Transport properties of a non-relativistic dilute Yukawa liquid

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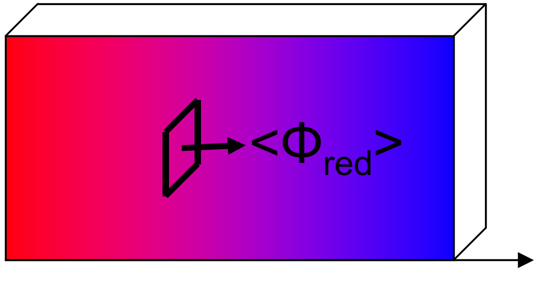
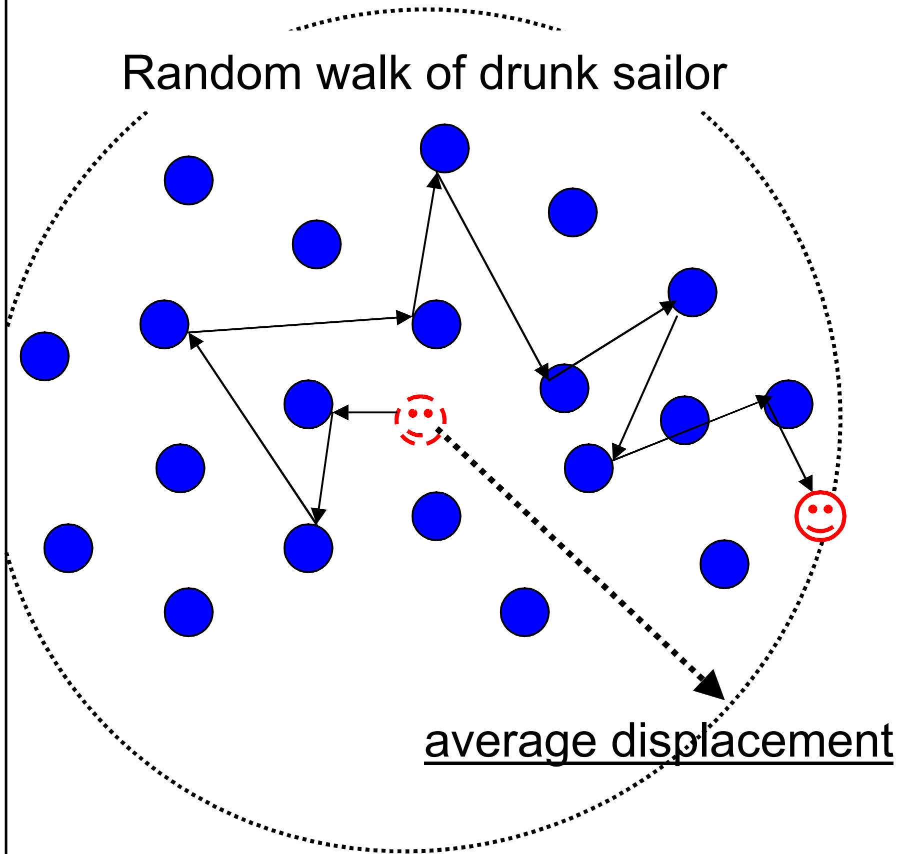
Content

- Introduction to transport phenomena
- Boltzman equation and the equation of change
- Enskog solution of Boltzman equation for a dilute system close to equilibrium
- Screened Coulomb potential: preliminary results for Yukawa liquid of C^{12}
- Relevance to Neutron Star physics and computer simulations (Horowitz & Caballero)

Diffusivity

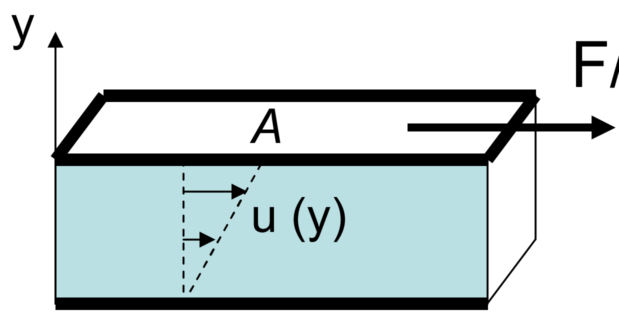
$\langle \Phi_{red} \rangle = D \; dn_{red} / dz$



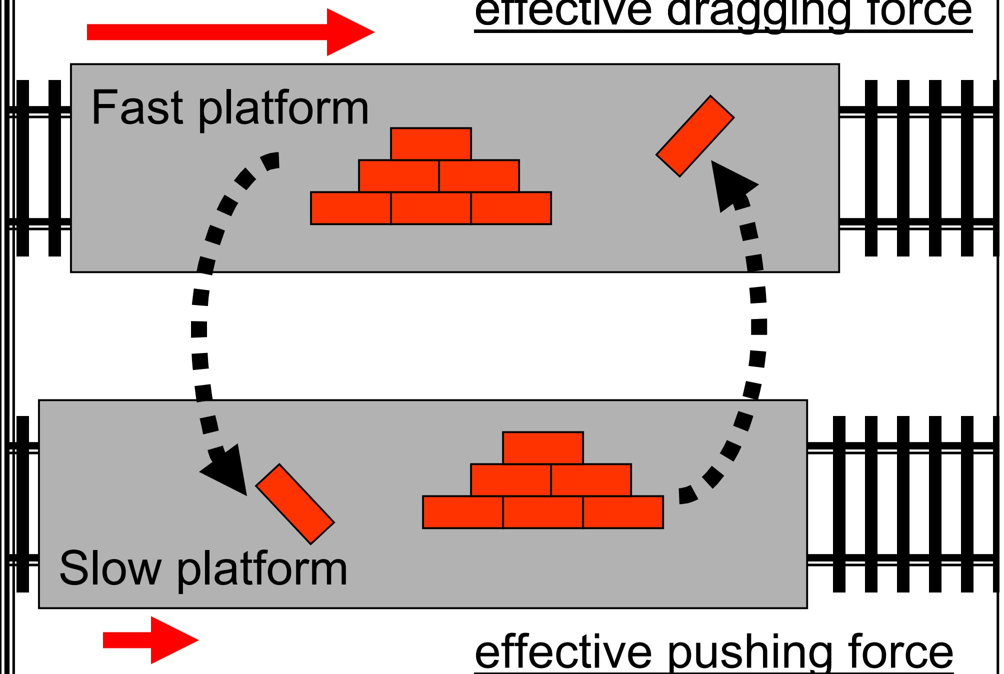


Shear viscosity

$F/A = \eta \; du/dy$



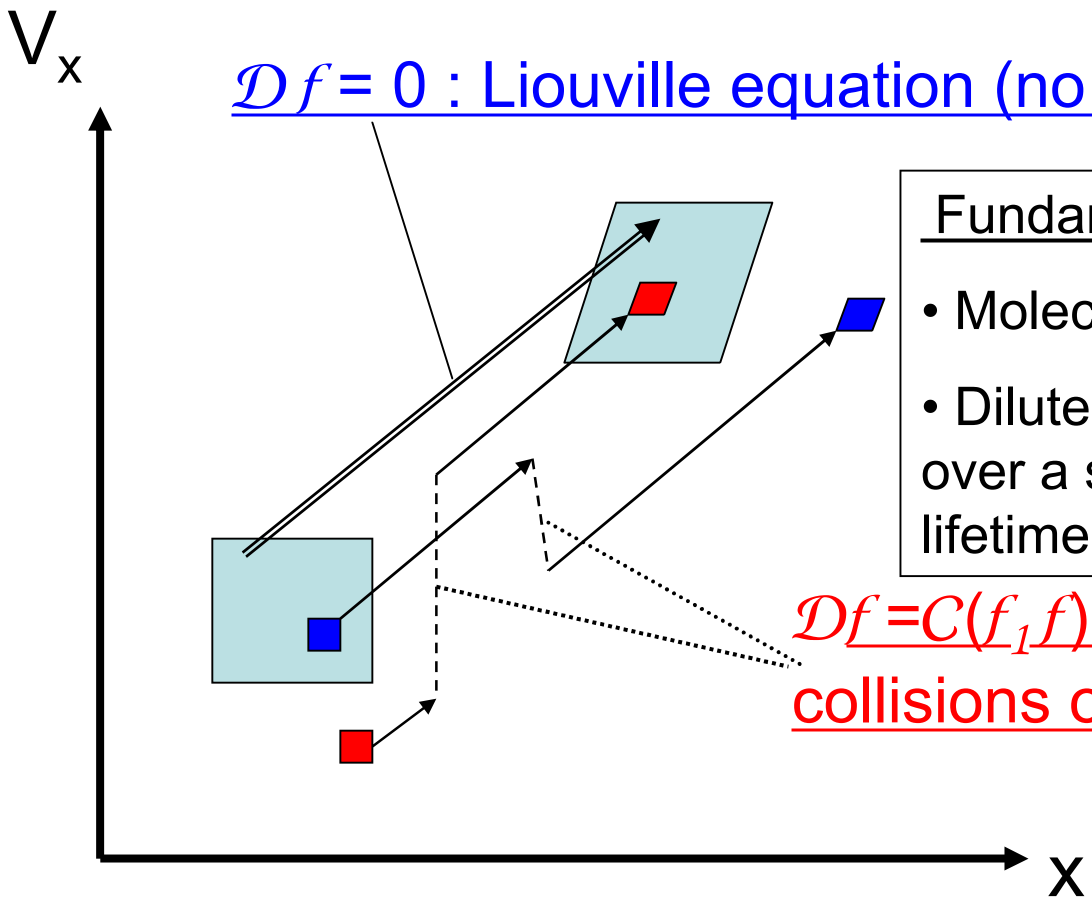
Classic Newtonian laminar flow



Boltzman equation for the particle distribution function: f (phase space)

Equations of motion → time evolution → operator $\mathcal{D}$

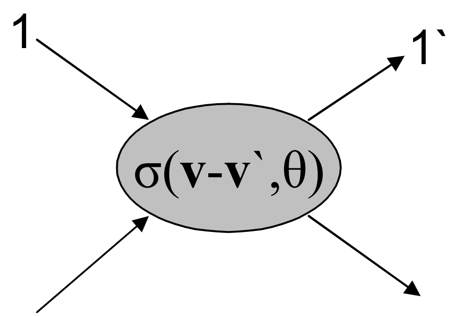
$\mathcal{D}f = 0$: Liouville equation (no collisions)



Fundamental assumptions:

- Molecular chaos – no correlations
- Dilute system – encounters occur over a small fraction of molecular lifetime

$\mathcal{D}f = \mathcal{C}(f_1 f)$: Boltzman equation (binary collisions only)



Equation of change for property ϕ

$$\int \phi\, \mathcal{D}f\, d\mathbf{v} = n \langle \Delta\phi \rangle$$

$$\langle \Delta\phi \rangle = n^{-1} \int \phi\, C(f_1 f)\, d\mathbf{v}$$

Table 14.2 Summary of phenomenological transport laws

Effect	Flux of particle property ϕ	Gradient	Coefficient	Law	Name of law	Approximate expression for coefficient
Diffusion	Number	$\frac{dn}{dz}$	Diffusivity D	$\mathbf{J}_n = -D \operatorname{grad} n$	Fick's law	$D = \frac{1}{3}\bar{c}l$
Viscosity	Transverse momentum	$M\frac{dv_x}{dz}$	Viscosity η	$\frac{F_x}{A} = J_{\mathbf{p}}^x = -\eta\frac{dv_x}{dz}$	Newtonian viscosity	$\eta = \frac{1}{3}\rho\bar{c}l$
Thermal conductivity	Energy	$\frac{d\rho_u}{dz} = \hat{C}_V\frac{dT}{dz}$	Thermal conductivity K	$\mathbf{J}_u = -K \operatorname{grad} \tau$	Fourier's law	$K = \frac{1}{3}\hat{C}_V\bar{c}l$
Electrical conductivity	Charge	$-\frac{d\varphi}{dz} = E_z$	Conductivity σ	$\mathbf{J}_q = \sigma\mathbf{E}$	Ohm's law	$\sigma = \frac{nq^2l}{M\bar{c}}$

SYMBOLS: n = number of particles per unit volume
$\bar{c}$ = mean thermal speed = $\langle |v| \rangle$
l = mean free path
$\hat{C}_V$ = heat capacity per unit volume
ρ_u = thermal energy per unit volume
F_x/A = shear force per unit area
φ = electrostatic potential
$\mathbf{E}$ = electric field intensity
q = electric charge
M = mass of particle
ρ = mass per unit volume
$\mathbf{p}$ = momentum

"Thermal Physics" Ch. Kittel & H. Kroemer

Enskog approximate solution of the Boltzman equation

System assumed to be only slightly disturbed from the Maxwell equilibrium state $f(0)$:

$$f = f(0) + f(1) + f(2) + \ldots$$

Boltzman equation: $F[f] = 0$

$$F[f] = F(0)[f(0)] + F(1)[f(0), f(1)] + F(2)[f(0), f(1), f(2)] + \ldots$$

$F(0)[f(0)] = 0 \rightarrow$ Maxwell distribution

$F(1)[f(0),f(1)] = 0 \rightarrow$ first approximation

$F(2)[f(0),f(1),f(2)] = 0 \rightarrow$ second approximation

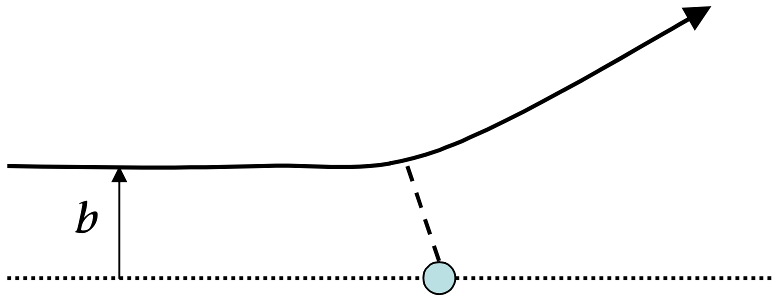
…

Classical vs quantum transport cross-section

The *transport cross-section of order n* is given by the integral

$$\phi^{(n)} = 2\pi \int_{-1}^{+1} d\cos\theta (1-\cos^n\theta) \frac{d\sigma(k,\theta)}{d\Omega}\Big|_{c.m.},$$

Classical case



$\sigma(k,\theta) = \pi b^2$

Quantum case

the orthogonality of the Legendre polynomials P_l

$$q^{(1)} \equiv \frac{\phi^{(1)}}{4\pi a^2} = \frac{2}{x^2} \sum_l{}' (2l+1)\sin^2(\delta_l),$$

$$q^{(2)} \equiv \frac{\phi^{(2)}}{4\pi a^2} = \frac{2}{x^2} \sum_l{}' \frac{(l+1)(l+2)}{(2l+3)} \sin^2(\delta_{l+2}-\delta_l),$$

- a – characteristic length for a potential
- $x = ka$ – dimensionless momentum variable
- l - quantum number for angular momentum
- δ_l – partial wave phase shifts

Statistics and Transport Integrals

$$q^{(n)}_{(s)} = \frac{s+1}{2s+1} q^{(n)}_{Bose} + \frac{s}{2s+1} q^{(n)}_{Fermi}, \quad \text{for integer } s,$$

$$q^{(n)}_{(s)} = \frac{s+1}{2s+1} q^{(n)}_{Fermi} + \frac{s}{2s+1} q^{(n)}_{Bose}, \quad \text{for half-integer } s.$$

$$\omega^{(n,t)}(T) \equiv \int_0^\infty d\gamma \, e^{-\gamma^2} \gamma^{2t+3} q^{(n)}(x),$$

$$\gamma = \frac{\hbar k}{\sqrt{2\mu k_B T}} = \frac{x}{\sqrt{2\pi}} \left(\frac{\lambda(T)}{a} \right).$$

$\lambda(T)$ – thermal De-Brogie wavelength

Diffusion and shear viscosity

$$\tilde{\mathscr{D}} = \frac{3h}{32\sqrt{2}\pi}\frac{1}{ma^3n},$$

$$\frac{[\mathscr{D}]_1}{\tilde{\mathscr{D}}} = \left(\frac{a}{\lambda(T)}\right)\frac{1}{\omega^{(1,1)}(T)},$$

$$\frac{[\mathscr{D}]_2}{[\mathscr{D}]_1} = 1 + \frac{(5\omega^{(1,1)}(T) - 2\omega^{(1,2)}(T))^2}{\omega^{(1,1)}(T)\left(30\omega^{(1,1)}(T) + 4\omega^{(1,3)}(T) + 8\omega^{(2,2)}(T)\right) - 4\left(\omega^{(1,2)}(T)\right)^2},$$

$$\tilde{\eta} = \frac{5h}{32\sqrt{2}\pi}\frac{1}{a^3},$$

$$\frac{[\eta]_1}{\tilde{\eta}} = \left(\frac{a}{\lambda(T)}\right)\frac{1}{\omega^{(2,2)}(T)},$$

$$\frac{[\eta]_2}{[\eta]_1} = 1 + \frac{3(7\omega^{(2,2)}(T) - 2\omega^{(2,3)}(T))^2}{2\left(\omega^{(2,2)}(T)\left(77\omega^{(2,2)}(T) + 6\omega^{(2,4)}(T)\right) - 6\left(\omega^{(2,3)}(T)\right)^2\right)},$$

Thermal conductivity

$$[\lambda_T]_1 = \frac{5}{2}[\eta]_1 \left(\frac{c_v(n,T)}{m}\right),$$

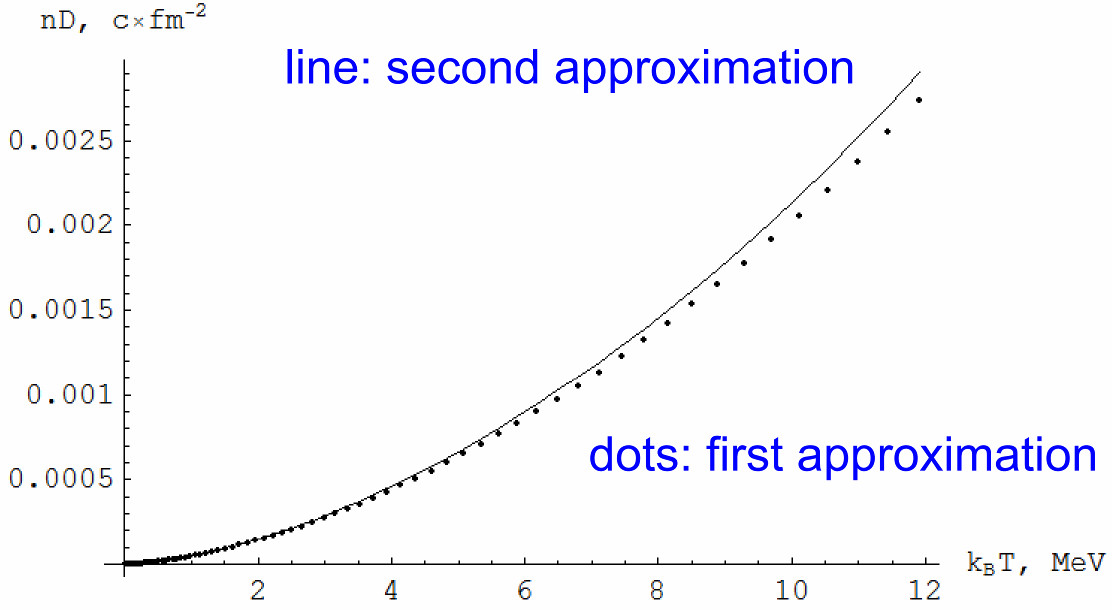
$$\tilde{\lambda}_T = \frac{25h}{64\sqrt{2}\pi}\frac{\tilde{c}_v(n)}{a^3 m},$$

$$\frac{[\lambda_T]_1}{\tilde{\lambda}_T} = \frac{c_v(n,T)}{\tilde{c}_v(n)}\left(\frac{a}{\lambda(T)}\right)\frac{1}{\omega^{(2,2)}(T)},$$

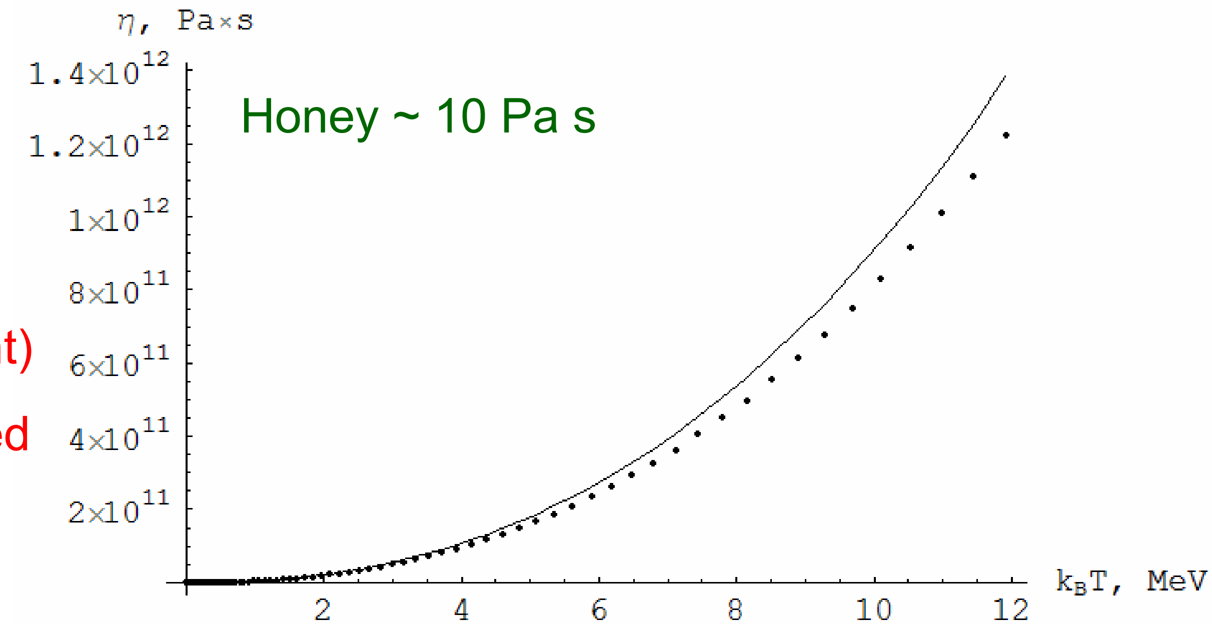
$$\frac{[\lambda_T]_2}{[\lambda_T]_1} = 1 + \frac{(7\omega^{(2,2)}(T) - 2\omega^{(2,3)}(T))^2}{4\left(\omega^{(2,2)}(T)\,(7\omega^{(2,2)}(T) + \omega^{(2,4)}(T)) - (\omega^{(2,3)}(T))^2\right)},$$

In order to calculate thermal conductivity one needs to invoke the virial expansion or other means to find specific heat capacity c_v

Results for C^{12} with $V(R)\rightarrow \exp[-R/a]/R$

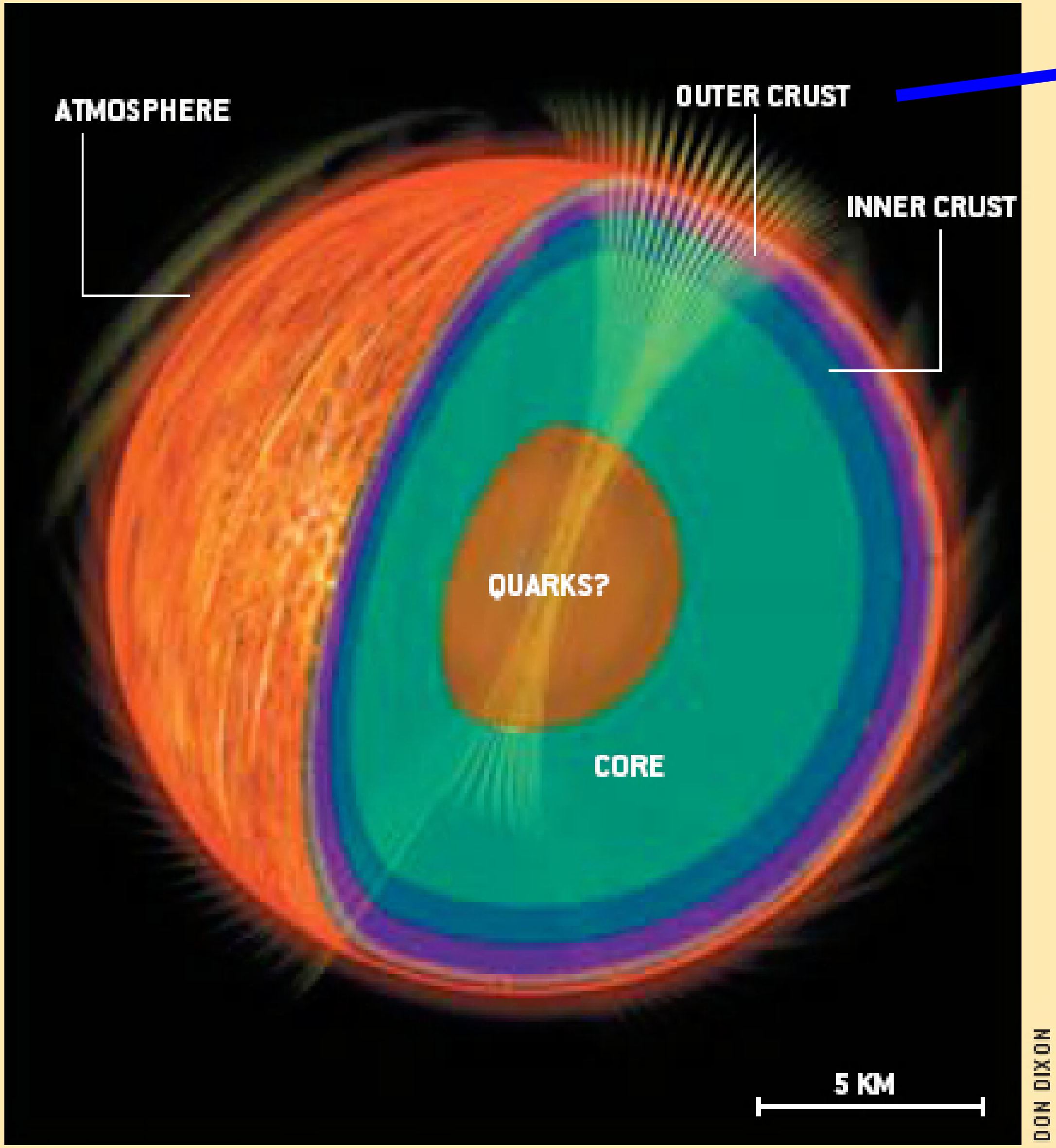


- "Low" temperatures
- Dilution parameter: $n\,a^3 < 1$
- Density independence
- Large number of partial waves



Ongoing work:

- Compare classical with quantum results
- Mixtures (multiple component)
- Study effects of magnetic filed
- + the virial gives η/s (T)



STRUCTURE OF A NEUTRON STAR can be inferred from theories of nuclear matter. Starquakes can occur in the crust, a lattice of atomic nuclei and electrons. The core consists mainly of neutrons and perhaps quarks. An atmosphere of hot plasma might extend a grand total of a few centimeters.

- Diffusion:
  - element segregation
- Viscosity:
  - rotation
  - seismic modes
- Thermal conductivity
  - cooling
  - temperature map

Classical molecular-dynamical simulations (Horowitz & Caballero) are to be compared with the Enskog approach for a dilute system with quantum and classical collision cross-sections, allowing a check of the low density regime of the system.

…to be continued

köszönöm תודה! děkuji

mahalo 고맙습니다

thank you

merci 谢谢 danke

Спасибо

Ευχαριστώ شكرا

どうもありがとう gracias