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SOME CHARACTERISTICS OF THE THERMAL NEUTRON SCATTERING PROBABILITY

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An explicit form for the function representing the probability that a neutron with velocity, $\underline{v}'$ shall be scattered into an element of volume in velocity space, d^3v about $\underline{v}$, by elastic collisions with atoms of arbitrary mass number, A, in a Maxwell-Boltzmann distribution characterized by a temperature, T, is derived. Analytical representations of this probability are presented for scattering cross sections which are either independent of relative speed or exhibit a Gaussion dependence. The scattering probability resulting from the former assumption is examined in some detail, and then employed in a calculation of the mean energy change per collision.

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The problem of formulating an internally consistent treatment of the neutron distribution in space and energy in finite systems reduces ultimately to the problem of solving in some approximation the transport equation:

$$\underline{v}\cdot\nabla\, n(\underline{r},\underline{v}) + \Sigma_t\, v\, n(\underline{r},\underline{v}) = S(\underline{r},\underline{v})$$

$$+ \int_{v'} \Sigma_s(v')\, v' n(\underline{r},\underline{v}')\, P(\underline{v}' \to \underline{v};\, T,\, A)\, d^3v' \quad . \qquad (1)$$

Clearly an attack upon this problem can proceed no further than the mere statement of it until at least some of the properties of the scattering probability,

$$P(\underline{v}' \to \underline{v};\, T,\, A)\, d^3v' \qquad (2)$$

have been delineated. The parametric dependence of this scattering probability upon moderator temperature, T, and mass number, A, is explicitly indicated.

It is the purpose of the work reported herein to:

(a) Obtain an explicit representation of this scattering probability based upon the assumptions that the moderator speed distribution is of the maxwell-Boltzmann type and that the scattering cross sections belong to a restricted class.

(b) Indicate some potentially interesting calculations which might be carried through more or less straightforwardly given an analytic form for the scattering probability.

The derivation of the scattering probability follows a procedure initially outlined by Jaffe[1]. An appropriate starting point may be taken to be a conventional[2] formulation of the rate/cm^3 of scattering of neutrons from all possible initial velocities into a particular element of volume in velocity space,

$$\int_{\underline{V}',\underline{\Omega}'_k} n(\underline{r},\underline{v}')\, d^3v' |\underline{v}'-V'|\, \sigma_s(|v'-V'|, \Omega'_k)\, d\Omega'_k M(\underline{V}')\, d^3V' \quad , \qquad (3)$$

where primes indicate pre-collision variables. We have defined $n(\underline{r},\underline{v}')\, d^3v' d^3r \equiv$ number of neutrons in d^3r about $\underline{r}$ with velocities in d^3v' about $\underline{v}'$; $M(\underline{V}')\, d^3V' \equiv$ number of scattering atoms/cm^3 with velocities in d^3V' about $\underline{V}$; (presumed constant in space); $\sigma_s\, (|\underline{v}'-\underline{V}'|, \Omega'_k)\, d\Omega'_k \equiv$ differential scattering cross section for neutrons scattered into an element of solid angle $d\Omega'_k$ measured in the center of mass coordinate system. The integral (3) requires some interpretation, and this is facilitated by examination of the schematic collision diagram illustrated in Figure 1.

Only elastic collisions are here envisaged. A coordinate transformation is now performed in the integrand of (3); i.e.,

$$\left\{ \underline{v}', \underline{V}', \underline{\Omega}'_k \right\} \rightarrow \left\{ \underline{v}', \underline{v}, \underline{\Omega}'_R \right\} \tag{4}$$

The integral now becomes

$$\int_{\underline{v}', \underline{\Omega}'_R} n(\underline{r}, \underline{v}')\, R'\, \sigma_s(R', \Omega'_R)\, M(\underline{V}')\, J\left(\frac{\underline{v}', \underline{V}', \underline{\Omega}'_k}{\underline{v}', \underline{v}, \Omega'_R}\right) d^3v'\, d\Omega'_R\, d^3v$$

$$= d^3v \int_{\underline{v}'} n(\underline{r}, \underline{v}')\, v' d^3v'\, \Sigma_s\,(v')\, P(\underline{v}' \rightarrow \underline{v};\, T, A), \tag{5}$$

where we have defined

$$\Sigma_s\,(v')\, P(\underline{v}' \rightarrow \underline{v};\, T, A)$$

$$\equiv \int_{\underline{\Omega}'_R} \frac{R'}{v'}\, \sigma_s\,(R', \underline{\Omega}'_R)\, M\,(\underline{V}')\, J\left(\frac{\underline{V}', \underline{\Omega}_k}{\underline{v}, \underline{\Omega}'_R}\right) d\Omega'_R \tag{6}$$

The evaluation of the Jacobian is straightforward but laborious[1].

One obtains

$$J\left(\frac{\underline{V}', \underline{\Omega}'_k}{\underline{v}, \underline{\Omega}'_R}\right) = \frac{1}{[2\beta \cos \gamma]^3}\,, \tag{7}$$

where the mass parameter β and the angle γ are defined in Figure 1. The relative speed, R', is related to the initial and final neutron velocities and the center of mass scattering angle, γ, by

$$R' = \frac{k}{2\beta \cos \gamma}\,, \tag{8}$$

where again the vector $\underline{k} = \underline{v} - \underline{v}'$ is illustrated in Figure 1. Also, from Figure 1, it is easily shown that

$$V'^2 = v'^2 + \frac{k^2}{(2\beta \cos \gamma)^2} - \frac{2\,kv'}{2\beta \cos \gamma}\Big[\cos \gamma \cos \zeta$$

$$+ \sin \gamma \,\mathrm{Sin}\,\zeta \cos (\varphi_{\underline{R}'} - \varphi_{\underline{v}'})\Big], \qquad (9)$$

where the angles $\varphi_{\underline{R}'}$ and $\varphi_{\underline{v}'}$ are appropriate azimuths for the vectors $\underline{R}'$ and $\underline{v}'$ measured relative to an arbitrary fixed coordinate system. If now we make the not very restrictive assumption that the differential cross section depends only upon the polar angle of scattering, γ; and observe that

$$\cos \zeta = \frac{v' - v\mu}{k} \qquad (10)$$

where μ is the cosine of the neutron scattering angle measured in the laboratory coordinate system; we see that the azimuthal integration for (6) may be readily performed[3]. The result is

$$\Sigma_s\,(v')\;P\,(\underline{v}' \rightarrow \underline{v};\;T,\,A)$$

$$= \frac{2\pi NsC}{(2\beta)^4}\;\frac{k}{v'}\int \sigma_s\,(v,v',\mu,\gamma)e^{-hD}\;\frac{J_o(ihB)\mathrm{Sin}\gamma d\gamma}{\cos^4\gamma}\;, \qquad (11)$$

where we have defined

Ns = total number of scattering atoms/cm^3,

$C = (h/\pi)^{3/2}$,

$h = M/2kT$,

$$D = v'^2 + \frac{k^2}{(2\beta \cos \gamma)^2} - \frac{kv' \cos \zeta}{\beta}$$

$$B = \frac{kv' \tan \gamma \mathrm{Sin}\,\zeta}{\beta}\;, \text{ and}$$

$J_o(X)$ = the zero order Bessel function of the first kind of argument X.

It is to be noted that the cross section depends upon v, v', and μ only through its dependence upon relative speed. For isotropic scattering in the center of mass it assumes the form

$$\sigma_s = \sigma_s \left(\frac{k}{2\beta \cos\gamma}\right) 4 \cos\gamma. \qquad (12)$$

More generally, the cross section is

$$\sigma_s (R', \Theta) \text{Sin}\, \Theta \, d\Theta$$

where Θ is the conventional C of M scattering angle. Thus if this be expanded in the usual series;

$$\sigma_s (R', \Theta) \text{Sin}\, \Theta \, d\Theta$$

$$= \sum_{\ell} \sigma_{s\ell} \left(\frac{k}{2\beta \cos\gamma}\right) 4 \cos\gamma \, (-1)^{\ell} P_{\ell} (\cos 2\gamma) \text{Sin}\, \gamma \, d\gamma$$

$$= \sigma_s (v, v', \mu, \gamma) \text{Sin}\, \gamma \, d\gamma. \qquad (13)$$

A form for the scattering cross section that has been found useful in the thermal range(4) is

$$\sigma_s (R', \gamma) = [\sigma_o + \sigma_1 e^{-pR'^2}] \, 4 \cos\gamma, \qquad (14)$$

where σ_o, σ_1 and p are constants to be fitted to the data. We will assume this form in what follows. Thus in the new coordinate system

$$\sigma_s (v, v', \mu, \gamma) = [\sigma_o + \sigma_1 e^{-p\left(\frac{k}{2\beta \cos\gamma}\right)^2}] \, 4 \cos\gamma \qquad (15)$$

and $\Sigma_s (v') \, P \, (\underline{v}' \rightarrow \underline{v}; \, T, A) = \Sigma_{so} \, P_o(\underline{v}' \rightarrow \underline{v}; \, T, A) + \Sigma_{s1} \, P_1(\underline{v}' \rightarrow \underline{v}; \, T, A)$

(16)

where

$$\Sigma_{so} = N_s \sigma_o,$$

$$\Sigma_{s1} = N_s \sigma_1;$$

and hence

P_o ($\underline{v}' \rightarrow \underline{v}$; T.A)

$$= \frac{8\pi}{(2\beta)^4} \left(\frac{h}{\pi} \right)^{3/2} \frac{k}{v'} \int_{\gamma=0}^{\pi/2} \frac{e^{-hD} J_o(ihB) \operatorname{Sin}\gamma \, d\gamma}{\cos^3\gamma} \qquad (17a)$$

P_1 ($\underline{v}' \rightarrow \underline{v}$; T,A)

$$= \frac{8\pi}{(2\beta)^4} \left(\frac{h}{\pi} \right)^{3/2} \frac{k}{v'} \int_{\gamma=0}^{\pi/2} \frac{e^{-hD-pR'^2} J_o(ihB) \operatorname{Sin}\gamma \, d\gamma}{\cos^3\gamma} \qquad (17b)$$

At this point we introduce a further variable transformation;

$$\xi = \tan \gamma .$$

Then if we define

$$X_1 = v'^2 - \frac{kv' \cos \zeta}{\beta} + \frac{k^2}{(2\beta)^2} ,$$

$$K_1 = hk^2 / (2\beta)^2 ,$$

$$X_2 = X_1 + pk^2/h \, (2\beta)^2 ,$$

$$K_2 = K_1 + pk^2 / (2\beta)^2 , \quad \text{and}$$

$$\eta = \frac{hk \, v' \operatorname{Sin} \zeta}{\beta} ,$$

we have

P_o ($\underline{v}' \rightarrow \underline{v}$; T,A)

$$= \frac{8\pi}{(2\beta)^4} \left(\frac{h}{\pi} \right)^{3/2} \frac{k}{v'} \frac{e^{-hX_1 + \eta^2/4K_1}}{2K_1} \qquad (18a)$$

and

P_1 ($\underline{v}' \rightarrow \underline{v}$; T,A)

$$= \frac{8\pi}{(2\beta)^4} \left(\frac{h}{\pi} \right)^{3/2} \frac{k}{v'} \frac{e^{-hX_2 + \eta^2/4K_2}}{2K_2} . \qquad (18b)$$

Formulae 18a,b provide us with explicit representations of the scattering kernel for the thermal region for a fair range of interesting cases. It should be noted in passing that the mass parameter, M, may be adjusted(4) in a given case to account at least partially for moderator thermal distributions for systems characterized by more degrees of freedom than those of pure translation.

The detailed discussion of the scattering probability, (18) that follows will be predicated upon the assumption that $\sigma_1 = 0$; i.e., that the scattering is isotropic in the center of mass and that the cross section is independent of the relative speed.

Returning to (18) and recalling (16) we see that[7]

$$P\,(\underline{v}' \rightarrow \underline{v};\ T,A) = \frac{1}{\beta^2}\sqrt{\frac{h}{\pi}}\ \frac{e^{-hX}}{kv'}\left(\Sigma_{so}/\Sigma_s(v')\right), \qquad (19)$$

where

$$X\,(\underline{v},\underline{v}') = \frac{\alpha}{\beta}v^2 + \frac{(\beta-\alpha)^2}{(2\beta)^2}(v^2 + v'^2) + 2\,\frac{\beta-\alpha}{(2\beta)^2}\,\underline{v}\circ\underline{v}'$$

$$-\ \frac{v^2v'^2 - (\underline{v}\circ\underline{v}')^2}{(v^2 + v'^2 - 2\underline{v}\bullet\underline{v}')}, \qquad (20a)$$

$$X\,(\underline{v},\underline{k}) = \frac{(\beta-\alpha)^2}{(2\beta)^2}k^2 - 2\frac{\beta-\alpha}{2\beta}\,\underline{v}\circ\underline{k} + \left(\frac{\underline{v}\circ\underline{k}}{k}\right)^2, \qquad (20b)$$

$$X\,(\underline{v}',\underline{k}) = \frac{k^2}{(2\beta)^2} + \frac{\underline{v}'\circ\underline{k}}{\beta} + \left(\frac{\underline{v}'\circ\underline{k}}{k}\right)^2. \qquad (20c)$$

This function is presented in a variety of forms; since, depending upon the nature of a given calculation, one rather than the others may be particularly appropriate.

The effective scattering cross section, $\Sigma_s(v')$, for the case considered herein is defined to be

$$\Sigma_s(v') = 4\pi \Sigma_{so} \int_{\underline{V}} \frac{|\underline{v}-\underline{V}|}{v} \left(\frac{h}{\pi}\right)^{3/2} e^{-hV^2} d^3V$$

$$= 4\pi \Sigma_{so} \left[\frac{e^{-hv'^2}}{\sqrt{\pi h}\; v'} + \left(1 + \frac{1}{2hv'^2}\right) \mathrm{erf}(\sqrt{h}\; v') \right]$$

$$= \Sigma_{so} Q(v') \quad . \tag{21}$$

Thus in this instance

$$P\,(\underline{v}' \to \underline{v};\ T,A) = \frac{1}{\beta^2} \sqrt{\frac{h}{\pi}} \quad \frac{e^{-hX}}{kv'\ Q(v')} \quad . \tag{22}$$

It is a straightforward matter to verify that the normalization of P is such that

$$\int_{\underline{v}} P\,(\underline{v}' \to \underline{v};\ T,A)\ d^3v = 1 \tag{23}$$

Another noteworthy property of the scattering probability follows from the observation that for neutrons in thermal equilibrium with their environment - hence distributed in velocities according to the Maxwell-Boltzmann law - the number scattering into d^3v per cm^3 per sec must equal the number scattering out of d^3v per cm^3 per sec; i.e.,

$$nv\,\Sigma_{so}\,Qd^3v = \int_{\underline{v}'} \Sigma_{so}\,Q'v'n'\,P\,(\underline{v}' \to \underline{v};\ T,A)\ d^3v\ d^3v' \ ,$$

which becomes

$$e^{-\frac{\alpha}{\beta} h\, v^2}\ v\, Q = \int_{\underline{v}'} (e^{-\frac{\alpha}{\beta} h\, v'^2}\ v'\ Q')\ P\,(\underline{v}' \to \underline{v};\ T,A) d^3v' . \tag{24}$$

That $e^{-\frac{\alpha}{\beta} hv^2}\ v\ Q$ is indeed an eigenfunction of P is most readily demonstrated by employing the form (20c) for X and then transforming the variables of integration according to

$$\underline{v}' \to \underline{v} - \underline{k}$$

and
$$d^3v' \to d^3k.$$

In order to exhibit the connection between the scattering probability as presented herein and the various forms of it that have been employed elsewhere for special purposes, it is convenient to expand it in the following manner:

$$P\ (\underline{v}' \to \underline{v};\ T,A) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu_o)\ P_\ell(v',v,T,A), \tag{25a}$$

where

$$\mu_o = \cos\ (\underline{v}',\underline{v}) \quad , \tag{25b}$$

and

$$P_\ell(v',v,T,A) = \int_{-1}^{1} P_\ell\ (\mu_o)\ P\ (\underline{v}' \to \underline{v};\ T,A)\ d\mu_o. \tag{25c}$$

We note firstly that $P_o(v',v,T,A)$ is the appropriate scattering probability for the infinite, homogeneous medium. The form of this function was first exhibited explicitly by Wigner and Wilkins(5), and may be readily reproduced here by direct integration of (25c).

The higher modes of the scattering probability are explicitly defined by (25c), but not in a form convenient for analytical investigation. They are obtainable approximately, however, in a form that somewhat illuminates the manner in which thermal motion begins to induce modifications in the near epithermal region. The approximating technique is essentially that of steepest descent and may be sketched as follows. Recalling eqn. (22), we have

$$P_\ell(v',v,T,A) = \frac{1}{\beta^2}\sqrt{\frac{h}{\pi}}\ \frac{1}{v'Q'} \int_{-1}^{1} \frac{d\mu_o}{k}\ P_\ell\ (\mu_o)\ e^{-hX} \quad . \tag{26}$$

Expand

$$X(\mu_o) \cong X(\mu_{oi}) + (\mu_o - \mu_{oi})^2 X''(\mu_{oi})/2$$

where the μ_{oi} are the physically significant roots of

$$X'(\mu_o) = \frac{\partial X}{\partial \mu_o} = 0 \quad .$$

There are two such roots and they are

$$\mu_{o1} = \frac{A+1}{2}\frac{v'}{v} - \frac{A-1}{2}\frac{v}{v'}; \quad v' \leq v \leq \frac{A+1}{A-1} v' \qquad (27a)$$

$$\mu_{o2} = \frac{A+1}{2}\frac{v}{v'} - \frac{A-1}{2}\frac{v'}{v}; \quad \frac{A-1}{A+1} v' \leq v \leq v' \; . \qquad (27b)$$

Assuming sufficient peaking of the Gaussian in the integrand so that $P_\ell(\mu_o)/k$ may be evaluated at the roots, μ_{o1} and μ_{o2}, one finds that

$$P_\ell(v',v,T.A) \cong \frac{(A+1)^2}{A} \frac{P_\ell(\frac{A+1}{2}\frac{v}{v'} - \frac{A-1}{2}\frac{v'}{v})}{v\, v'^2\, Q'} \; ; \quad \frac{A-1}{A+1} v' \leq v \leq v' \; ,$$

$$\cong \frac{(A+1)^2}{A} \frac{P_\ell(\frac{A+1}{2}\frac{v'}{v} - \frac{A-1}{2}\frac{v}{v'}) e^{-\frac{h(v^2-v'^2)}{A}}}{v\, v'^2\, Q'} \; ;$$

$$v' \leq v \leq \frac{A+1}{A-1} v' \; , \qquad (28)$$

$$\cong 0 \text{ otherwise.}$$

In the limit as $\sqrt{hv'}$ becomes large, the portion of this result appropriate for an infinite, homogeneous medium reduces to the usual one for the fast region; i.e.,

$$2\pi\, P_o(v',v,T,A) v^2 = \frac{(A+1)^2}{2A} \frac{v}{v'^2} \; ; \quad \frac{A-1}{A+1} v' \leq v \leq v' \; ,$$

$$= 0; \text{ otherwise,} \qquad (29)$$

since

$$\lim_{\sqrt{hv'} \to \infty} Q' \to 4\pi .$$

Furthermore, since Q' is an increasing function of decreasing $\sqrt{h}\, v'$, it is seen that the initial modifications in the scattering probability are a decrease in the probability of scattering down in speed and an introduction of the possibility of scattering up.

Finally, a parameter of potential interest in the investigation of the thermalizing process, which is explicitly accessible here, is the mean energy of neutrons after a collision; or equivalently the mean energy loss per collision, in the thermal range(6). If we define $< E_f >_{E'}$ to be the mean final energy of neutrons scattered at an energy E' , then

$$< E_f >_{E'} = \int_{\underline{v}} P\,(\underline{v}' \rightarrow \underline{v};\ T,A)\ d^3v \left(\frac{1}{2}\ mv^2\right) . \tag{30}$$

The evaluation of this integral is tedious but straightforward. The result for the mean energy loss per collision is

$$E' - < E_f >_{E'} = 2\,\alpha\beta\, E' + \frac{\beta kT}{A\Psi}(\alpha - 4\beta)\, e^{-y} + \frac{2\beta\ kT\psi}{A\Psi}\left[(\alpha - 4\beta)\sqrt{y} - (\alpha + 4\beta)\frac{1}{2\sqrt{y}}\right] , \tag{31a}$$

where

$$\Psi(y) = e^{-y} + \left[2\sqrt{y} + \frac{1}{\sqrt{y}}\right]\psi(y) , \tag{31b}$$

and

$$\psi(y) = \int_0^{\sqrt{y}} e^{-x^2} dx;\quad y = AE'/kT. \tag{31c}$$

It is observed that

$$\begin{aligned}\lim_{y\rightarrow\infty}\ [E' - < E_f >_{E'}] &\rightarrow 2\,\alpha\,\beta\, E' - kT\,\frac{4A-1}{(A+1)^2} \\ &\rightarrow 2\,\alpha\,\beta\, E'\end{aligned} \tag{32a}$$

$$\lim_{y \to 0} \; [E' - \langle E_f \rangle_{E'}] \to - \frac{4AkT}{(A+1)^2} \quad . \tag{32b}$$

The result embodied in (32a) is the same as that obtained by invoking at the outset the assumption that the struck particles are at rest before each collision; whereas (32b) implies that neutrons whose energies are small compared to thermal gain energy on the average in each collision; as, indeed, must be the case.

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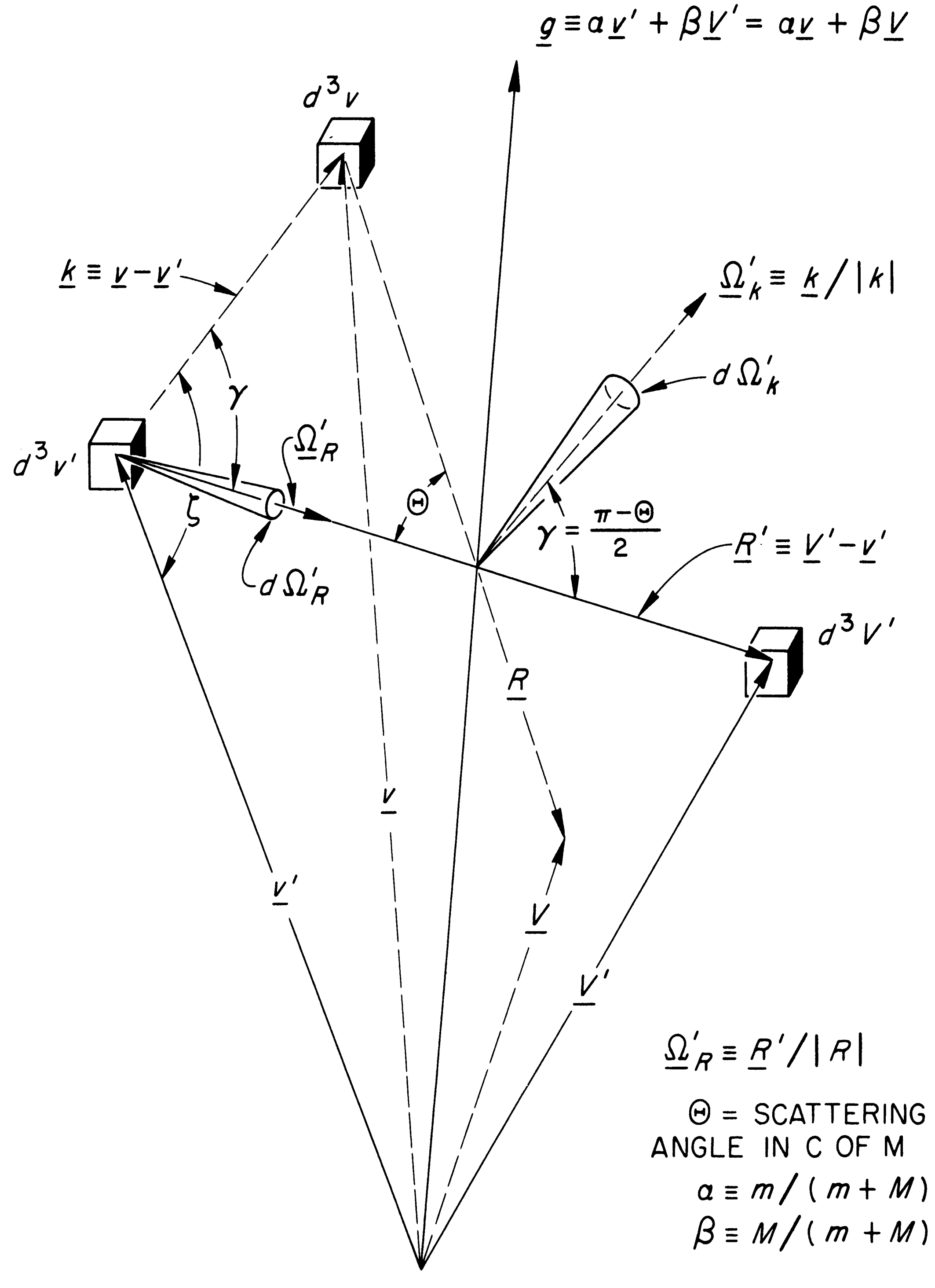
g ≡ αv' + βV' = αv + βV
d³v
k ≡ v − v'
Ω'_k ≡ k/|k|
dΩ'_k
γ
Ω'_R
d³v'
ζ
dΩ'_R
Θ
γ = (π − Θ)/2
R' ≡ V' − v'
d³V'
R
v
v'
V
V'
Ω'_R ≡ R'/|R|
Θ = SCATTERING ANGLE IN C OF M
α ≡ m/(m + M)
β ≡ M/(m + M)

Fig. 1.