

On half-space problems for the discrete Boltzmann equation

N. BERNHOFF

Karlstad University - 651 88 Karlstad, Sweden

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Summary. — We study typical half-space problems of rarefied gas dynamics, including the problems of Milne and Kramer, for the discrete Boltzmann equation (a general discrete velocity model, DVM, with an arbitrary finite number of velocities). Then the discrete Boltzmann equation reduces to a system of ODEs. The data for the outgoing particles at the boundary are assigned, possibly linearly depending on the data for the incoming particles. A classification of well-posed half-space problems for the homogeneous, as well as the inhomogeneous, linearized discrete Boltzmann equation is made. In the non-linear case the solutions are assumed to tend to an assigned Maxwellian at infinity. The conditions on the data at the boundary needed for the existence of a unique (in a neighborhood of the assigned Maxwellian) solution of the problem are investigated. In the non-degenerate case (corresponding, in the continuous case, to the case when the Mach number at the Maxwellian at infinity is different of -1 , 0 and 1) implicit conditions are found. Furthermore, under certain assumptions explicit conditions are found, both in the non-degenerate and degenerate cases. An application to axially symmetric models is also studied.

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1. – Introduction

Half-space problems for the Boltzmann equation are of great importance in the study of the asymptotic behavior of the solutions of boundary value problems of the Boltzmann equation for small Knudsen numbers, see ref. [1] and references therein. Mathematical results on the half-space problem for the Boltzmann equation for a single-component gas are reviewed in ref. [2]. In this paper we consider corresponding problems for the general discrete velocity model (DVM), *i.e.* where the velocity is assumed to be able to take only an arbitrary finite number of different values. The Boltzmann equation can be approximated by DVMs, see *e.g.* refs. [3] and [4], and these approximations can be solved by numerical methods. The study of DVMs can also give a better conceptual understanding and new ideas for the continuous case. The half-space problems discussed in this paper are an example where one can find clear similarities between the discrete and continuous cases. For example, the number of additional conditions needed for well-posedness in the discrete case agrees with the results in the continuous case. In the planar stationary case, the discrete Boltzmann equation reduces to a system of ordinary differential equations. We review here results on this problem from refs. [5, 6] and [7].

Half-space problems for the linearized Boltzmann equation are well investigated, see ref. [2] and references therein. In ref. [8] Ukai, Yang and Yu studied the non-linear problem with inflow boundary condition for a hard sphere gas, assuming that the solutions tend to an assigned Maxwellian at infinity. The conditions on the data at the boundary needed for the existence of a unique (in a neighborhood of the assigned Maxwellian) solution of the problem are investigated. In the cases when the Mach number at the Maxwellian at infinity is different of -1 , 0 and 1 the number of conditions needed is found. Ukai considered in ref. [9] the same problem for the discrete Boltzmann equation, in the case corresponding to the case when the Mach number at the Maxwellian at infinity is less than -1 for the full Boltzmann equation. This result was generalized by Kawashima and Nishibata in ref. [10], where they still considered inflow boundary condition, and in ref. [11], for different boundary condition. However, Kawashima and Nishibata still assumed some quite restrictive conditions in refs. [10] and [11].

This paper is organized as follows: In sect. **2**, we introduce the planar stationary discrete Boltzmann equation and review some of its properties. We also review, in Theorem 1, the results in ref. [5] on the dimensions of the stable, unstable and center manifolds of the system of ODEs. These results are used to investigate the number of additional conditions needed to obtain well-posedness of the half-space problems in sect. **3**. The linearized problems are discussed in subsect. **3.1** based on results in ref. [6]. Here we also present and briefly discuss the boundary conditions. The non-linear problems are discussed in subsect. **3.2** based on results in ref. [7].

All results in this paper are valid for an arbitrary finite number of velocities. Similar results can also be obtained for DVMs for mixtures. Existence of weak shock wave solutions for the discrete Boltzmann equation has also been proved based on the same ideas in ref. [12].

2. – Discrete Boltzmann equation

The planar stationary system for the discrete Boltzmann equation (DBE) reads

$$(1) \quad B \frac{dF}{dx} = Q(F, F),$$

where $V = \{\xi_1, \dots, \xi_n\} \subset \mathbf{R}^d$, with $\xi_i = (\xi_i^1, \dots, \xi_i^d)$, is a finite set of velocities, $B = \text{diag}(\xi_1^1, \dots, \xi_n^1)$, and $F = (F_1, \dots, F_n)$, with $F_i = F_i(x) = F(x, \xi_i)$, and $x \in \mathbf{R}_+$. We assume that $\xi_i^1 \neq 0$, for $i = 1, \dots, n$.

For a function $g = g(\xi)$ (possibly depending on more variables than ξ), we identify g with its restrictions to the points $\xi \in V$, *i.e.* $g = (g_1, \dots, g_n)$, with $g_i = g(\xi_i)$.

The collision operator $Q(F, F)$ in (1) is given by the bilinear expressions

$$(2) \quad Q_i(F, F) = \sum_{j,k,l=1}^n \Gamma_{ij}^{kl} (F_k F_l - F_i F_j),$$

where it is assumed that the collision coefficients Γ_{ij}^{kl} satisfy the relations $\Gamma_{ij}^{kl} = \Gamma_{ji}^{kl} = \Gamma_{kl}^{ij} \geq 0$, with equality unless the conservation laws

$$(3) \quad \xi_i + \xi_j = \xi_k + \xi_l \quad \text{and} \quad |\xi_i|^2 + |\xi_j|^2 = |\xi_k|^2 + |\xi_l|^2$$

are satisfied (preservation of momentum and energy).

We consider below (even if this restriction is not necessary in our general context) only normal DVMS. That is, DVMS without spurious (or non-physical) collision invariants, *i.e.* any collision invariant is of the form $\phi = a + \mathbf{b} \cdot \xi + c|\xi|^2$, for some constant $a, c \in \mathbf{R}$ and $\mathbf{b} \in \mathbf{R}^d$. Methods of their construction are described in refs. [13, 14] and [15].

For DVMS the Maxwellian distributions are of the form

$$(4) \quad M = \exp[\phi] = A \exp[\mathbf{b} \cdot \xi + c|\xi|^2], \quad \text{with} \quad A = \exp[a] > 0,$$

where ϕ is a collision invariant. The latter equality in eq. (4) is due to the assumption of normal DVMS.

Given a Maxwellian M we denote

$$(5) \quad F = M + M^{1/2}f,$$

in eq. (1), and obtain

$$(6) \quad B \frac{df}{dx} + Lf = S(f, f),$$

where $Lf = -2M^{-1/2}Q(M, M^{1/2}f)$, and $S = S(f, f) = M^{-1/2}Q(M^{1/2}f, M^{1/2}f)$. The linearized collision operator ($n \times n$ matrix) L is symmetric and semi-positive, and the null-space $N(L)$ of L is (for normal DVMS) given by

$$(7) \quad N(L) = \text{span}(M^{1/2}, M^{1/2}\xi^1, \dots, M^{1/2}\xi^d, M^{1/2}|\xi|^2).$$

Furthermore, the quadratic part $S(f, f)$ is orthogonal to $N(L)$.

The diagonal matrix B is (under our assumptions) non-singular. If we denote $f|_{x=0} = f_0$, then we can rewrite eq. (6) as

$$(8) \quad f(x) = \exp[-xB^{-1}L]f_0 + \int_0^x \exp[(\sigma - x)B^{-1}L][S(f, f)](\sigma) d\sigma.$$

We now denote by n^\pm , where $n^+ + n^- = n$, and m^\pm , with $m^+ + m^- = q$, the numbers of positive and negative eigenvalues (counted with multiplicity) of the matrices B and $B^{-1}L$ respectively, and by m^0 the number of zero eigenvalues of $B^{-1}L$. Moreover, we denote by k^+ , k^- , and l the numbers of positive, negative, and zero eigenvalues of the $p \times p$ matrix K ($p = d+2$ for normal DVMS), with entries $k_{ij} = \langle y_i, y_j \rangle_B = \langle y_i, By_j \rangle$, such that $\{y_1, \dots, y_p\}$ is a basis of the null-space of L , *i.e.* for normal DVMS $\text{span}(y_1, \dots, y_p) = N(L) = \text{span}(M^{1/2}, M^{1/2}\xi^1, \dots, M^{1/2}\xi^d, M^{1/2}|\xi|^2)$. Here and below, we denote by $\langle \cdot, \cdot \rangle$ the Euclidean scalar product on \mathbf{R}^n and we also denote $\langle \cdot, \cdot \rangle_B = \langle \cdot, B \cdot \rangle$. Note that the numbers k^+ , k^- , and l do not depend on the specific choice of the basis $\{y_1, \dots, y_p\}$.

In applications, the number p of collision invariants is usually relatively small compared to n (note that formally $n = \infty$ for the continuous Boltzmann equation whereas $p \leq 5$). Also, the matrix B is diagonal and therefore all its eigenvalues are known. This explains the importance of the following result by Bobylev and Bernhoff in ref. [5] (see also ref. [6]).

Theorem 1. The numbers of positive, negative and zero eigenvalues of $B^{-1}L$ are given by

$$(9) \quad \begin{cases} m^+ = n^+ - k^+ - l, \\ m^- = n^- - k^- - l, \\ m^0 = p + l. \end{cases}$$

In the proof of Theorem 1 a basis

$$(10) \quad u_1, \dots, u_q, y_1, \dots, y_k, z_1, \dots, z_l, w_1, \dots, w_l$$

of \mathbf{R}^n , such that

$$(11a) \quad y_i, z_r \in N(L), \quad B^{-1}Lw_r = z_r \quad \text{and} \quad B^{-1}Lu_\alpha = \lambda_\alpha u_\alpha,$$

$$(11b) \quad \langle u_\alpha, u_\beta \rangle_B = \lambda_\alpha \delta_{\alpha\beta}, \quad \text{with} \quad \lambda_1, \dots, \lambda_{m^+} > 0 \quad \text{and} \quad \lambda_{m^++1}, \dots, \lambda_q < 0,$$

$$(11c) \quad \langle y_i, y_j \rangle_B = \gamma_i \delta_{ij}, \quad \text{with} \quad \gamma_1, \dots, \gamma_{k^+} > 0 \quad \text{and} \quad \gamma_{k^++1}, \dots, \gamma_k < 0,$$

$$(11d) \quad \langle u_\alpha, z_r \rangle_B = \langle u_\alpha, w_r \rangle_B = \langle u_\alpha, y_i \rangle_B = \langle w_r, y_i \rangle_B = \langle z_r, y_i \rangle_B = 0,$$

$$(11e) \quad \langle w_r, w_s \rangle_B = \langle z_r, z_s \rangle_B = 0 \quad \text{and} \quad \langle w_r, z_s \rangle_B = \delta_{rs},$$

is constructed. Then for any $h \in \mathbf{R}^n$, we obtain

$$(12) \quad \exp[-xB^{-1}L]h = \sum_{i=1}^k \mu_i y_i + \sum_{j=1}^l ((\eta_j - x\alpha_j)z_j + \alpha_j w_j) + \sum_{r=1}^q \beta_r \exp[-\lambda_r x] u_r,$$

where $\mu_i = \langle h, y_i \rangle_B / \langle y_i, y_i \rangle_B$, $\beta_r = \langle h, u_r \rangle_B / \lambda_r$, $\alpha_j = \langle h, z_j \rangle_B$ and $\eta_j = \langle h, w_j \rangle_B$.

For the continuous Boltzmann equation (with $d = 3$), if we have made the expansion (5) around a non-drifting Maxwellian $M = (\rho/(2\pi T)^{3/2}) \exp[-|\xi|^2/2T]$: $k^+ = k^- = 1$ and $l = 3$; and we can choose: $y_1 = (\xi^1/\sqrt{2T} + |\xi|^2/(\sqrt{30T}))M^{1/2}$, $y_2 = (-\xi^1/\sqrt{2T} + |\xi|^2/(\sqrt{30T}))M^{1/2}$, $z_1 = (\sqrt{5/2} - |\xi|^2/(\sqrt{10T}))M^{1/2}$, $z_2 = (\xi^2/\sqrt{T})M^{1/2}$, $z_3 = (\xi^3/\sqrt{T})M^{1/2}$; and, at least up to a constant: $w_j = L^{-1}\xi^1 z_j$.

3. – Half-space problems

3.1. Linearized problem. – First we consider the inhomogeneous (or homogeneous if $g = 0$) linearized problem

$$(13) \quad B \frac{df}{dx} + Lf = g,$$

where $g = g(x) \in L^1(\mathbf{R}_+, \mathbf{R}^n)$, with one of the boundary conditions

(O) the solution tends to zero at infinity, *i.e.* $f(x) \rightarrow 0$ as $x \rightarrow \infty$;

(P) the solution is bounded, *i.e.* $|f(x)| < \infty$ for all $x \in \mathbf{R}_+$;

(Q) the solution can be slowly increasing, *i.e.* $|f(x)| \exp[-\epsilon x] \rightarrow 0$ as $x \rightarrow \infty$, for all $\epsilon > 0$;

at infinity. The boundary condition (O) corresponds to the case when we have made the expansion (5) around a Maxwellian M , such that $F \rightarrow M$ as $x \rightarrow \infty$. The boundary conditions (P) and (Q) are the boundary conditions in the Milne and Kramers problem, respectively. In the case of boundary condition (O) at infinity we additionally assume that

$$(14) \quad g(x) \in N(L)^\perp \text{ for all } x \in \mathbf{R}_+.$$

We can, without loss of generality, assume that

$$(15) \quad B = \begin{pmatrix} B_+ & 0 \\ 0 & B_- \end{pmatrix},$$

where $B_+ = \text{diag}(\xi_1^1, \dots, \xi_{n^+}^1)$ and $B_- = -\text{diag}(\xi_{n^++1}^1, \dots, \xi_n^1)$, with $\xi_1^1, \dots, \xi_{n^+}^1 > 0$ and $\xi_{n^++1}^1, \dots, \xi_n^1 < 0$. We also define the projections $R_+ : \mathbf{R}^n \rightarrow \mathbf{R}^{n^+}$ and $R_- : \mathbf{R}^n \rightarrow \mathbf{R}^{n^-}$, by

$$(16) \quad R_+ s = s^+ = (s_1, \dots, s_{n^+}) \quad \text{and} \quad R_- s = s^- = (s_{n^++1}, \dots, s_n)$$

for $s = (s_1, \dots, s_n)$.

The original boundary condition at $x = 0$

$$(17) \quad F^+(0) = C_0 F^-(0) + a_0,$$

where C_0 is a given $n^+ \times n^-$ matrix and $a_0 \in \mathbf{R}^{n^+}$, leads after the expansion (5) to the general boundary condition

$$(18) \quad f^+(0) = C f^-(0) + h_0,$$

where $C = M_+^{-1/2} C_0 M_-^{1/2}$ is an $n^+ \times n^-$ matrix and $h_0 = M_+^{-1/2} (C_0 M^- - M^+ + a_0) \in \mathbf{R}^{n^+}$, with $M_+^{-1/2} = \text{diag}(M_1^{-1/2}, \dots, M_{n^+}^{-1/2})$ and $M_-^{1/2} = \text{diag}(M_{n^++1}^{1/2}, \dots, M_n^{1/2})$, see refs. [6] and [7]. We introduce the operator $\mathcal{C} : \mathbf{R}^n \rightarrow \mathbf{R}^{n^+}$, given by $\mathcal{C} = R_+ - C R_-$. In order to be able to obtain existence and uniqueness of solutions of the linearized half-space problems, we will assume that the matrix C fulfills either the condition

$$(19) \quad \dim \mathcal{C} U_+ = m^+, \quad \text{with} \quad U_+ = \text{span}(u_1, \dots, u_{m^+}),$$

as we consider boundary condition (O) at infinity, or the condition

$$(20) \quad \dim \mathcal{C} X_+ = n^+, \quad \text{with} \quad X_+ = \text{span}(u_1, \dots, u_{m^+}, y_1, \dots, y_{k^+}, z_1, \dots, z_l),$$

as we consider boundary condition (P) or (Q) at infinity.

If we assume inflow boundary condition, *i.e.* $C_0 = 0$, then $C = 0$ and $h_0 = M_+^{-1/2} (a_0 - M^+)$.

Let $n^- = n^+$. The discrete version of the Maxwell-type boundary conditions reads

$$(21) \quad F^+(0) = C_0 F^-(0), \quad \text{with} \quad C_0 = (1 - \alpha)I + \alpha C_{0d}, \quad 0 \leq \alpha \leq 1,$$

where I is the identity matrix and C_{0d} is the $n^+ \times n^+$ matrix, with the elements $c_{0d,ij} = \xi_{n^++j}^1 M_{0i} / \langle B_- M_0^-, 1 \rangle$ for some Maxwellian M_0 . The cases $\alpha = 0$ and $\alpha = 1$ correspond to specular and diffuse reflection, respectively. After the expansion (5), the Maxwell-type boundary conditions read

$$(22a) \quad f^+(0) = C_M f^-(0) + h_0, \quad \text{with } C_M = (1 - \alpha) M_+^{-1/2} M_-^{1/2} + \alpha C_d, \quad 0 \leq \alpha \leq 1,$$

$$(22b) \quad h_0 = M_+^{-1/2} ((1 - \alpha) M^- + \alpha (\langle B_- M^-, 1 \rangle / \langle B_- M_0^-, 1 \rangle) M_0^+ - M^+),$$

where C_d is the matrix with the elements $c_{d,ij} = \xi_{n^++j}^1 M_i^{-1/2} M_{n^++j}^{1/2} M_{0i} / \langle B_- M_0^-, 1 \rangle$, see also refs. [6] and [7]. We have the following existence result from ref. [6].

Theorem 2. i) Assume that the conditions (14) and (19) are fulfilled and that

$$(23) \quad h_0, C \exp[xB^{-1}L]B^{-1}g(x) \in \mathcal{CU}_+ \text{ for all } x \in \mathbf{R}_+.$$

Then the system (13) with the boundary conditions (O) and (18) has a unique solution.

ii) Assume that the condition (20) is fulfilled. Then the system (13) with the boundary conditions (Q) and (18) has a unique solution with the asymptotic flow

$$(24) \quad f_A(x) = \sum_{i=1}^k \mu_i y_i + \sum_{j=1}^l ((\eta_j - x\alpha_j) z_j + \alpha_j w_j),$$

if the $k^- + l$ parameters $\mu_{k^++1}, \dots, \mu_k$ and $\alpha_1, \dots, \alpha_l$ are prescribed.

If we assume boundary condition (P) instead of (Q), then we have to prescribe $\alpha_1 = \dots = \alpha_l = 0$ above.

Especially, for the homogeneous system, where $g = 0$, condition (23) is reduced to $h_0 \in \mathcal{CU}_+$.

One can easily prove, see refs. [6] and [7], that condition (19) is fulfilled, if $C^T B_+ C \leq B_-$ on $R_- U_+$, and similarly that condition (20) is fulfilled, if $C^T B_+ C < B_-$ on $R_- X_+$. It follows immediately that if $C = 0$, then conditions (19) and (20) are fulfilled. Furthermore, if we assume that $n^+ = n^-$ and that we have a set of velocities V , such that $\xi_{i+n^+} = (-\xi_i^1, \dots, \xi_i^d)$, $\xi_i^1 > 0$, and that we have made the expansion (5) around a non-drifting Maxwellian M , *i.e.* with $\mathbf{b} = \mathbf{0}$ in eq. (4), then condition (19) is fulfilled for the Maxwell-type boundary conditions, see ref. [6],

$$(25) \quad f^+(0) = C_M f^-(0), \quad \text{with } C_M = (1 - \alpha)I + \alpha C_{0d}, \quad 0 \leq \alpha \leq 1,$$

where I is the identity matrix and C_{0d} is the $n^+ \times n^+$ matrix, with the elements $c_{d,ij} = \xi_j^1 M_i^{1/2} M_j^{1/2} / \langle B_+ M^+, 1 \rangle$. Moreover, if $\alpha \neq 0$, then also condition (20) is fulfilled.

3.2. Weakly non-linear problem. – We now consider the full non-linear system

$$(26) \quad B \frac{df}{dx} + Lf = S(f, f),$$

where the solution tends to zero at infinity.

We add, following the structure in [8] for the full Boltzmann equation, a damping term $-\gamma P_0^+ f$ to the right-hand side of the system (26) and obtain

$$(27) \quad B \frac{df}{dx} + Lf = S(f, f) - \gamma P_0^+ f,$$

where $\gamma > 0$ and $P_0^+ f = \sum_{i=1}^{k^+} (\langle f(x), y_i \rangle_B / \langle y_i, y_i \rangle_B) y_i + \sum_{j=1}^l \langle f(x), w_j \rangle_B z_j$.

First we consider the corresponding linearized inhomogeneous system

$$(28) \quad B \frac{df}{dx} + Lf = g - \gamma P_0^+ f,$$

where $g = g(x) : \mathbf{R}_+ \rightarrow \mathbf{R}^n$ is a given function such that $g(x) \in N(L)^\perp$ for all $x \in \mathbf{R}_+$. We can under the assumptions that condition (20) is fulfilled and that all necessary integrals exist prove the existence of a unique solution to the system (28), with the boundary conditions (O) and (18), see ref. [7]. Thereafter, we can use contraction mapping arguments to prove the following result, see ref. [7].

Theorem 3. Let condition (20) be fulfilled. Then there is a positive number δ_0 , such that if

$$(29) \quad |h_0| \leq \delta_0,$$

then the system (27) with the boundary conditions (O) and (18) has a locally unique solution $f = f(x)$.

We can now note that, if $\langle S(f, f), w_j \rangle = 0$ for $j = 1, \dots, l$, then the solution of Theorem 3 is a solution of the problem (26), (O), (18) if and only if $P_0^+ f(0) = 0$. Thereafter, we can use arguments similar to the ones in [8] for the continuous Boltzmann equation to prove the following theorem, see ref. [7].

Theorem 4. Let condition (20) be fulfilled, and suppose that $\langle S(f(x), f(x)), w_j \rangle = 0$ for $j = 1, \dots, l$, and that $\langle h_0, h_0 \rangle_{B_+}$ is sufficiently small. Then with $k^+ + l$ conditions on h_0 , the system (26) with the boundary conditions (O) and (18) has a locally unique solution.

We obtain implicit conditions on h_0 and have, if $l \geq 1$ (corresponding, in the continuous case, to the case when the Mach number at the Maxwellian at infinity is 0 or ± 1) some quite restrictive conditions on the quadratic part. If we consider the system (26) directly we can by using contraction mapping arguments obtain the following result, see ref. [7].

Theorem 5. Let condition (19) be fulfilled and assume that

$$(30) \quad h_0, \mathcal{C} \exp[xB^{-1}L]B^{-1}S(f(x), f(x)) \in \mathcal{C}U_+$$

for all $x \in \mathbf{R}_+$, with $U_+ = \text{span}(u : Lu = \lambda Bu, \lambda > 0) = \text{span}(u_1, \dots, u_{m^+})$. Then there is a positive number δ_0 , such that if $|h_0| \leq \delta_0$, then the system (26) with the boundary conditions (O) and (18) has a locally unique solution.

Here we have $k^+ + l$ explicit conditions on h_0 , but also, if $k^+ + l \geq 1$ (corresponding, in the continuous case, to the case when the Mach number at the Maxwellian at infinity is ≥ -1), in general some restrictive conditions on the quadratic part (depending on the matrix C and the DVM). However, these conditions can be better than the ones in Theorem 4 if $l \geq 1$.

These results extend, by both more general boundary conditions and more general assumptions, previous results for the discrete Boltzmann equation by Ukai in ref. [9], and Kawashima and Nishibata in refs. [10] and [11], and include also (for DVMs) the results obtained by Ukai *et al.* in ref. [8] for the full Boltzmann equation, see ref. [7].

For a class of axially symmetric models, with some extra symmetry condition on the collision coefficients, we can prove the following theorem, using Theorem 5, if we have made the expansion (5) around a non-drifting Maxwellian M , see ref. [7].

Theorem 6. Let $h_0 \in (R_+ - R_-)U_+$, where $U_+ = \text{span}(u_1^+, \dots, u_{N-d-1}^+)$. Then there is a positive number δ_0 , such that if $|h_0| \leq \delta_0$, then the system (26) with the boundary conditions (O) and $(R_+ - R_-)f(0) = h_0$ has a locally unique solution $f = f(x)$.

The same problem, for $d = 2$, has been studied by Babovsky in ref. [16], but then under the quite restrictive condition $\langle S(f, f), w_i \rangle = 0$ for $i = 1, 2$. See also ref. [17] for the continuous case.

All our results can be extended in a natural way, to yield also for singular matrices B , if $N(L) \cap N(B) = \{0\}$, see refs. [6] and [7].

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