PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF Olin 103

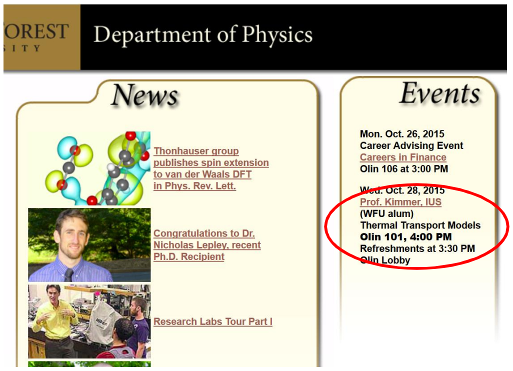
Plan for Lecture 25:

Introduction to hydrodynamics

(Chap. 9 in F & W)

1. Incompressible fluids
2. Isentropic fluids

11	Fri, 9/18/2015	Chap. 3 & 6	Hamiltonian formalism	#11
12	Mon, 9/21/2015	Chap. 3 & 6	Hamiltonian formalism	#12
13	Wed, 9/23/2015	Chap. 3 & 6	Hamiltonian Jacobi transformations	#13
14	Fri, 9/25/2015	Chap. 4	Small oscillations	#14
15	Mon, 9/28/2015	Chap. 4	Normal modes of motion	#15
16	Wed, 9/30/2015	Chap. 7	Wave motion	#16
17	Fri, 10/02/2015	Chap. 7 & App. A	Contour Integration	#17
18	Mon, 10/05/2015	Chap. 7	Fourier transforms	#18
19	Wed, 10/07/2015	Chap. 7	Laplace transforms	#19
20	Fri, 10/09/2015	Chap. 7	Green's functions	Start exam
	Mon, 10/12/2015		No class	Take home exam
	Wed, 10/14/2015		No class	Exam due before 10/19/2015
	Fri, 10/16/2015		Fall break -- no class	
21	Mon, 10/19/2015	Chap. 5	Motion of Rigid Bodies	#20
22	Wed, 10/21/2015	Chap. 5	Motion of Rigid Bodies	#21
23	Fri, 10/23/2015	Chap. 8	Motion of Elastic membranes	#22
24	Mon, 10/26/2015	Chap. 9	Hydrodynamics	#23
25	Wed, 10/28/2015	Chap. 9	Hydrodynamics	#24
	Wed, 12/02/2015		Student presentations I	
	Fri, 12/04/2015		Student presentations II	
	Mon, 12/07/2015		Begin Take-home final	



WFU Physics Colloquium

TITLE: Effect of interfacial adhesive layers on thermal transport in model systems

SPEAKER: Christopher J. Kimmer, (WFU alum)

School of Natural Sciences,
Indiana University Southeast

TIME: Wednesday October 28, 2015 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

The thermal properties of nanoscale systems often critically depend on phonon scattering at internal interfaces. The Kapitza conductance of an interface provides an overall measure of this scattering, and the ability to design systems with a prescribed or maximal conductance requires a deeper understanding of how interfacial properties effect this quantity. Experimental challenges with measurements of thermal properties at the nanoscale along with the need for predictive models to aid in systems design invites computer simulation to play a prominent role in the study of phonon-mediated thermal transport in these systems. One proposed approach to enhancing thermal transport across an interface is to include so-called adhesive layers with vibrational properties intermediate to those on either side of the interface. We focus on the effects of adhesion layers by considering model bicrystalline systems on diamond lattices interacting via the Stillinger-Weber interatomic potential. We vary the thickness, atomic mass, and interfacial bonding to conduct a study of the effect of these parameters on the interfacial conductance. The systems are characterized using the "direct method", a non-equilibrium molecular dynamics approach. We find the strongest enhancement in transport at weak interfacial bonding and discuss the implications of this result.

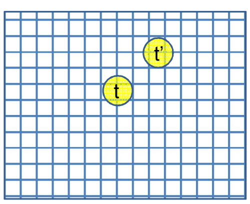
Newton's equations for fluids

Use **Euler** formulation; properties described in terms of stationary spatial grid

Variables: Density $\rho(x,y,z,t)$

Pressure $p(x,y,z,t)$

Velocity $\mathbf{v}(x,y,z,t)$



Particle at t: $\mathbf{r}, t$

Particle at t': $\mathbf{r}+\mathbf{v}\delta t, t'$

$$t' = t + \delta t$$

Euler analysis -- continued

Particle at t: $\mathbf{r}, t$

Particle at t': $\mathbf{r}+\mathbf{v}\delta t, t'$ where $\delta t = t' - t$

For $f(\mathbf{r},t)$:

$$\frac{df}{dt} = \lim_{\delta t \to 0}\left(\frac{f(\mathbf{r},t') - f(\mathbf{r},t)}{\delta t} + \frac{f(\mathbf{r}+\mathbf{v}\delta t,t) - f(\mathbf{r},t)}{\delta t}\right)$$

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + (\mathbf{v}\cdot\nabla) f$$

Some details on the velocity potential

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{\partial \rho}{\partial t} + \rho(\nabla \cdot \mathbf{v}) + (\nabla \rho) \cdot \mathbf{v} = 0$$

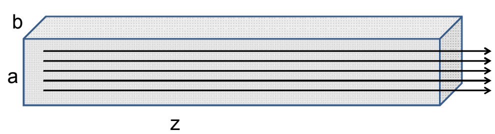
For incompressible fluid: $\rho = (\text{constant})$

$$\Rightarrow \nabla \cdot \mathbf{v} = 0$$

Irrotational flow: $\nabla \times \mathbf{v} = 0 \qquad \Rightarrow \mathbf{v} = -\nabla \Phi$

$$\Rightarrow \nabla^2 \Phi = 0$$

Example – uniform flow



$$\nabla^2 \Phi = 0$$

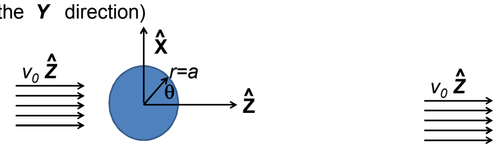
$$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} + \frac{\partial^2 \Phi}{\partial z^2} = 0$$

Possible solution:

$$\Phi = -v_o z$$

$$\mathbf{v} = -\nabla \Phi = v_o \hat{\mathbf{z}}$$

Example – flow around a long cylinder (oriented in the ***Y*** direction)



$$\nabla^2 \Phi = 0$$

$$\left. \frac{\partial \Phi}{\partial r} \right|_{r=a} = 0$$

Laplace equation in cylindrical coordinates

($r,\theta,$ defined in x-z plane; y representing cylinder axis)

$$\nabla^2\Phi = 0 = \frac{1}{r}\frac{\partial}{\partial r} r\frac{\partial \Phi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\Phi}{\partial\theta^2} + \frac{\partial^2\Phi}{\partial y^2}$$

In our case, there is no motion in the y dimension

$$\Rightarrow \Phi(r,\theta,y) = \Phi(r,\theta)$$

From boundary condition : $v_z(r\rightarrow\infty) = v_0$

$$\frac{\partial\Phi}{\partial z}(r\rightarrow\infty) = -v_0 \qquad \Rightarrow \Phi(r\rightarrow\infty,\theta) = -v_0 r\cos\theta$$

Note that : $\frac{\partial^2\cos\theta}{\partial\theta^2} = -\cos\theta$

Guess form : $\Phi(r,\theta) = f(r)\cos\theta$

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Necessary equation for radial function

$$\frac{1}{r}\frac{\partial}{\partial r} r\frac{\partial f}{\partial r} - \frac{1}{r^2} f = 0$$

$f(r) = Ar + \frac{B}{r}$ where A, B are constants

Boundary condition on cylinder surface :

$$\left.\frac{\partial\Phi}{\partial r}\right|_{r=a} = 0$$

$$\frac{df}{dr}(r=a) = 0 = A - \frac{B}{a^2}$$

$$\Rightarrow B = Aa^2$$

Boundary condition at ∞ : $\Rightarrow A = -v_0$

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$$\Phi(r,\theta) = -v_0\left(r + \frac{a^2}{r}\right)\cos\theta$$

$$v_r = -\frac{\partial\Phi}{\partial r} = v_0\left(1 - \frac{a^2}{r^2}\right)\cos\theta$$

$$v_\theta = -\frac{1}{r}\frac{\partial\Phi}{\partial\theta} = -v_0\left(1 + \frac{a^2}{r^2}\right)\sin\theta$$

For 3-dimensional system, consider a spherical obstruction

Laplacian in spherical polar coordinates:

$$\nabla^2\Phi = 0 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\varphi^2}$$

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Spherical system continued:

Laplacian in spherical polar coordinates:

$$\nabla^2\Phi = 0 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\varphi^2}$$

In terms of spherical harmonic functions:

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)Y_{lm}(\theta,\phi) = -l(l+1)Y_{lm}(\theta,\phi)$$

In our case:

$$Y_{10}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$\Phi(r,\theta,\phi) = f(r)Y_{lm}(\theta,\phi)$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{df}{dr}\right) - \frac{l(l+1)}{r^2}f = 0$$

(Continue analysis for homework)

Solution of Euler's equation for fluids

$$\frac{\partial\mathbf{v}}{\partial t} + \nabla\left(\tfrac{1}{2}v^2\right) - \mathbf{v}\times(\nabla\times\mathbf{v}) = \mathbf{f}_{applied} - \frac{\nabla p}{\rho}$$

Consider the following restrictions:

1. $(\nabla\times\mathbf{v}) = 0$ "irrotational flow"
   $\Rightarrow \mathbf{v} = -\nabla\Phi$
2. $\mathbf{f}_{applied} = -\nabla U$ conservative applied force
3. $\rho = \text{(constant)}$ incompressible fluid

$$\frac{\partial(-\nabla\Phi)}{\partial t} + \nabla\left(\tfrac{1}{2}v^2\right) = -\nabla U - \frac{\nabla p}{\rho}$$

$$\Rightarrow \nabla\left(\frac{p}{\rho} + U + \tfrac{1}{2}v^2 - \frac{\partial\Phi}{\partial t}\right) = 0$$

Bernoulli's integral of Euler's equation for constant ρ

$$\nabla\left(\frac{p}{\rho} + U + \tfrac{1}{2}v^2 - \frac{\partial\Phi}{\partial t}\right) = 0$$

Integrating over space:

$$\frac{p}{\rho} + U + \tfrac{1}{2}v^2 - \frac{\partial\Phi}{\partial t} = C(t)$$

where $\mathbf{v} = -\nabla\Phi(\mathbf{r},t) = -\nabla\left(\Phi(\mathbf{r},t) + C(t)\right)$

$$\Rightarrow \frac{p}{\rho} + U + \tfrac{1}{2}v^2 - \frac{\partial\Phi}{\partial t} = C_0 \qquad \text{Bernoulli's theorem}$$

For incompressible fluid

Solution of Euler's equation for fluids -- isentropic

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla\left(\tfrac{1}{2}v^2\right) - \mathbf{v}\times(\nabla\times\mathbf{v}) = \mathbf{f}_{applied} - \frac{\nabla p}{\rho}$$

Consider the following restrictions:

1. $(\nabla\times\mathbf{v}) = 0$ "irrotational flow"
   $\Rightarrow \mathbf{v} = -\nabla\Phi$
2. $\mathbf{f}_{applied} = -\nabla U$ conservative applied force
3. $\rho \neq$ (constant) isentropic fluid

A little thermodynamics

First law of thermodynamics: $dE_{\text{int}} = dQ - dW$

For isentropic conditions: $dQ = 0$

$dE_{\text{int}} = -dW = -pdV$

Solution of Euler's equation for fluids – isentropic (continued)

$dE_{\text{int}} = -dW = pdV$

In terms of mass density: $\rho = \frac{M}{V}$

For fixed M and variable V: $d\rho = -\frac{M}{V^2}dV$

$$dV = -\frac{M}{\rho^2}d\rho$$

In terms in intensive variables: Let $E_{\text{int}} = M\varepsilon$

$$dE_{\text{int}} = Md\varepsilon = -dW = -pdV = M\frac{p}{\rho^2}d\rho$$

$$d\varepsilon = \frac{p}{\rho^2}d\rho \qquad \left(\frac{\partial\varepsilon}{\partial\rho}\right)_{dQ=0} = \frac{p}{\rho^2}$$

Solution of Euler's equation for fluids – isentropic (continued)

$$\left(\frac{\partial\varepsilon}{\partial\rho}\right)_{dQ=0} = \frac{p}{\rho^2}$$

Consider: $\nabla\varepsilon = \left(\frac{\partial\varepsilon}{\partial\rho}\right)_{dQ=0}\nabla\rho = \frac{p}{\rho^2}\nabla\rho$

Rearranging: $\nabla\left(\varepsilon + \frac{p}{\rho}\right) = \frac{\nabla p}{\rho}$

Solution of Euler's equation for fluids – isentropic (continued)

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla\left(\tfrac{1}{2}v^2\right) - \mathbf{v}\times\left(\nabla\times\mathbf{v}\right) = \mathbf{f}_{applied} - \frac{\nabla p}{\rho}$$

$$\frac{\nabla p}{\rho} = \nabla\left(\varepsilon + \frac{p}{\rho}\right)$$

$$\nabla\times\mathbf{v} = 0 \qquad \mathbf{v} = -\nabla\Phi \qquad \mathbf{f}_{applied} = -\nabla U$$

$$\frac{\partial\left(-\nabla\Phi\right)}{\partial t} + \nabla\left(\tfrac{1}{2}v^2\right) = -\nabla U - \nabla\left(\varepsilon + \frac{p}{\rho}\right)$$

$$\Rightarrow \nabla\left(\varepsilon + \frac{p}{\rho} + U + \tfrac{1}{2}v^2 - \frac{\partial\Phi}{\partial t}\right) = 0$$

Summary of Bernoulli's results

For incompressible fluid

$$\nabla\left(\frac{p}{\rho} + U + \tfrac{1}{2}v^2 - \frac{\partial\Phi}{\partial t}\right) = 0$$

For isentropic fluid with internal energy density ε

$$\nabla\left(\varepsilon + \frac{p}{\rho} + U + \tfrac{1}{2}v^2 - \frac{\partial\Phi}{\partial t}\right) = 0$$

Application of fluid equations to the case of air in equilibrium plus small perturbation

Newton - Euler equation of motion :

$$\frac{\partial \mathbf{v}}{\partial t} + \left(\mathbf{v}\cdot\nabla\right)\mathbf{v} = \mathbf{f}_{applied} - \frac{\nabla p}{\rho}$$

Continuity equation : $\frac{\partial \rho}{\partial t} + \nabla\cdot\left(\rho\mathbf{v}\right) = 0$

Near equilibrium :

$$\rho = \rho_0 + \delta\rho$$

$$p = p_0 + \delta p$$

$$\mathbf{v} = 0 + \delta\mathbf{v}$$

$$\mathbf{f}_{applied} = 0$$

Equations to lowest order in perturbation :

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v} = \mathbf{f}_{applied} - \frac{\nabla p}{\rho} \quad \Rightarrow \quad \frac{\partial \delta\mathbf{v}}{\partial t} = -\frac{\nabla \delta p}{\rho_0}$$

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0 \quad \Rightarrow \quad \frac{\partial \delta\rho}{\partial t} + \rho_0 \nabla\cdot\delta\mathbf{v} = 0$$

In terms of the velocity potential :

$$\delta\mathbf{v} = -\nabla\Phi$$

$$\frac{\partial \delta\mathbf{v}}{\partial t} = -\frac{\nabla \delta p}{\rho_0} \quad \Rightarrow \nabla\left(-\frac{\partial\Phi}{\partial t} + \frac{\delta p}{\rho_0}\right) = 0$$

$$\frac{\partial \delta\rho}{\partial t} + \rho_0 \nabla\cdot\delta\mathbf{v} = 0 \quad \Rightarrow \frac{\partial \delta\rho}{\partial t} - \rho_0\nabla^2\Phi = 0$$

Expressing pressure in terms of the density :

$p = p(s,\rho) = p_0 + \delta p$ where s denotes the (constant) entropy

$p_0 = p(s,\rho_0)$

$$\delta p = \left(\frac{\partial p}{\partial \rho}\right)_s \delta\rho \equiv c^2\delta\rho$$

$$\nabla\left(-\frac{\partial\Phi}{\partial t} + \frac{\delta p}{\rho_0}\right) = 0 \quad \Rightarrow -\frac{\partial\Phi}{\partial t} + c^2\frac{\delta\rho}{\rho_0} = (\text{constant})$$

$$\Rightarrow -\frac{\partial^2\Phi}{\partial t^2} + \frac{c^2}{\rho_0}\frac{\partial \delta\rho}{\partial t} = 0$$

$$\frac{\partial \delta\rho}{\partial t} - \rho_0\nabla^2\Phi = 0 \quad \Rightarrow \frac{\partial^2\Phi}{\partial t^2} - c^2\nabla^2\Phi = 0$$

Wave equation for air :

$$\frac{\partial^2\Phi}{\partial t^2} - c^2\nabla^2\Phi = 0$$

Here, $c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s$

$\mathbf{v} = -\nabla\Phi$

Note that, we also have :

$$\frac{\partial^2 \delta\rho}{\partial t^2} - c^2\nabla^2\delta\rho = 0$$

$$\frac{\partial^2 \delta p}{\partial t^2} - c^2\nabla^2\delta p = 0$$

Boundary values :

Impenetrable surface with normal $\hat{\mathbf{n}}$ moving at velocity $\mathbf{V}$:

$$\hat{\mathbf{n}}\cdot\mathbf{V} = \hat{\mathbf{n}}\cdot\delta\mathbf{v} = -\hat{\mathbf{n}}\cdot\nabla\Phi$$

Free surface :

$$\delta p = 0 \quad \Rightarrow \rho_0\frac{\partial \Phi}{\partial t} = 0$$

Analysis of wave velocity in an ideal gas:

$$c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s$$

Equation of state for ideal gas :

$$pV = NkT \qquad N = \frac{M}{M_0}$$

$$p = \frac{M}{V}\frac{k}{M_0}T = \rho\frac{k}{M_0}T$$

$$k = 1.38\times 10^{-23}\,J/k$$

M_0 = average mass of each molecule

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Internal energy for ideal gas :

$$E = \frac{f}{2}NkT = M\varepsilon \qquad \varepsilon = \frac{f}{2}\frac{k}{M_0}T = \frac{f}{2}\frac{p}{\rho}$$

In terms of specific heat ratio : $\gamma \equiv \frac{C_p}{C_V}$

$$dE = dQ - dW$$

$$C_V = \left(\frac{dQ}{dT}\right)_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{f}{2}\frac{Mk}{M_0}$$

$$C_p = \left(\frac{dQ}{dT}\right)_p = \left(\frac{\partial E}{\partial T}\right)_p + p\left(\frac{\partial V}{\partial T}\right)_p = \frac{f}{2}\frac{Mk}{M_0} + \frac{Mk}{M_0}$$

$$\gamma = \frac{C_p}{C_V} = \frac{\frac{f}{2}+1}{\frac{f}{2}} \qquad \Rightarrow \frac{f}{2} = \frac{1}{\gamma - 1}$$

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Internal energy for ideal gas :

$$E = \frac{1}{\gamma-1}NkT = M\varepsilon \qquad \varepsilon = \frac{1}{\gamma-1}\frac{k}{M_0}T = \frac{1}{\gamma-1}\frac{p}{\rho}$$

Internal energy for ideal gas under isentropic conditions :

$$d\varepsilon = -\frac{p}{M}dV = \frac{p}{\rho^2}d\rho$$

$$\left(\frac{\partial \varepsilon}{\partial \rho}\right)_s = \frac{p}{\rho^2} = \frac{\partial}{\partial \rho}\left(\frac{1}{\gamma-1}\frac{p}{\rho}\right)_s = \left(\frac{\partial p}{\partial \rho}\right)_s \frac{1}{(\gamma-1)\rho} - \frac{p}{(\gamma-1)\rho^2}$$

$$\Rightarrow \left(\frac{\partial p}{\partial \rho}\right)_s = \frac{p\gamma}{\rho}$$

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Alternative derivation:

Isentropic or adiabatic equation of state:

$$\frac{dp}{p} = \gamma \frac{d\rho}{\rho} \qquad \Rightarrow \frac{p}{p_0} = \left(\frac{\rho}{\rho_0}\right)^{\gamma}$$

$$\left(\frac{\partial p}{\partial \rho}\right)_s = \frac{p\gamma}{\rho}$$

Linearized speed of sound

$$c_0^{\ 2} = \left(\frac{\partial p}{\partial \rho}\right)_{s,p_0,\rho_0} = \frac{p_0\gamma}{\rho_0}$$

$$c_0^{\ 2} \approx \frac{1.5 \cdot 1.013 \times 10^5\, Pa}{1.3 kg/m^3} \qquad c_0 \approx 340 \text{ m/s}$$

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Density dependence of speed of sound for ideal gas:

$$c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s = \frac{p\gamma}{\rho}$$

$$\frac{p}{p_0} = \left(\frac{\rho}{\rho_0}\right)^{\gamma}$$

$$c^2 = \frac{p_0\gamma}{\rho_0}\frac{p/p_0}{\rho/\rho_0} = c_0^2\left(\frac{\rho}{\rho_0}\right)^{\gamma-1}$$

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