METHOD OF MARKOV CHAINS SIMULATION IN INCOHERENT RADIATION TRANSFER THEORY

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A numerical solution of the Fredholm linear integral equation of the 2-nd kind by the Monte-Carlo method, which is directly applicable to obtaining various functionals in the theory of incoherent radiation and neutron transfer, is suggested. The method resembles a well-known statistics quota sample realized in a generalized space of variable dimension. The necessary distribution of states according to a set of subspaces is achieved by means of the Markov Chain Technique. The numerical calculation, made for the particular case of breaking up into subspaces of photon scattering of various multiplicities, reveals the high efficiency of the method in comparison with the known estimate by collisions for not very large mean values of photon scattering, $\overline{N}$, in the medium.

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1. Introduction

The necessity to calculate radiation characteristics allowing for various nonequilibrium processes is more often met nowadays in fields such as atrophysics, atmospheric optics, low-temperature plasma, gasdynamic lasers and radiation gasdynamics. In many problems, however, one has to take into account the radiating gas motion, spatial inhomogeneity of gasdynamic fields, frequency redistribution, etc. In general case similar problems compel a scientist to solve integro-differential equations with a complicated kernel under the given velocity-, temperature- and pressure-fields.

The incoherent radiation resonance scattering by two-level atoms is the simplest problem of this kind in physics [1, 2]. While considering real radiating particles for instance such as diatomic molecules [3, 4], an equation for the vibrational energy density defining the source function of the transfer equation differs only in the kernel structure of the integro-differential equation as follows from [5, 6]. Problems of radiation transfer in scattering media [7] as well as the theory of neutron transport [8] are also solved by equations of the same type.

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In what follows, we develop the method of numerical solution of Fredholm linear integral equation of the 2-nd kind which can be applied directly to the above-mentioned problems taking into consideration that in the stationary case the original integro-differential equation reduces to an integral one through the Green function of the transfer operator.

The basic difference between the proposed approach and classical Monte-Carlo methods [8–10] is in the essential use of the uniform Markov chains theory. This method is the development of the approach, introduced by the authors in the previous paper [11]. The whole calculation procedure becomes more simple and effective as the calculation of the constant normalization of the obtainable state sequence $\{a_S\}$ is needless.

2. Calculation of functionals by the Markov chains method

Radiation characteristics such as radiation flux density, intensity, etc. are of considerable interest. They are linear functionals defined by a Fredholm equation of the 2-nd kind [11]:

$$\varepsilon(\vec{r}) = \int_V K(\vec{r}, \vec{r}')\varepsilon(\vec{r}')d\vec{r}' + \varphi(\vec{r}). \tag{1}$$

Therefore, it is reasonable to formulate the direct calculation technique for linear functionals F of the form:

$$F = \int_V f(\vec{r})\varepsilon(\vec{r})d\vec{r}, \tag{2}$$

where $f(\vec{r})$ is the arbitrary nonnegative function defining the sought after radiation characteristic.

Bearing in mind that the kernel norm of Eq. (1) is below unity we may set down the desired functional F as the Neumann series

$$F = \sum_{n=1}^{\infty} \int_V \dots \int_V f(\vec{r}_1)K(\vec{r}_1, \dots, \vec{r}_n)\varphi(\vec{r}_n)d\vec{r}_1 \dots d\vec{r}_n, \tag{3}$$

where $K(\vec{r}_1) \equiv 1$, $K(\vec{r}_1, \dots, \vec{r}_n) \equiv K(\vec{r}_1, \vec{r}_2) \dots K(\vec{r}_{n-1}, \vec{r}_n)$. Introduce the set of spaces $A_n = V \otimes V \otimes V \otimes \dots \otimes V$ for $n = 1, 2, \dots$ each A_n being presented in the form of a union of non-crossing spaces $A_{n\beta}$:

$$A_n = \bigcup_\beta A_{n\beta}.$$

Let $\{a_S\}$ be some sequence of points $a \equiv (\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n)$, $N(a) \equiv n$, satisfying the following: The points $a_S \in A_{n\beta}$ are distributed with some positive probability density $\pi_{n\beta}(a)$:

$$\int_{(A_{n\beta})} \dots \int \pi_{n\beta}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n)d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_n = 1, \tag{4}$$

at $M \to \infty$, $M_{n\beta}/M \to P_{n\beta}$, where $P_{n\beta}$ are the fixed non-zero probabilities $\sum_{n\beta} P_{n\beta} = 1$, $M_{n\beta}$ is the number of points $a_S \in A_{n\beta}$, $M = \sum_{n\beta} M_{n\beta}$. To allow for these definitions on the

basis of the law of large numbers an expression for the functional (3) with M large enough takes the form:

$$F = \sum_{n=1}^{\infty} \sum_{\beta} \sum_{a_S \in A_{n\beta}} \frac{f(a_S)K(a_S)}{M_{n\beta}\pi_{n\beta}(a_S)} \varphi(a_S), \tag{5}$$

where

$$f(a) \equiv f(\vec{r}_1), \quad K(a) \equiv K(\vec{r}_1, \ldots, \vec{r}_n), \quad \varphi(a) \equiv \varphi(\vec{r}_n).$$

To derive formula (5) one should proceed in (3) from integration over $a_S \in A_{n\beta}$ to summation over $a_S \in A_{n\beta}$, noting that at $M \to \infty$ an average volume per single sequence state $a_S \in A_{n\beta}$ is equal to $\varrho_{n\beta}(a) = (M_{n\beta}\pi_{n\beta}(a))^{-1}$. An introduced breaking up of the set of spaces A_n into $A_{n\beta}$ resembles a well-known method of quota sample [9] and serves for the decrease of dispersion. Consider now in detail the following case of the space A_n breaking up:

$$A_{n\beta} = V_\beta \otimes \underbrace{V \otimes V \otimes \ldots \otimes V}_{n-1}, \quad V = \bigcup_{\beta} V_\beta.$$

Define $\pi_{n\beta}(a)$ at $N(a) = n$ as:

$$\pi_{n\beta}(a) = \frac{f_0(a)K_0(a)}{f_{0\beta}}, \quad K_0(a) \equiv K_0(\vec{r}_1, \vec{r}_2) \ldots K_0(\vec{r}_{n-1}, \vec{r}_n), \tag{6}$$

where

$$f_0(a) \equiv f_0(\vec{r}_1), \quad f_{0\beta} = \int_{V_\beta} f_0(\vec{r})d\vec{r}, \quad \int_V K_0(\vec{r}, \vec{r}')d\vec{r}' = 1.$$

Correspondingly, Eq. (5) at sufficiently large M will take the form

$$F = \sum_{n\beta} \frac{f_{0\beta}}{M_{n\beta}} \sum_{a_S \in A_{n\beta}} \frac{f(a_S)K(a_S)}{f_0(a_S)K_0(a_S)} \varphi(a_S). \tag{7}$$

Thus in the limit $M \to \infty$ formula (7) gives an exact value of the functional F for the specified sequence $\{a_S\}$. Note, that for convenience $f_0(\vec{r})$ and $K_0(\vec{r}, \vec{r}')$ should be chosen such that

$$f_0(\vec{r}) \simeq f(\vec{r}), \quad K_0(\vec{r}, \vec{r}') \simeq \frac{K(\vec{r}, \vec{r}')}{\int_V K(\vec{r}, \vec{r}')d\vec{r}'}. \tag{8}$$

The form of Eq. (7) is especially simple when relations (8) are exact equalities. The remaining arbitrariness in choice of probabilities $P_{n\beta}$ is used to decrease the dispersion of the functional F.

It is known [9] that as $M \to \infty$ the dispersion DF goes to zero when the sequence $\{a_S\}$ is distributed with density in proportion to the integrand in Eq. (3). Hence, it appears that for the sake of dispersion decrease the following choice of $P_{n\beta}$ is advisable:

$$P_{n\beta} = \frac{1}{F} \int_{V_\beta} \int_V \ldots \int_V f(\vec{r}_1)K(\vec{r}_1, \ldots, \vec{r}_n)\varphi(\vec{r}_n)d\vec{r}_1 \ldots d\vec{r}_n. \tag{9}$$

Thus, one should construct the sequence $\{a_S\}$, its subsequent $a_k \in A_{n\beta}$ being distributed with the probability density (6). As $M \to \infty$ $M_{n\beta}/M$ tends to $P_{n\beta}$, defined by formula (9). For this purpose we can use the results of paper [11], describing the method of obtaining the $\{a_S\}$ sequence based on the theory of uniform Markov chains. By this method the arbitrary distribution of the sequence $\{a_S\}$ may be realized in the limit when the statistical sample volume tends to infinity.

We define the probability density of the a-to-b-state transition $W(a, b)$, satisfying the conditions of the fundamental limiting theorem [12] as well as the balance and normalization equations, as

$$P(a)W(a, b) = P(b)W(b, a),$$

$$\sum_{m=1}^{\infty} \int_V \dots \int_V W(\vec{r}_1, \dots, \vec{r}_n; \vec{r}'_1, \dots, \vec{r}'_m) d\vec{r}'_1 \dots d\vec{r}'_m = 1. \tag{10}$$

By Eq. (3) the probability density $P(a)$ is chosen as:

$$P(a) = \frac{1}{F} f(a)K(a)\varphi(a). \tag{11}$$

By [11] the solution of a set of equations (10) general enough for further purposes is of the form:

$$W(a, b) = \Delta(a, b)\pi(b)w(a, b), \tag{12}$$

where at $N(a) \neq 1$, $a \neq b$

$$\Delta(a, b) = \sigma\delta_{N(a),N(b)} + \frac{(1-\sigma)}{2}\delta_{N(a),N(b)-1} + \frac{(1-\sigma)}{2}\delta_{N(a),N(b)+1} \tag{13}$$

and, correspondingly, at $N(a) = 1$, $a \neq b$

$$\Delta(a, b) = \frac{(1+\sigma)}{2}\delta_{N(a),N(b)} + \frac{(1-\sigma)}{2}\delta_{N(a),N(b)-1}. \tag{14}$$

Here, σ is the free theoretical parameter $0 < \sigma < 1$ which is often set equal to 1/3. $\delta_{N(a),N(b)}$ is the Kroneker symbol. $\pi(a)$ is the probability density which is chosen proportional to $\pi_{n\beta}(a)$ at $a \in A_{n\beta}$:

$$\pi(a) = \frac{f_0(a)K_0(a)}{\sum_\beta f_{0\beta}}, \quad \int_V \dots \int_V \pi(\vec{r}_1, \dots, \vec{r}_n) d\vec{r}_1 \dots d\vec{r}_n = 1. \tag{15}$$

The conditional transition probability $w(a, b)$ at the known final state b can be defined either symmetrically

$$w(a, b) = \frac{f(b)K(b)\varphi(b)/f_0(b)K_0(b)}{f(a)K(a)\varphi(a)/f_0(a)K_0(a) + f(b)K(b)\varphi(b)/f_0(b)K_0(b)},$$

or asymmetrically

$$w(a, b) = \begin{cases} 1, & \tilde{w}_{ab} \geqslant 1, \\ \tilde{w}_{ab}, & \tilde{w}_{ab} < 1, \end{cases} \tag{16}$$

where

$$\tilde{w}(a, b) = \frac{f(b)K(b)\varphi(b)}{f_0(b)K_0(b)} \cdot \frac{f_0(a)K_0(a)}{f(a)K(a)\varphi(a)}. \tag{17}$$

Note, that an asymmetrical definition of the conditional transition probability is more preferable as in this case the transition frequency to new states is increased.

Describe now an explicit construction procedure of the sequence $\{a_S\}$ with simultaneous calculation of the unknown functional (7). Let a certain state a_k of the sequence $\{a_S\}$ be known. Each additional state is generated from its immediate predecessor in the following manner. First, by Eqs. (13), (14) we select $N(a_{k+1})$. At $N(a_k) \neq 1$ with probability σ we set $N(a_{k+1}) = N(a_k)$, with probability $(1-\sigma)/2$ we set $N(a_{k+1}) = N(a_k)-1$ and also with probability $(1-\sigma)/2$ we set $N(a_{k+1}) = N(a_k)+1$. By analogy at $N(a_k) = 1$, with probability $(1+\sigma)/2$ we set $N(a_{k+1}) = N(a_k)$ and with probability $(1-\sigma)/2$ we set $N(a_{k+1}) = N(a_k)+1$. Then we construct the state a_{k+1} itself with the probability density $\pi(a)$ (15). With the probability density $f_0(a)/\sum_\beta f_{0\beta}$ we select at first $\vec{r}_1$, then with the probability density $K_0(\vec{r}_1, \vec{r}_2)$ and the known $\vec{r}_1$ we select $\vec{r}_2$, etc. The process terminates at $n = N(a_{k+1})$ and as a result we find $a_{k+1} = (\vec{r}_1, \ldots, \vec{r}_n)$. Finally, we examine the realization of the transition $a_k \to a_{k+1}$. With that end in view the probability $w(a_k, a_{k+1})$ defined by Eqs. (16), (17) is computed and compared with the proper pseudorandom fraction ξ (uniform on the interval (0, 1)). If the transition appears to be an allowed one, (if $\xi \leqslant w(a_k, a_{k+1})$) then to find a_{k+2} we repeat the procedure described starting from the already known state a_{k+1}. In the opposite case (if $\xi > w(a_k, a_{k+1})$) the state a_{k+1} is generated for the second time with the probability density $\pi_{n\beta}(a)$ where $n = N(a_k)$, $\beta = \beta(a_k)$ and one finally gets a_{k+1}. The transition to the next state, however, is carried out in this case on the basis of the previous state a_k, i.e. as if $a_{k+1} = a_k$. If the next transition $a_k \to a_{k+2}$ proves to be forbidden as well, then a_{k+2} is generated again with the density $\pi_{n\beta}(a)$ at $n = N(a_{k+1})$, $\beta = \beta(a_{k+1})$ resulting in a_{k+2}, the transition to a_{k+3} being carried out from the state a_k: $a_k \to a_{k+3}$, etc. As the initial state a_1 of the sequence $\{a_S\}$ being generated can be an arbitrary one, for the sake of convenience the density $\pi(a)$ at $N(a) = 1$ may be used.

The calculation of the functional F goes simultaneously with the generation $\{a_S\}$. Therefore, it is advisable to have two memory cells for each pair of numbers (n, β). In the process of $\{a_S\}$ generation one serves for the $M_{n\beta}$ number storage, the other stores the sum

$$\sum_{a_S \in A_{n\beta}} \frac{f(a_S)K(a_S)}{f_0(a_S)K_0(a_S)} \varphi(a_S).$$

When the generation of $\{a_S\}$ is ceased by Eq. (7), the functional F is obtained by summation.

Note also that in those cases when the transition appears to be forbidden the calculated term $f(a_S)K(a_S)\varphi(a_S)/f_0(a_S)K_0(a_S)$ in the forbidden state a_S should be placed in additional memory cells. Henceforth, they can be used instead of a supplementary generation if forbidden transitions occur.

The technique described is applied readily to the case when the function $f(\vec{r})$ governs some density either on a line or a surface belonging to V. In this case similarly to [11] in all the formulae instead of $\vec{r}_1$ the new variable S_1, will be given, defined on the corresponding null set. In other respects the calculation procedure for F remains unchanged.

3. The comparison of various methods. Numerical results

To investigate the comparative efficiency of the above method named for brevity the MC (Markov Chains) method and other methods to be mentioned, consider the simplest integral equation

$$\varepsilon(\tau) = \int_0^{\tau_0} \frac{R^*}{2} \exp(-|\tau-\tau'|)\varepsilon(\tau')d\tau' + \varphi_0. \tag{18}$$

The choice is explained by an opportunity to find an analytical solution and to evaluate strictly enough the accuracy of various methods. Note, that transition to multidimensional spaces with V-volume any configuration and arbitrary complicated kernel K in the framework of the methods considered causes no difficulties. Eq. (19) describes the vibrational energy density distribution as diffusion approximation [6] in a homogeneous flat layer of an efficient optical depth τ_0 and the photon survival probability in an elementary scattering act R^*. An average by layer density of the vibrational energy will be taken as the functional

$$F = \frac{1}{\tau_0} \int_0^{\tau_0} \varepsilon(\tau)d\tau. \tag{19}$$

In what follows, for the sake of simplicity the breaking up of A_n into subspaces $A_{n\beta}$ is not used.

Assuming by Eq. (8)

$$f_0 = f = \frac{1}{\tau_0}$$

and

$$K_0(\tau, \tau') = \frac{\exp(-|\tau'-\tau|)}{\kappa(\tau)}, \quad \kappa(\tau) = \int_0^{\tau_0} \exp(-|\tau-\tau'|)d\tau',$$

we come to the following representation of the functional (19)

$$F = \varphi_0 \sum_{n=1}^{\max n} M_n^{-1} \left(\frac{R^*}{2}\right)^{n-1} \sum_{a_S \in A_n} \kappa(a_S), \tag{20}$$

where

$$a \equiv (\tau_1, \tau_2, \ldots, \tau_n), \quad \kappa(a) \equiv \kappa(\tau_1)\kappa(\tau_2) \ldots \kappa(\tau_{n-1}).$$

The above MC method accuracy can be easily improved by increasing the number of M_n states in Eq. (20), the total number of trajectories under generation remaining the same. Aiming at this, we introduce an extended state sequence $\{a'_S\}$ enclosing into $a_S \in A_n$ the initial sections $(\tau_1, \ldots, \tau_n)$ of all the $\{a_S\}$ sequence states for which $N(a_S) > n$. The dispersion of F is likely to decrease due to an increase of M_n. To calculate F using $\{a'_S\}$ it is sufficient to substitute a_S into Eq. (20) for a'_S, M_n denoting the number of states $a'_S \in A_n$.

For reasons of convenience the calculation of F based on the sequence $\{a'_S\}$ is called the Modified Markov Chains (MMC) method. In the following the accuracies of MC and MMC methods are compared with the well-known estimator by collisions [8, 9, 10] which is presented as the classical (Cl) method. The probability density of the photon trajectory by the Cl method is taken as

$$\pi_{cl}(a) = f_0(\tau_1)S(\tau_1)K_1(\tau_1, \tau_2) \ldots S(\tau_{m-1})K_1(\tau_{m-1}, \tau_m)\,[1 - S(\tau_m)],$$

$$K_1(\tau, \tau') = \exp(-\alpha|\tau - \tau'|) \Big/ \int_0^{\tau_0} \exp(-\alpha|\tau - \tau'|)d\tau', \quad \alpha = \text{const},$$

here $S(\tau)$ is the probability of trajectory continuation in the point τ (scattering), m is the random number of the final trajectory point and α defines the difference of the mean free path of the photon being modelled from the true one, which is 1. Note, that at $\alpha = 1$ $K_1(\tau, \tau') \equiv K_0(\tau, \tau')$.

Tables I, II give values of $\delta F(T)$:

$$\delta F(T) = F^{-1}M^{-1} \sum_{i=1}^{M} |F - F_i|,$$

which is an average relative deviation for the counting time T. The latter was set equal 30 minutes for all variants in the computer BESM-6. Here $\bar{N}$ is the theoretical value of

TABLE I

Relative accuracy of F-functional calculation by Cl method as a function of $S(\tau)$ and α; $\tau_0 = 6$, $R^* = 0.999$, $\bar{N} = 6.97$

$S(\tau)$	α	δF
$S(\tau) = \text{const} = 0.95$	1	4.10×10^{-4}
$S(\tau) = S_t(\tau)$	1	1.82×10^{-3}
$S(\tau) = \text{const} = 0.75$	1	1.21×10^{-2}
$S(\tau) = \text{const} = 0.95$	0.2	1.27×10^{-2}
$S(\tau) = S_t(\tau)$	0.2	2.32×10^{-2}
$S(\tau) = \text{const} = \bar{S}_t = 0.83$	0.2	4.32×10^{-2}
$S(\tau) = \text{const} = 0.75$	0.1	4.50×10^{-2}
$S(\tau) = S_t(\tau)$	0.05	2.95×10^{-2}
$S(\tau) = 2 - \exp(-\alpha\tau) - \exp[-\alpha(\tau_0 - \tau)]$	0.05	2.90×10^{-1}

TABLE II

Relative accuracy of F-functional calculation by MC, MMC, Cl methods for various mean scattering numbers of photon $\bar{N}$

Method	$\tau_0 = 1$ $\bar{N} = 1.58$	$\tau_0 = 2$ $\bar{N} = 2.33$	$\tau_0 = 3$ $\bar{N} = 3.24$	$\tau_0 = 6$ $\bar{N} = 6.97$	$\tau_0 = 12$ $\bar{N} = 18.6$	$\tau_0 = 24$ $\bar{N} = 57.1$
Cl	5.12×10^{-4}	6.40×10^{-4}	1.60×10^{-3}	1.82×10^{-3}	1.22×10^{-3}	1.40×10^{-2}
MC	1.92×10^{-4}	3.62×10^{-4}	5.08×10^{-4}	1.30×10^{-3}	1.20×10^{-2}	1.40×10^{-1}
MMC	6.20×10^{-5}	2.70×10^{-4}	1.99×10^{-4}	8.97×10^{-4}	1.10×10^{-2}	1.35×10^{-1}

an average photon scattering number in the medium for each variant of τ_0, R^* values. Table I gives the behaviour of δF calculated by the Cl method depending on various assignments of $S(\tau)$ and α at $\tau_0 = 6$ and $R^* = 0.999$. The true, $S_t(\tau)$ and the mean true, $\bar{S}_t$ probabilities of scattering are defined by

$$S_t(\tau) = \frac{R^*}{2}\kappa(\tau), \qquad \bar{S}_t = \frac{1}{\tau_0}\int_0^{\tau_0} S_t(\tau)d\tau.$$

Table II presents values of δF calculated by three methods Cl, MC, MMC according to an optical thickness of the layer τ_0 at $R^* = 0.999$, one of the best variants $S(\tau) = S_t(\tau)$, $\alpha = 1$ being chosen in Cl method.

The results given in Table I indicate the importance of the proper choice of $S(\tau)$, α by all Monte-Carlo methods using trajectories with absorption. It is clear also that an understating or overstating of an average scattering probability with respect to $\bar{S}_t$ as well as the changing of an average free path with respect to the true one results as a rule in a decrease in accuracy. It should be noted that in practice an evaluation of $S_t(\tau)$ and the true average free path is usually troublesome while in MC and MMC methods the problem of summation of the Neumann series terms with various scattering multiplicity is solved efficiently enough "automatically".

Table II indicates that for not very large values of $\bar{N} \gtrsim 10$ the MC and MMC methods yield better results in comparison with the Cl method. The Cl method accuracy exceeds that of MC and MMC methods only for large mean values of $\bar{N}$.

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