ECE-656: Fall 2011

Lecture 31:

Balance Equation Approach: II

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outline

1) **Review of L30**
2) Energy balance equation
3) Energy flux balance equation
4) Terminating the hierarchy
5) Summary

(Reference: Chapter 5, Lundstrom, FCT)

moment of *f*

Physical quantities are moments of $f\left(\vec{r},\vec{p},t\right)$

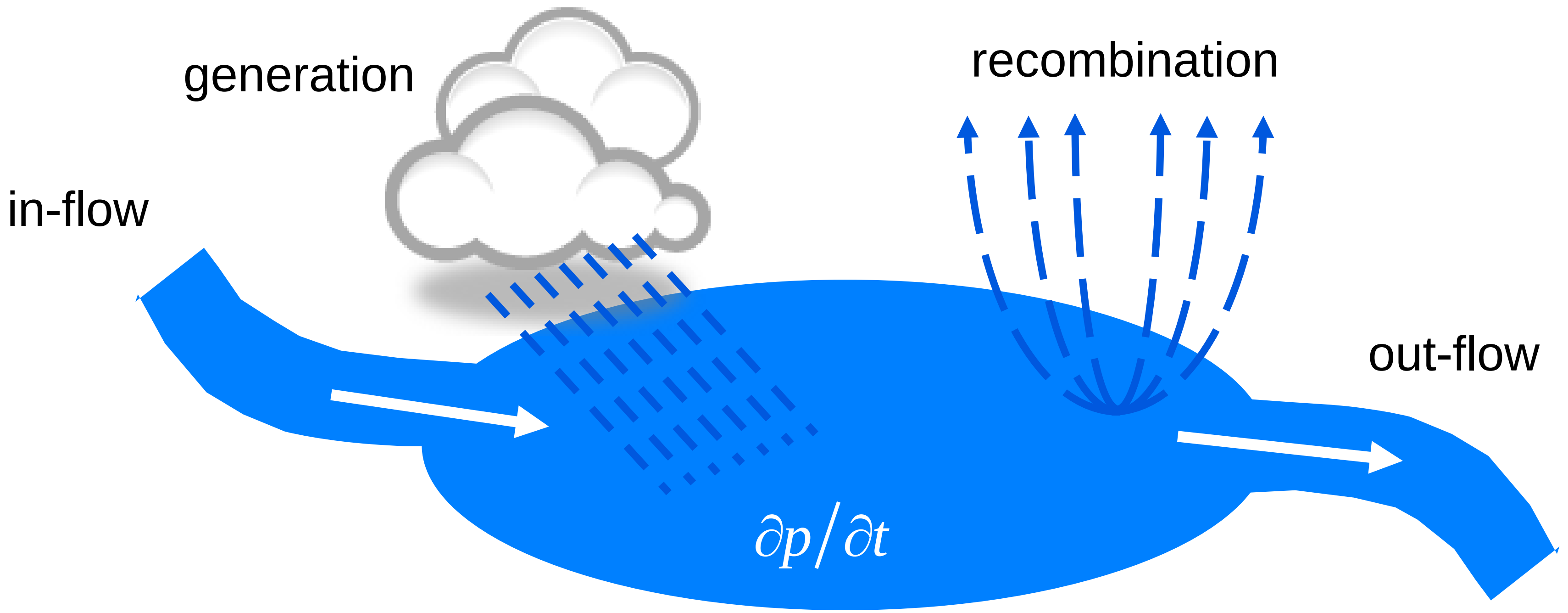
$$n_{\phi}\left(\vec{r},t\right)=\sum_{\vec{p}}\phi\left(\vec{p}\right)f\left(\vec{r},\vec{p},t\right)$$

e.g. $$\vec{J}_{n}\left(\vec{r},t\right)=\sum_{\vec{p}}\left(-q\right)\vec{\upsilon}\,f\left(\vec{r},\vec{p},t\right)$$

Can we bypass solving the BTE and solve directly for the physical quantities of interest?

the continuity equation

A familiar balance equation: $$\frac{\partial p}{\partial t} = -\nabla \bullet \frac{\vec{J}_p}{q} + G_p - R_p$$



in-flow -out-flow = - divergence of flux

balance equations for physical quantities

$$\frac{\partial p}{\partial t} = -\nabla \bullet \frac{\vec{J}_p}{q} + G_p - R_p \quad \rightarrow \quad \frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - R_\phi$$

$$n_\phi(x,t) = \frac{1}{L^d}\sum_p \phi(p) f\left(x,p,t\right)$$

$\phi\left(\vec{p}\right) = 1: \quad n_\phi(\vec{r},t) = n(\vec{r},t)$ electron continuity equation

$\phi\left(\vec{p}\right) = \left(-q\right)\vec{\upsilon}\left(\vec{p}\right): \quad n_\phi(\vec{r},t) = \vec{J}_n(\vec{r},t)$ current balance equation

$\phi\left(\vec{p}\right) = E\left(\vec{p}\right): \quad n_\phi(\vec{r},t) = W(\vec{r},t)$ kinetic energy balance equation

putting it all together

$$\sum_{\vec{p}} \phi(\vec{p}) \left\{ \frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} - \frac{q\mathcal{E}_x}{\hbar} \frac{\partial f}{\partial k_x} = \hat{C} f \right\}$$

$$\frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - R_\phi$$

$$n_\phi(x,t) = \frac{1}{L^d} \sum_{\vec{p}} \phi(\vec{p}) f(x, \vec{p}, t)$$

$$G_\phi = -q\mathcal{E}_x \left\{ \frac{1}{L^d} \sum_{\vec{p}} \frac{\partial \phi}{\partial p_x} f \right\}$$

$$F_{\phi x} \equiv \frac{1}{L^d} \sum_{\vec{p}} \phi(\vec{p}) \upsilon_x f(x, \vec{p}, t)$$

$$R_\phi \equiv \frac{n_\phi - n_\phi^0}{\langle \tau_\phi \rangle}$$

0th moment of the BTE

$$\phi(p) = 1$$

$$\frac{\partial n_\phi}{\partial t} = -\frac{dF_{\phi x}}{dx} + G_\phi - R_\phi \quad \rightarrow \frac{\partial n}{\partial t} = -\frac{d\left[J_{nx}/(-q)\right]}{dx}$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}\frac{dJ_{nx}}{dx}$$

In steady-state, the current is constant because we have assumed that there is no generation-recombination of electrons.

1st moment of the BTE

$$\phi(p) = p_x$$

$$n_\phi(x,t) = P_x \qquad F_\phi = W_{xx} = n\frac{\langle p_x \upsilon_x \rangle}{2} \qquad R_\phi = \frac{P_x}{\langle \tau_m \rangle} \qquad G_\phi = (-q)n\mathcal{E}_x$$

$$P_x = n\langle p_x \rangle$$

"momentum balance equation"

$$\frac{\partial n_\phi}{\partial t} = -\frac{dF_{\phi x}}{dx} + G_\phi - R_\phi \quad \rightarrow \frac{\partial P_x(x,t)}{\partial t} = -\frac{d(2W_{xx})}{dx} - nq\mathcal{E}_x - \frac{P_x}{\langle \tau_m \rangle}$$

current equation

$$\frac{\partial P_x(x,t)}{\partial t} = -\frac{d(2W_{xx})}{dx} - nq\mathcal{E}_x - \frac{P_x}{\langle \tau_m \rangle}$$

$$P_x = n\langle p_x \rangle = nm^*\langle \upsilon_x \rangle \qquad J_{nx} = (-q)n\langle \upsilon_x \rangle \qquad J_{nx} = \frac{(-q)}{m^*}P_x$$

$$J_{nx} + \langle \tau_m \rangle \frac{\partial J_{nx}(x,t)}{\partial t} = nq\mu_n\mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

$$\mu_n \equiv \frac{q\langle \tau_m \rangle}{m^*}$$

drift-diffusion equation

$$J_{nx} + \langle \tau_m \rangle \frac{\partial J_{nx}(x,t)}{\partial t} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

assume:

$$\langle \tau_m \rangle \frac{\partial J_{nx}(x,t)}{\partial t} << J_{nx}$$

$$\frac{q\langle \tau_m \rangle}{m^*} = \mu_n \qquad \mu_n \approx 1000\ \text{cm}^2/\text{V-s}, \qquad m^* = m_0 \rightarrow \langle \tau_m \rangle = 0.5\ \text{ps}$$

$$f << \frac{1}{\langle \tau_m \rangle} = 2\ \text{THz}$$

DD equation with temperature gradients

assume:

$$\langle \tau_m \rangle \frac{\partial J_{nx}(x,t)}{\partial t} << I_x \qquad W_{xx} = n\left\langle \frac{1}{2} m^* \upsilon_x^2 \right\rangle \approx n\frac{k_B T_e}{2}$$

$T_e \neq \text{constant}$

$$J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

$$2\mu_n \frac{dW_{xx}}{dx} = 2\mu_n \frac{d}{dx}\left(n\frac{k_B T_e}{2} \right) = \mu_n \frac{d}{dx}\left(n\, k_B T_e \right)$$

$$n = N_C e^{(F_n - E_C)/k_B T_e} = \frac{1}{4}\left(\frac{2m^* k_B T_e}{\pi \hbar^2} \right)^{3/2} e^{(F_n - E_C)/k_B T_e} = n(x, T_e)$$

DD equation with temperature gradients (ii)

$$J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

$$2\mu_n \frac{dW_{xx}}{dx} = \mu_n \frac{d}{dx}\left(n\ k_B T\right) = \mu_n \left[k_B T \frac{\partial n}{\partial x} + n\ k_B \frac{dT_e}{dx} + k_B T_e \frac{\partial n}{\partial T_e} \frac{dT_e}{dx} \right]$$

$$n = \frac{1}{4}\left(\frac{2m^* k_B T_e}{\pi \hbar^2} \right)^{3/2} e^{(F_n - E_C)/k_B T_e}$$

$$2\mu_n \frac{dW_{xx}}{dx} = k_B T_e \mu_n \frac{\partial n}{\partial x} + n k_B \mu_n \left[\frac{3}{2} - \frac{\left(F_n - E_C\right)}{k_B T_e} \right] \frac{dT_e}{dx}$$

final current equation

$$J_{nx} = nq\mu_n \mathcal{E}_x + qD_n \frac{dn}{dx} - S_T \frac{dT_e}{dx}$$

$$\mu_n = \frac{q\langle \tau_m \rangle}{m^*}$$

$$D_n = \frac{k_B T_e}{q} \mu_n$$

$$S_T = n_L q \mu_n \frac{k_B}{(-q)} \left[\frac{3}{2} - \eta_F \right]$$

(Soret coefficient)

Note error in eqn. (5.101), p. 236 of Lundstrom, FCT.

Seebeck coefficient

assume $dn/dx = 0$, and solve for $\mathcal{E}_x$:

$$J_{nx} = nq\mu_n \mathcal{E}_x + qD_n \frac{dn}{dx} - S_T \frac{dT_e}{dx}$$

$$\mathcal{E}_x = \frac{J_{nx}}{nq\mu_n} + \frac{S_T}{nq\mu_n}\frac{dT_e}{dx}$$

$$\mathcal{E}_x = \rho_n J_{nx} + S_n \frac{dT_e}{dx}$$

$$S_n = \frac{k_B}{(-q)}\left[\frac{3}{2} - \eta_F\right]$$

recall: Lecture 12

$$S_{3D} = \frac{k_B}{(-q)}\left[(r+2) - \eta_F\right]$$

$$\lambda(E) = \lambda_0 \left(E/k_B T\right)^r$$

recap: moments of the BTE

$$\frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} - \frac{q\mathcal{E}_x}{\hbar}\frac{\partial f}{\partial k_x} = \hat{C} f \rightarrow \frac{\partial n_\phi}{\partial t} = -\nabla \bullet \vec{F}_\phi + G_\phi - R_\phi$$

1) 0th moment: $\phi(p_x) = 1 = p_x{}^0$ $\qquad \frac{\partial n}{\partial t} = \frac{dJ_{nx}}{dx}$

2) 1st moment: $\phi(p_x) = (-q)\frac{p_x{}^1}{m^*}$

$$J_{nx} + \tau_m \frac{\partial J_{nx}(x,t)}{\partial t} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

Now we need an equation for *W_{xx}* ….

terminating the hierarchy

$$W_{xx} = \frac{1}{\Omega}\sum_{\vec{p}} \frac{p_x \upsilon_x}{2} f\left(x, \vec{p}, t\right) = n u_{xx} \quad u_{xx} \approx \frac{k_B T_e}{2}$$

But what is T_e? Answer: Near equilibrium: $T_e \approx T_L$

$$W_{xx} = n\frac{k_B T_e}{2}$$

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2nd moment of the BTE

$$\phi(\vec{p}) = E(\vec{p}) \qquad n_\phi(x,t) = \frac{1}{\Omega}\sum_{\vec{p}} \phi(\vec{p}) f(x,\vec{p},t)$$

$$n_\phi = W = \frac{1}{\Omega}\sum_{\vec{p}} E(\vec{p}) f = n\langle E \rangle = nu$$

$$W(x,t) = \frac{1}{\Omega}\sum_{\vec{p}} E(\vec{p}) f(x,\vec{p},t) \qquad W_{xx} = \frac{1}{\Omega}\sum_{\vec{p}} \frac{p_x \upsilon_x}{2} f(x,p_x,t)$$

2nd moment of the BTE

$$\phi(p) = E\left(p\right) \qquad n_\phi(x,t) = \frac{1}{L}\sum_p \phi(p) f\left(x,p,t\right) = W$$

$$F_{\phi x} \equiv \frac{1}{\Omega}\sum_{\vec{p}} \phi\left(\vec{p}\right)\upsilon_x f\left(x,\vec{p},t\right) = \frac{1}{L}\sum_{\vec{p}} E\left(\vec{p}\right)\upsilon_x f\left(x,\vec{p},t\right) = F_{Wx}$$

$$G_\phi = -q\mathcal{E}_x\left\{\frac{1}{\Omega}\sum_{\vec{p}}\frac{\partial\phi}{\partial p_x} f\right\} = -q\mathcal{E}_x\left\{\frac{1}{\Omega}\sum_{\vec{p}}\frac{\partial E\left(\vec{p}\right)}{\partial p_x} f\right\} = J_{nx}\mathcal{E}_x$$

$$R_\phi \equiv \frac{n_\phi - n_\phi^0}{\left\langle\tau_\phi\right\rangle} = \frac{W - W_0}{\left\langle\tau_E\right\rangle}$$

2nd moment of the BTE

$$\phi(p) = p_x \upsilon_x / 2 \qquad n_\phi(x,t) = W(x,t) \qquad F_\phi = F_{Wx} \qquad G_\phi = J_{nx}\mathcal{E}_x$$

$$\frac{\partial n_\phi}{\partial t} = -\frac{dF_{\phi x}}{dx} + G_\phi - R_\phi \quad \Rightarrow \frac{\partial W(x,t)}{\partial t} = -\frac{dF_{Wx}}{dx} + J_{nx}\mathcal{E}_x - \frac{(W - W_0)}{\langle \tau_E \rangle}$$

recap

$$\frac{\partial n(x,t)}{\partial t} = -\frac{d\left[J_{nx}/(-q)\right]}{dx}$$

0th moment of BTE

$$\langle \tau_m \rangle \frac{\partial J_{nx}(x,t)}{\partial t} + J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

1st moment of BTE

$$\frac{\partial W(x,t)}{\partial t} = -\frac{dF_{Wx}}{dx} + J_{nx}\mathcal{E}_x - \frac{(W - W_0)}{\langle \tau_E \rangle}$$

2nd moment of BTE

Now we need an equation for F_W!

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energy flux balance equation

$$\phi(p) = E\left(p\right)\upsilon_x \qquad n_\phi(x,t) = \frac{1}{\Omega}\sum_{\vec{p}}\phi(\vec{p})\, f\left(x,\vec{p},t\right) = F_{Wx}$$

$$F_{\phi x} \equiv \frac{1}{\Omega}\sum_{\vec{p}}\left(E(\vec{p})\upsilon_x\right)\upsilon_x\, f\left(x,\vec{p},t\right) \equiv n\left\langle E\upsilon_x^2\right\rangle$$

$$F_{\phi x} = n\left\langle E\upsilon_x^2\right\rangle = X_{xx}$$

$$G_\phi = -q\mathcal{E}_x\left\{\frac{1}{\Omega}\sum_{\vec{p}}\frac{\partial\phi}{\partial p_x}\, f\right\} = -\frac{q\mathcal{E}_x}{m^*}\left\{2W_{xx} + W\right\}$$

(parabolic bands)

$$R_\phi \equiv \frac{n_\phi - n_\phi^0}{\left\langle\tau_\phi\right\rangle} = \frac{F_W}{\left\langle\tau_{F_W}\right\rangle}$$

energy flux balance equation

$$\frac{\partial n_\phi}{\partial t} = -\frac{dF_{\phi x}}{dx} + G_\phi - R_\phi \quad \rightarrow \frac{\partial F_{Wx}}{\partial t} = -\frac{dX_{xx}}{dx} - \frac{q}{m^*}\left(2W_{xx} + W\right)\mathcal{E}_x - \frac{F_{Wx}}{\left\langle \tau_{F_W} \right\rangle}$$

Now we need an equation for X_{xx}!

$$F_{\phi x} \equiv \frac{1}{\Omega}\sum_{\vec{p}}\left(E(\vec{p})\upsilon_x\right)\upsilon_x f\left(x,\vec{p},t\right) \equiv n\left\langle E\upsilon_x^2\right\rangle = X_{xx}$$

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the four balance equations

$$\frac{\partial n(x,t)}{\partial t} = -\frac{d\left[J_{nx}/(-q)\right]}{dx}$$

0th moment of BTE

$$\langle \tau_m \rangle \frac{\partial J_{nx}}{\partial t} + J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

1st moment of BTE

$$\frac{\partial W(x,t)}{\partial t} = -\frac{dF_{Wx}}{dx} + J_{nx}\mathcal{E}_x - \frac{(W - W_0)}{\langle \tau_E \rangle}$$

2nd moment of BTE

$$\frac{\partial F_{Wx}}{\partial t} = -\frac{dX_{xx}}{dx} - \frac{q}{m^*}(2W_{xx} + W)\mathcal{E}_x - \frac{F_{Wx}}{\langle \tau_{F_W} \rangle}$$

3rd moment of BTE

terminating at the 1st moment

$$\frac{\partial n}{\partial t} = -\frac{d\left[J_{nx}/(-q)\right]}{dx}$$

0th moment of BTE

$$\langle \tau_m \rangle \frac{\partial J_{nx}(x,t)}{\partial t} + J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

1st moment of BTE

$$W_{xx} \approx \frac{W}{3} \approx n\frac{u_0}{3}$$

assume: $\langle \tau_m \rangle \partial J_{nx}(x,t)/\partial t << J_{nx}$ $\quad W_{xx} \approx \frac{k_B T_L}{2}$ $\quad T_L(x) \approx \text{constant}$

$$J_{nx} = nq\mu_n \mathcal{E}_x + k_B T_L \mu_n \frac{dn}{dx} = nq\mu_n \mathcal{E}_x + qD_n \frac{dn}{dx}$$

$$D_n \equiv \left(k_B T_L/q\right)\mu_n$$

terminating at the second moment

$$\frac{\partial n}{\partial t} = -\frac{d\left[J_{nx}/(-q)\right]}{dx}$$

0th moment of BTE

$$\langle \tau_m \rangle \frac{\partial J_{nx}(x,t)}{\partial t} + J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

1st moment of BTE

$$\frac{\partial W(x,t)}{\partial t} = -\frac{dF_{Wx}}{dx} + J_{nx}\mathcal{E}_x - \frac{(W - W_0)}{\langle \tau_E \rangle}$$

2nd moment of BTE

We need to approximate F_W in terms of the 3 unknowns

approximating the third moment

$$\frac{\partial F_{Wx}}{\partial t} = -\frac{dX_{xx}}{dx} - \frac{q}{m^*}\left(2W_{xx} + W\right)\mathcal{E}_x - \frac{F_{Wx}}{\left\langle \tau_{F_W} \right\rangle}$$

$$F_W + \left\langle \tau_{F_W} \right\rangle \frac{\partial F_{Wx}}{\partial t} = -\left\langle \tau_{F_W} \right\rangle \frac{dX_{xx}}{dx} - \frac{5}{3}\frac{q\left\langle \tau_{F_W} \right\rangle}{m^*} W\mathcal{E}_x \qquad \left(W_{xx} \approx W/3\right)$$

$$\left\langle \tau_{F_W} \right\rangle \partial F_{Wx}/\partial t << F_{Wx}$$

$$X_{xx} \approx \frac{1}{\Omega}\sum_{\vec{p}}\left(E(\vec{p})\upsilon_x^2\right) f_S\left(x, \vec{p}, t\right) = \frac{10}{3}\frac{k_B T_e}{m^*} W$$

the energy flux

$$F_W + \langle \tau_{F_W} \rangle \frac{\partial F_{Wx}}{\partial t} = -\frac{5}{3}\frac{q\langle \tau_{F_W} \rangle}{m^*} W \mathcal{E}_x - \frac{10}{3}\frac{q\langle \tau_{F_W} \rangle}{m^*} \frac{d\left(\frac{k_B T_e}{q} W\right)}{dx}$$

$$F_{Wx} = -\frac{5}{3}\mu_E W \mathcal{E}_x - \frac{10}{3}\mu_E \frac{d\left(W k_B T_e / q\right)}{dx}$$

$$\mu_E = \frac{q\langle \tau_{F_W} \rangle}{m^*} \qquad W \approx n\frac{k_B T_e}{2}$$

four balance equations

$$\frac{\partial n}{\partial t} = -\frac{d\left[J_{nx}/(-q)\right]}{dx}$$

electron continuity equation

$$J_{nx} = nq\mu_n \mathcal{E}_x + 2\mu_n \frac{dW_{xx}}{dx}$$

current equation

$$\frac{\partial W(x,t)}{\partial t} = -\frac{dF_{Wx}}{dx} + J_{nx}\mathcal{E}_x - \frac{(W - W_0)}{\tau_E}$$

energy-balance equation

$$F_{Wx} = -\frac{5}{3}\mu_E W \mathcal{E}_x - \frac{10}{3}\mu_E \frac{d\left(W k_B T_e / q\right)}{dx}$$

energy-flux equation

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summary

1) The first moment of the BTE gives the current continuity equation.

2) The second moment gives the current density.

3) The third moment gives the kinetic energy.

4) Each moment involves the next moment – the hierarchy must be terminated.

unfinished business

1) Can we define temperature more clearly?

questions?

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