Comment on "Energy partitioning and particle spectra in multicomponent collision cascades"

Zhu Lin Zhang*
Department of Mathematics and Physics, Anhui University of Science and Technology, Huainan, China
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Four equations proposed by Vicanek *et al.* have been studied based on the pertinent transport equation. Several difficulties have been found at using them and three corresponding revised ones have been derived rigorously for arbitrary particle interaction potentials.

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In 1993, Vicanek, Conrad, and Urbassek (called VCU in this work) proposed a system of differential equations [Eqs. (7) in VCU's paper] for approximate energy distributions of recoil atoms in collision cascades in composite media.[1] Besides, VCU derived three other equations, for deposited energy sharing, particle slowing down density, and the number of recoils [Eqs. (14), (20), and (21) in VCU's paper]. In this work, VCU's equations will be studied carefully based on the transport theory and several difficulties will be shown using these equations. The author will show that the approximate differential equations may not be suitable "for arbitrary particle interaction potentials" at least. It will be shown that VCU's three other equations directly contradict the transport theory and the corresponding revised ones will be given exactly.

I. BASIC TRANSPORT THEORY

Consider a random, infinite medium with c_jN atoms of type j (atomic number Z_j, atomic mass M_j) per unit volume $(j=1,2,\ldots,n)$. c_j $(0\leqslant c_j\leqslant 1;\ \Sigma_j c_j=1)$ is the concentration of j atoms, and N the atomic density (atoms/cm^3). Let the particle flux $\Psi_{ij}(E_0,E)$ be the average number of j atoms moving with energy in the interval (E,dE) in a collision cascade initiated by an i atom starting with an initial energy E_0. $\Psi_i(E)\equiv\Psi_{1i}(E_0,E)$ satisfies the forward Boltzmann equation[1]

$$N\sum_j \int dT\{c_j\sigma_{ij}(E+T,T)\Psi_i(E+T)+c_i\sigma_{ji}(E+T,E)\times\Psi_j(E+T)-c_j\sigma_{ij}(E,T)\Psi_i(E)\}+\delta_{i1}\delta(E-E_0)=0, \tag{1}$$

with the obvious initial condition $\Psi_i(E>E_0)=0$. Where $d\sigma_{ij}(E,T)\equiv\sigma_{ij}(E,T)dT$ is the differential cross section for scattering between a moving i atom and a j atom at rest. Here, E and T represent the energies of the scattered and recoiling atom, respectively.

Freezing collision densities were introduced and derived asymptotically by Roosendaal *et al.* for a monatomic medium.[2] Following their track, taking into account all recoils exited into $(E',E'+dE')$ from rest and all recoils deexited into $(E',E'+dE')$ from energy above threshold energy E in a single collision, a "frozen in" picture of the cascade for $E'\leqslant E<E_0$ is obtained. Thus, it is natural to define the energy sharing $\omega_{ij}(E_0,E)$ (Refs. 3 and 4) and the particles slowing down density $\chi_{ij}(E_0,E)$,[1,3] respectively, as follows:

$$\sum_k c_k\int_0^{E_0} d\sigma_{ik}(E_0,T)[\omega_{ij}(E_0,E)-\omega_{ij}(E_0-T,E)-\omega_{kj}(T,E)]=0, \tag{2}$$

$$\sum_k c_k\int_0^{E_0} d\sigma_{ik}(E_0,T)[\chi_{ij}(E_0,E)-\chi_{ij}(E_0-T,E)-(1-\theta(E-T))\chi_{kj}(T,E)]=0, \tag{3}$$

with conditions

$$\omega_{ij}(E_0,E\geqslant E_0)/E_0=\chi_{ij}(E_0,E\geqslant E_0)=\delta_{ij}, \tag{4}$$

where $\theta(x\geqslant 0)=1$ and $\theta(x<0)=0$. Since E is set up as a threshold energy, a particle with energies above E is able to create a cascade and slows down to energy $\leqslant E$, then keeps on moving with its final energy E' and no longer creates any cascade. The conditions (4) are critical to solving Eqs. (2) and (3). In physics, the following idea is absolutely inacceptable: a particle with energy $E'>E$ suddenly disappears after it slows down to energy $E'\leqslant E$.

Taking Eq. (4) into account, comparing Eqs. (2) and (3) to Eq. (1) respectively, one obtains

$$\omega_i(E)=[1-\theta(E-E_0)]\,\overline{\omega_i}(E)+E_0\delta_{i1}\theta(E-E_0), \tag{5}$$

$$\chi_i(E)=[1-\theta(E-E_0)]\overline{\chi_i}(E)+\delta_{i1}\theta(E-E_0), \tag{6}$$

where $\omega_i(E)\equiv\omega_{1i}(E_0,E)$ and $\chi_i(E)\equiv\chi_{1i}(E_0,E)$. We also obtain

$$\overline{\omega_i}(E)\equiv N\sum_j \int_E^{E_0}dE'\left[\Psi_j(E')c_i\int_0^E\sigma_{ji}(E',T)TdT+\Psi_i(E')c_j\int_{E'-E}^{E'}\sigma_{ij}(E',T)(E'-T)dT\right],$$

$$\overline{\chi_i}(E)\equiv\int_E^{E_0}dE'\Psi_i(E')N\sum_j c_j\int_{E'-E}^{E'}\sigma_{ij}(E',T)dT.$$

Differentiating Eqs. (5) and (6) with respect to E and using Eq. (1), one obtains

$$-\frac{d\omega_i(E)}{dE}+N\sum_j [\Psi_i(E)c_jS_{ij}(E)-\Psi_j(E)c_iS_{ji}(E)]=0 \tag{7}$$

$$-\frac{d\chi_i(E)}{dE}=F_i(E) \tag{8}$$

exactly, where $F_i(E)dE$ was defined by VCU as the number of i atoms set in motion at energy (E,dE) due to collisions by moving atoms of any kind

$$F_i(E)=\int_E^{E_0} dE' Nc_i\sum_j \Psi_j(E')\sigma_{ji}(E',E).$$

II. DIFFICULTIES IN VCU'S PAPER

Difficulty 1. About the particle spectra $\Psi_i(E)$: VCU proposed a system of differential equations[1]

$$\begin{aligned} &N\sum_j [-c_jS_{ij}(E)\Psi_i(E)+c_iS_{ji}(E)\Psi_j(E)] \\ &\quad+\frac{d}{dE}N\sum_j [c_j\sigma_{ij}^s(E)E^2\Psi_i(E)+c_i\sigma_{ji}^r(E)E^2\Psi_j(E)] \\ &\quad+E\delta_{i1}\delta(E-E_0)=0 \end{aligned} \tag{9}$$

to approximate Eq. (1) and advocated that "this is possible for arbitrary particle interaction potentials." For the cases of "detailed balance" simulated by two[5] of VCU's equations by using same parameters in the general power cross section ($\tilde{C}_{11}=\tilde{C}_{22}=1$, $\tilde{C}_{12}=\tilde{C}_{21}=100$, etc.), the present author solved Eq. (9) and got nonphysics negative particle spectra.[3] Therefore, at least for these cases, Eq. (9) cannot predict even approximate particle spectra. Since the range of validity of Eq. (9) has never been given, these bad examples may weaken the conclusion in VCU's paper.[1]

Difficulty 2. About deposited energy sharing $\omega_i(E)$ and slowing down density $\chi_i(E)$: VCU defined the deposited energy sharing and slowing down density as

$$\omega_i(E)=\overline{\omega_i}(E) \quad\text{and}\quad \chi_i(E)=\overline{\chi_i}(E), \tag{10}$$

respectively.[1] Differentiating Eqs. (10) with respect to E and using Eq. (1), VCU obtained

$$\begin{aligned} &-\frac{d\omega_i(E)}{dE}+N\sum_j [\Psi_i(E)c_jS_{ij}(E)-\Psi_j(E)c_iS_{ji}(E)] \\ &\quad=E\delta_{i1}\delta(E-E_0), \end{aligned} \tag{11}$$

$$-\frac{d\chi_i(E)}{dE}=F_i(E)+\delta_{i1}\delta(E-E_0). \tag{12}$$

One may notice that Eqs. (11) and (12) are strictly equivalent to Eqs. (7) and (8), respectively for $E<E_0$, as long as

$$\omega_i(E\geqslant E_0)/E_0=\chi_i(E\geqslant E_0)=0. \tag{13}$$

However, Eq. (13) violates both energy and particle number conservation. From a mathematical point of view, taking Eq. (13) rather than Eq. (4) into account, and comparing Eqs. (2) and (3) to Eq. (1), respectively, one only can get $\omega_i(E)/E_0 =\chi_i(E)=0$ which directly contradicts their beginning assumptions (10). From a physics point of view, Eq. (13) means that a particle suddenly disappears after the particle with energy $E'>E$ slows down to energy $E'\leqslant E$, which is absolutely inacceptable. Therefore, Eqs. (11) and (12) are not those from VCU's but new Eqs. (7) and (8) are strictly equivalent to the original transport equations.

Difficulty 3. About the total number of recoils N_i: The total number of recoils generated above some displacement threshold energy $E_d>E$ was derived exactly by the present author,[3]

$$N_i=\int_{E_d}^{E_0} dE' Nc_i\sum_j \Psi_j(E')\int_0^{E_d}\sigma_{ji}(E',T)dT.$$

Directly integrating yields

$$\int_{E_d}^{E_0} dE\, F_i(E)=\int_{E_d}^{E_0} dE' Nc_i\sum_j \Psi_j(E')\int_{E_d}^{E'}\sigma_{ji}(E',T)dT,$$

which is not the total number N_i of recoils. In addition, it is easy to see that Eqs. (21) in VCU's paper,

$$\int_{E_d}^{E_0} dE\, F_i(E)=\chi_i(E_d)-\delta_{i1},$$

also cannot be tenable.

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*Corresponding author. Email address: hnzhangbch@mail.ahbbptt.net.cn

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