In this range Scheme 2 appears promising; however, some means of accelerating its rate of convergence is necessary if it is to be used profitably. Scheme 4—not used in this work because it cannot be applied to the neutron transport problem due to the approximation of the basis $\phi(v, \mu)$ by $\phi_e(v_i, \mu)$ —used in conjunction with Scheme 3, represents our solution of the half-range problem, when its orthogonality relations are unknown, in terms of the corresponding full-range properties. Problems having a

denumerable basis set are not limited by the above restriction and are typical candidates for the application of this FR solution of their HR problems, e.g., the Fokker-Planck equation for Brownian motion referred to in this paper.

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NOTE ADDED IN PROOF

In schemes employing full range weight function, it appears more appropriate to use the positive zeros of full range orthogonal polynomials as collocation points rather than the zeros of shifted polynomials as done here.

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