Transport properties of a non-relativistic dilute Yukawa liquid

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Content

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

\[ \langle \Phi_{\text{red}} \rangle = D \frac{d n_{\text{red}}}{dz} \]

Shear viscosity

\[ \frac{F}{A} = \eta \frac{du}{dy} \]

Random walk of drunk sailor

Average displacement

Effective dragging force

Effective pushing force

Classic Newtonian laminar flow
Boltzman equation for the particle distribution function: \( f \) (phase space)

**Equations of motion \( \rightarrow \) time evolution \( \rightarrow \) operator \( \mathcal{D} \)**

\[ \mathcal{D} f = 0 : \text{Liouville equation (no collisions)} \]

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

\[ \mathcal{D} f = C(f, f) : \text{Boltzman equation (binary collisions only)} \]
Equation of change for property $\phi$

$$\int \phi \, Df \, dv = n \langle \Delta \phi \rangle$$

$$\langle \Delta \phi \rangle = n^{-1} \int \phi \, C(f_{1}f) \, dv$$

**Table 14.2 Summary of phenomenological transport laws**

<table>
<thead>
<tr>
<th>Effect</th>
<th>Flux of particle property $\phi$</th>
<th>Gradient</th>
<th>Coefficient</th>
<th>Law</th>
<th>Name of law</th>
<th>Approximate expression for coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion</td>
<td>Number</td>
<td>$\frac{dn}{dz}$</td>
<td>Diffusivity $D$</td>
<td>$J_n = -D \text{ grad } n$</td>
<td>Fick’s law</td>
<td>$D = \frac{1}{2} \bar{c} l$</td>
</tr>
<tr>
<td>Viscosity</td>
<td>Transverse momentum</td>
<td>$M \frac{dv_x}{dz}$</td>
<td>Viscosity $\eta$</td>
<td>$\frac{F_x}{A} = J_{p} = -\eta \frac{dv_x}{dz}$</td>
<td>Newtonian viscosity</td>
<td>$\eta = \frac{1}{3} \rho \bar{c} l$</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>Energy</td>
<td>$\frac{d\rho_u}{dz} = \bar{C}_v \frac{dT}{dz}$</td>
<td>Thermal conductivity $K$</td>
<td>$J_{u} = -K \text{ grad } \tau$</td>
<td>Fourier’s law</td>
<td>$K = \frac{1}{2} \bar{C}_v \bar{c} l$</td>
</tr>
<tr>
<td>Electrical conductivity</td>
<td>Charge</td>
<td>$-\frac{d\phi}{dz} = E_z$</td>
<td>Conductivity $\sigma$</td>
<td>$J_q = \sigma E$</td>
<td>Ohm’s law</td>
<td>$\sigma = \frac{nq^2 l}{Mc}$</td>
</tr>
</tbody>
</table>

**Symbols:**
- $n$ = number of particles per unit volume
- $\bar{c}$ = mean thermal speed = $\langle \bar{v} \rangle$
- $l$ = mean free path
- $\bar{C}_v$ = heat capacity per unit volume
- $\rho_u$ = thermal energy per unit volume
- $F_x/A$ = shear force per unit area
- $\phi$ = electrostatic potential
- $E$ = electric field intensity
- $q$ = electric charge
- $M$ = mass of particle
- $\rho$ = mass per unit volume
- $p$ = momentum

“Thermal Physics” Ch. Kittel & H. Kroemer
Enskog approximate solution of the Boltzmann equation

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

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

Boltzmann 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

\[ \ldots \]
Classical vs quantum transport cross-section

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

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

**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
- $\delta_l$ – partial wave phase shifts
Statistics and Transport Integrals

\[
q_{(s)}^{(n)} = \frac{s+1}{2s+1} q_{\text{Bose}}^{(n)} + \frac{s}{2s+1} q_{\text{Fermi}}^{(n)}, \quad \text{for integer } s,
\]

\[
q_{(s)}^{(n)} = \frac{s+1}{2s+1} q_{\text{Fermi}}^{(n)} + \frac{s}{2s+1} q_{\text{Bose}}^{(n)}, \quad \text{for half-integer } s.
\]

\[
\omega^{(n,t)}(T) \equiv \int_{0}^{\infty} d\gamma \, e^{-\gamma^2} \gamma^{2t+3} q^{(n)}(x),
\]

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

\(\lambda(T)\) – thermal De-Broglie wavelength
Diffusion and shear viscosity

$$\tilde{\mathcal{D}} = \frac{3h}{32\sqrt{2\pi m}} \frac{1}{a^3 n},$$

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

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

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

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

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

Honey $\sim 10$ Pa s
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
Спасибо
thank you
mercì 谢谢 danke
Ευχαριστώ شكرا
どうもありがとうございます gracias