

PHY 770 -- Statistical Mechanics
12:00* - 1:45 PM TR Olin 107

Instructor: Natalie Holzwarth (Olin 300)
Course Webpage: <http://www.wfu.edu/~natalie/s14phy770>

Lecture 22

Chap. 9 – Transport coefficients

- Linearized Boltzmann equation
- Systematic approximation of the transport coefficients

*Partial make-up lecture -- early start time

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1	Thur: 03/06/2014	APS Meeting	Take-home exam (no class meeting)	
	Tue: 03/11/2014		Spring break (no class meeting)	
	Thur: 03/13/2014		Spring break (no class meeting)	
14	Tue: 03/18/2014	Chap. 6	Fermi and Bose particles (class 12-1:45 PM; Exam due)	#13 03/25/2014
15	Thur: 03/20/2014	Chap. 6	Interacting particles (class 12-1:45 PM)	#14 03/25/2014
16	Tue: 03/25/2014	Chap. 7	Langevin equation (class 12-1:45 PM)	#15 04/01/2014
17	Thur: 03/27/2014	Chap. 7	Fokker-Planck equation (class 12-1:45 PM)	#16 04/03/2014
18	Tue: 04/01/2014	Chap. 7	Linear Response (class 12-1:45 PM)	#17 04/10/2014
19	Thur: 04/03/2014	Chap. 9	Transport theory (class 12-1:45 PM)	#18 04/10/2014
20	Tue: 04/08/2014	Chap. 9	The Boltzmann Equation (class 12-1:45 PM)	#19 04/10/2014
21	Thur: 04/10/2014	Chap. 9	The Boltzmann Equation (class 12-1:45 PM)	#20 04/17/2014
22	Tue: 04/15/2014	Chap. 9	The Boltzmann Equation (class 12-1:45 PM)	#21 04/17/2014
23	Thur: 04/17/2014		Review and highlights (class 12-1:45 PM)	
24	Tue: 04/22/2014		Review and highlights (class 12-1:45 PM)	
	Thur: 04/24/2014		Presentations Part I (class 11-1:45 PM)	
	Tue: 04/29/2014		Presentations Part II (class 11-1:45 PM)	

Signup schedule for presentations available this afternoon. Please list the title of your presentation when you sign up.

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 WAKE FOREST UNIVERSITY Department of Physics

News

- 
Prof. Carroll named APS Fellow
- 
Protein research led by Prof. Cho featured in news
- 
Prof. Thonhauser receives Award for Excellence in Research

Events

- Wed, Apr. 16, 2014**
Organic electronics
Prof. Conrad, App. State
4:00 PM in Olin 101
Reception: 3:30 PM in Olin Lobby
- Wed, Apr. 23, 2014**
Honors Presentations I
4:00 PM in Olin 101
Reception: 3:30 PM in Olin Lobby
- Wed, Apr. 30, 2014**
Honors Presentations II +
4:00 PM in Olin 101
Reception: 3:30 PM in Olin Lobby

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WFU Physics Colloquium

TITLE: Advances in Organic Electronics

SPEAKER: Professor Brad Conrad,
Department of Physics and Astronomy,
Appalachian State University

TIME: Wednesday April 16, 2014 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

Organic semiconductors offer the promise of low-cost devices on arbitrary surfaces, transparent displays, efficient OLEDs, and even biodegradable photovoltaics. Through chemical engineering, the physical and electronic properties of these new materials can be tailored to meet specific requirements and investigate interesting condensed matter physics. In this colloquium I will have a lively introduction to organic semiconductors, explore some recent advances, and briefly discuss our recent work on small organic molecule solar cells.

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The Boltzmann equation:

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_r + \frac{\mathbf{F}}{m} \cdot \nabla_v \right) f(\mathbf{r}, \mathbf{v}, t) = \left(\frac{\partial f}{\partial t} \right)_{coll}$$

With:

$$\left(\frac{\partial f}{\partial t} \right)_{coll} = \int d\Omega_{CM} \int d^3 v_2 |\mathbf{v}_2 - \mathbf{v}| \frac{d\sigma_{CM}}{d\Omega_{CM}} (f(\mathbf{r}, \mathbf{v}', t) f(\mathbf{r}, \mathbf{v}_2', t) - f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_2, t))$$

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The Boltzmann equation:

In the notation of your textbook:
 $f(\mathbf{r}, \mathbf{v}, t) \rightarrow f(\mathbf{r}, \mathbf{p}, t)$

$$\left(\frac{\partial f}{\partial t} \right)_{coll} = \int d\Omega_{CM} \int d^3 p_2 g \sigma_{cm}(b, g) (f(\mathbf{r}, \mathbf{p}', t) f(\mathbf{r}, \mathbf{p}_2', t) - f(\mathbf{r}, \mathbf{p}, t) f(\mathbf{r}, \mathbf{p}_2, t))$$

where b = impact parameter of collision
where $g \equiv |\mathbf{v}_2 - \mathbf{v}|$

Detailed solution for a dilute gas of N identical particles of mass m in volume V in absence of external force ($\mathbf{F}=0$). In order to help the analysis, we will imagine that $\frac{N}{2}$ the particles are “normal” with label “N” and $\frac{N}{2}$ the particles are “tracers” with label “T”. The density of particles is denoted $n_0=N/V$.

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The Boltzmann equation – approximation by linearization

Assume that the system is near equilibrium and define:

$$f(\mathbf{r}, \mathbf{p}, t) = f^0(\mathbf{p})(1 + h(\mathbf{r}, \mathbf{p}, t))$$

$$\text{In our case, } f^0(\mathbf{p}) = f_N^0(\mathbf{p}) = f_T^0(\mathbf{p}) = \frac{n_0}{2} \left(\frac{\beta}{2\pi m} \right)^{3/2} e^{-\beta p^2/(2m)}$$

Define the possible collision cross sections for $\{a, b, c, d\} \leftrightarrow \{N, T\}$

$$\sigma_{a,b,c,d} = \begin{cases} \sigma(b,g)_{cm} & \text{for } a,b:c,d = NN : NN, TT : TT, TN : TN, NT : NT \\ 0 & \text{otherwise} \end{cases}$$

Abbreviate:

$$h_{i,a} \equiv h_a(\mathbf{r}, \mathbf{p}_i, t) \quad \text{for } a=N \text{ or } T.$$

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Linearized Boltzmann equation for normal and tracer particles

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_r \right) h_N(\mathbf{r}, \mathbf{p}_1, t) = \left(\frac{\partial f^1}{\partial t} \right)_{coll,N}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_r \right) h_T(\mathbf{r}, \mathbf{p}_1, t) = \left(\frac{\partial f^1}{\partial t} \right)_{coll,T}$$

$$\left(\frac{\partial f^1}{\partial t} \right)_{coll,N} \equiv \sum_{a,b,c} \int d^3 p_2 \int d\Omega g \sigma_{a,b,c,d} f^0(\mathbf{p}_2) (h_{1,a} + h_{2,b} - h_{1,N} - h_{2,c})$$

$$\left(\frac{\partial f^1}{\partial t} \right)_{coll,T} \equiv \sum_{a,b,c} \int d^3 p_2 \int d\Omega g \sigma_{a,b,c,d} f^0(\mathbf{p}_2) (h_{1,a} + h_{2,b} - h_{1,T} - h_{2,c})$$

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Linearized Boltzmann equation for normal and tracer particles

It is convenient to define the sum and difference distributions:

$$h^+ \equiv h_N + h_T \quad \text{and} \quad h^- \equiv h_N - h_T$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_r \right) h^+(\mathbf{r}, \mathbf{p}_1, t) = \left(\frac{\partial f^1}{\partial t} \right)_{coll,+} \equiv \hat{\mathbf{C}}_1^+ h^+(\mathbf{r}, \mathbf{p}_1, t)$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_r \right) h^-(\mathbf{r}, \mathbf{p}_1, t) = \left(\frac{\partial f^1}{\partial t} \right)_{coll,-} \equiv \hat{\mathbf{C}}_1^- h^-(\mathbf{r}, \mathbf{p}_1, t)$$

$$\left(\frac{\partial f^1}{\partial t} \right)_{coll,+} \equiv 2 \int d^3 p_2 \int d\Omega g \sigma(b, g) f^0(\mathbf{p}_2) (h_{1'}^+ + h_{2'}^+ - h_1^+ - h_2^+) \quad \text{_____}$$

$$\left(\frac{\partial f^1}{\partial t} \right)_{coll,-} \equiv 2 \int d^3 p_2 \int d\Omega g \sigma(b, g) f^0(\mathbf{p}_2) (h_{1'}^- - h_1^-) \quad \text{_____}$$

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Linearized Boltzmann equation for normal and tracer particles – remarkable properties of collision operators

Define the special inner product:

$$\langle \phi, \chi \rangle = \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p_1 e^{-\beta p_1^2/(2m)} \phi(\mathbf{p}_1) \chi(\mathbf{p}_1)$$

$$\hat{\mathbf{C}}_1^+ \chi(\mathbf{r}, \mathbf{p}_1, t) = 2 \int d^3 p_2 \int d\Omega g \sigma(b, g) f^0(\mathbf{p}_2) (\chi_{1'} + \chi_{2'} - \chi_1 - \chi_2)$$

Note that for an arbitrary function $\chi(\mathbf{r}, \mathbf{p}_1, t)$:

$$\langle \chi, \hat{\mathbf{C}}_1^+ \chi \rangle = -\frac{N}{4V} \left(\frac{\beta}{2\pi m} \right)^3 \times$$

$$\int d^3 p_1 \int d^3 p_2 \int d\Omega g \sigma(b, g) e^{-(\beta/(2m))(p_1^2 + p_2^2)} (\chi_{1'} + \chi_{2'} - \chi_1 - \chi_2)^2$$

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Linearized Boltzmann equation for normal and tracer particles – remarkable properties of collision operators -- continued

Similar identity for difference collision operator

$$\hat{\mathbf{C}}_1^- \chi(\mathbf{r}, \mathbf{p}_1, t) = 2 \int d^3 p_2 \int d\Omega g \sigma(b, g) f^0(\mathbf{p}_2) (\chi_{1'} - \chi_1)$$

Note that for an arbitrary function $\chi(\mathbf{r}, \mathbf{p}_1, t)$:

$$\langle \chi, \hat{\mathbf{C}}_1^- \chi \rangle = -\frac{N}{2V} \left(\frac{\beta}{2\pi m} \right)^3 \times$$

$$\int d^3 p_1 \int d^3 p_2 \int d\Omega g \sigma(b, g) e^{-(\beta/(2m))(p_1^2 + p_2^2)} (\chi_{1'} - \chi_1)^2$$

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Linearized Boltzmann equation for normal and tracer particles – remarkable properties of collision operators – continued

Summary of results:

$$\langle \chi, \hat{\mathbf{C}}_1^+ \chi \rangle = -\frac{N}{4V} \left(\frac{\beta}{2\pi m} \right)^3 \times$$

$$\int d^3 p_1 \int d^3 p_2 \int d\Omega g \sigma(b, g) e^{-(\beta/(2m))(p_1^2 + p_2^2)} (\chi_{1'} + \chi_{2'} - \chi_1 - \chi_2)^2$$

\Rightarrow Eigenvalues of $\hat{\mathbf{C}}_1^+$ are ≤ 0

with 5 degenerate eigenvalues of 0 for $\chi \propto 1, p_x, p_y, p_z, \frac{p^2}{2m}$

$$\langle \chi, \hat{\mathbf{C}}_1^- \chi \rangle = -\frac{N}{2V} \left(\frac{\beta}{2\pi m} \right)^3 \times$$

$$\int d^3 p_1 \int d^3 p_2 \int d\Omega g \sigma(b, g) e^{-(\beta/(2m))(p_1^2 + p_2^2)} (\chi_{1'} - \chi_1)^2$$

\Rightarrow Eigenvalues of $\hat{\mathbf{C}}_1^- \leq 0$, with zero eigenvector $\chi \propto 1$

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Analysis of the diffusion coefficient

The difference in the tracer and normal particle densities at (\mathbf{r}, t) :

$$\begin{aligned} m(\mathbf{r}, t) &= n_N(\mathbf{r}, t) - n_T(\mathbf{r}, t) = \int d^3 p_i f^0(\mathbf{p}_i) h^-(\mathbf{r}, \mathbf{p}_i, t) \\ h^- &\equiv h_N - h_T \\ \left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla_r \right) h^-(\mathbf{r}, \mathbf{p}_i, t) &= \hat{\mathbf{C}}_i^- h^-(\mathbf{r}, \mathbf{p}_i, t) \\ \int d^3 p_i f^0(\mathbf{p}_i) \left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla_r \right) h^-(\mathbf{r}, \mathbf{p}_i, t) &= \int d^3 p_i f^0(\mathbf{p}_i) \hat{\mathbf{C}}_i^- h^-(\mathbf{r}, \mathbf{p}_i, t) = 0 \\ \Rightarrow \frac{\partial m(\mathbf{r}, t)}{\partial t} + \nabla_r \cdot \mathbf{J}^D(\mathbf{r}, t) &= 0 \quad \text{where } \mathbf{J}^D(\mathbf{r}, t) \equiv \int d^3 p_i f^0(\mathbf{p}_i) \mathbf{v}_i h^-(\mathbf{r}, \mathbf{p}_i, t) \end{aligned}$$

Assume Fick's law: $\mathbf{J}^D(\mathbf{r}, t) = -D \nabla_r m(\mathbf{r}, t)$

$$\Rightarrow \frac{\partial m(\mathbf{r}, t)}{\partial t} = D \nabla_r^2 m(\mathbf{r}, t)$$

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Analysis of the diffusion coefficient

Need to solve the equation:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla_r \right) h^-(\mathbf{r}, \mathbf{p}_i, t) = \hat{\mathbf{C}}_i^- h^-(\mathbf{r}, \mathbf{p}_i, t)$$

Let $h^-(\mathbf{r}, \mathbf{p}_i, t) = \Psi_n^-(\mathbf{k}, \mathbf{p}) e^{i\mathbf{k} \cdot \mathbf{r} - i\omega_n t}$

$$(\hat{\mathbf{C}}_i^- - i\mathbf{v}_i \cdot \mathbf{k}) \Psi_n^-(\mathbf{k}, \mathbf{p}) = -i\omega_n \Psi_n^-(\mathbf{k}, \mathbf{p})$$

Assume that $k = |\mathbf{k}|$ is small (long wavelength case)

$$\omega_n \approx \omega_n^{(0)} + k\omega_n^{(1)} + k^2\omega_n^{(2)} \dots$$

$$\Psi_n^-(\mathbf{k}, \mathbf{p}) \approx \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) + k\Psi_n^{(-1)}(\mathbf{k}, \mathbf{p}) + k^2\Psi_n^{(-2)}(\mathbf{k}, \mathbf{p}) \dots$$

Assuming $\langle \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) | \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) \rangle = \delta_{nn'}$:

$$\omega_n^{(0)} = i \langle \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) | \hat{\mathbf{C}}_i^- | \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) \rangle$$

$$\omega_n^{(1)} = \langle \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) | \mathbf{v}_i \cdot \hat{\mathbf{k}} | \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) \rangle, \text{ etc...}$$

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Analysis of the diffusion coefficient -- continued

Recall that $\hat{\mathbf{C}}_i^-$ has one zero eigenvalue and choose $\Psi_0^-(\mathbf{k}, \mathbf{p}) = \Psi_0^+(\mathbf{k}, \mathbf{p}) = 1$

$$\omega_0^{(0)} = i \langle \Psi_0^{(-0)}(\mathbf{k}, \mathbf{p}) | \hat{\mathbf{C}}_i^- | \Psi_0^{(-0)}(\mathbf{k}, \mathbf{p}) \rangle = 0$$

$$\omega_0^{(1)} = \langle \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) | \mathbf{v}_i \cdot \hat{\mathbf{k}} | \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) \rangle = \frac{1}{m} \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p_i e^{-\beta p_i^2/(2m)} \mathbf{p}_i \cdot \hat{\mathbf{k}} = 0$$

$$\omega_0^{(2)} = - \langle \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) | (\mathbf{v}_i \cdot \hat{\mathbf{k}} - \omega_0^{(1)}) | \hat{\mathbf{C}}_i^- + \omega_0^{(0)} \rangle^{-1} (\mathbf{v}_i \cdot \hat{\mathbf{k}} - \omega_0^{(1)}) | \Psi_n^{(-0)}(\mathbf{k}, \mathbf{p}) \rangle$$

$$= - \frac{1}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p_i e^{-\beta p_i^2/(2m)} \mathbf{p}_i \cdot \hat{\mathbf{k}} (\hat{\mathbf{C}}_i^-)^{-1} \mathbf{p}_i \cdot \hat{\mathbf{k}}$$

$$D = - \frac{1}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p_i e^{-\beta p_i^2/(2m)} \mathbf{p}_i \cdot \hat{\mathbf{k}} (\hat{\mathbf{C}}_i^-)^{-1} \mathbf{p}_i \cdot \hat{\mathbf{k}}$$

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Analysis of the diffusion coefficient -- continued

$$D = -\frac{1}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p_i e^{-\beta p_i^2/(2m)} \mathbf{p}_i \cdot \hat{\mathbf{k}} (\hat{\mathbf{C}}_p)^{-1} \mathbf{p}_i \cdot \hat{\mathbf{k}}$$

For convenience, let $\hat{\mathbf{k}} = \hat{\mathbf{x}}$ and define $\Delta_x \equiv (\hat{\mathbf{C}}_p)^{-1} p_x$

$$D = -\frac{1}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x \Delta_x$$

Define Sonine polynomials (relatives of Laguerre polynomials)

$$S_q^n(x) \equiv \sum_{l=0}^n (-1)^l \frac{\Gamma(q+n+1)x^l}{\Gamma(q+l+1)(n-l)!l!}$$

$$\text{Note that: } \int_0^\infty dx e^{-x} S_q^n(x) S_{q'}^{n'}(x) = \frac{\Gamma(q+n+1)}{n!} \delta_{n,n'}$$

$$\text{Expand: } \Delta_x = p_x \sum_{n=0}^\infty d_n S_q^n \left(\frac{\beta p^2}{2m} \right)$$

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Analysis of the diffusion coefficient -- continued

$$D = -\frac{1}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x \Delta_x$$

$$\text{Expand: } \Delta_x = p_x \sum_{n=0}^\infty d_n S_q^n \left(\frac{\beta p^2}{2m} \right)$$

$$\Rightarrow D = -\frac{1}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \sum_{n=0}^\infty d_n \int d^3 p e^{-\beta p^2/(2m)} p_x^2 S_{3/2}^n \left(\frac{\beta p^2}{2m} \right) = -\frac{1}{m\beta} d_0$$

Evaluation of coefficient d_0 :

$$\Delta_x \equiv (\hat{\mathbf{C}}_p)^{-1} p_x \Rightarrow \hat{\mathbf{C}}_p^{-1} \Delta_x = p_x$$

$$\hat{\mathbf{C}}_p p_x \sum_{n=0}^\infty d_n S_{3/2}^n \left(\frac{\beta p^2}{2m} \right) = p_x$$

$$\left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x S_{3/2}^{n'} \left(\frac{\beta p^2}{2m} \right) \hat{\mathbf{C}}_p^{-1} p_x \sum_{n=0}^\infty d_n S_{3/2}^n \left(\frac{\beta p^2}{2m} \right)$$

$$= \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x^2 S_{3/2}^{n'} \left(\frac{\beta p^2}{2m} \right)$$

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Analysis of the diffusion coefficient -- continued

Evaluation of coefficient d_0 :

$$\left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x S_{3/2}^{n'} \left(\frac{\beta p^2}{2m} \right) \hat{\mathbf{C}}_p^{-1} p_x \sum_{n=0}^\infty d_n S_{3/2}^n \left(\frac{\beta p^2}{2m} \right)$$

$$= \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x^2 S_{3/2}^{n'} \left(\frac{\beta p^2}{2m} \right)$$

$$\sum_{n=0}^\infty D_{n'n} d_n = \frac{m}{\beta} \delta_{n',0}$$

$$\text{where } D_{n'n} \equiv \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x S_{3/2}^{n'} \left(\frac{\beta p^2}{2m} \right) \hat{\mathbf{C}}_p p_x S_{3/2}^n \left(\frac{\beta p^2}{2m} \right)$$

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Analysis of the diffusion coefficient -- continued

Approximation of equation by truncation to $\nu+1$:

$$\sum_{n=0}^{\nu} D_{n,n} \approx \frac{m}{\beta} \delta_{n,0}$$

$$D = -\frac{1}{\beta^2} \nu \lim_{\nu} (D^\nu)_{00}$$

Lowest order: $\nu=0$

$$D_{00} = \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x \hat{C}_p^- p_x$$

Evaluation for the case of scattering from a hard sphere of radius a :

$$D_{00} = \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x \hat{C}_p^- p_x = -\frac{3}{32} \frac{\beta^2}{n_0 a^2} \sqrt{kT}$$

$$\Rightarrow D = \frac{3}{32} \frac{1}{n_0 a^2} \sqrt{\frac{kT}{\pi m}}$$

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Analysis of Viscosity and Thermal Conductivity

For these transport coefficients, we need to evaluate the total scattering operator.

Thermal conductivity: $K =$

$$-\frac{n_0 k}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} \left(\frac{\beta p^2}{2m} - \frac{5}{2} \right) p_x (\hat{C}_1^+)^{-1} \left(\frac{\beta p^2}{2m} - \frac{5}{2} \right)$$

$$\text{Shear viscosity: } \eta = -\frac{n_0 \beta}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x p_y (\hat{C}_1^+)^{-1} (p_x p_y)$$

Previously, we have shown:

$$\langle \chi, \hat{C}_1^+ \chi \rangle = -\frac{N}{4V} \left(\frac{\beta}{2\pi m} \right)^3 \times \int d^3 p_i \int d^3 p_j \int d\Omega g(\sigma(b,g)) e^{-(\beta/(2m))(p_i^2 + p_j^2)} (\chi_1 + \chi_2 - \chi_1 - \chi_2)^2$$

\Rightarrow Eigenvalues of \hat{C}_1^+ are ≤ 0

$$\text{with 5 degenerate eigenvalues of 0 for } \chi \propto 1, p_x, p_y, p_z, \frac{p^2}{2m}$$

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Analysis of viscosity and thermal conductivity -- continued

Need to solve the equation:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_r \right) h^+(\mathbf{r}, \mathbf{p}_1, t) = \hat{C}_1^+ h^+(\mathbf{r}, \mathbf{p}_1, t)$$

$$\text{Let } h^+(\mathbf{r}, \mathbf{p}_1, t) = \Psi_n^+(\mathbf{k}, \mathbf{p}) e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_n t}$$

$$(\hat{C}_1^+ - i\mathbf{v}_1 \cdot \mathbf{k}) \Psi_n^+(\mathbf{k}, \mathbf{p}) = -i\omega_n \Psi_n^+(\mathbf{k}, \mathbf{p})$$

For this case, we are interested in solutions near $k=0$; the 5 zero eigenstates

$\hat{C}_1^+ \phi = 0$ are:

$$\phi_1 = 1 \quad \phi_2 = \sqrt{\frac{\beta}{m}} p_x \quad \phi_3 = \sqrt{\frac{\beta}{m}} p_y \quad \phi_4 = \sqrt{\frac{\beta}{m}} p_z \quad \phi_5 = \sqrt{\frac{2}{3}} \left(-\frac{3}{2} + \frac{\beta}{2m} p^2 \right)$$

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Analysis of viscosity and thermal conductivity -- continued

$$(\hat{C}_1^+ - i\mathbf{v}_1 \cdot \mathbf{k}) \Psi_n^+(\mathbf{k}, \mathbf{p}) = -i\omega_n \Psi_n^+(\mathbf{k}, \mathbf{p})$$

Assume that $k \equiv |\mathbf{k}|$ is small (long wavelength case)

$$\omega_n \approx \omega_n^{(0)} + k\omega_n^{(1)} + k^2\omega_n^{(2)} \dots$$

$$\Psi_n^+(\mathbf{k}, \mathbf{p}) \approx \Psi_n^{+(0)}(\mathbf{k}, \mathbf{p}) + k\Psi_n^{+(1)}(\mathbf{k}, \mathbf{p}) + k^2\Psi_n^{+(2)}(\mathbf{k}, \mathbf{p}) \dots$$

It is convenient to construct functions so that $\langle \Psi_n^{+(0)}(\mathbf{k}, \mathbf{p}) | \Psi_{n'}^{+(0)}(\mathbf{k}, \mathbf{p}) \rangle = \delta_{nn'}$:

For the 5 states: $\omega_n^{(0)} = 0$

By construction: $\omega_n^{(1)} = 0$

$$\Rightarrow \omega_n = k^2\omega_n^{(2)}$$

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Analysis of viscosity and thermal conductivity -- continued

Following Eqs. 9.121-9.124 of your text and using:

$$\phi_1 = 1 \quad \phi_2 = \sqrt{\frac{\beta}{m}} p_x \quad \phi_3 = \sqrt{\frac{\beta}{m}} p_y \quad \phi_4 = \sqrt{\frac{\beta}{m}} p_z \quad \phi_5 = \sqrt{\frac{2}{3}} \left(-\frac{3}{2} + \frac{\beta}{2m} p^2 \right)$$

$$\Psi_1^{(0)+} = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{3}{5}} \phi_1 + \sqrt{\frac{2}{5}} \phi_3 + \phi_2 \right)$$

$$\Psi_2^{(0)+} = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{3}{5}} \phi_1 + \sqrt{\frac{2}{5}} \phi_3 - \phi_2 \right)$$

$$\Psi_3^{(0)+} = \phi_3 \quad \Psi_4^{(0)+} = \phi_4$$

$$\Psi_5^{(0)+} = \left(-\sqrt{\frac{2}{5}} \phi_1 + \sqrt{\frac{3}{5}} \phi_3 \right)$$

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Analysis of thermal conductivity -- continued

Following Sect. 9.7.3 of your text, we can write the thermal conductivity coefficient:

$$K = -\frac{n_0 k}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \sum_{n=0}^{\infty} a_n \int d^3 p e^{-\beta p^2/(2m)} \left(\frac{\beta p^2}{2m} - \frac{5}{2} \right) p_x^2 S_{3/2}^n \left(\frac{\beta p^2}{2m} \right)$$

$$= \frac{5n_0 k}{2m\beta} a_1 \quad \text{where } \sum_{n=0}^{\infty} M_{nn} a_n = -\frac{5m}{2\beta} \delta_{n',1}$$

$$\text{and } M_{n'n} \equiv \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x S_{3/2}^{n'} \left(\frac{\beta p^2}{2m} \right) \hat{C}_{\mathbf{p}}^* p_x S_{3/2}^n \left(\frac{\beta p^2}{2m} \right)$$

Estimate for hard sphere scattering of radius a

$$K = \frac{75k}{256a^2} \sqrt{\frac{kT}{m\pi}}$$

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Analysis of shear viscosity-- continued

Following Sect. 9.7.4 of your text, we can write the shear viscosity coefficient:

$$\eta = -\frac{n_0 \beta}{m^2} \left(\frac{\beta}{2\pi m} \right)^{3/2} \sum_{n=0}^{\infty} b_n \int d^3 p e^{-\beta p^2/(2m)} p_x^2 p_y^2 S_{5/2}^n \left(\frac{\beta p^2}{2m} \right)$$

$$= -\frac{n_0}{\beta} b_0 \quad \text{where } \sum_{n=0}^{\infty} N_{n'n} b_n = \frac{m^2}{\beta^2} \delta_{n',0}$$

and $N_{n'n} \equiv \left(\frac{\beta}{2\pi m} \right)^{3/2} \int d^3 p e^{-\beta p^2/(2m)} p_x p_y S_{5/2}^{n'} \left(\frac{\beta p^2}{2m} \right) \hat{C}_p^* p_x p_y S_{5/2}^n \left(\frac{\beta p^2}{2m} \right)$

Estimate for hard sphere scattering of radius a

$$\eta = \frac{5}{64a^2} \sqrt{\frac{mkT}{\pi}}$$