# **Ionization Structure & Numerics of Protoplanetary Disks**



### Steven A. Balbus

Ecole Normale Supérieure Physics Department Paris, France

### FORMATION and EVOLUTION OF PROTOSTELLAR DISKS

Problem is central to understanding star and planet formation.

Initial collapse of a rotating molecular cloud is likely to be planar, not spherical, with a condensed pressurized core and an extended rotating repository of angular momentum. Identify with protostar and protostellar disk.

Early infall stages will be strongly self-gravitating. Deep spiral structure in disk effective at angular momentum transport. Disk turbulence by infall will *not* be effective, for reasons we shall see.

### FUNDAMENTALS OF ACCRETION DISKS

• Modern accretion disk theory began in the 1960's from the attempts of Lynden-Bell, Rees, Thorne and others to establish observational signatures from hot gas in orbit around black holes.

• Applications of this formalism to the solar nebula (and protostellar disks more generally), pioneered by Lin and Papaloizou, began in earnest around 1980.

• A quarter of a century later, we still lack a "vanilla" model!

### **DISK MODEL**, version 0.1

• The equation of hydrostatic equilibrium is:

$$\frac{\nabla P}{\rho} = -\nabla \Phi + R\Omega^2 \mathbf{e}_{\mathbf{R}}$$

If  $\Omega = \Omega(R)$ , right side is exact gradient. Constant density and constant pressure surfaces coincide. We may thus define an enthalpy function  $H(\rho) = \int dP/\rho$ .

$$H(\rho) + \Phi - \int R' \Omega^2(R') dR' = \text{Constant}$$

## TO FIX IDEAS,

take  $v_{rot}^2 = GM \cos \alpha / R$ , where  $\alpha$  is a parameter. This is sub-Keplerian. Hydrostatic equation becomes:

 $H(\rho) - GM/r + GM \cos\alpha/R =$ 

 $H(\rho) + GM/r$  [ (cos $\alpha$ /cos $\lambda$ ) - 1 ] = Constant (Note that accretion velocity does not enter into HSE.)







If the free energy of differential rotation is extracted, dissipated, and radiated locally, the fundamental equation is:

 $\nabla \bullet F_{rad} = - T_{R\phi} \quad d\Omega/d \ln R$ ,

Where  $T_{R\phi} = \langle \rho(u_R | u_{\phi} - u_{AR} | u_{A\phi}) \rangle$  is a mean averaged correlation. In alpha models,  $T_{R\phi} = \alpha P$ , with  $\alpha$  constant. The equations states that:

 $\int F_{rad} \cdot dA = - \int T_{R\phi} d\Omega / d \ln R dV$ 

Recall:

 $F_{rad} = - [16\sigma T^{3}/3\kappa_{r}\rho] \partial T/\partial z e_{z}$ where  $\kappa_{r}$  is the opacity ( $\kappa_{r} \sim 1 \text{ cm}^{2} \text{ g}^{-1}$ ). Hence,  $\partial /\partial z [16\sigma T^{3}/3\kappa_{r}\rho \partial /\partial z] T = T_{R\phi} d\Omega/d \ln R$  $= \alpha P d\Omega/d \ln R$ 

Consider the case of constant opacity  $\kappa_r$ ...

With optical depth  $d\tau = -\kappa_r \rho dz$ , equation takes the form :

$$d^2y/d\tau^2 = -A y^{1/4},$$

y=T<sup>4</sup>, dy/d $\tau$  = (3/4 $\sigma$ ) **F**<sub>rad</sub>, A=(3 $\alpha$ k/4 $\sigma$ k<sub>r</sub>m) |d $\Omega$ /d ln R| Integrating, (dy/d $\tau$ )<sup>2</sup> = - (8A T<sup>5</sup>/5) + CONST.

At the disk surface  $(dy/d\tau)^2 = (3T_{eff}^4 / 4)^2$ , hence :

CONST =  $(8A T_{eff}^5 / 5) + (3T_{eff}^4 / 4)^2$ , and  $(dy/d\tau)^2 = (8A/5) (T_{eff}^5 - T^5) + (3T_{eff}^4 / 4)^2$ 

 $(dy/d\tau)^2 = (8A/5) (T_{eff}^5 - T^5) + (3T_{eff}^4 / 4)^2$ 

T gradient  $\Downarrow$  as T  $\Uparrow$ ; T maximum when

 $T_{MAX}^{5} = T_{eff}^{5} + (128A/45)^{-1} T_{eff}^{8}$ 

At R =1 AU, M = 1  $M_{\odot}$ , this gives:

 $T_{MAX} \sim 600 \ (\kappa_r \ / \ \alpha_{-2})^{1/5} \ (T_{eff} \ / \ 152)^{8/5} \ K$ 

Interesting, because T > 1000K required for self-consistent MRI . . .

I max

Τ

 $(dy/d\tau)^2 = (8A/5) (T_{eff}^5 - T^5) + (3T_{eff}^4 / 4)^2$ 

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#### OTHER ASSUMPTIONS ARE POSSIBLE:

 $\alpha$  models are not the only possibility---nor are they are necessarily the most promising.

« $\beta$  models» (Zahn & coworkers) are based on the prescription

 $T_{R\phi} = \beta (R d\Omega / d \ln R)^2$ ,  $\beta = const.$ 

Invoked for hydrodynamic turbulence, scaling might just apply to MRI saturation as well.

Numerics suggest  $v_A \approx \text{constant}$  in space. (Galaxy as well...)

Then 
$$T_{R\phi} = \gamma \rho$$
,  $\gamma = a$  *dimensional* const.

#### A (SAMPLE) COMPLETE MODEL:

 $\sigma T_{eff}^{4} = 3 \text{ GM } M_{DOT} / 8\pi R^{3} = \alpha c_{S}^{2} (3/4) \Omega \Sigma$ 

 $T_{MAX}^{5} = T_{eff}^{5} + (128A/45)^{-1} T_{eff}^{8}$ 

 $A = (3\alpha k/4\sigma \kappa_r m) |d\Omega/d \ln R|$ 

Three equations to solve for  $T_{eff}$  ,  $T_{MAX}$  , and  $~\Sigma,~given$   $\alpha$  and  $M_{DOT.}$ 

#### A (SAMPLE) COMPLETE MODEL:

$$\begin{split} \sigma T_{eff}^{4} &= \ 3 \ GM \ M_{DOT} \ / \ 8\pi R^{3} \ = \alpha \ c_{S}^{2} \ (3/4) \ \Omega \Sigma \\ T_{MAX}^{5} &= T_{eff}^{5} + \ (128A/45)^{-1} \quad T_{eff}^{8} \end{split}$$

RESULTS:  $T_c = 589 \text{ K} (\alpha_{-2})^{-1/5} \kappa_r^{1/5} M_{DOT-7}^{2/5} R_{AU}^{-9/10}$ 

 $T_{eff} = 152 \text{ K} \text{ M}_{\text{DOT-7}}^{1/4} \text{ R}_{\text{AU}}^{-3/4}$ 

 $\Sigma = 965 \text{ g cm}^{-2} (\alpha_{-2})^{-4/5} \kappa_r^{-1/5} M_{\text{DOT}^{-7}}^{3/5} R_{\text{AU}}^{-3/5}$ 

 $\rho = 6.68 \times 10^{-10} \text{ g cm}^{-3} (\alpha_{-2})^{-9/10} \kappa_r^{-3/10} \text{ M}_{\text{DOT-7}}^{2/5} \text{ R}_{\text{AU}}^{-33/20}$ 

### **POSSIBLE IONIZATION SOURCES**

1. Cosmic Rays (Gammie 1996, Sano et al. 2000)

2. Radioactive Isotopes (many studies)

3. Chromospheric X-rays (Igea & Glassgold 1999, Fromang et al. 2002, Ilger & Nelson 2006abc)

Cosmic rays uncertain, excluded by stellar winds and possibly by plasma instabilities. Radioactivity ultimately too small. X-rays are both a potent source *and* observed. **IONIZATION STRUCTURE OF α-MODELS** (Fromang et al. 2002, Ilger & Nelson 2006a)

- Ionization depends upon details of chemistry (nature of atomic and molecular species) as well as presence of dust grains.
- 2. Simple models tend to be to "optimistic": predict higher levels and more extended active zone.
- 3. Submicron dust grains are MRI-killers, chemistry less important. But:
- 4. Suppresing the MRI leads to quiesence and dust settling which turns the MRI back on, which mixes the dust back in...!

Table A.1. List of gaseous	species includin	g free electrons	and grain
particles with different elec	tric excess charg	es.	

$H^+$	Н	H <sub>2</sub>	$H_2^+$	$H_3^+$
He	$He^+$	C	$\mathbf{C}^{\overline{+}}$	CH
$CH^+$	CH <sub>2</sub>	$CH_2^+$	$N^+$	Ν
$CH_3^+$	$NH^+$	CH <sub>3</sub>	NH	$CH_4^+$
$NH_2^+$	0	NH <sub>2</sub>	$O^+$	$CH_4$
OH	NH <sub>3</sub>	$NH_3^+$	$OH^+$	$CH_5^+$
$H_2O$	$NH_4^+$	$H_2O^+$	$H_3O^+$	Mg
$C_2$	$C_2^+$	$Mg^+$	$C_2H^+$	$C_2H$
CN	$C_2H_2$	$CN^+$	$C_2H_2^+$	HCN
$C_{2}H_{3}^{+}$	HNC	$C_2H_3$	$HCN^+$	$H_2NC^+$
$Si^+$	$HCNH^+$	$CO^+$	CO	Si
$N_2^+$	N <sub>2</sub>	$C_{2}H_{4}^{+}$	SiH <sup>+</sup>	$HCO^+$
HCO	SiH	$HN_2^+$	$NO^+$	$H_2CO^+$
SiH <sub>2</sub>	NO	$SiH_2^+$	$H_2CO$	$H_3CO^+$
SiH <sub>3</sub>	$SiH_3^+$	S+	CH <sub>3</sub> OH <sup>+</sup>	$SiH_4$
CH <sub>3</sub> OH	$O_2^+$	S	$SiH_4^+$	$O_2$
$HS^+$	$CH_3OH_2^+$	HS	$SiH_5^+$	$H_2S$
$H_2S^+$	$H_3S^+$	C <sub>3</sub>	C <sub>3</sub> +	C <sub>3</sub> H
$C_3H^+$	$C_3H_2$	$C_{3}H_{2}^{+}$	$C_2N^+$	$CNC^+$
$C_3H_3$	$C_{3}H_{3}^{+}$	$C_3H_4$	$SiC^+$	$C_3H_4^+$
SiC	$C_2O^+$	HCSi	$HC_2O^+$	HCSi <sup>+</sup>
$CH_3CN^+$	$C_3H_5^+$	CH <sub>3</sub> CN	$CH_2CO$	$SiN^+$
SiN	$CH_2CO^+$	$H_4C_2N^+$	$CH_3CO^+$	HNSi
HNSi <sup>+</sup>	$CO_2^+$	$SiO^+$	CS	SiO
$CO_2$	$CS^+$	HCS	$HCO_2^+$	SiOH <sup>+</sup>
$HCS^+$	$NS^+$	NS	$H_2CS$	$H_2CS^+$
$H_3CS^+$	$HNS^+$	$C_4^+$	$SO^+$	SO
$C_4$	$HSO^+$	$C_4H^+$	$C_4H$	$C_3N$
$C_4H_2^+$	$C_3N^+$	$C_4H_2$	$HC_3N^+$	$HC_3N$
$C_3O^+$	C <sub>3</sub> O	$H_2C_3N^+$	$HC_3O^+$	$C_3H_2O^+$
$H_3C_3O^+$	$C_2S^+$	$C_2S$	Fe <sup>+</sup>	Fe
$HC_2S^+$	SiS	$OCS^+$	SiO <sub>2</sub>	$SiS^+$
OCS	$HSiS^+$	$HOCS^+$	$SO_2^+$	$SO_2$
S <sub>2</sub>	$HSO_2^+$	$H_4C_4N^+$	$H_{2}S_{2}^{+}$	C <sub>3</sub> S
$C_3S^+$	$HC_3S^+$	$C_7^+$	e <sup>-</sup>	gr
gr <sup>2-</sup>	gr <sup>-</sup>	gr <sup>+</sup>	gr <sup>2+</sup>	

# List of gaseous species from Ilger & Nelson 2006a



**Fig. 6.** The effective X-ray ionisation rate  $\zeta_{\text{eff}}$  per hydrogen nucleus (including contributions due to thermal ionisation of potassium). The disk parameters are  $\alpha = 10^{-2}$  and  $\dot{M} = 10^{-7} M_{\odot} \text{ yr}^{-1}$ . The contour lines refer to values of  $\zeta_{\text{eff}}$ :  $10^{-19}$ ,  $10^{-21}$ , and  $10^{-23} \text{ s}^{-1}$ .

#### Ilger and Nelson standard model of ionization structure

The boundary between the active and dead zones is unstable.

In a turbulent system, a classical method of modeling the fluctuation amplitude y is to use a "Landau Equation:"

 $dy/dt = [\gamma - \eta(T)] y - Ay^3$ 

Where  $\gamma$  is a linear growth rate,  $\eta$  a damping rate --- here T dependent! --- and A is a nonlinear saturation term, possibly T dependent.

Cooling:  $dT/dt = Wy^2 - C(T)$ 

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Cooling:  $dT/dt = Wy^2 - C(T)$  $-T_{R\phi} d\Omega/dlnR$ 

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Where  $\gamma$  is a linear growth rate,  $\eta$  a damping rate --- here T dependent! --- and A is a nonlinear saturation term, possibly T dependent.

Cooling:  $dT/dt = Wy^2 - C(T)$ T-dependent cooling function

The boundary between the active and dead zone is unstable.

For protostellar disks,  $\eta(T) = 234 T^{1/2} (n_n / n_e) cm^2 s^{-1}$ , where  $n_n/n_e$  is *very* T-sensitive.

Result:  $\eta(T) \sim T^{-1/4} \exp(T_0/T)$ . Take A=constant.

The steady state  $\gamma = \eta(T_0)$ ,  $W y_0^2 = C(T_0)$  is **unstable** if either

 $\partial C/\partial T < 0$ , or  $\partial \eta/\partial T < 0$ , (Balbus & Lesaffre 2006).

Active-inactive interface is therefore a region of instability!

The physical reasoning is simple:

If  $\partial C/\partial T < 0$ , the cooling increases as the temperature decreases, T decreases more, a runaway ensues (Field 1965.)

If  $\partial \eta / \partial T < 0$ , increasing the temperature decreases the resistivity and *raises* the fluctuation amplitude y. The turbulent heating then goes up, which raises the temperature even more.

This behavior is not limited to protostellar disks: Dwarf Novae may also have dead zones. Both DN and PSD show outbursts.



### INNER REGIONS OF SOLAR NEBULA

#### *Nonlinear Calculation by P. Lesaffre* Phase space



### **SUMMARY**

- 1. If accretion velocity is small, v<sub>rot</sub> (R), gross disk structure is relatively simple.
- 2. Accretion mass flux may exhibit complicated structure.
- 3. Ionization is *certainly* complex. Sensitive to molecular chemistry and grain physics.
- 4. Grains kill MRI, but killing MRI settles grains. Self-consistent solution needed.
- 5. Despite uncertainty, magnetic decoupling is likely on scales of 10 AU. Vertical, temporal extent uncertain.

### SUMMARY

6. Active-decoupled boundary is unstable, and may be the site of eruptive behavior, and different disk states.

# **IV. Numerical Simulations**



### Steven A. Balbus

Ecole Normale Supérieure Physics Department Paris, France

### **EFFECTS OF MHD TURBULENCE**

- 1. Self-consistent models involve HSE and a decoupled mass conservation equation,  $\nabla \cdot (\rho \mathbf{v}) = 0$ .
- 2. Simplest models take a radial mass flux,  $\rho r^2 v_R = Const.$
- 3. An obvious generalization is to try  $\rho \mathbf{v} = \nabla \Phi$ ,  $\nabla^2 \Phi = 0$  with  $\Phi \sim 1/r + P_2(\cos\theta) / r^3 + ...$
- Quadrupolar structure is natural because turbulent forcing is quadrupolar, <v<sub>i</sub> v<sub>i</sub> - v<sub>Ai</sub> v<sub>Ai</sub> > ∂v<sub>i</sub>/∂v<sub>i</sub>. Non-alpha.
- 5. Seen in simulations. Potential importance for mixing.



## NUMERICAL SIMULATIONS OF PROTOSTELLAR DISKS

### NUMERICAL SIMULATIONS OF PROTOSTELLAR DISKS

Only the tiniest pieces have been attempted: Ohmic dissipation, Hall MHD (Stone, Sano and coworkers).

## WHY NOT MORE?

- 1. Dynamic range requirements.
- 2. Chemistry coupled to dynamics is not yet feasible, even in very local models.
- 3. Radiation dynamics is in its infancy (Hirose, Krolik & Stone 2006).

Long history of MHD polytropic simulations. Let us start with the "Shearing Box:"















Equations of motion for shearing box:

$$\frac{Dv_{x}}{Dt} - 2\Omega v_{y} = -x \frac{d\Omega^{2}}{d\ln R} - \frac{\partial P}{\partial x} + (\mathbf{J} \times \mathbf{B})_{x} \qquad \text{(radial)}$$

$$\frac{Dv_{y}}{Dt} + 2\Omega v_{x} = -\frac{\partial P}{\partial y} + (\mathbf{J} \times \mathbf{B})_{y} \qquad \text{(azimuthal)}$$

$$\frac{Dv_{z}}{Dt} = -\frac{\partial P}{\partial z} + (\mathbf{J} \times \mathbf{B})_{z} \qquad \text{(vertical)}$$



2D shearing box simulation from Hawley & Balbus 1992: Angular momentum contours.



Simulation of convection in shearing box (Stone & Balbus 96)





FIG. 2.—Top: Time history of the vertical kinetic energy during the three-dimensional evolution of a convectively unstable accretion disk with a vertical structure given in Fig. 1 and with an ad hoc heating source added at the disk midplane. *Bottom*: Time history of the Reynolds stress normalized by the pressure at the disk midplane.

The stress tensor of a convectively driven shearing box is negative (Stone & Balbus 1996)!

α

- 1. Very different behaviors depending on whether mean  $B_z$  vanishes or not. Turbulence cannot destroy mean **B** in SBS.
- 2. Early 2D simulations with  $\langle B_z \rangle$  did not saturate! Instead, Exponentially growing streams formed:



- In 3D, "channel solution" is K-H unstable (Goodman and Xu 1994), breaks down. K-H is critical for turbulent cascade.
- 4. Finite  $\langle B_z \rangle$  simulations in 3D show higher  $T_{R\phi}$  than finite  $\langle B_R \rangle$  or  $\langle B_{\phi} \rangle$ . If zero initial mean field, no evidence of convergence. From Hawley, Gammie, Balbus 1995:



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- 5. Restricted dynamical range of SB allows more complex MHD. For PSDs, Ohmic and Hall effects most interesting.
- 6. Most detailed studies of dissipation by T. Sano and collaborators. Key parameter is Lundquist number:

 $\text{Re}_{\text{M}} = v_{\text{A}}^2 / \eta \Omega$ 

In  $B_z$  simulations, this must exceed unity to avoid Ohmic dissipation.



From Sano et al. 2001



Over longer time scales,  $B_z$  runs show highly fluctuating time signals, reminiscent of Shot Noise.

#### **SHEARING BOX STATE OF THE ART:**

Recently, the first "Shakura-Sunyaev model" has been constructed from first principles (Hirose, Krolik, Stone 2006; Blaes et al. 2006 for spectra).

Full energy equation, including radiation transport. Vertical stratification. Energy "dissipated" goes into heating gas, radiatively diffused and lost through surface. Kramers op.

No explicit resistivity or viscosity, so energy not truly dissipated. Instead, lost at grid scale and recycled as heat.

Photosphere occurs at z=7 ( $c_S/\Omega$ ), very high [cf. 3 ( $c_S/\Omega$ ) in Analytic models]. Significant departures from Planckian. Magnetic pressure dominates at high latitude.

### **GLOBAL MODELS**

Global Models of accretion disks began in 1998 (Armitage), and were developed by Hawley (2000).

Pacynski-Wiita potential  $1/|r - r_g|$ , developed for black holes, used almost universally (infalling boundary condition at finite r).

Extremely demanding of computational resources, simple polytropes so far, a few runs with resistive heating. Used for PSDs, BHDs alike!

### **GLOBAL MODELS**

Typically, hard EOS accrete with great difficulty, isothermal less so. Bound and unbound equipotential surfaces all converge:

This means it is easy for blackflow to move from bound to unbound surfaces, simulations often reveal jets from this region; start thermal, become MHD.

### **GLOBAL MODELS**

A quasi-Keplerian disk & jet structure readily emerge from pressure supported tori as initial conditions.

Beyond this, there is no regularity: *highly fluctuating* both spatially and temporally. Underlying average structure is very difficult to extract.  $T_{R\phi}$ , a correlated average of fluctuations, is impossible to describe in a simple way, certainly is NOT  $\alpha P$ .

Radial mixing is efficient in simulations. If representative of PSDs, a result of considerable practical importance.

Fluctuation Equation:

$$\boldsymbol{\nabla} \cdot \left( \frac{\gamma \rho}{\gamma - 1} \langle \delta \boldsymbol{v} \, \delta \tau \rangle \right) + \frac{\tau}{\gamma - 1} \langle \rho \boldsymbol{v} \rangle \cdot \boldsymbol{\nabla} \ln P \rho^{-\gamma} = -Q^{-} - T_{R\phi} \frac{d\Omega}{d \ln R}$$

$$\tau = kT/\mu, \ T_{R\phi} = \rho \langle \delta \boldsymbol{v} \delta v_{\phi} - \boldsymbol{v}_{A} v_{A\phi} \rangle$$
$$\frac{\gamma \rho}{\gamma - 1} \langle \delta \boldsymbol{v} \, \delta \tau \rangle = \langle \delta P \, \delta \boldsymbol{v} \rangle \quad \text{(acoustic)}$$
$$= C_P \langle \delta \boldsymbol{v} \delta T \rangle \text{ (isobaric.)}$$

Dominant balances (4 out of 4!/2!2! = 6):

$$-Q^{-} = T_{R\phi} \frac{d\Omega}{d\ln R} \text{ (classical disk theory)}$$
$$\boldsymbol{\nabla} \cdot \left(\frac{\gamma \rho}{\gamma - 1} \langle \delta \boldsymbol{v} \, \delta \tau \rangle \right) = -T_{R\phi} \frac{d\Omega}{d\ln R} \text{ (wave action)}$$
$$\frac{\tau}{\gamma - 1} \langle \rho \boldsymbol{v} \rangle \cdot \boldsymbol{\nabla} \ln P \rho^{-\gamma} = -Q^{-} \text{ (classical cooling flow.)}$$
$$\frac{\tau}{\gamma - 1} \langle \rho \boldsymbol{v} \rangle \cdot \boldsymbol{\nabla} \ln P \rho^{-\gamma} = -T_{R\phi} \frac{d\Omega}{d\ln R} \text{ (RIAF's)}$$

#### Global Simulations of the MRI, Hawley 2000





#### Meridional Plane

#### **Equatorial Plane**

disk and jet by *John Hawley* 



#### PLANET IN A DISK (NELSON & PAPALOIZOU 2005):



30  $M_{\oplus}$  planet in laminar disk.

#### PLANET IN A DISK (NELSON & PAPALOIZOU 2005):



30  $M_{\oplus}$  planet in *turbulent* disk.



 $M_{\oplus}$  planet in *turbulent* disk: midplane.



Torques on  $M_{\oplus}$  planet. Blue: outer Green: inner Red: net. Highly stochastic, long term behavior unresolved.

# SUMMARY

- 1. Realistic PSD simulations not yet feasible.
- 2. Numerics indicate a highly fluctuating flow. Analytic prescriptions unimpressive, but not obvious how to improve them.
- Two broad approaches: shearing box and global disks. (There is nothing in between, despite occasional attempts to "improve" shearing box.)
- 4. Local simulations: small dynamic range, more complex physics, e.g. Ohmic, Hall MHD; radiative losses.
- 5. Global simulations: extended dynamic range, simple EOS.

# SUMMARY

- 6. Gross morphology of global simulations *do* show some regularity: Keplerian disk, mixing, "corona," jet.
- 7. More detailed structure (e.g. transport via  $T_{R\phi}$ ) is *not* simple: no obvious  $\alpha$  prescription from simulations.
- 8. Planet migration is dominated by MHD turbulence, *when present.*
- 9. The PSD problem has yet to be addressed. Mixing of active and decoupled zones, temperature sensitive resistivity, radiation are the heart of PSDs---even a restricted combination would be of interest.