Mach cones in dusty plasmas: analytical models vs. computer simulation

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## OUTLINE

Introduction to Dusty Plasma Physics Structures and Waves in Dust Layers Mach Cones in Dust Layers Excited by: moving laser & external particle Experiment, analytical models & simulation > Polarization Forces on External Particle Details of Modeling and Simulation

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## What is a dusty plasma?



- + small particle of solid matter
  - absorbs electrons and ions
  - becomes negatively charged
  - Debye shielding



## **Dust Charging Processes**

> electron and ion collection
> secondary emission
> UV induced photoelectron emission



$$\Sigma I = I_e + I_i + I_{sec} + I_{pe} = 0$$

#### The Charge on a Dust Grain

In typical lab plasmas  $I_{sec} = I_{pe} = 0$ 

Electron thermal speed >> ion thermal speed so the grains charge to a negative potential  $V_s$  relative to the plasma, until the condition  $I_{e} = I_{i}$  is achieved.



#### Assembly of highly charged dust particles immersed in a partially ionized plasma



Yukawa potential

#### Where are Dusty Plasmas?

#### In Nature

In man-made facilities

In research laboratory

#### Examples of Dusty Plasmas in Nature





## Safety issues for fusion !



#### Dust:

- activated
- retains tritium
- ITER safety limit: 350 kg Tungsten dust

#### Fire & chemical explosion



#### Hydrogen:

- stored in dust
- released during accidental exposure to:
  - air
  - steam
- ITER safety limit: 6 kg dust allowed on hot surfaces

Phil Sharpe Fusion Safety Program, Idaho National Laboratory

Dust in Fusion Plasmas Workshop 2005

#### Semiconductor Manufacturing



silane  $(SiH_4) + Ar + O_2 \rightarrow SiO_2$  particles

**Credit: Merlino** 

#### Number of publications on Dusty Plasma



# Voyager's images of radial spokes rotating around Saturn's B ring



13

## Discovery by Selwyn at IBM in 1989 during plasma etching of Si wafer



#### Silicon wafer

#### Lower electrode

Dust grain ~20µm

## Schematics of Selwyn's experiment



## Schematics of Selwyn's experiment



#### Levitation of dust particles in plasma sheath



#### Levitation of dust particles in plasma sheath



Power off

#### Examples of dust in laboratory

Grown spontaneously during gas discharge



Purchased from a vendor

#### **Typical laboratory parameters**

- Discharge conditions. gas: Ar, power:~10 W, pressure: 1~X00 Pa, frequency ~10 MHz
- Plasma density: 10<sup>8</sup>~10<sup>9</sup> cm<sup>-3</sup>
- > Electron temperature: 1~5 eV
- > Size of dust particle: ~1-10 μm
- Inter-particle distance: ~ 0.1-1 mm
- Dust charge (negative) : 10<sup>3</sup>~10<sup>4</sup> e
- Mass of dust particle: ~ 10<sup>-10</sup> g

## Why study Dusty Plasma?

#### Solar system

- Rings of Saturn
- Comet tails



#### Manufacturing

- Particle contamination (Si wafer processing)
- Nanomaterial synthesis

#### **Basic physics**

- Coulomb (plasma) crystals
- Waves





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#### "Discovery" of Plasma Crystals

- Thomas, Morfill, Demmel and Goree et al., Phys. Rev. Lett. 73, 652 (1994).
- > Chu and Lin, Phys. Rev. Lett. 72, 4009 (1994).
- Hayashi and Tachibana, Jpn. J. Appl. Phys. 33, L804 (1994).
- Melzer, Trottenberg and Piel, Phys. Lett., A 191, 301 (1994).

#### Observations of 3D plasma crystals Experimental snapshots



200µm

•:1st layer O:2nd layer O:3rd layer

24

#### Three states of 2D plasma crystal

Experimental movie of 2D plasma crystal in solid, liquid and gas states





#### From Complex Plasma Laboratory of Sydney

# Excitation of waves in 2D dust crystal: experimental scheme



#### Sinusoidally excited longitudinal wave



Nunomura et al. Phys. Rev. E 2002

#### Wave processes in dust layers

Dust Acoustic Wave Experiment

J. B. Pieper and J. Goree 26 February 1996

gas pressure: 100 mtorr (Kr) frequency: 1.0 Hz frame time: 1/30 sec

1 mm

#### Wave processes in dust layers

Dust Acoustic Wave Experiment

J. B. Pieper and J. Goree 26 February 1996

gas pressure: 100 mtorr (Kr) frequency: 3.0 Hz frame time: 1/30 sec

1 mm

#### Phonon spectrum



Nunomura et al. PRL 2002



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#### Mach cones



Mach cone angle



cone

Supersonic disturbance

Acoustic wavefronts

# Ship's wake



#### Mach cones in dusty plasmas

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#### Havnes 1995

Existence predicted theoretically, for Saturn's rings

#### Samsonov 1999

Discovered experimentally in lab, by external charged particle Melzer & Nunomura 2000

Excitation of Mach cones in lab, by moving laser spot
## Wake pattern determined by dispersion relation



Has both features:

- Mach Cone
- Lateral & transverse wakes



Mach cone



#### Lateral & transverse wakes

Credit: Goree

### Mach cone by moving laser spot: experimental scheme



#### Mach cone excitation by laser spot



4mm

*M*=*V*/*C*<sub>*L*</sub> = 1.29 Nosenko *et al.* PRL 2002

#### Mach cone in 2D Dusty Plasma

**Experimental video** 



A. Melzer, S. Nunomura, D. Samsonov, Z. W. Ma, and J. Goree, Phys. Rev. E 62, 4162 (2000)

# Mach cone by moving external charged particle: experiment



Samsonov, et al., Phys. Rev. Lett. 83, 3649 (1999)

#### **Experimental snapshots**



#### Samsonov, et al., Phys. Rev. Lett. 83, 3649 (1999)

# Mach cone excited by external charge: experimental velocity field

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#### **Problem definition**



#### Physical model: 2D Yukawa system

- Electrons and ions provide Debye screening
- Neutral particles provide damping and determine the system temperature
- Dust particles undergo Brownian motion and interact with each other via Yukawa potential

#### Physical model: 2D Yukawa system

 $\kappa = a / \lambda_D$ Screening parameter $\Gamma = \frac{Q^2 / a}{k_B T}$ Interparticle coupling coefficient $\gamma$ Damping coefficient

#### Typically $\Gamma \gg 1 \rightarrow$ strongly coupled system

Experimental support: Konopka, Morfill, and Ratke, Phys. Rev. Lett. 84, 891 (2000) Hebner, Riley, Johnson, Ho, and Buss, Phys. Rev. Lett. 87, 235001 (2001).

#### **Problem definition**

- Perturbation of the dust layer
  - Polarization
  - Mach cone excitation
- Induced forces acting on test particle
  - Stopping force
  - Image force
  - Transverse forces

#### Analytical models

 Random-Phase-Approximation (RPA)
Quasi-Localized Charge Approximation (QLCA)

• Kalman and Golden, PRA 41, 5516 (1990)

Computer simulation
Brownian Dynamics (BD)

#### Induced dust density: QLCA vs. RPA



### Algorithms for BD simulation

#### > Euler-like

• Ermak, J. Chem. Phys. 62, 4189 (1975)

#### > Beeman-like:

• Allen, Mol. Phys., 66, 3039 (1980)

#### > Verlet-like

- Van Gunsteren and Berendsen, Mol. Phys. 45, 637 (1982)
- > Gear-Like Predictor-Corrector
  - Hou, Miskovic and Wang, in preparation

#### Simulations provide information on:

- > Equilibrium states
  - Crystal structures (radial distribution function)
  - Phonon spectra
  - Time-correlations
- Non-Equilibrium interactions
  - Excited Mach Waves in the plane
  - Forces on the test particle(s)

#### Test: energy conservation



#### **Test: velocity distribution**

Liquid state with  $\Gamma = 360$  and  $\kappa = 2$ 





 $\kappa = 1$ 

#### Statics: radial distribution function



#### A double check: static structure

**Comparison with previous MD simulation** 



MD data from: Kalman et al., PRL 92, 065001 (2004)

### Dynamics: phonon energy spectra



# Mach cone excited by external charge: experimental velocity field

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# Mach cone excited by external charge: BD simulation



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### Forces on the moving particle



#### Induced potential (hydrodynamic model)



#### Stopping force on the moving particle



### Position dependent stopping force from BD sim.



## Evaluating the mean stopping force from the cumulative force



Mean stopping force











#### Variance of stopping force


# Probability distribution of stopping force - straggling



Bars : direct measurements of simulation data red lines: Gaussian distributions with the above-calculated means and variances.

### BD sim. of the image force



### **Total perpendicular force**



## Repulsive (unperturbed) force



### Image force: h=2.0





### Image force: h=0.5



### Image force: h=0.2



Projectile-target coupling strength  $\Theta(h, r, v) = \frac{V_{td}}{V_{dd} + m_d v^2 / 2}$  $\max\{V_{td}\} = \frac{|Q_t Q_d|}{h} \exp(-\frac{h}{\lambda_p})$  $V_{dd} = \frac{Q_d^2}{a} \exp(-\kappa)$ 

> **Θ « 1 criterion for validity of linear theory (QLCA & RPA)**

### Conclusions

Strong-coupling effects described well by QLCA but RPA fails except at high speeds

Non-linear effects in the projectile-target interactions not described by QLCA & RPA



# Experimental vicinage effect





### Experimental vicinage effect



Experimental image by Nosenko et al.

Produced by *two* laser spots moving parallel to each other over dust layer

Credit: Nosenko et al.

### **Test of Linear Superposition**

+



### **Experimental image 1**



### Experimental image 2



Synthesized

### **Test of Linear Superposition**





#### Experimental image

#### Synthesized image

Agreement  $\Rightarrow$  linear superposition is true

## BD sim. of transversal forces











# Thanks for

# your attention!

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# Analytical models of dust layer response

> Hydrodynamic model, gives the RPA dielectric function

Dielectric response theory using QLCA

# Hydrodynamic model

$$\begin{split} \frac{\partial \sigma_{\rm d}(\mathbf{r},t)}{\partial t} + \nabla_{\parallel} \cdot \left[\sigma_{\rm d}(\mathbf{r},t)\mathbf{u}_{\rm d}(\mathbf{r},t)\right] &= 0, \end{split} \begin{array}{l} \text{Correlation effects} \\ \frac{\partial \mathbf{u}_{\rm d}(\mathbf{r},t)}{\partial t} + \mathbf{u}_{\rm d}(\mathbf{r},t) \cdot \nabla_{\parallel} \mathbf{u}_{\rm d}(\mathbf{r},t) &= \frac{eZ_{\rm d}}{m_{\rm d}} \nabla_{\parallel} \Phi(\mathbf{R},t) \Big|_{z=0} + \frac{\mathbf{F}_{int}}{m_{\rm d}} \\ &+ \frac{eZ_{\rm d}}{m_{\rm d}c} \left[\mathbf{u}_{\rm d}(\mathbf{r},t)\mathbf{B}_{0}\right] + \frac{\mathbf{F}_{\rm ext}}{m_{\rm d}} - \gamma \mathbf{u}_{\rm d}(\mathbf{r},t), \\ \nabla^{2} \Phi(\mathbf{R},t) &= -4\pi e \left[n_{\rm i}(\mathbf{R},t) - n_{\rm e}(\mathbf{R},t) - Z_{\rm d}\sigma_{\rm d}(\mathbf{r},t)\delta(z)\right], \end{split}$$

$$n_{\rm e} = n_0 \exp(e\Phi/k_{\rm B}T_{\rm e}), n_{\rm i} = n_0 \exp\left(-e\Phi/k_{\rm B}T_{\rm i}\right)$$

Linearization:  $\Phi(\mathbf{R}, t) = \Phi_0(z) + \Phi_1(\mathbf{R}, t)$ , etc.

# Response of the dust layer $\Phi_{\text{ind}}(\mathbf{K}, \omega) = \begin{bmatrix} 1 \\ \varepsilon_L(\mathbf{k}, \omega) \end{bmatrix} \Phi_{\text{ext}}(\mathbf{K}, \omega)$

$$\Phi_{\text{ext}}(\mathbf{r}, z, t) = \frac{Q_t Q_d}{\sqrt{(\mathbf{r} - \mathbf{v}t)^2 + (z - h)^2}} e^{\left(-\kappa\sqrt{(\mathbf{r} - \mathbf{v}t)^2 + (z - h)^2}\right)}$$

 $\mathbf{k} = \{k_x, k_y\}$  $\mathbf{K} = \{k_x, k_y, k_z\}$ 

### Dielectric function of the system

$$\varepsilon_{L}(\mathbf{k},\omega) = 1 - \frac{\omega_{0}^{2}(\mathbf{k})}{\omega^{2} - (\sigma_{d0} / m_{d})G(\mathbf{k},\omega)}$$

$$\omega_0^2(\mathbf{k}) = \frac{\omega_{pd}^2 (k\lambda_D)^2}{\sqrt{1 + (k\lambda_D)^2}}$$

$$p_{pd}^2 = \frac{2\pi Q_d^2 \sigma_{d0}}{m_d \lambda_D}$$

 $G(\mathbf{k},\omega) = \begin{cases} 0 & \text{RPA} \\ D_L(\mathbf{k}) & \text{QLCA} \end{cases}$ 

### Formulae

$$\Phi_{\text{ind}}(\mathbf{r}, z, t) = \frac{1}{(2\pi)^4} \int d^3 \mathbf{K} d\omega \Phi_{\text{ind}}(\mathbf{K}, \omega) e^{i\mathbf{K}\cdot\mathbf{R}-i\omega t}$$

$$F_{st}(v) = Q_t \frac{\partial \Phi_{ind}(\mathbf{r}, z, t)}{\partial x}\Big|_{z=h, \mathbf{r}=\mathbf{v}t}$$

### Stopping force (power)

$$F_{im}(v) = Q_t \frac{\partial \Phi_{ind}(\mathbf{r}, z, t)}{\partial z}\Big|_{z=h, \mathbf{r}=\mathbf{v}}$$

**Image force** 

## Quasi-Localized Charge Approxim.

$$\zeta_j(t)$$

$$\sigma_{d1}(\mathbf{r},t) = \sum_{j=1}^{N_d} \left\langle \rho(\mathbf{r}_j + \boldsymbol{\zeta}_j(t)) - \rho(\mathbf{r}_j) \right\rangle, \quad \mathbf{u}_{d1}(\mathbf{r},t) = \sum_{j=1}^{N_d} \left\langle \frac{d\boldsymbol{\zeta}_j(t)}{dt} \right\rangle,$$

$$-\omega^{2}\zeta_{\mathbf{k}}(\omega) = -\left[\mathbf{D}(\mathbf{k}) + \frac{\sigma_{d0}\phi(k)}{m_{d}}\mathbf{k}\mathbf{k}\right]:\zeta_{\mathbf{k}}(\omega) + i\gamma\omega\zeta_{\mathbf{k}}(\omega) + \frac{\sigma_{d0}}{(m_{d}N_{d})^{1/2}}\mathbf{F}_{ext}(\mathbf{k},\omega),$$

$$D_L(k) = \frac{\omega_{pd}^2 \lambda_D^2}{2} \int_0^\infty dr \frac{g(r) - 1}{r^2} \exp\left(-\frac{r}{\lambda_D}\right) \left[ \left(1 + \frac{r}{\lambda_D} + \frac{r^2}{\lambda_D^2}\right) - \left(4 + \frac{4r}{\lambda_D} + \frac{2r^2}{\lambda_D^2}\right) J_0(kr) + \left(6 + \frac{6r}{\lambda_D} + \frac{2r^2}{\lambda_D^2}\right) \frac{J_1(kr)}{kr} \right],$$

## Induced dust density: QLCA vs. RPA



Mean stopping force



## **Brownian Dynamics simulation**



### **BD** simulation

Based on Langevin equation



# Algorithms for BD simulation

### > Euler-like

• Ermak, J. Chem. Phys. 62, 4189 (1975)

### > Beeman-like:

• Allen, Mol. Phys., 66, 3039 (1980)

### > Verlet-like

- Van Gunsteren and Berendsen, Mol. Phys. 45, 637 (1982)
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### Euler-like method

$$\mathbf{v}(t) = \mathbf{v}_0 e^{-\gamma t} + \frac{t}{m} \mathbf{F}_0 \frac{1 - e^{-\gamma t}}{\gamma t} + \mathbf{R}_{\mathbf{v}}(t),$$
  
$$\mathbf{r}(t) = \mathbf{r}_0 + t \mathbf{v}_0 \frac{1 - e^{-\gamma t}}{\gamma t} + \frac{t^2 \mathbf{F}_0}{m \gamma t} \left[ 1 - \frac{1 - e^{-\gamma t}}{\gamma t} \right] + \mathbf{R}_{\mathbf{r}}(t),$$

$$\mathbf{R}_{\mathbf{v}}(t) = \sqrt{\frac{k_B T}{m}} (1 - e^{-\gamma t}) \mathbf{N}_{\mathbf{v}}(0, 1);$$
  
$$\mathbf{R}_{\mathbf{r}}(t) = \sqrt{\frac{2k_B T}{m}} [1 - 2\frac{1 - e^{-\gamma t}}{\gamma t} + \frac{1 - e^{-2\gamma t}}{2\gamma t}] \mathbf{N}_{\mathbf{r}}(0, 1)$$

### **Euler-like method**

 $\mathbf{F}_0 = \mathbf{F}(0)$  is a constant

Euler-like method: when  $\gamma \rightarrow 0$  it recovers the Euler method

 $\mathbf{r}(t) = \mathbf{a}_{0} + a_{1}\mathbf{N}_{1}(0,1)$   $\mathbf{v}(t) = \mathbf{b}_{0} + b_{1}\mathbf{N}_{1}(0,1) + b_{2}\mathbf{N}_{2}(0,1),$   $\mathbf{a}_{0} = \text{mean}\{\mathbf{r}\}; \qquad \mathbf{a}_{1}^{2} = \text{var}\{\mathbf{r}\};$  $\mathbf{b}_{0} = \text{mean}\{\mathbf{v}\}; \qquad \mathbf{b}_{1}^{2} = \frac{\text{cov}\{\mathbf{v},\mathbf{r}\}}{\sqrt{\text{var}\{\mathbf{r}\}}}; \qquad \mathbf{b}_{2}^{2} = \text{var}\{\mathbf{v}\} - \mathbf{a}_{1}^{2}$
#### **Beeman-like method**

 $\mathbf{F} \approx \mathbf{F}(0) + \mathbf{F}'(0)t \qquad \mathbf{F}'(0) \approx \left[\mathbf{F}(0) - \mathbf{F}(-t)\right]/t$ 

 $\mathbf{r}(t) = \mathbf{a}_0 + a_1 \mathbf{N}_{\mathbf{v}}(0, 1)$  $\mathbf{v}(t) = \mathbf{b}_0 + b_1 \mathbf{N}_{\mathbf{v}}(0, 1) + b_2 \mathbf{N}_{\mathbf{r}}(0, 1),$ 

$$\mathbf{a}_{0} = \operatorname{mean}\{\mathbf{r}\} = \mathbf{r}_{0} + c_{a}t\mathbf{v}_{0} + c_{b}t^{2}\frac{\mathbf{F}(0)}{m} + c_{c}t^{2}\frac{\mathbf{F}(-t)}{m},$$
  
$$\mathbf{b}_{0} = \operatorname{mean}\{\mathbf{v}\} = c_{d}\mathbf{v}_{0} + c_{e}t\frac{\mathbf{F}(t)}{m} + c_{f}t\frac{\mathbf{F}(0)}{m} + c_{g}t\frac{\mathbf{F}(-t)}{m},$$

### **Beeman-like method**

when  $\gamma \rightarrow 0$  it recovers the Beeman method

$$\begin{split} c_{a} &= c_{1}, \qquad c_{d} = c_{0}, \qquad c_{0} = e^{-\gamma t} \\ c_{b} &= c_{2} + c_{3}, \qquad c_{e} = c_{2} - c_{0}c_{3}/c_{1}, \qquad c_{1} = (1 - c_{0})/\gamma t \\ c_{c} &= -c_{3}, \qquad c_{f} = c_{1} - c_{2} + 2c_{0}c_{3}/c_{1}, \qquad c_{2} = (1 - c_{1})/\gamma t \\ c_{g} &= -c_{0}c_{3}/c_{1}, \qquad c_{3} = (1/2 - c_{2})/\gamma t \end{split}$$

# Boundary and initial conditions

Boundary conditions

 Periodic boundary with a force cutoff

Initial conditions

 Random positions and velocities, or
 Previous results

Particle number: N=1000~2000

# Going beyond Yukawa inter-dust interaction potential

Dust particles immersed in plasma sheath with ion flow and non-homogeneous distribution of electron & ion density, and electric field

# Ion wake: vertical alignment of dust particles in plasma sheath



# Ion wake and inter-dust interactions



Equipotential curves from PIC simulation by Lampe et al<sub>4</sub>

# Ion wake and inter-dust interactions



Equipotential curves from PIC simulation by Lampe et als

# Ion wake and inter-dust interactions







#### Wake riding effect for two particles in sheath



# Effects of sheath on ion wake



## Hydrodynamic model for ions

 $\boldsymbol{\nabla} \cdot [n_i(\mathbf{r})\mathbf{u}_i(\mathbf{r})] = 0$ 

$$\mathbf{u}_i(\mathbf{r}) \cdot \boldsymbol{\nabla} \mathbf{u}_i(\mathbf{r}) = -\frac{Z_i e}{m_i} \boldsymbol{\nabla} \Phi(\mathbf{r}) - \nu \mathbf{u}_i(\mathbf{r})$$

$$\nabla^{2}\Phi(\mathbf{r}) = -4\pi [en_{i}(\mathbf{r}) - en_{e}(\mathbf{r}) - Q_{d}\delta(\mathbf{r} - \mathbf{r}_{d})]$$

#### Linearize about sheath values for:

$$n_{i0}(z), u_{i0}(z), n_{e0}(z), \mathbf{E}_0(z)$$

## Effects of sheath on ion wake



Inhomogeneous sheath

Homogeneous plasma

# Thanks for

# your attention!