Molecular dynamics simulations of strongly coupled plasmas

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7 January 2011

Max Planck Institute for the Physics of Complex Systems

Molecular dynamics simulations of strongly coupled plasmas

Results obtained in collaboration with:

- G. J. Kalman - Boston College, USA
- P. Hartmann - RISSP Budapest, Hungary
- K. Kutasi - RISSP Budapest, Hungary
- K. I. Golden - University of Vermont, USA
- J. Goree - University of Iowa, USA
- M. Rosenberg - UCSD, USA
- S. Kyrkos - Boston College / Le Moyne College, USA
- M. Bonitz, T. Ott - Christian Albrechts University, Kiel, Germany
- P. Bakshi - Boston College, USA

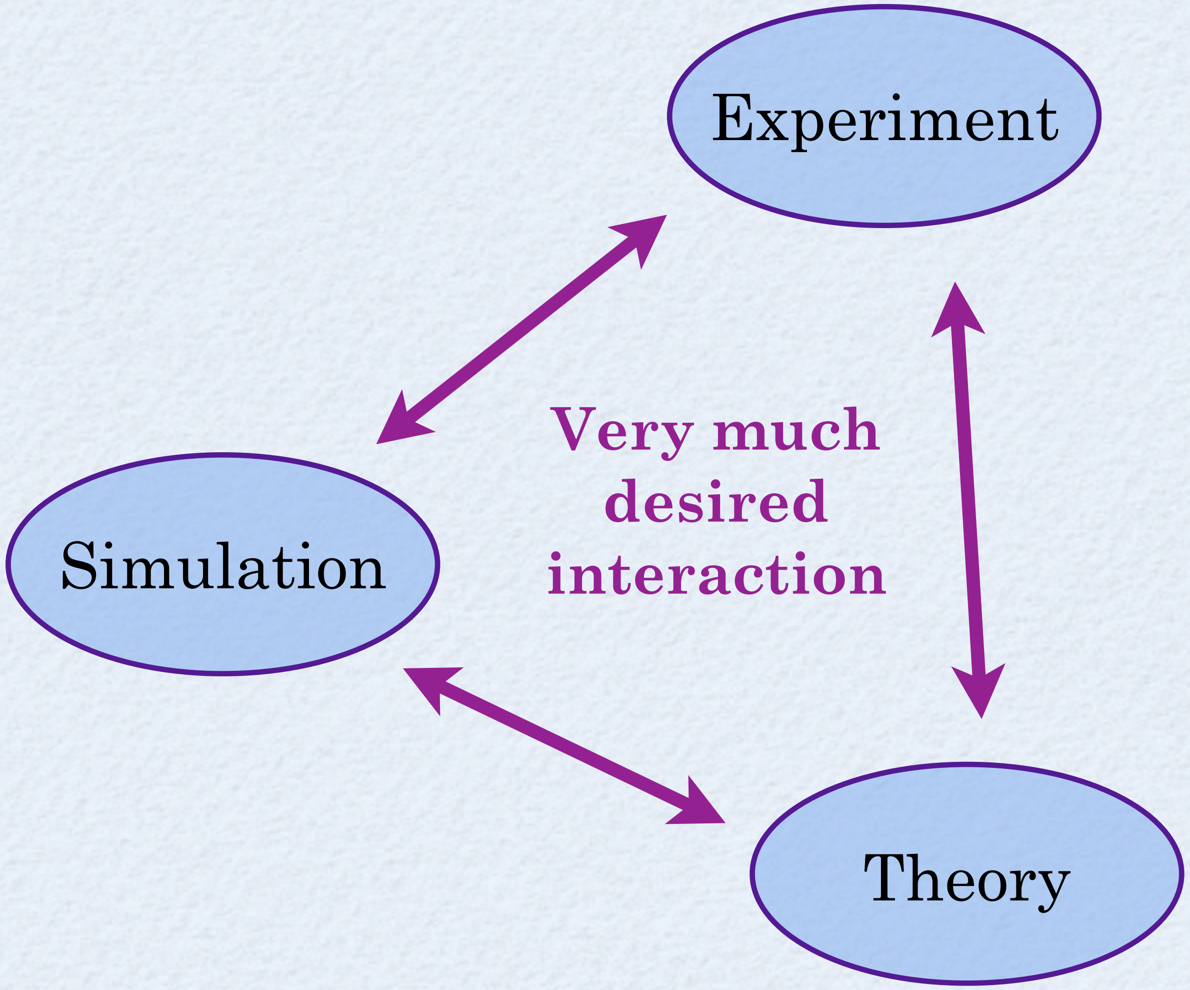
Supported by:

- NSF / MTA (HU Academy of Sciences) / OTKA (HU Sci. Research Fund)

Outline

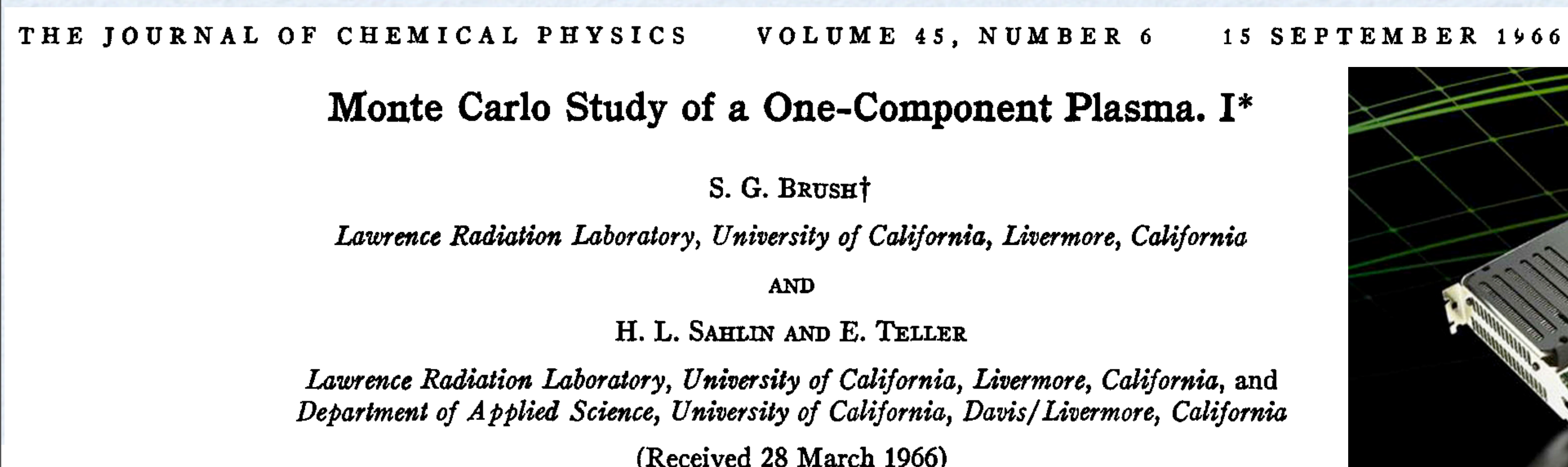
- Why do we need simulations?
- Systems of interest
- Basics of Molecular Dynamics (MD) simulations
- What do we learn from MD?
- Structural & thermodynamical properties
- Localization and transport
- Collective excitations

Why do we need simulations?



- *Simulations are useful*
  - for checking theoretical results
  - for cases where no theoretical results are available
  - for understanding experimental observations
- *Simulations allow:*
  - identification of important processes
  - visualization of the system
- *Most dramatic advance of resources is experienced in the field of simulations*

Dramatic advance of resources


THE JOURNAL OF CHEMICAL PHYSICS VOLUME 45, NUMBER 6 15 SEPTEMBER 1966

Monte Carlo Study of a One-Component Plasma. I*

S. G. Brush†

Lawrence Radiation Laboratory, University of California, Livermore, California

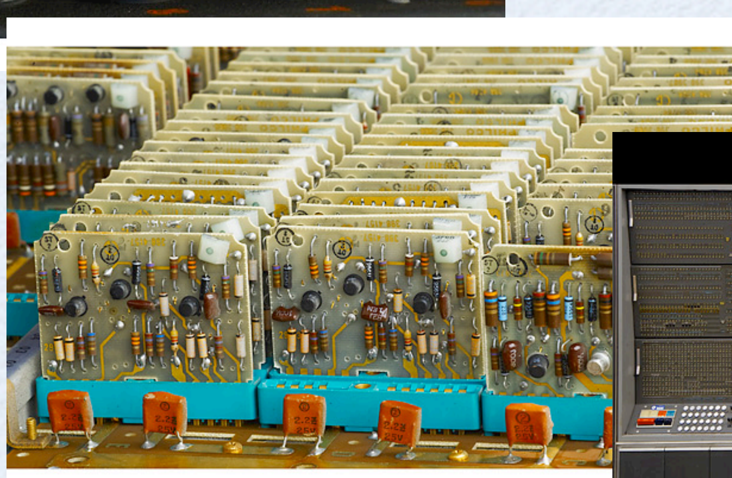
AND

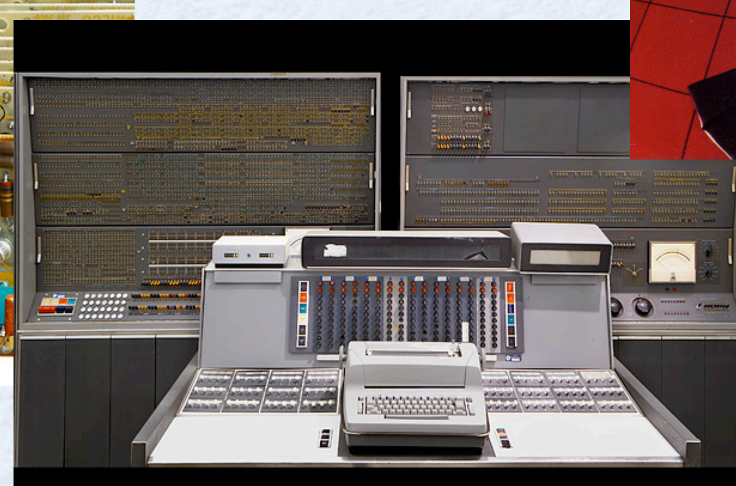
H. L. Sahlin and E. Teller

Lawrence Radiation Laboratory, University of California, Livermore, California, and
Department of Applied Science, University of California, Davis/Livermore, California

(Received 28 March 1966)

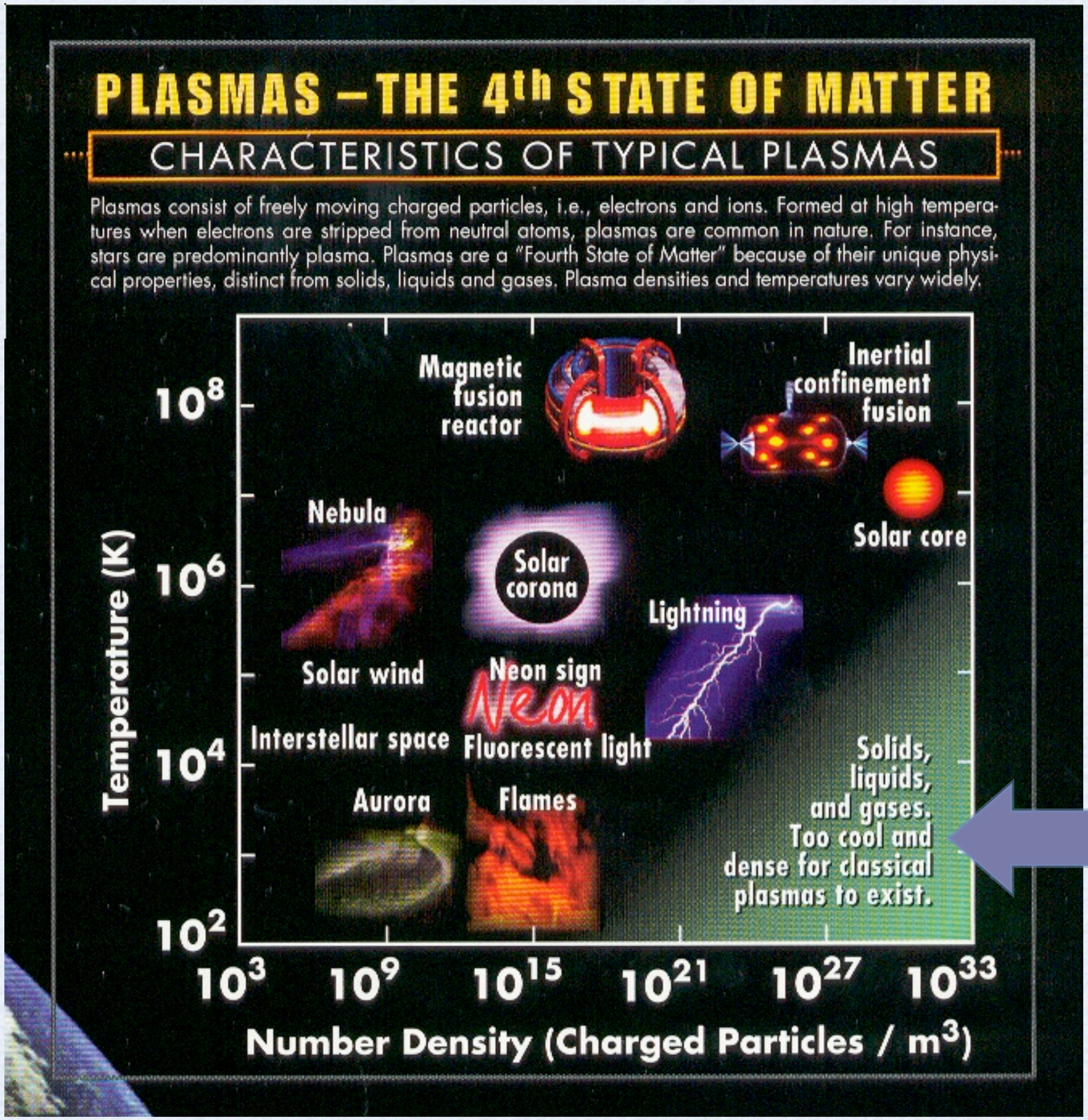
been made of a plasma of heavy ions immersed in a uniform neutralizing back-
from 32 to 500 particles, with periodic boundary conditions, were used. The
ented in terms of a dimensionless parameter $\Gamma=(4\pi n/3)^{\frac{1}{3}}[(Ze)^2/kT]$, where
per cubic centimeter), T is the temperature (degrees K
ronic charge, and Z is the atomic number. Thermody
ere obtained for values of Γ ranging from 0.05 to 100
(MC) method.





Pioneering MD simulations in the 1970s-80s
(OCP, BIM, statics, dynamics, transport, etc.)

Systems of interest

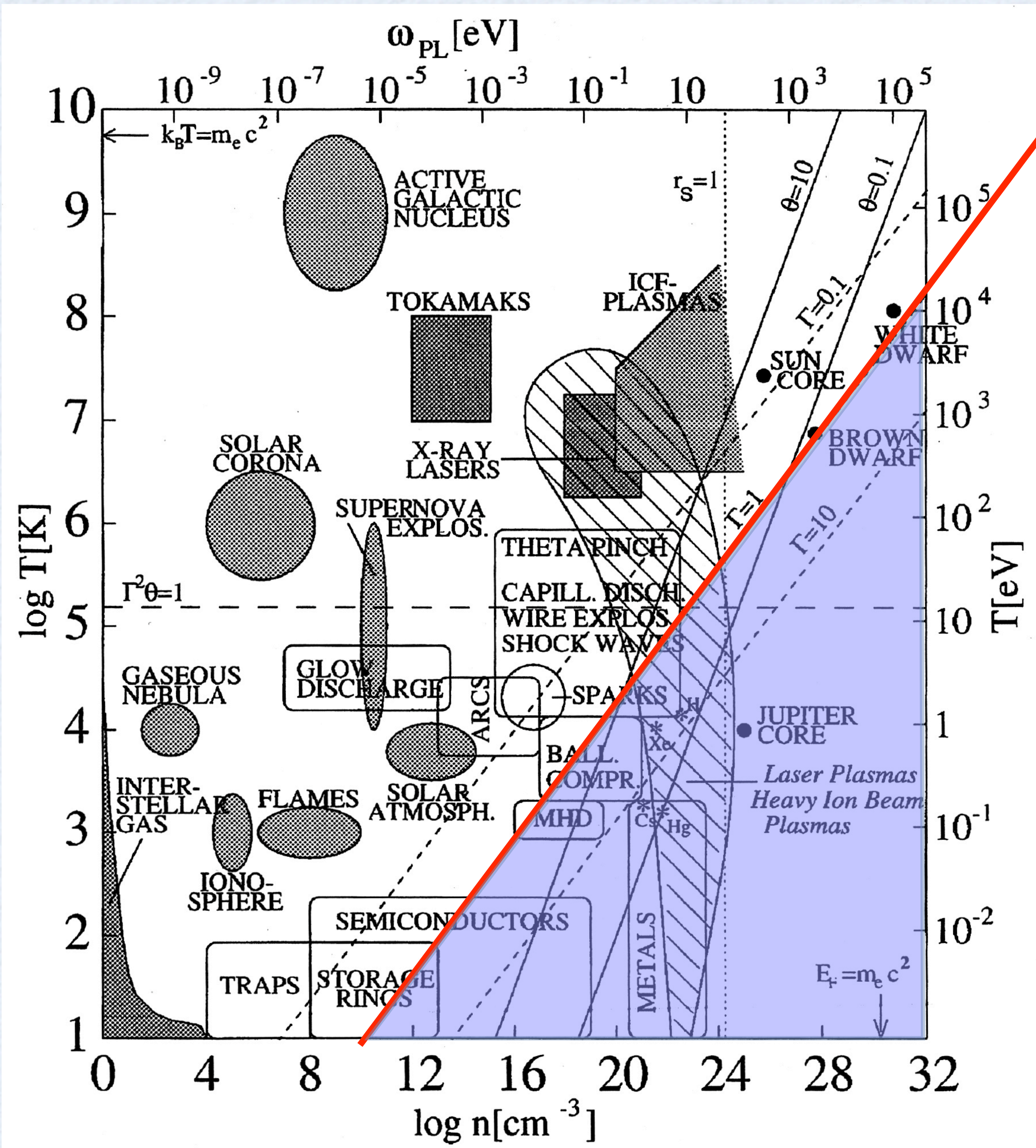


Classification of plasmas

from the
American Physical Society
"fusion chart"

Is there really not much here to look for ???

Plasmas.... a better phase diagram



$\Gamma = 1$

Consider for a moment the interaction between a single type of particles (ion-ion)

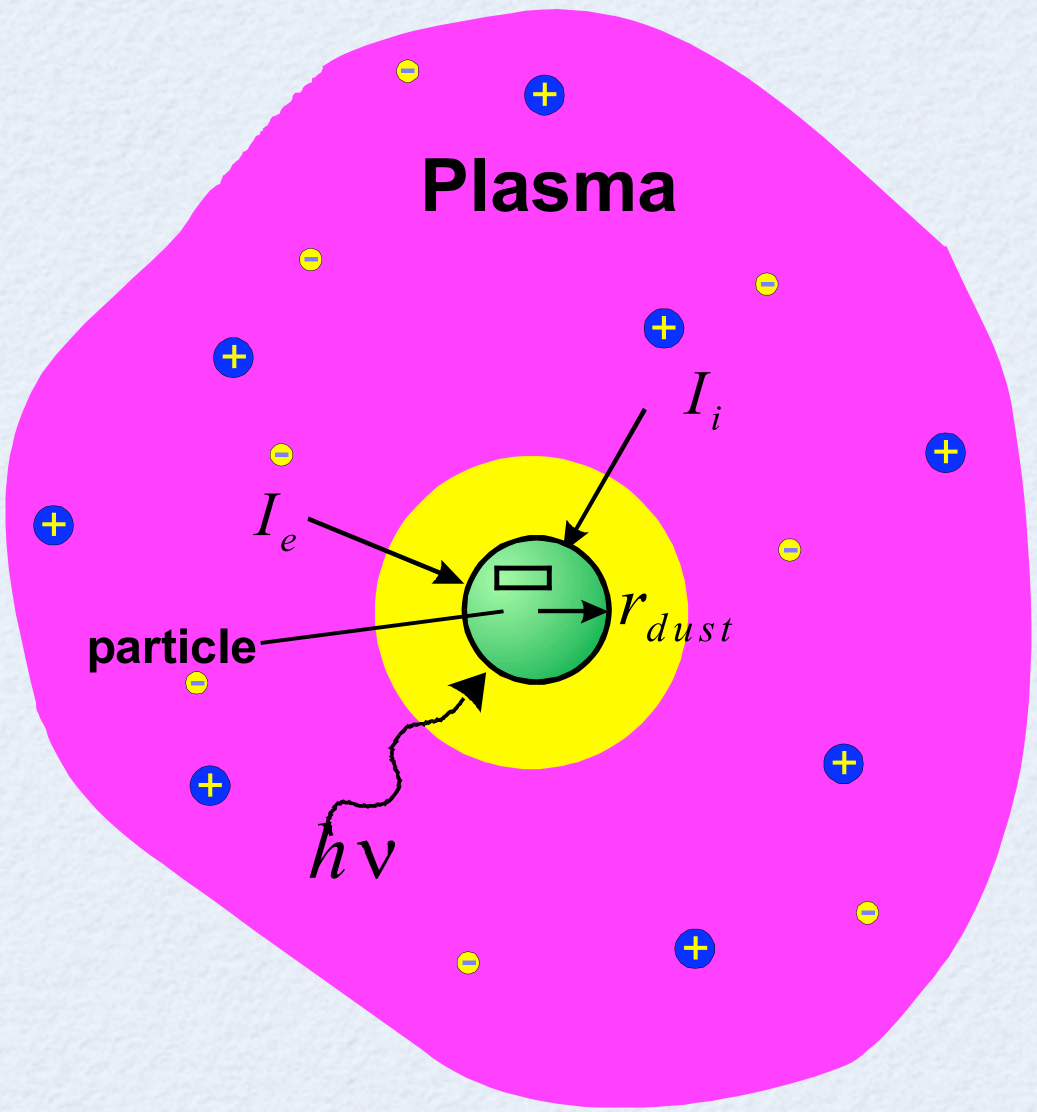
$$\Gamma = \frac{V_{\mathrm{POT}}}{V_{\mathrm{KIN}}}$$

STRONGLY COUPLED PLASMAS

R. Redmer, Phys. Reports 282, 35 (1997)

Complex (dusty) plasmas: one-component plasma (OCP) model

OCP model: only one type of species is considered explicitly, the presence and effects of other species are accounted for by the potential



Characteristic energies (Coulomb):

$$V_{\mathrm{KIN}} = kT \qquad V_{\mathrm{POT}} = \frac{Q^2}{4\pi\varepsilon_0 a}$$

a : Wigner-Seitz radius

Coupling parameter:

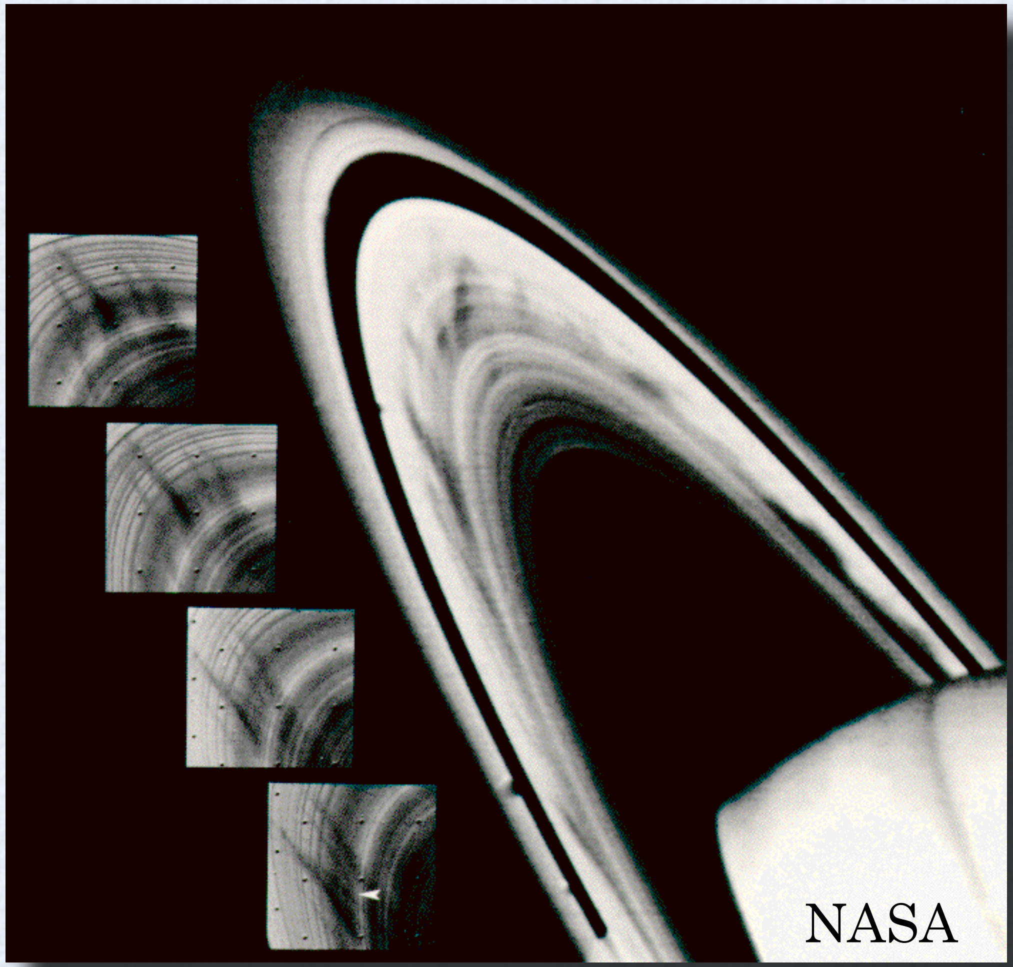
$$\boxed{\Gamma = \frac{V_{\mathrm{POT}}}{V_{\mathrm{KIN}}} = \frac{1}{4\pi\varepsilon_0}\frac{Q^2}{akT}}$$

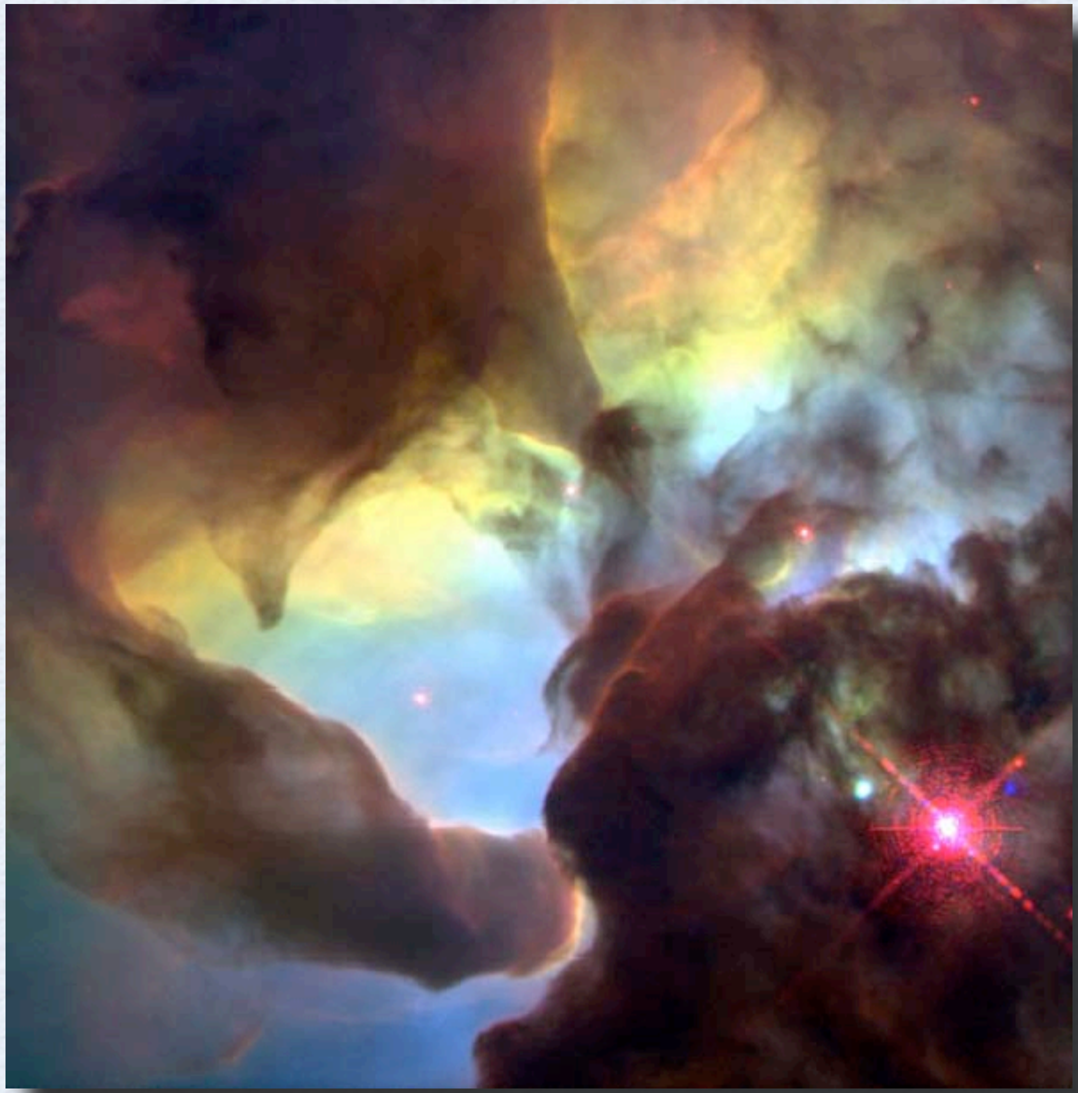
Debye / Yukawa potential & screening parameter:

$$\Phi(r) = \frac{1}{4\pi\varepsilon_0}\frac{Q\exp\left(-r/\lambda_{\mathrm{D}}\right)}{r} \quad , \quad \boxed{\kappa = \frac{a}{\lambda_{\mathrm{D}}}}$$

Dusty plasmas in space

1980s: Voyager2 images of Saturn rings show ”spokes” formed of fine dust particles and influenced by electromagnetic fields
→ charged dust



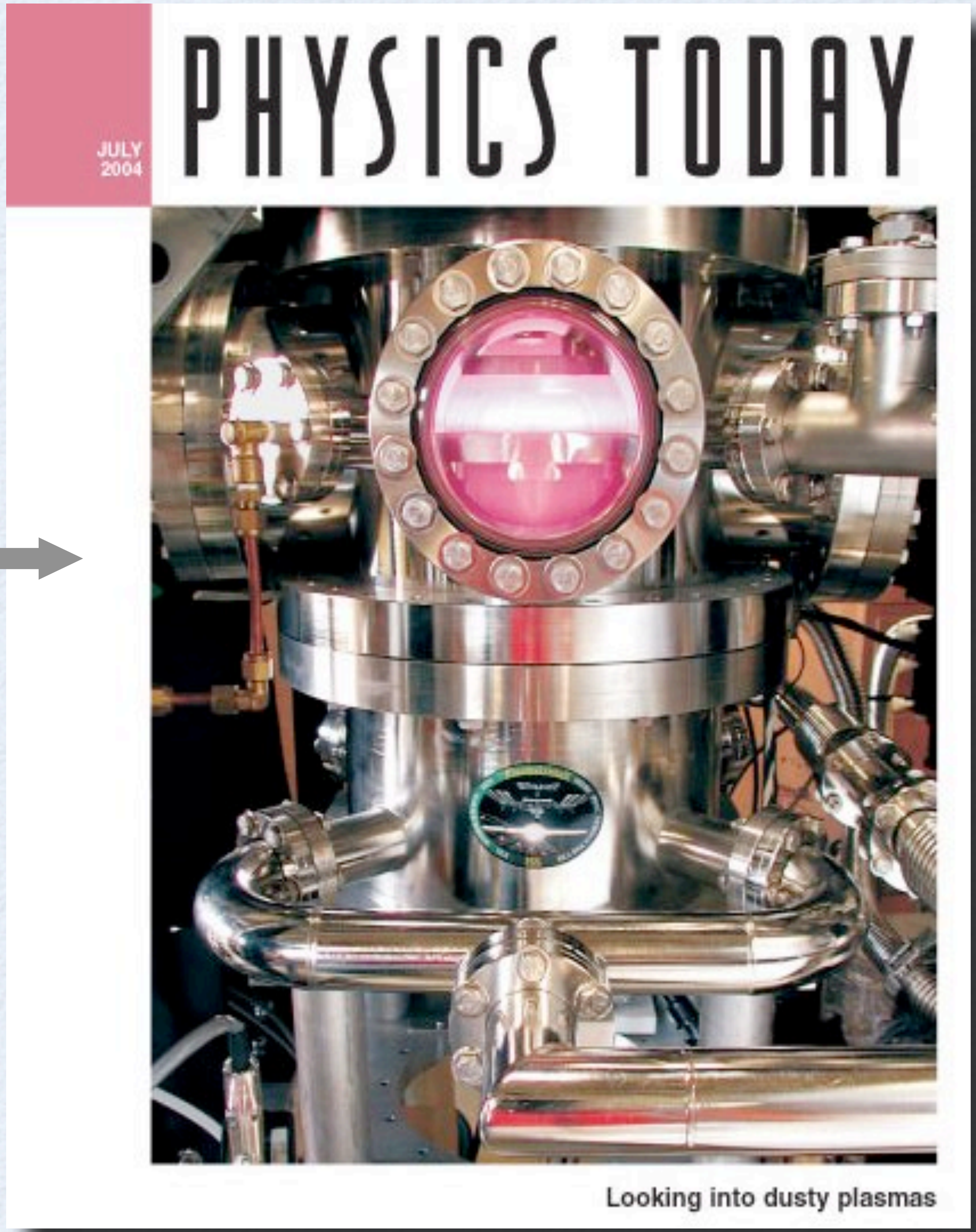


Charging of fine particles due to UV radiation
Lagoon Nebula (Hubble)

Dusty plasmas in laboratory

Discovery of micron-sized dust particle formation in a reactive plasma over wafers:
G. S. Selwyn, J. Singh, R. S. Bennett,
J. Vac. Sci. Technol. A7, 2758 (1989).

"Dusty plasmas in the Laboratory, Industry and Space"
Robert L. Merlino and John A. Goree
Physics Today, pp. 32 - 38, July 2004



Dust can grow in a plasma or can be introduced

Molecular Dynamics (MD) basics

Equilibrium & non-equilibrium MD

We let the system evolve according to interactions

Perturb the system and measure response

Molecular Dynamics (MD) simulation basics

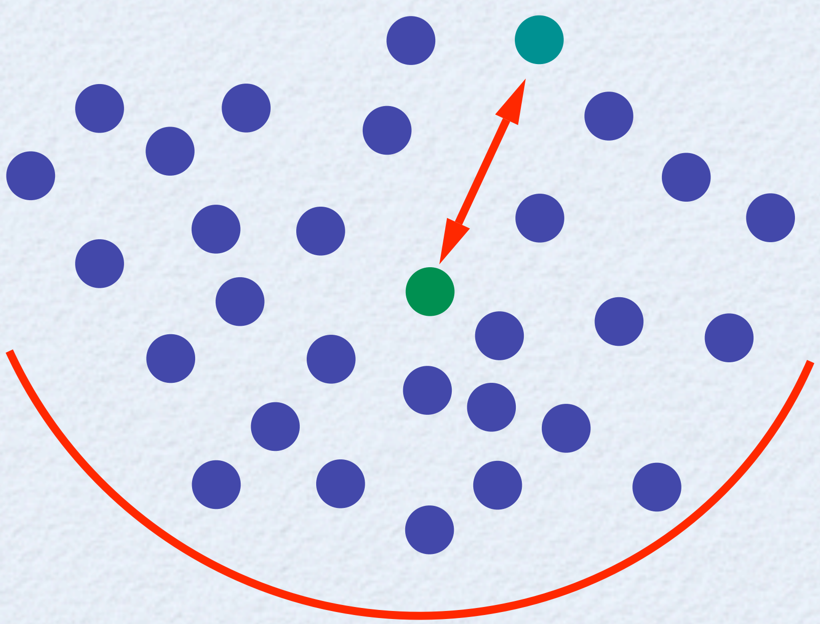
Equilibrium MD

SIMULATION CORE + MEASUREMENTS

Time evolution of phase space trajectories of an ensemble of N particles

Calculate quantities of interest from phase space coordinates

Example: finite system with external confinement:



$$m\ddot{\mathbf{r}}_i = \sum_{i \neq j} \mathbf{F}_{i,j}(t) + \mathbf{F}_{\mathrm{ext}}(t) - m\eta\mathbf{v}_i(t) + \mathbf{R}$$

$$\mathbf{F}_{i,j} = -\frac{\partial \phi(r_{ij})}{\partial r}$$

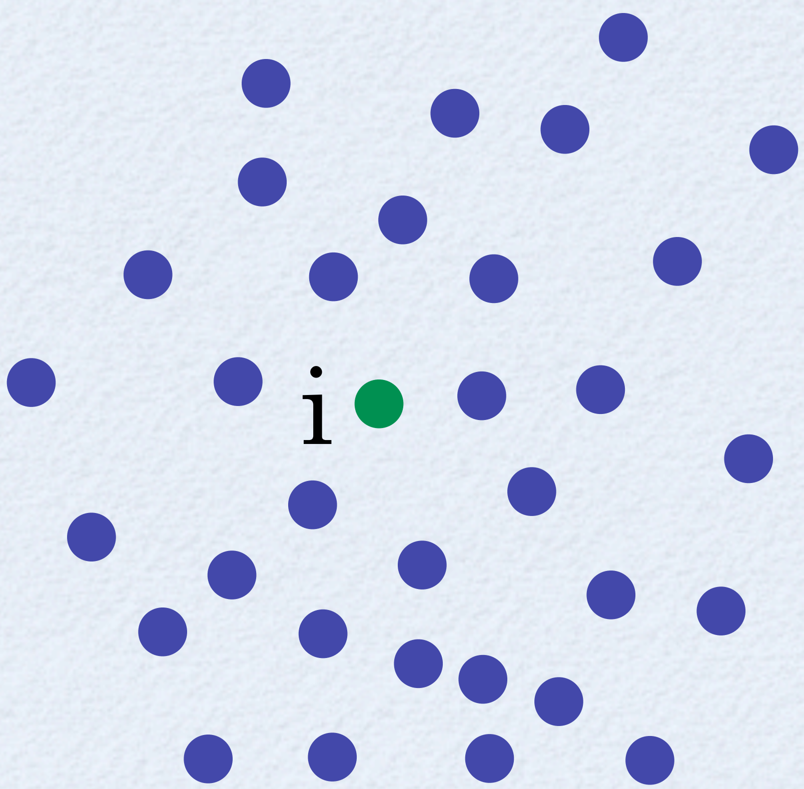
$$\mathbf{F}_{\mathrm{ext}} = -fr^2 \ \text{(e.g.)}$$

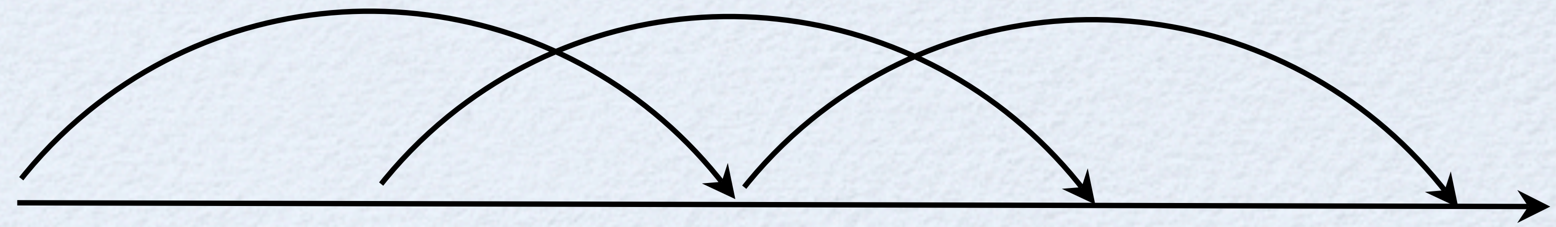
Friction

Brownian randomly fluctuating force (Langevin force)

Molecular Dynamics (MD) simulation basics

Integration of the equation of motion (“leapfrog scheme”)





$$\mathbf{v}_i\left(t-\frac{\Delta t}{2}\right) \qquad \mathbf{r}_i(t) \qquad \mathbf{v}_i\left(t+\frac{\Delta t}{2}\right) \qquad \mathbf{r}_i(t+\Delta t)$$

time

$$\mathbf{v}_i\left(t+\frac{\Delta t}{2}\right) = \mathbf{v}_i\left(t-\frac{\Delta t}{2}\right) + \frac{\mathbf{F}_i(t)}{m}\Delta t$$

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i\left(t+\frac{\Delta t}{2}\right)$$

$$m\ddot{\mathbf{r}}_i = \sum_{i\neq j}\mathbf{F}_{i,j}(t) + \mathbf{F}_{\text{ext}}(t) - m\eta\mathbf{v}_i(t) + \mathbf{R}$$

How to calculate $\sum \mathbf{F}_{i,j}(t)$?

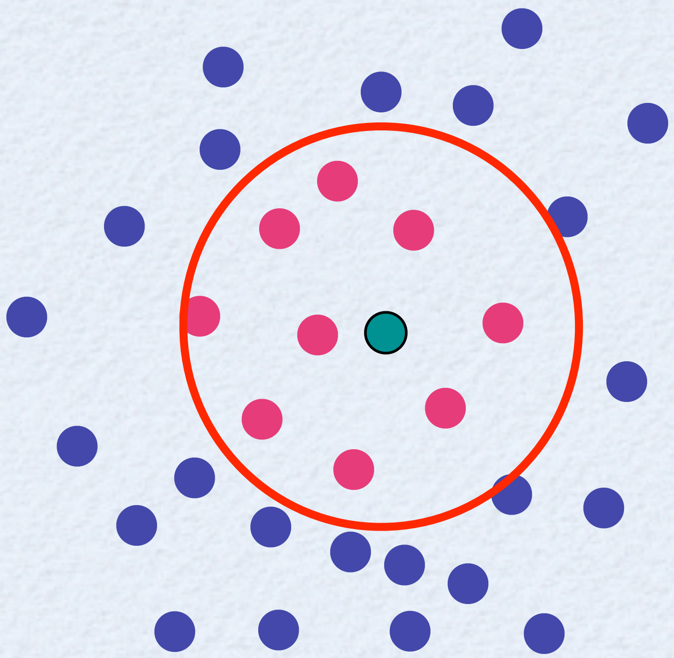
Molecular Dynamics (MD) simulation basics

Short – range interaction potentials

Interaction is considered only between “closely-separated” pairs of particles (cutoff radius)

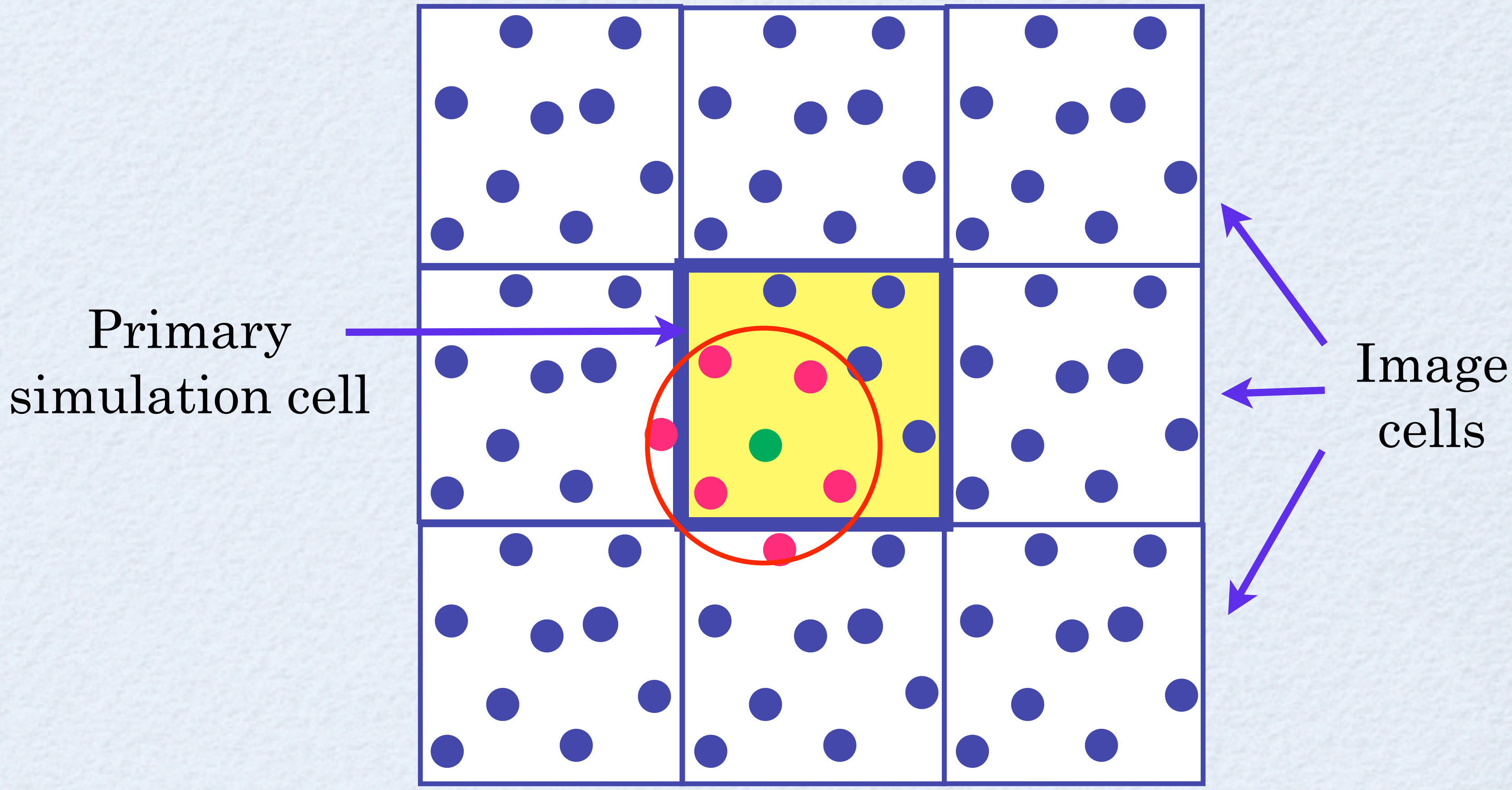
$$\mathbf{F}_i(t) = \sum_{r_{ij}<r_C} \mathbf{F}_{i,j}(t)$$

Finite system



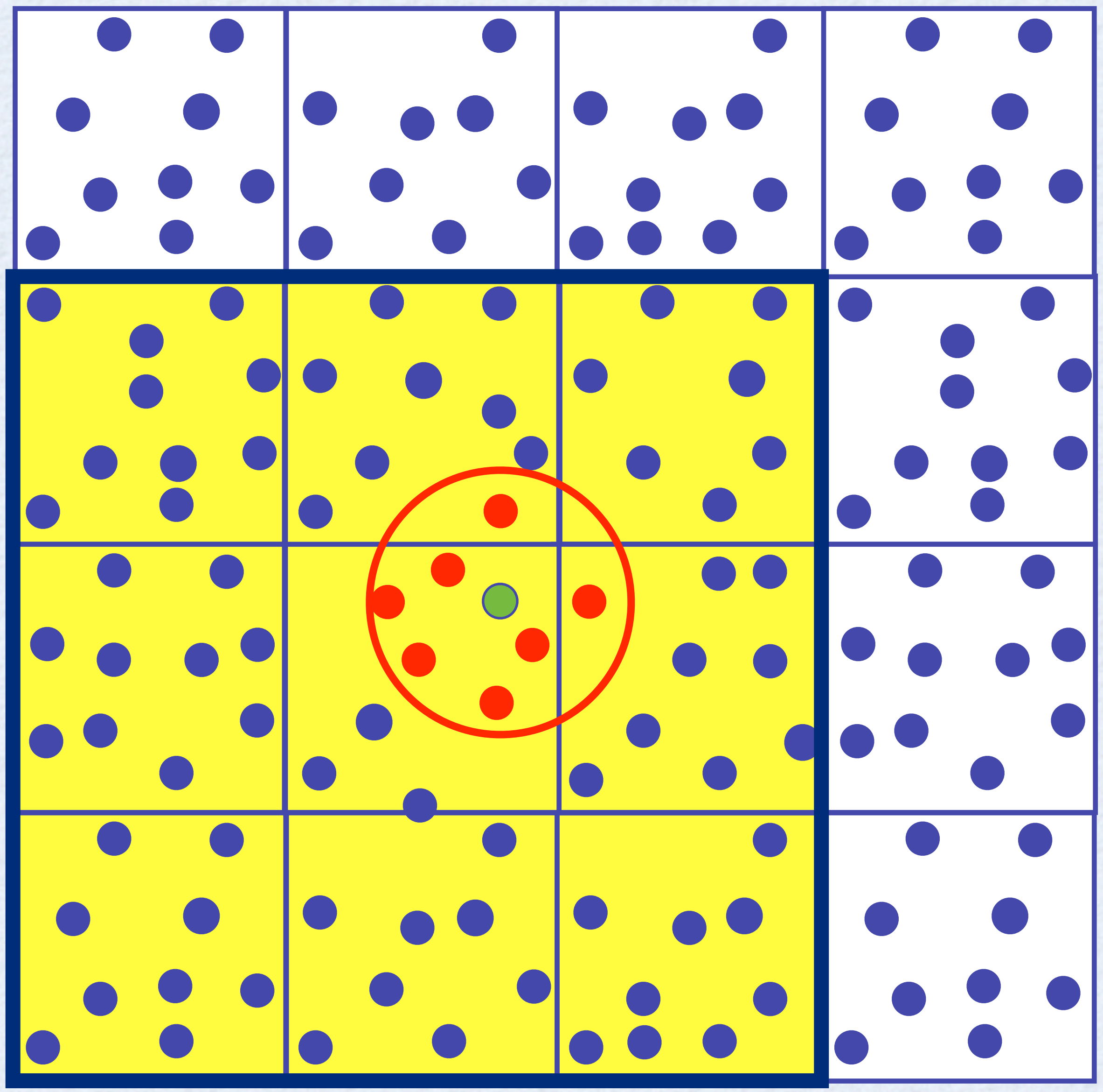
Infinite system

PERIODIC BOUNDARY CONDITIONS



Molecular Dynamics (MD) simulation basics

How to find the neighbors?



Primary simulation cell (yellow)

Image chaining mesh cells (white)

- For particle i (i=1...N) : check every other particle j if they are neighbors
- **Use chaining mesh**

Molecular Dynamics (MD) simulation basics

How to find the neighbors?

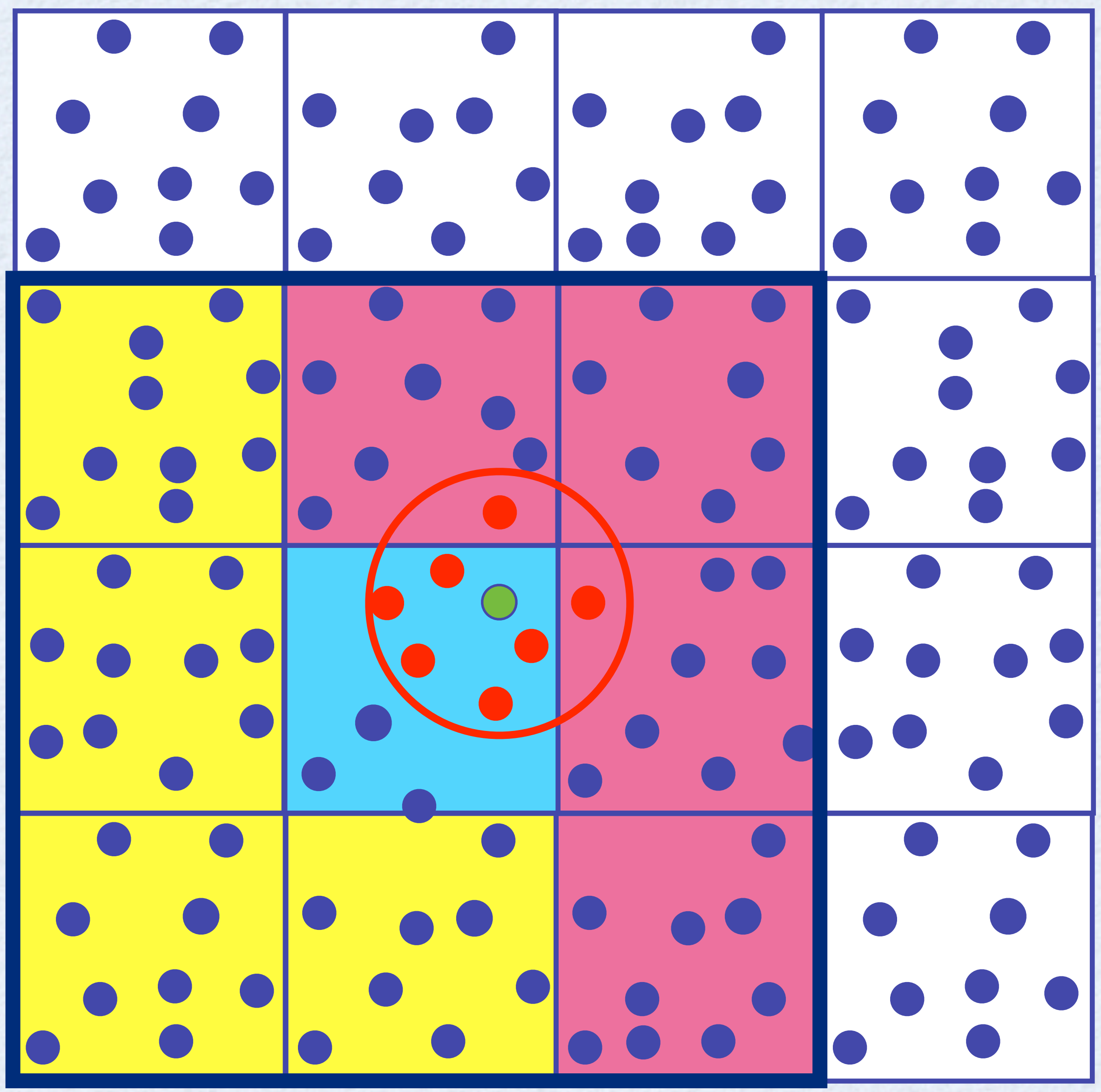


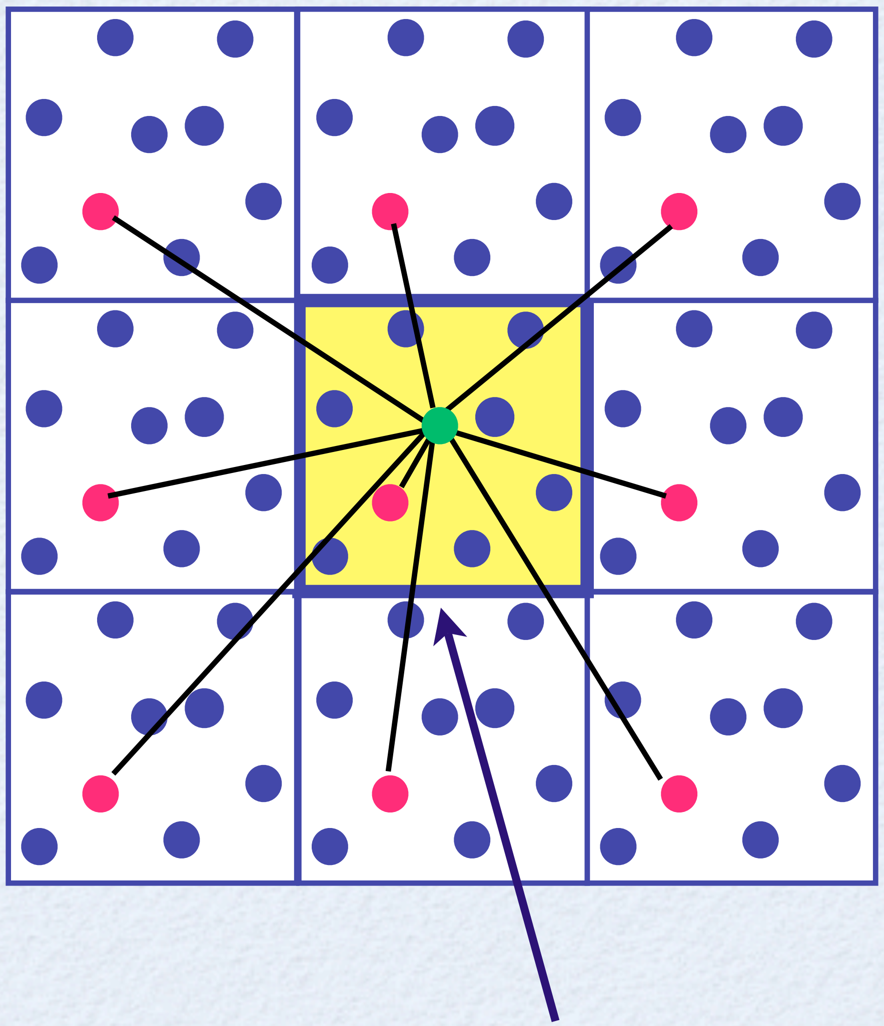
Image chaining mesh cells (white)

- For particle i (i=1...N) : check every other particle j if they are neighbors
- **Use chaining mesh**

- Create a list of particles in each cell, $L(m,n)$
- go over all cells, for each particle i in cell (m,n) → all neighbors are in cells (m,n), $(m,n+1)$, $(m+1,n)$, $(m+1,n+1)$, $(m+1,n-1)$ [i.e. own cell and half of the neighboring cells, due to symmetry]

D. Frenkel and B. Smit, Understanding Molecular Dynamics Simulations (Academic Press, 2001)

Molecular Dynamics (MD) simulation basics



Primary simulation cell (yellow)

Long – range interaction potentials

(e.g. Coulomb):

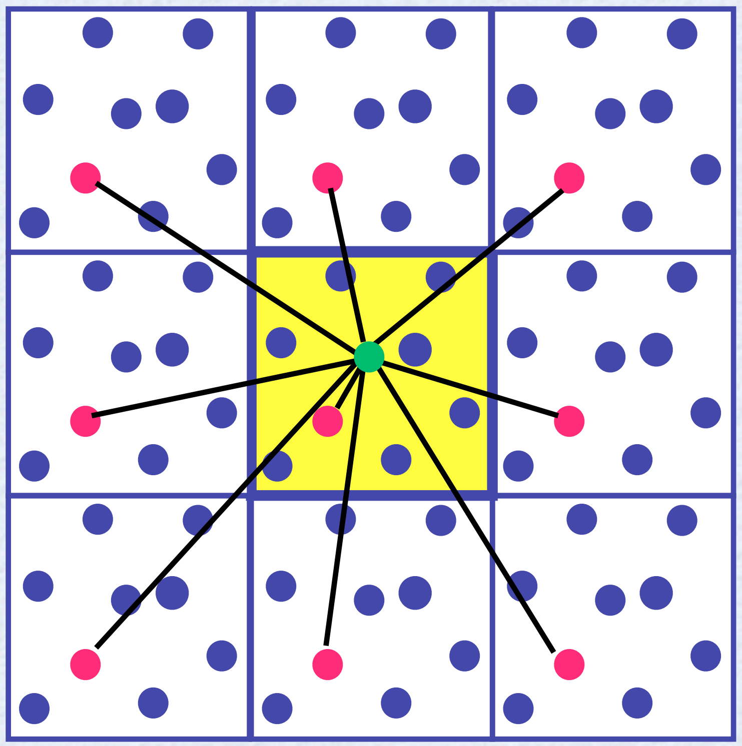
Not possible to find cutoff radius, "tricks" are needed

$$\mathbf{F}_i(t) = \sum_{\text{cell+images}} \mathbf{F}_{i,j}(t)$$

Possible solutions:

- Ewald summation
- Particle-Particle, Particle-Mesh (PPPM, P3M) method (Hockney & Eastwood)

Molecular Dynamics (MD) simulation basics



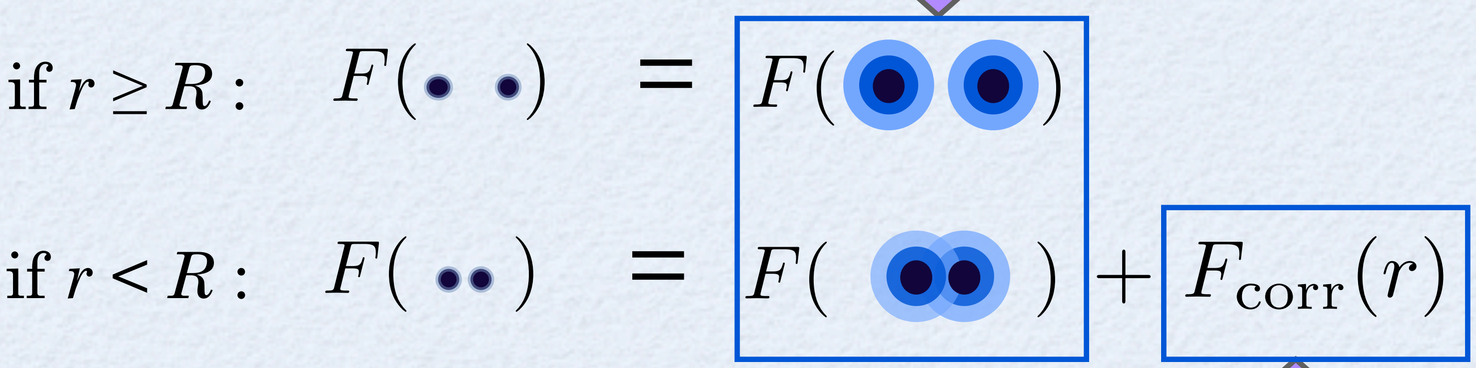
The PPPM method

uses finite size charge clouds

$$\rho(r) = \rho_0\left(1 - \frac{r}{R}\right)$$

$$\int_0^R \rho(r)\mathrm{d}V = Q$$

Fourier transform is band-limited, the interaction between clouds can be represented on a mesh in **k**-space, images are included (PM)

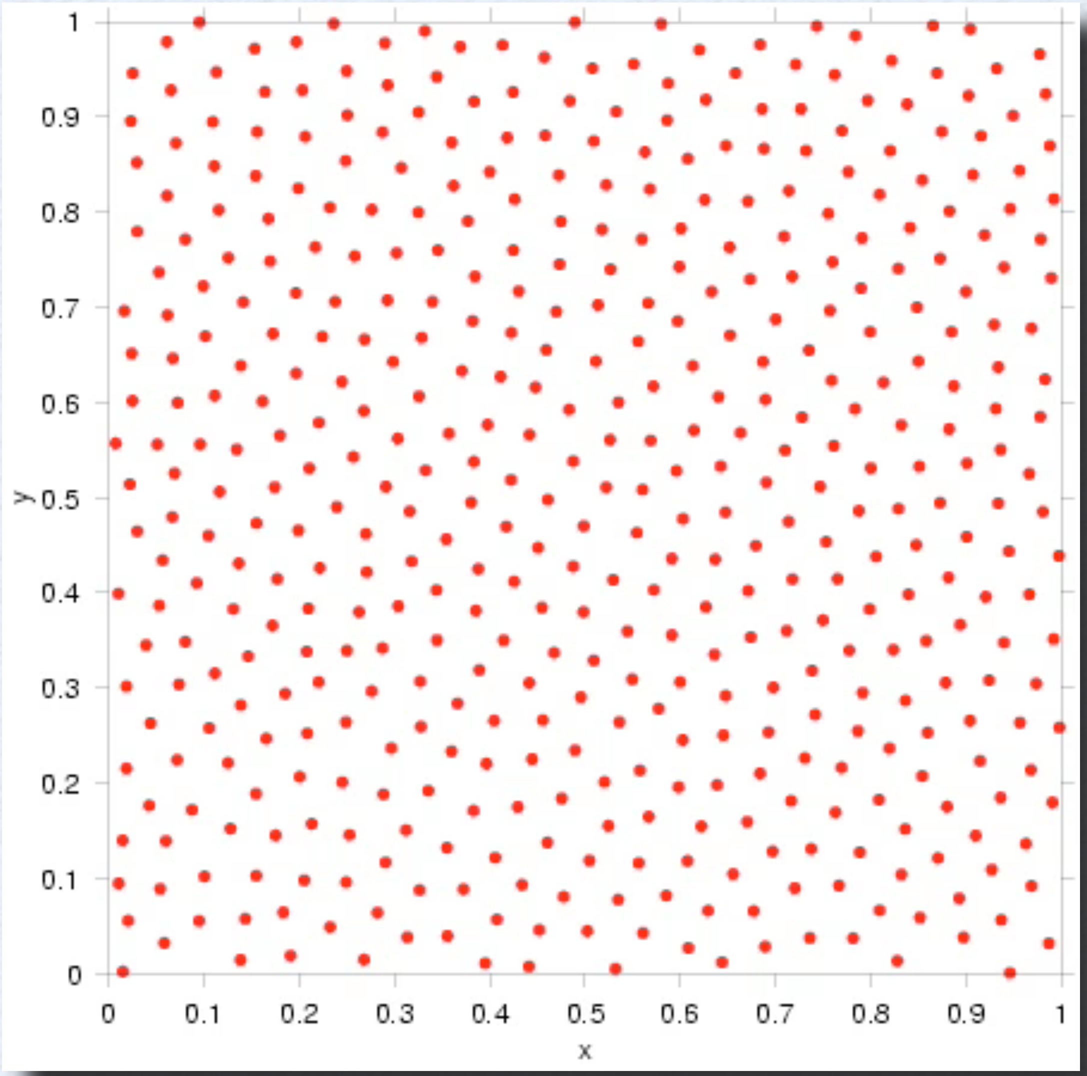


Hockney R W and Eastwood J W 1981
Computer Simulation Using Particles
(New York: McGraw-Hill)

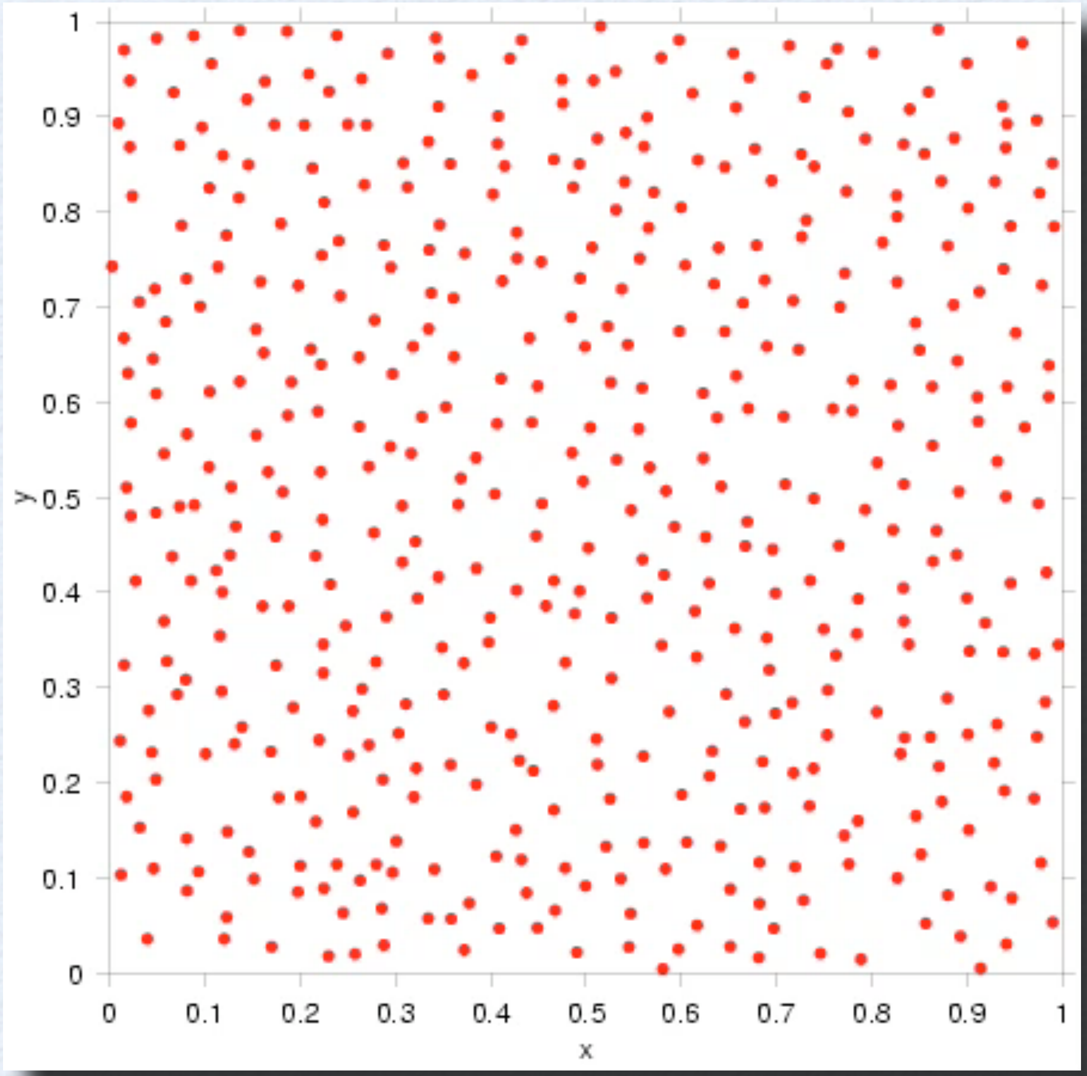
Correction force, to be applied for closely separated neighbors only (PP, chaining mesh)

Molecular Dynamics : What do we see?

Γ=120, κ=1



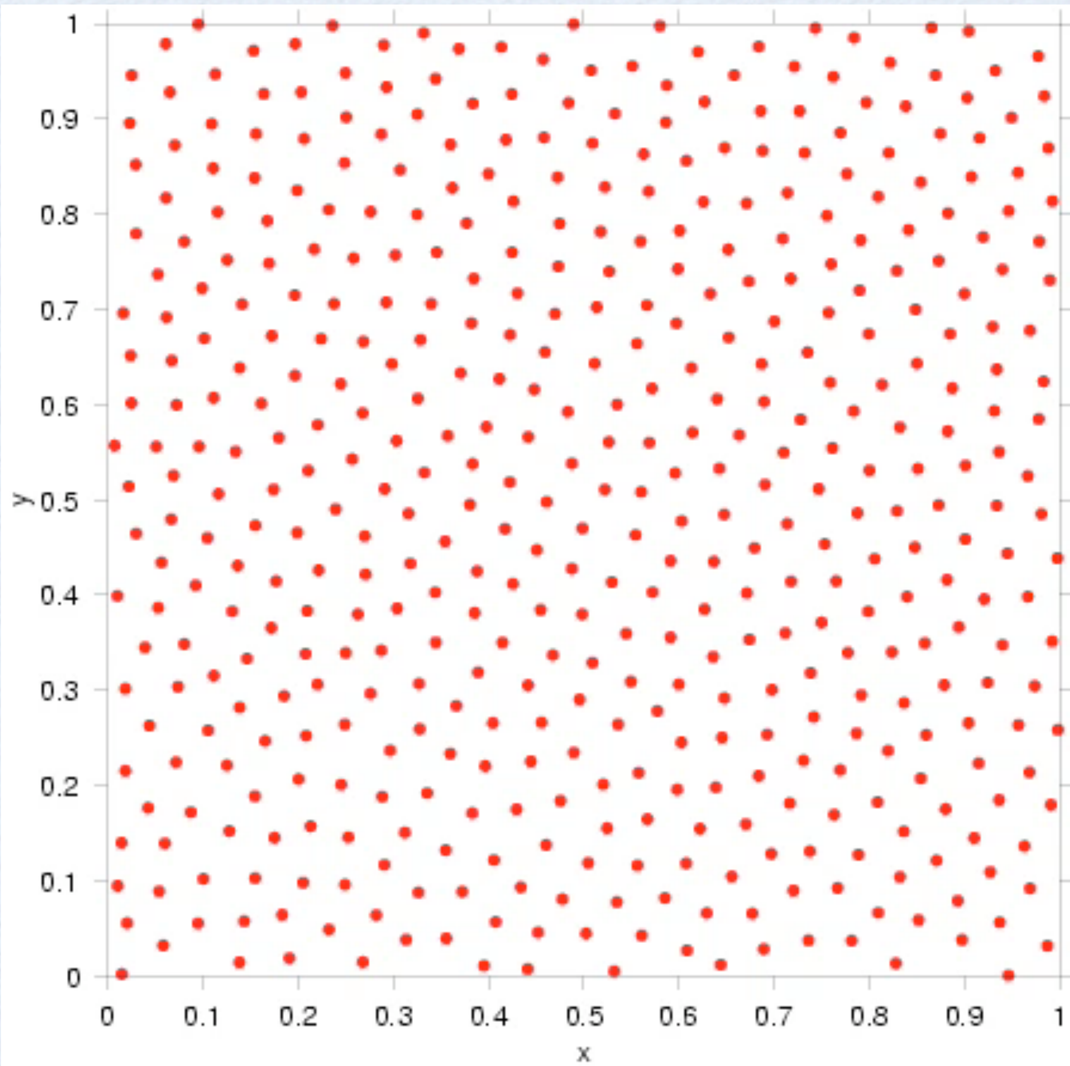
Γ=5, κ=1



2D frictionless Yukawa liquids

Molecular Dynamics : What do we learn?

A LOT



Phase space coordinates

Correlation functions

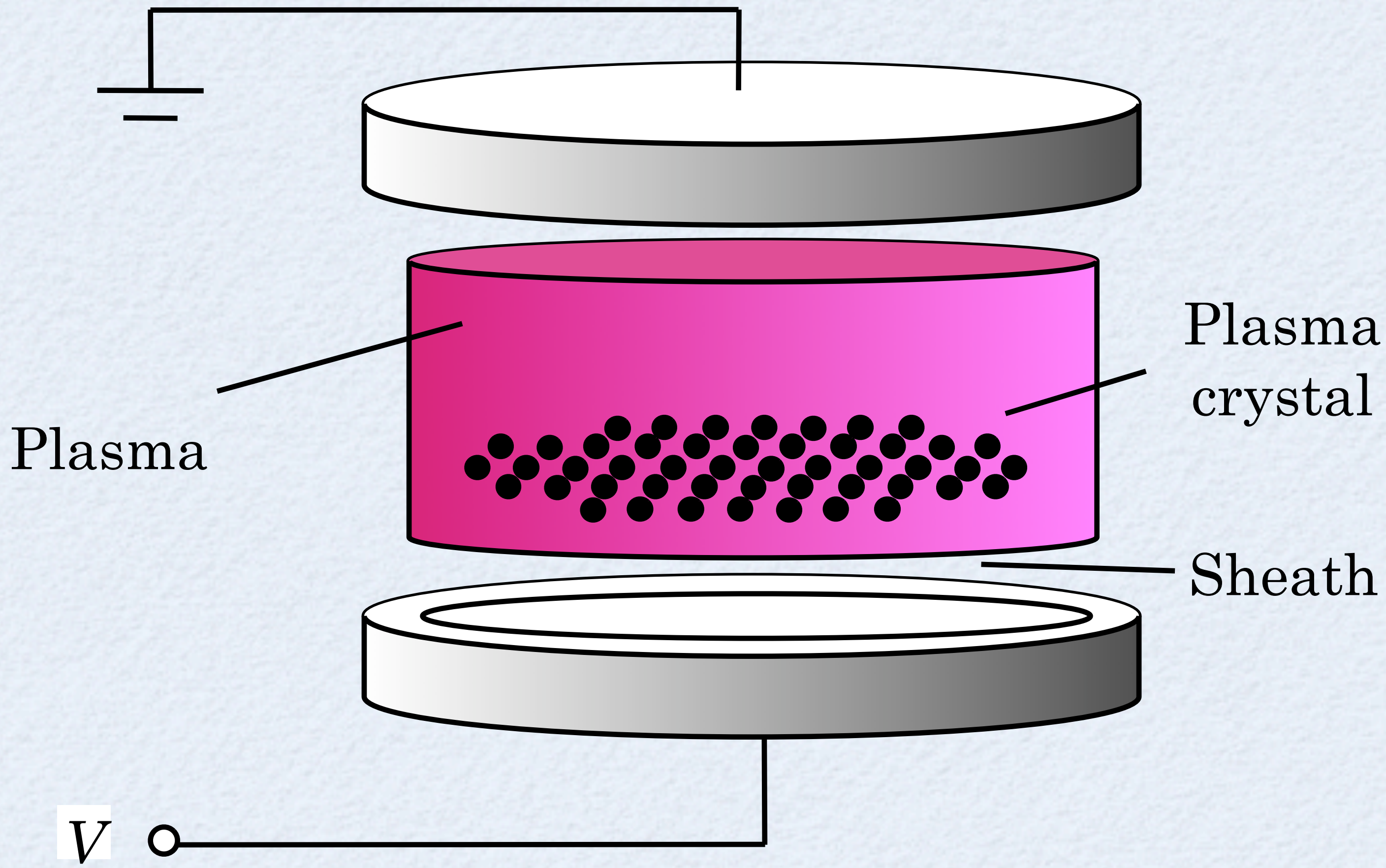
Structure

Thermodynamic quantities

Calculation of transport parameters

Identification of collective modes

It's real: experimental realization of 2D dusty plasma



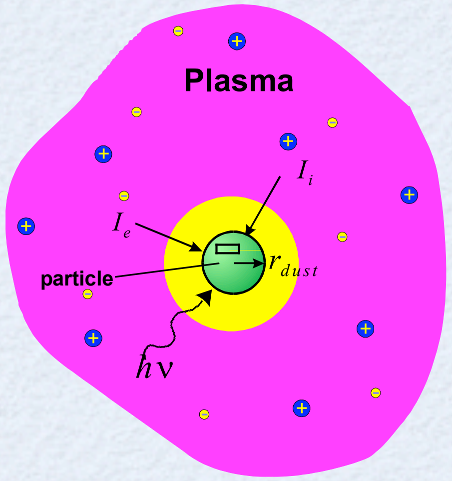
$$\Phi(r) = \frac{1}{4\pi\varepsilon_0}\frac{Q\exp\left(-r/\lambda_{\mathrm{D}}\right)}{r} \quad , \quad \kappa = \frac{a}{\lambda_{\mathrm{D}}}$$

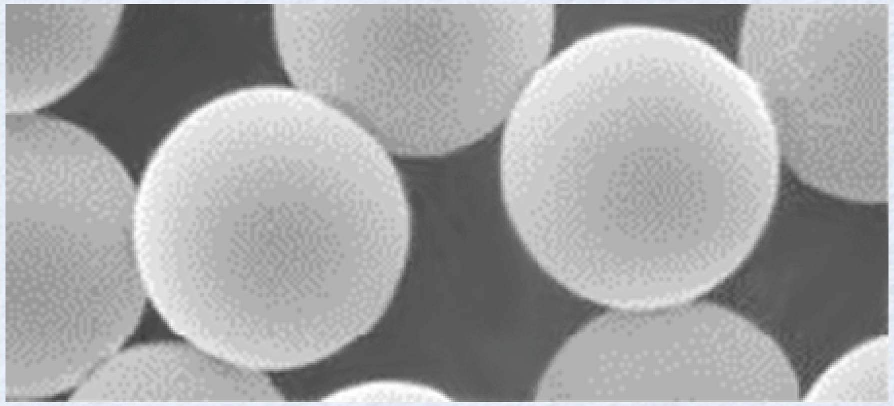
- Dust particles dispersed in a glow discharge plasma acquire a charge of ~ $10^4\, q_e$
- Dust layer is levitated due to the balance between electrostatic force and gravity
- Interaction: screened Coulomb (Yukawa) potential
- Crystallization at high Γ
- Quasi-2D confinement
- Extensive experimental work from early 1990s (Morfill, Thomas, Goree, Fortov, Piel, et al., ...) in the crystal and liquid phases

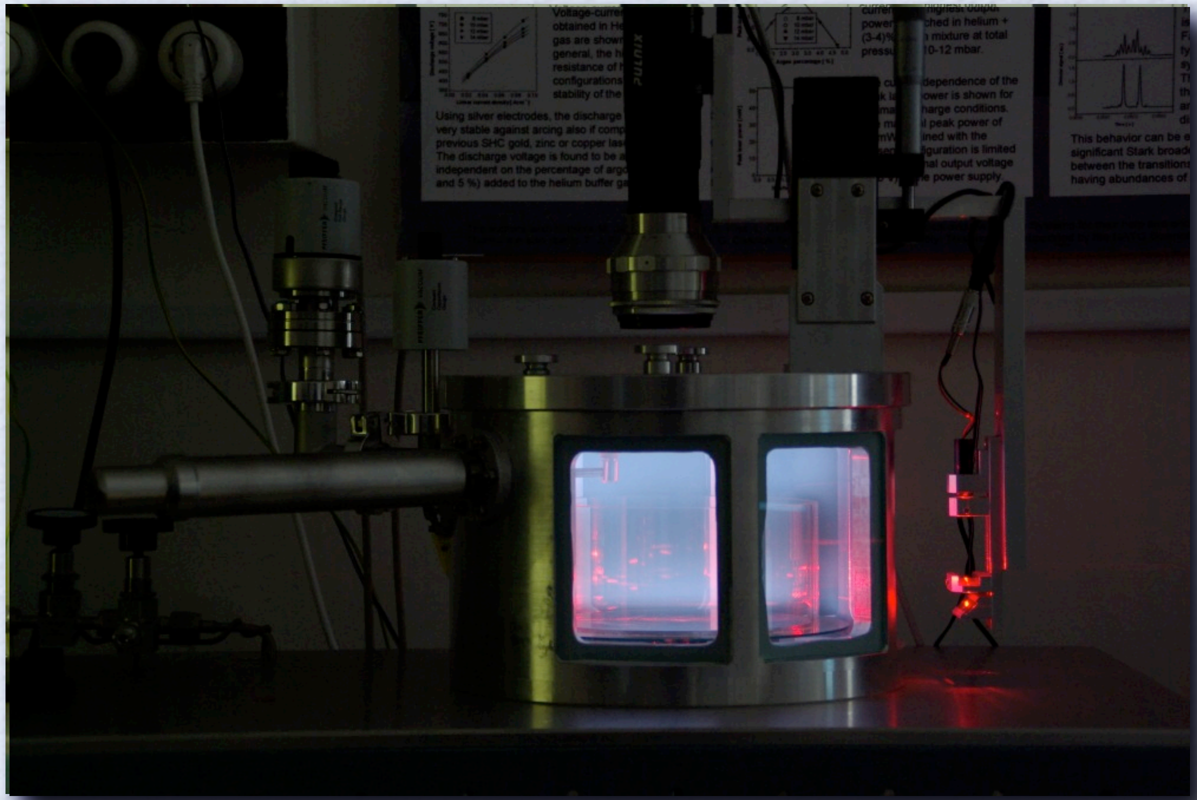
Experimental realization of 2D dusty plasma

melamine-formaldehyde microspheres

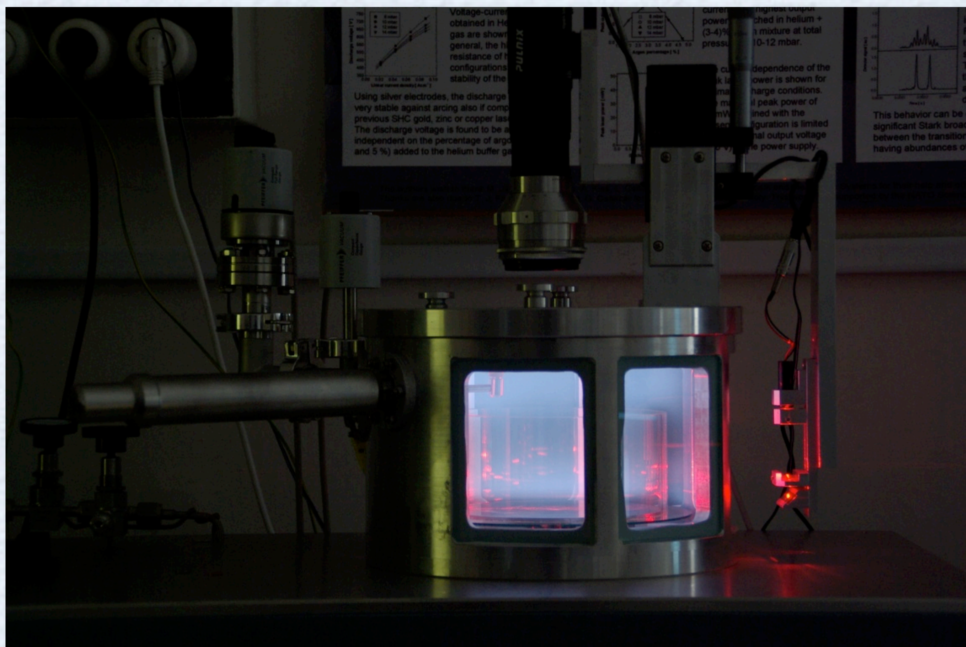
Dusty plasma experiment in RISSP, Budapest (P. Hartmann)

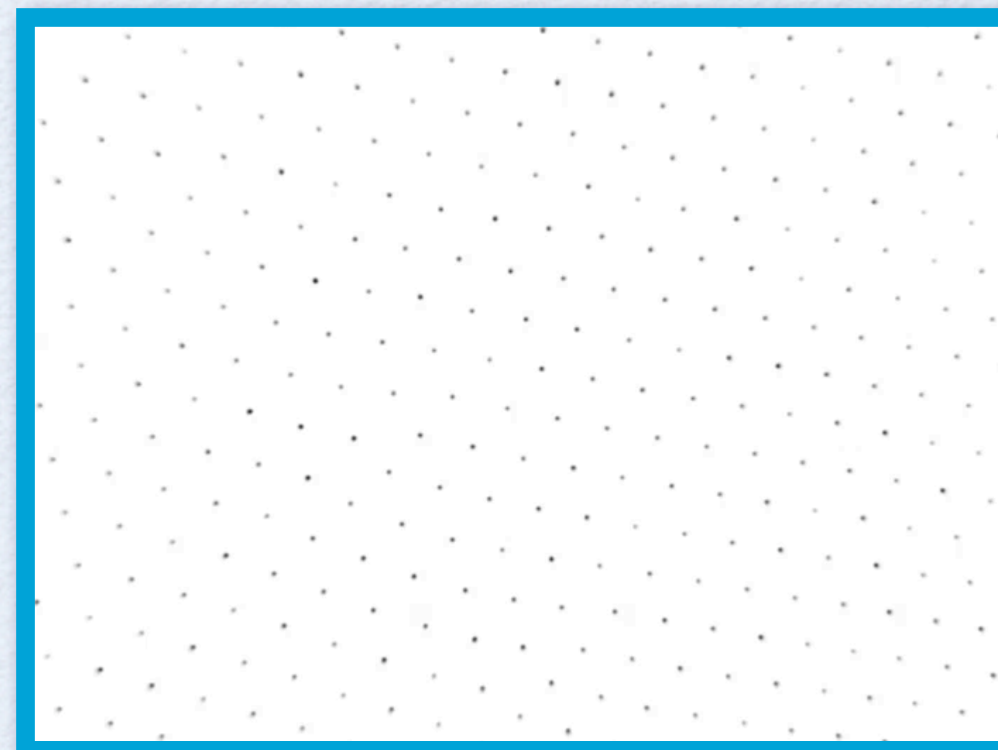




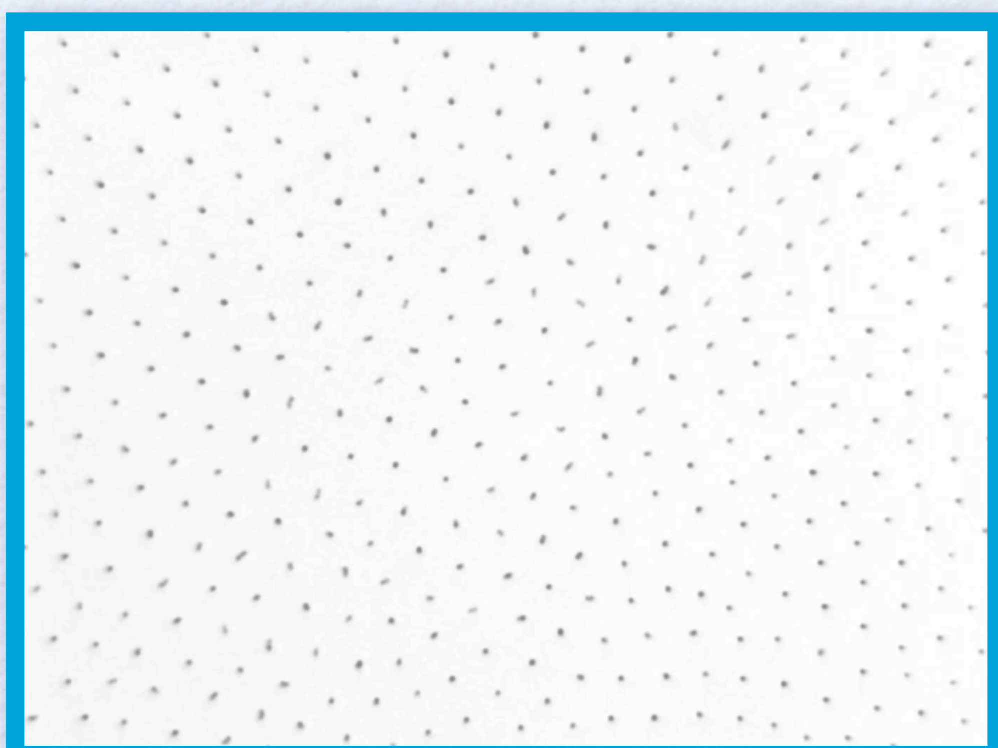


Experimental realization of 2D dusty plasma





Crystallized phase



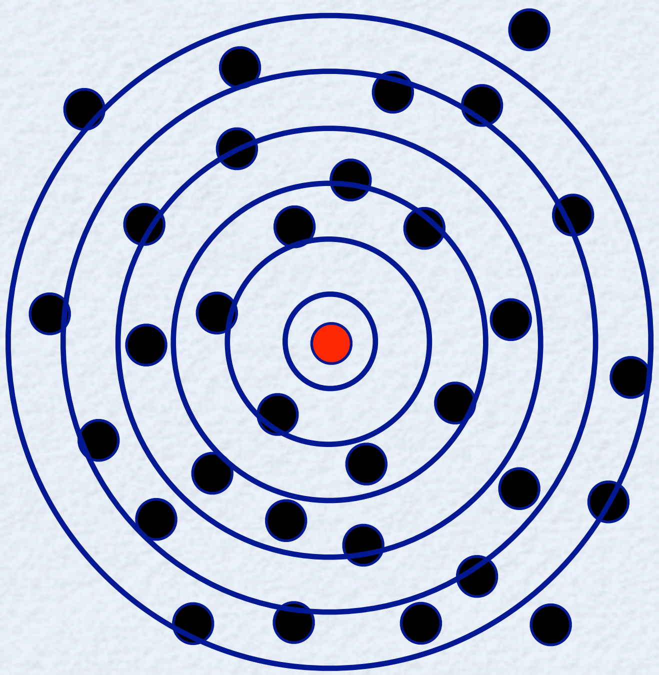
Oscillations near melting

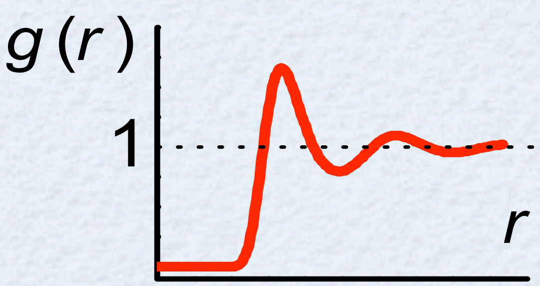
Structural and thermodynamic properties

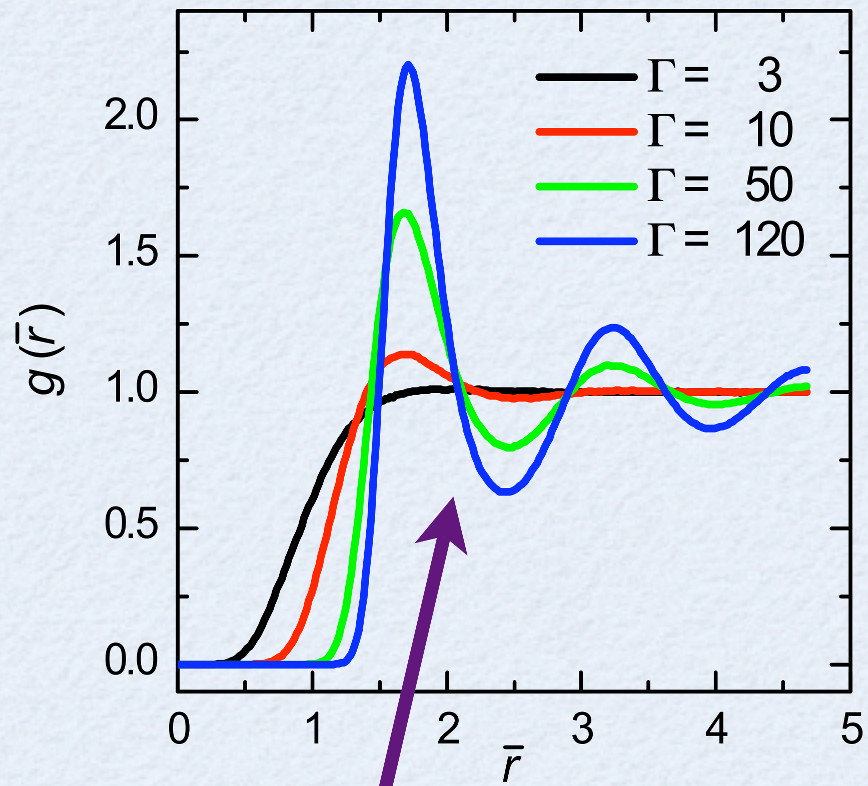
Pair correlation & thermodynamic properties

Pair correlation function

e.g. 3D Coulomb OCP
(one-component plasma)







Strong correlation,
liquid-like structure
at high coupling

- Energy:

$$\frac{E}{N} = \frac{3}{2} k_{\mathrm{B}} T + \frac{n}{2} \int_0^\infty \varphi(r) g(r)\ 4\pi r^2 \mathrm{d}r$$

- Pressure:

$$p = n k_{\mathrm{B}} T - \frac{n^2}{6} \int_0^\infty \frac{\partial \varphi(r)}{\partial r} g(r)\ 4\pi r^3 \mathrm{d}r$$

- Isothermal compressibility:

$$k_{\mathrm{B}} T \left(\frac{\partial n}{\partial p} \right)_T = 1 + n \int_0^\infty [g(r) - 1]\ 4\pi r^2 \mathrm{d}r$$

Phase transitions: 3D Coulomb / Yukawa systems

Coulomb
(Monte Carlo)

S. G. Brush, H. L. Sahlin and E. Teller,
J. Chem. Phys. 45, 2102 (1966).

$\Gamma \cong 125$

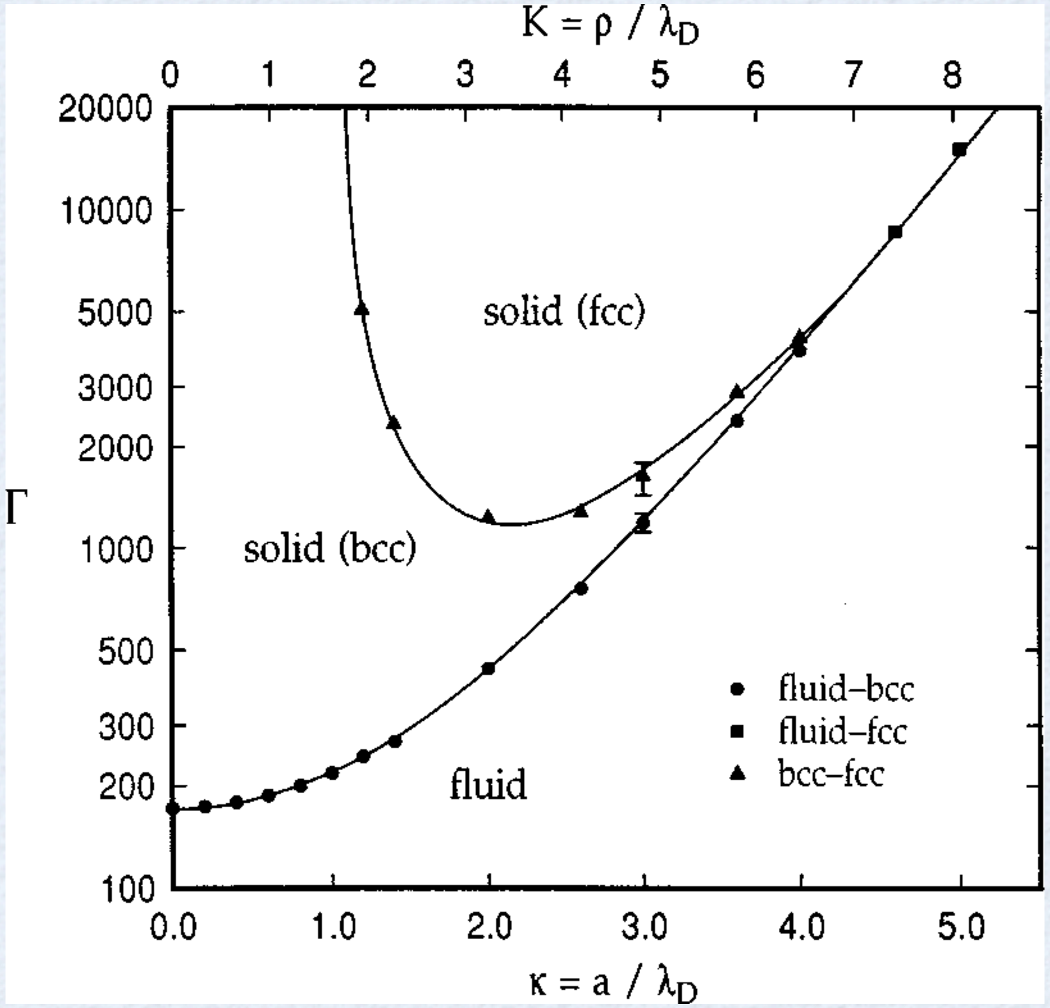
E. L. Pollock and J. P. Hansen
Phys. Rev. A 8, 3110 (1973)

G. S. Stringfellow, H. E. DeWitt and W. L. Slattery,
Phys. Rev. A 41, 1105 (1990).

$\Gamma \cong 175$

Yukawa

S. Hamaguchi, R.T. Farouki and D.H.E. Dubin,
Phys. Rev. E 56, 4671 (1997).



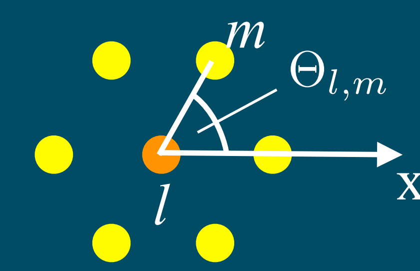
Solid to liquid transition in 2D

Phases in two dimensions:

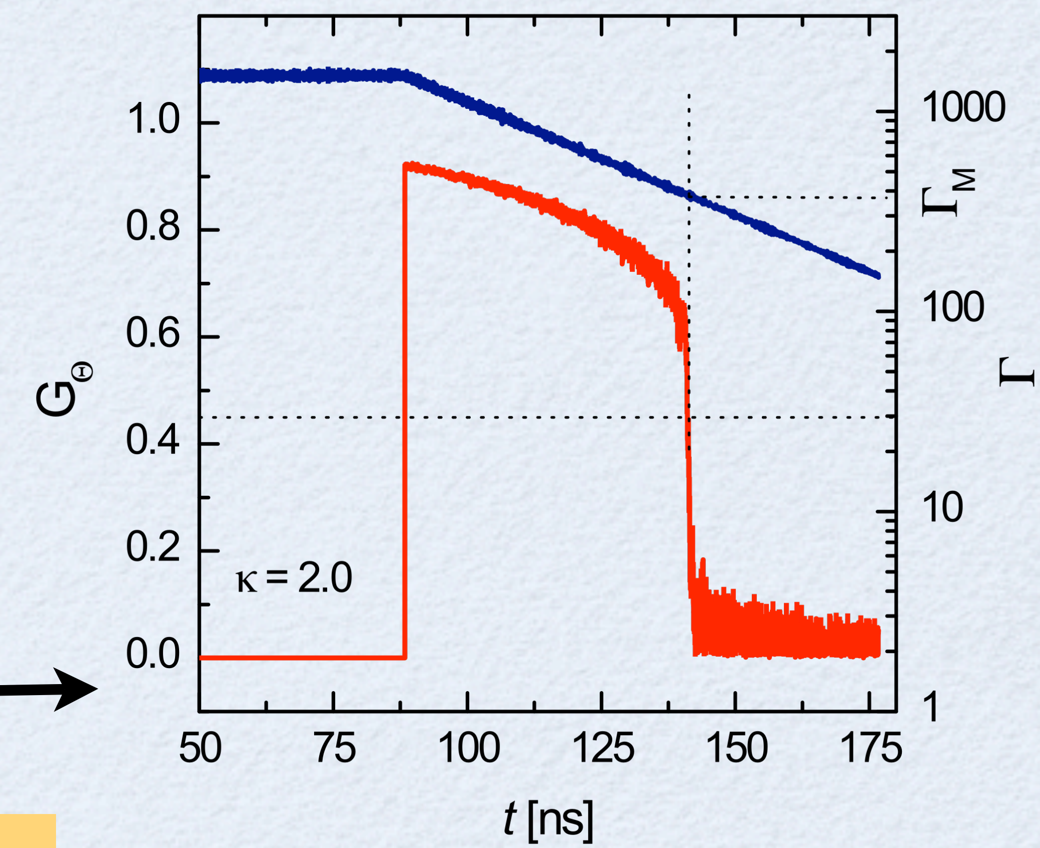
- Theoretical finding: “There is no exact long-range order in one and two dimensions for $T \neq 0$” [Ginzburg, Landau, Goldstone, Peierls, Penrose, Bogoliubov; ~1950]
- But: finite sized systems can develop crystal-like stable structures for $T > 0$
- No thermodynamic limit - need for finite particle thermodynamics
- Continuous temperature dependence of measured quantities
- ??? Nature of solid-liquid phase transition ???
- Possible multi-phase melting (unproven theory) intermediate “hexatic” phase

Bond-angular order parameter

$$G_\Theta = \frac{1}{N}\left|\sum_{l=1}^{N}\frac{1}{6}\sum_{m=1}^{6}\exp(i6\Theta_{l,m})\right|^2$$



“Melting experiment”



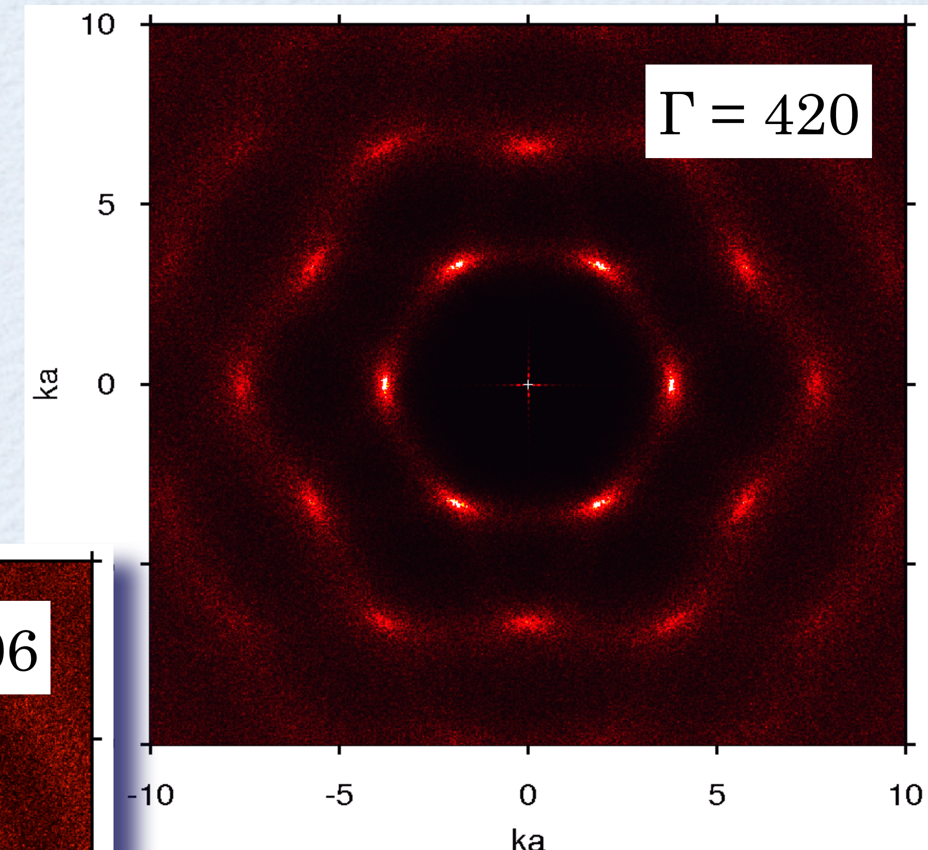
P. Hartmann, G. J. Kalman, Z. Donkó, and K. Kutasi, Phys. Rev. E 72, 026409 (2005)

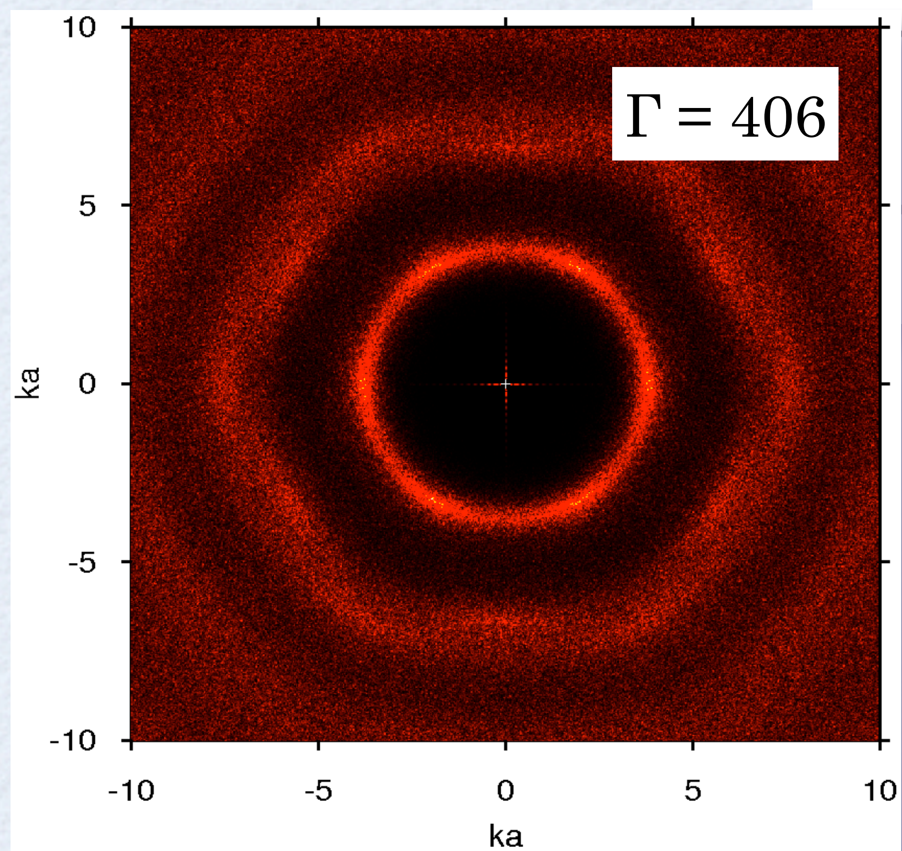
Much more careful studies are required (under way)

Solid to liquid transition in 2D

Investigated quantities:

- Bond angular order parameter
- Einstein frequency distributions
- Angular distribution of Einstein frequencies
- Potential energy
- Long-range behavior of $g(r)$
- Peak amplitude of $S(k)$
- Diffraction patterns - $S(\mathbf{k})$





WORK IN PROGRESS

P. Hartmann, Z. Donkó, P. Bakshi, G. J. Kalman, S. Kyrkos, IEEE Trans. Plasma Sci., 35 332 (2007)

Localization and transport phenomena

Quasi-localization: an important feature of the strongly coupled liquid state

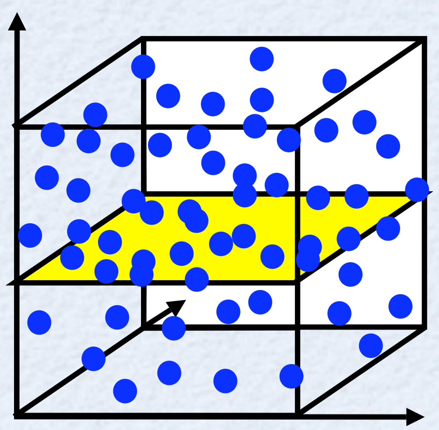
PHYSICS OF PLASMAS VOLUME 7, NUMBER 1 JANUARY 2000

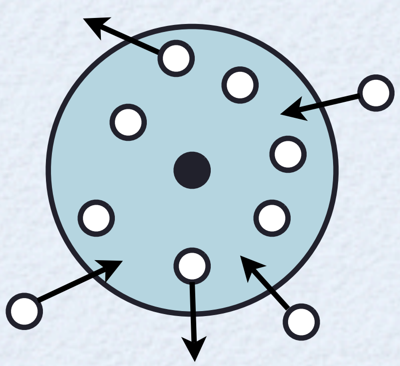
Quasilocalized charge approximation in strongly coupled plasma physics

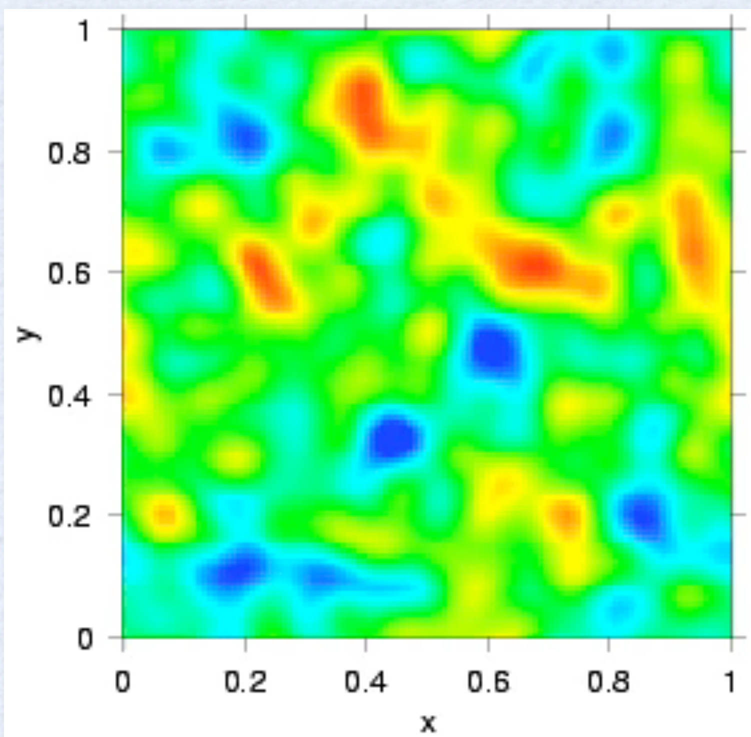
Kenneth I. Golden
Department of Mathematics and Statistics, Department of Physics, University of Vermont, Burlington, Vermont 05401-1455

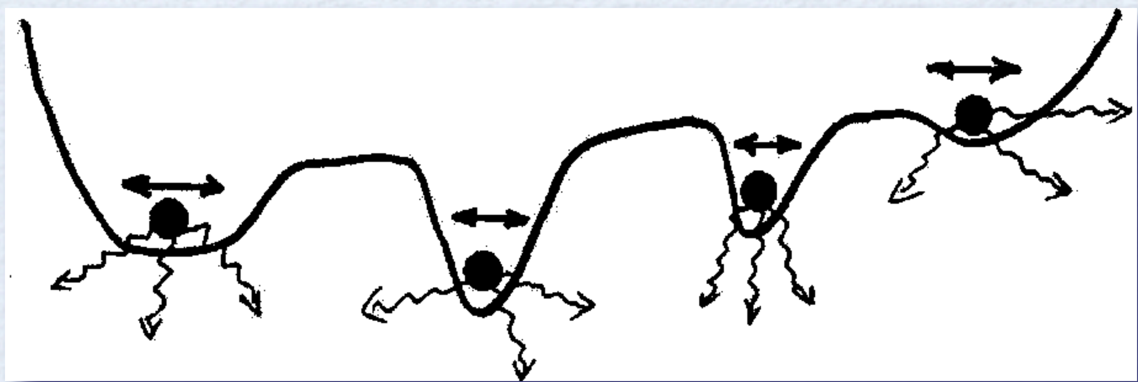
Gabor J. Kalman
Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467

Static $g(r)$ → Dynamics









- Localized oscillation of particles in local minima of the potential surface

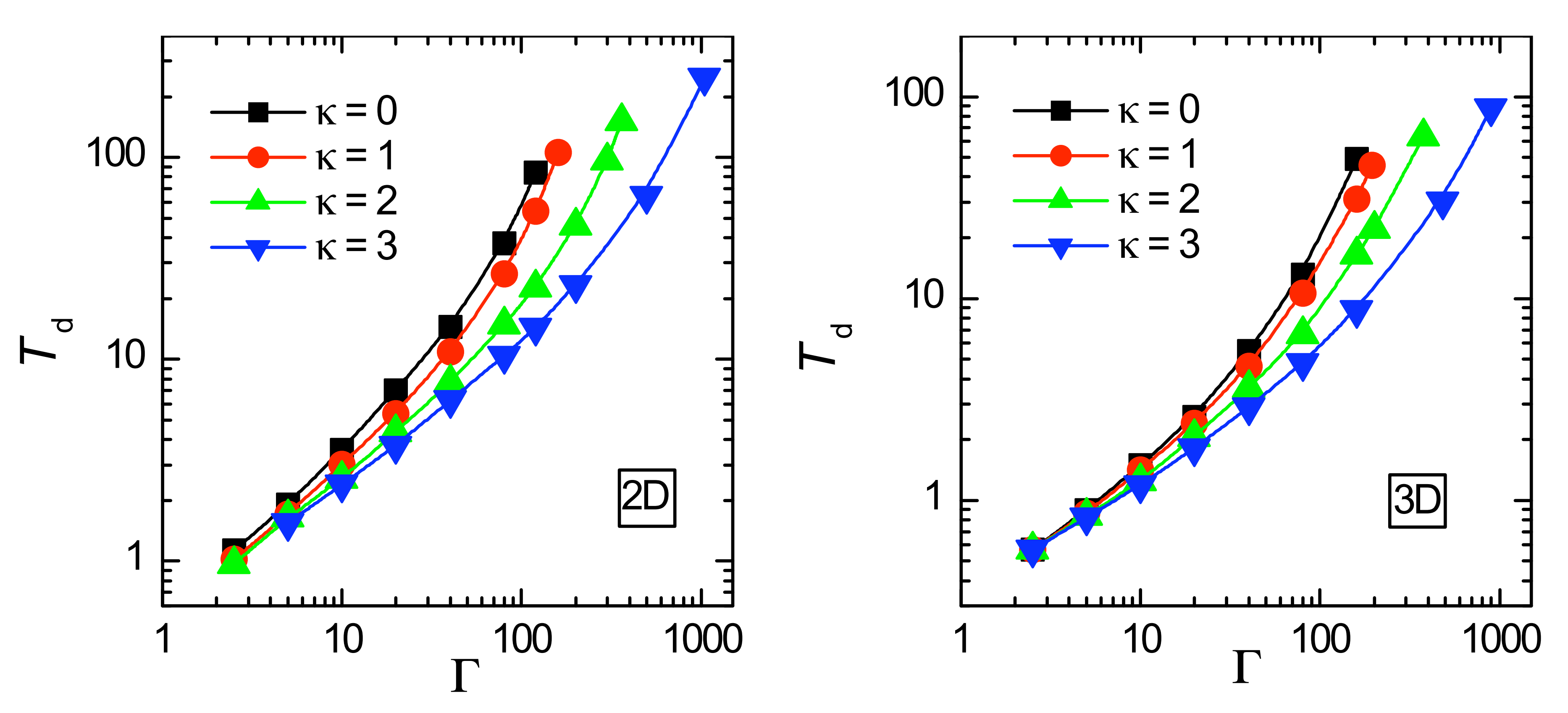
- Slow deformation of the potential surface due to particle diffusion

- Localized state covers several plasma oscillation cycles

Quantification:
CAGE CORRELATION FUNCTION

Quasi-localization in the strongly coupled liquid phase

Time needed for the *decorrelation* of the surroundings of the particles (in units of ω_p^{-1})



Localization covers several plasma oscillation cycles

Assumptions of QLCA tested

Z. Donkó, G.J. Kalman, K.I. Golden, Phys. Rev. Lett. 88, 225001 (2002),
Z. Donkó, P. Hartmann, G.J. Kalman, Physics of Plasmas 10, 1563 (2003).

The properties of the systems critically depend on the caging:

J. Daligault, "*Liquid-State Properties of a One-Component Plasma*",
Phys. Rev. Lett. 96, 065003 (2006)

Measurements of transport coefficients

Equilibrium Molecular Dynamics:

Measure correlation functions

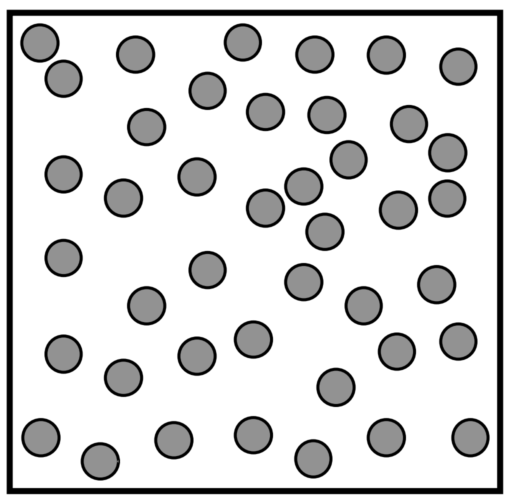
$D = \frac{1}{2}\int_0^\infty C_v \mathrm{d}t$	$C_v \equiv \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle$	VACF
$\eta = \frac{1}{VkT}\int_0^\infty C_\eta \mathrm{d}t$	$C_\eta \equiv \langle P_{xy}(t) P_{xy}(0) \rangle$	SACF
$\lambda = \frac{1}{VkT^2}\int_0^\infty C_\lambda \mathrm{d}t$	$C_\lambda \equiv \langle J_{Qx}(t) J_{Qx}(0) \rangle$	EACF

Non-Equilibrium Molecular Dynamics:

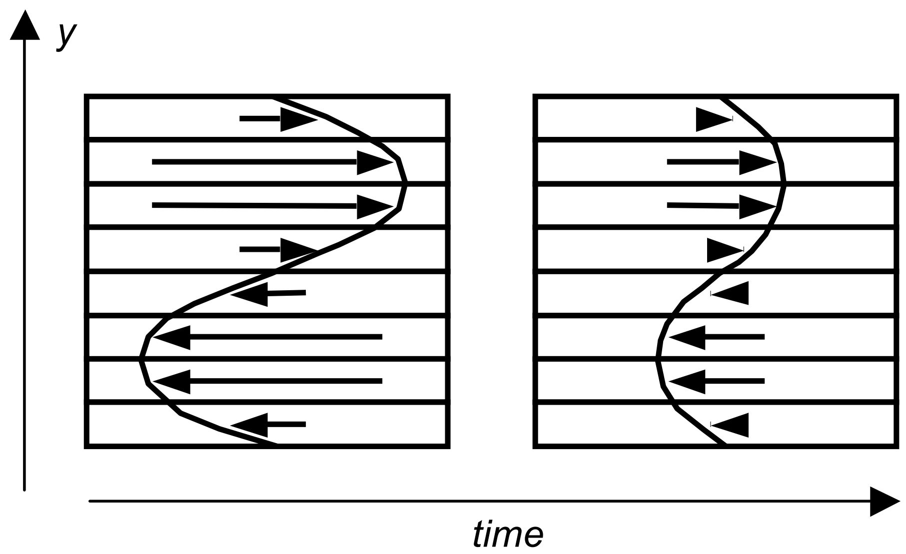
Perturb the system and measure the response

“Measurement” of transport coefficients: Shear viscosity

Equilibrium MD



Nonequilibrium (transient perturbation) MD



$$P^{xy} = \sum_{i=1}^{N}\left[m v_{ix} v_{iy} - \frac{1}{2}\sum_{j\neq i}^{N} \frac{x_{ij} y_{ij}}{r_{ij}} \frac{\partial \phi(r_{ij})}{\partial r_{ij}} \right]$$

$$\eta = \frac{1}{VkT}\int_0^\infty \langle P^{xy}(t) P^{xy}(0)\rangle \mathrm{d}t$$

$$W(y_k) = W_{M0}\sin\left(\frac{2\pi y_k}{L}\right) \qquad \frac{\partial v_x}{\partial t} = \frac{\eta}{\rho}\,\frac{\partial^2 v_x}{\partial y^2}$$

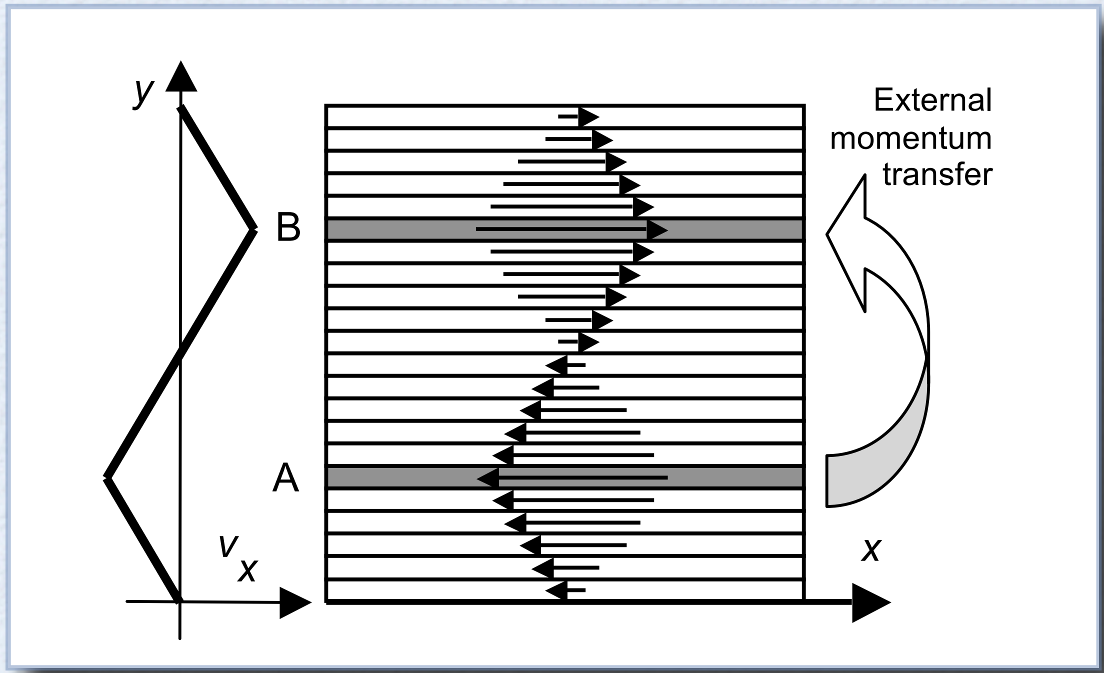
$$W(y,t) = W_{M0}\ \sin\left(\frac{2\pi y}{L}\right)\exp\left(-\frac{t-t_0}{\tau}\right)$$

$$\eta = \frac{\rho}{\tau}\left(\frac{L}{2\pi}\right)^2$$

Z. Donkó and B. Nyíri, Phys. Plasmas 7, 45 2000
K. Y. Sanbonmatsu and M. S. Murillo, Phys. Rev. Lett. 86, 1215 2001.

"Measurement" of transport coefficients: Shear viscosity

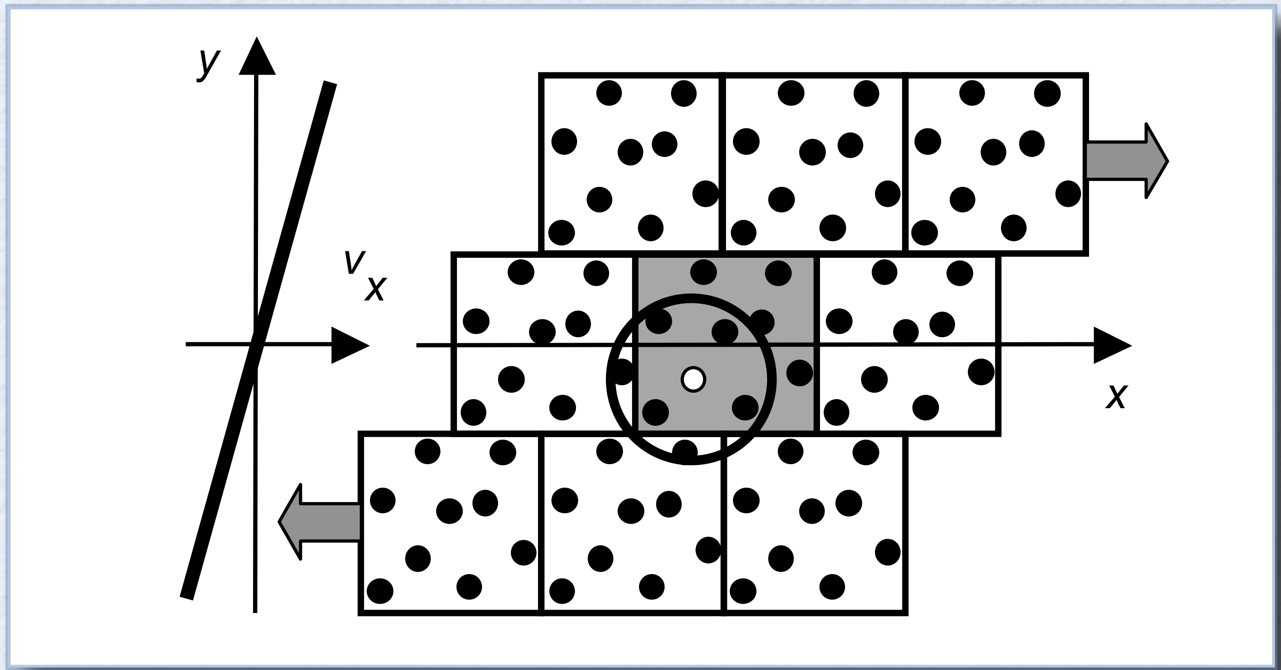
Reverse Molecular Dynamics



$$\eta \frac{dv_x(y)}{dy} = \frac{\Delta p}{2t_{\mathrm{sim}}S}$$

F. Müller-Plathe,
Phys. Rev. E 59, 4894 (1999).

Homogeneous Shear Algorithm

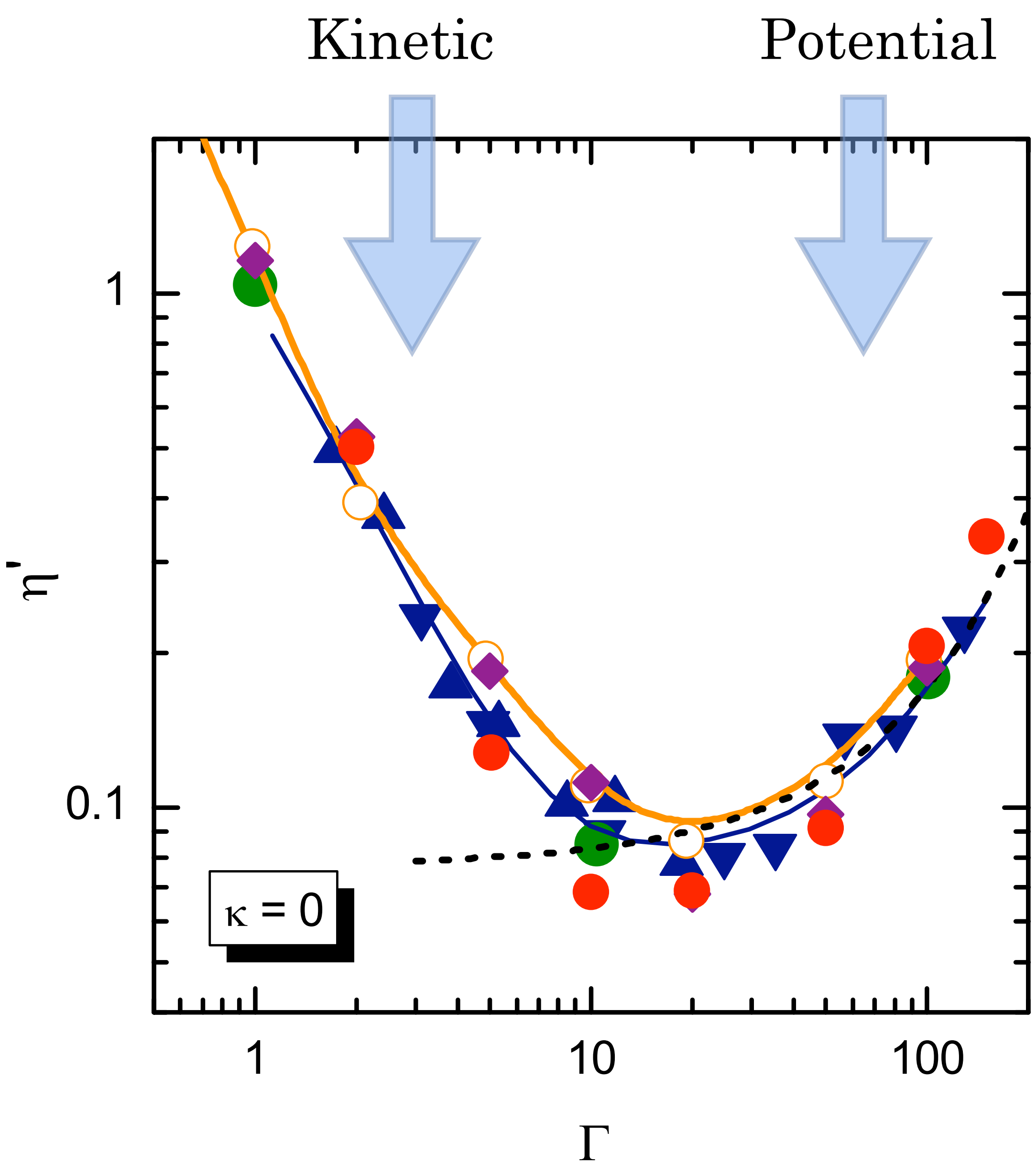


$$\frac{d\mathbf{r}_i}{dt} = \frac{\tilde{\mathbf{p}}_i}{m} + \gamma y_i \hat{\mathbf{x}} \qquad \frac{d\tilde{\mathbf{p}}_i}{dt} = \mathbf{F}_i - \gamma \tilde{p}_{yi}\hat{\mathbf{x}} - \alpha \tilde{\mathbf{p}}_i$$

$$\eta = -\lim_{t\to\infty} \frac{\langle P^{xy}(t)\rangle}{\gamma}$$

D. J. Evans and G. P. Morriss, "*Statistical mechanics of nonequilibrium liquids*" (Academic Press, 1990)

Shear viscosity of 3D Coulomb liquids



$$P^{xy} = \sum_{i=1}^{N} \left[m v_{ix} v_{iy} - \frac{1}{2} \sum_{j \neq i}^{N} \frac{x_{ij} y_{ij}}{r_{ij}} \frac{\partial \phi(r_{ij})}{\partial r_{ij}} \right]$$

Equilibrium MD:

- B. Bernu, P. Vieillefosse, and J. P. Hansen, Phys. Lett. A 63, 301 (1977); B. Bernu and P. Vieillefosse, Phys. Rev. A 18, 2345 (1978)
- S. Bastea, Phys. Rev. E 71, 056405 (2005)
- J. Daligault, Phys. Rev. Lett. 96, 065003 (2006) (Scaled) high Γ Arrhenius fit
- G. Salin and J.-M. Caillol, Phys. Rev. Lett. 88, 065002 (2002); G. Salin and J.-M. Caillol, Phys. Plasmas 10, 1220 (2003) (κ = 0.01)
- T. Saigo and S. Hamaguchi, Phys. Plasmas 9, 1210 (2002) (κ = 0.1)

Transient perturbation MD:

- Donkó & Nyiri (*N* = 8192) Phys. Plasmas 7, 45 (2000) (*N* = 8192)
- Donkó & Nyiri (*N* = 8192) Phys. Plasmas 7, 45 (2000) (*N* = 1024)

$$\eta' = \frac{\eta}{m n \omega_{\mathrm{p}} a^2}$$

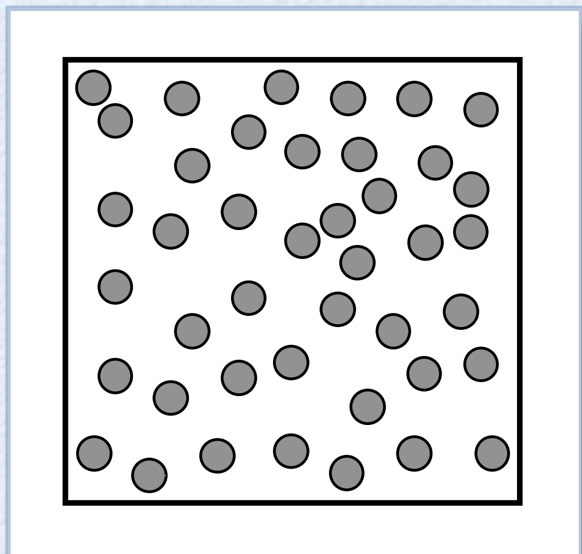
Complex shear viscosity of 3D Coulomb liquids

$$\boxed{\eta(\omega) = \eta'(\omega) - i\eta''(\omega)}$$

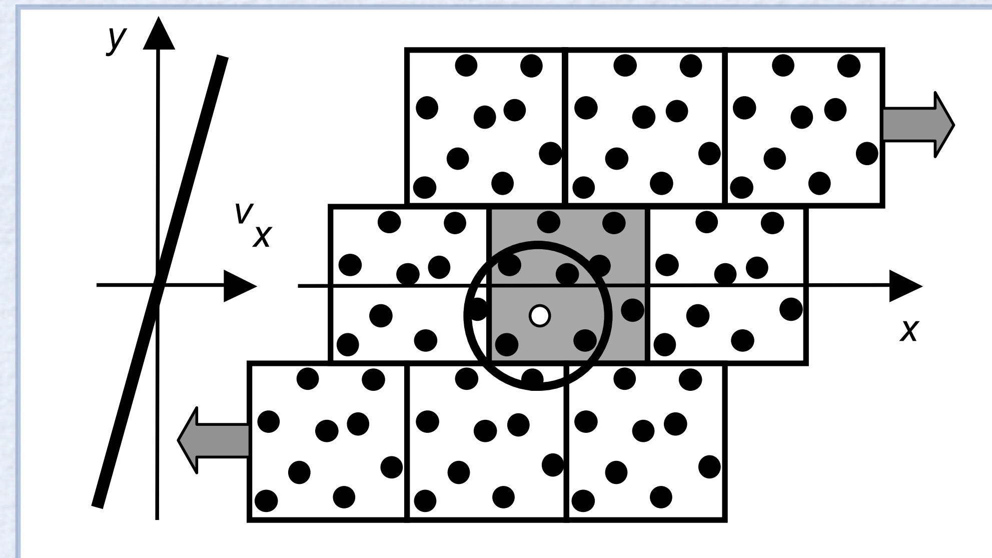
Viscous dissipation

Elasticity

Equilibrium MD



Homogeneous Shear Algorithm



$$P_{xy} = \sum_{i=1}^{N}\left[m v_{ix} v_{iy} - \frac{1}{2}\sum_{j\neq i}^{N} \frac{x_{ij} y_{ij}}{r_{ij}} \frac{\partial \phi(r_{ij})}{\partial r_{ij}} \right]$$

$$C_\eta(t) = \langle P_{xy}(t) P_{xy}(0) \rangle$$

$$\boxed{\eta(\omega) = \frac{1}{VkT}\int_0^\infty C_\eta(t) e^{\mathrm{i}\omega t}\mathrm{d}t}$$

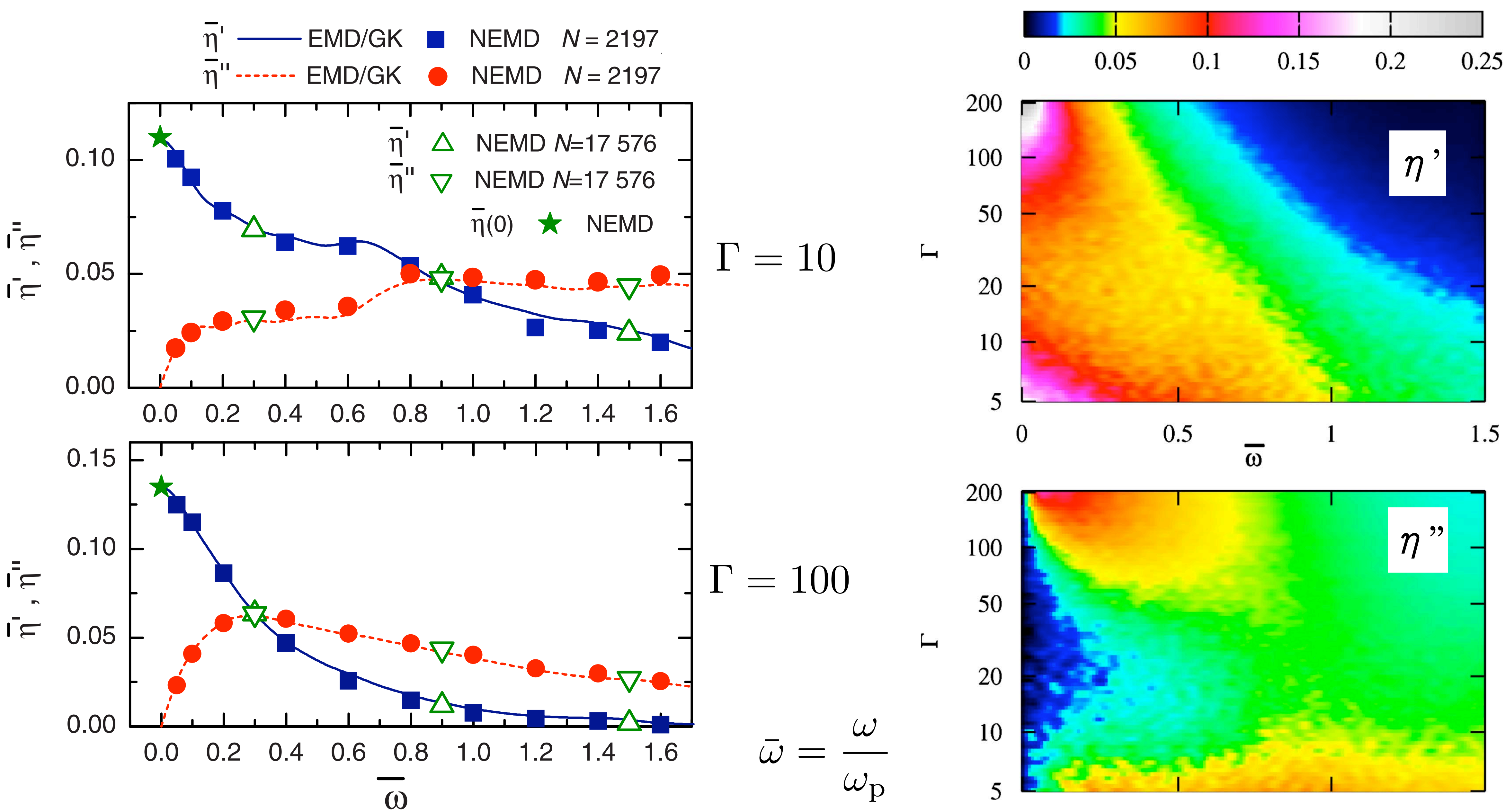
Laplace-Fourier transform
in the GK integral

$$\frac{d\mathbf{r}_i}{dt} = \frac{\tilde{\mathbf{p}}_i}{m} + \gamma y_i \hat{\mathbf{x}} \qquad \frac{d\tilde{\mathbf{p}}_i}{dt} = \mathbf{F}_i - \gamma \tilde{p}_{yi}\hat{\mathbf{x}} - \alpha \tilde{\mathbf{p}}_i$$

$$\boxed{\gamma(t) = \gamma_0 \cos(\omega t)}$$

Harmonic shear perturbation,
measure *phase* and *amplitude* of P_{xy}

Complex shear viscosity of 3D Yukawa liquids

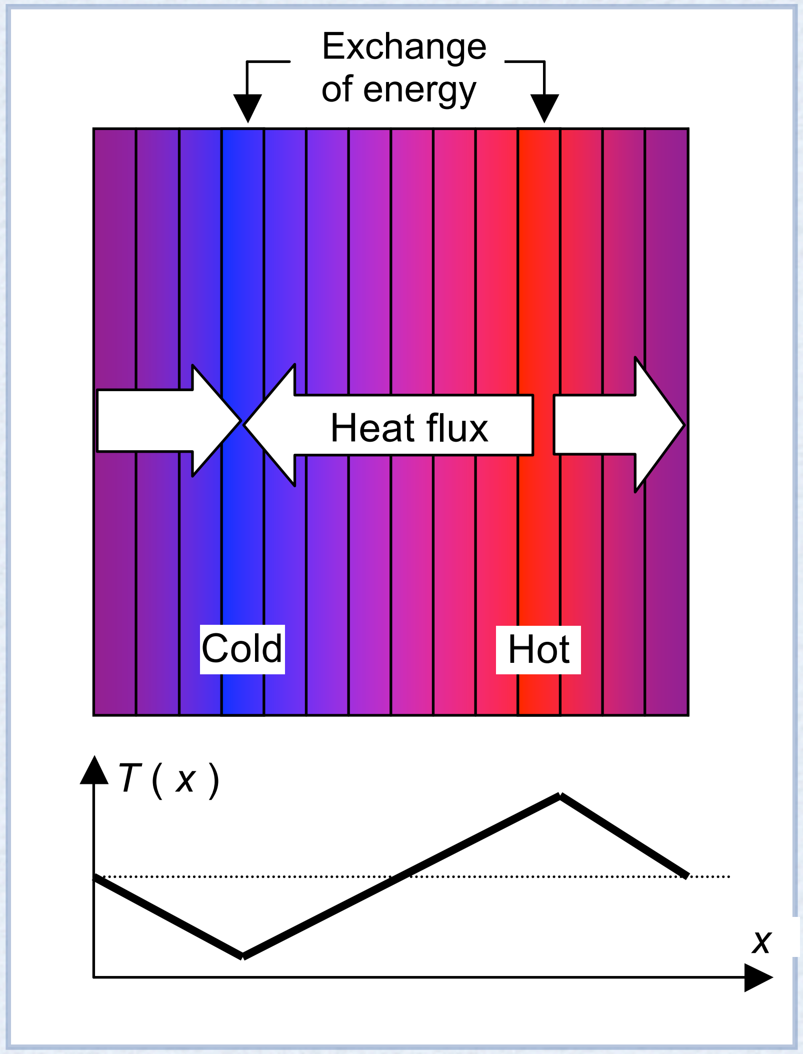


Viscous → elastic transition

Z. Donkó, J. Goree, H. Hartmann, Phys. Rev. E 81, 056404 (2010)

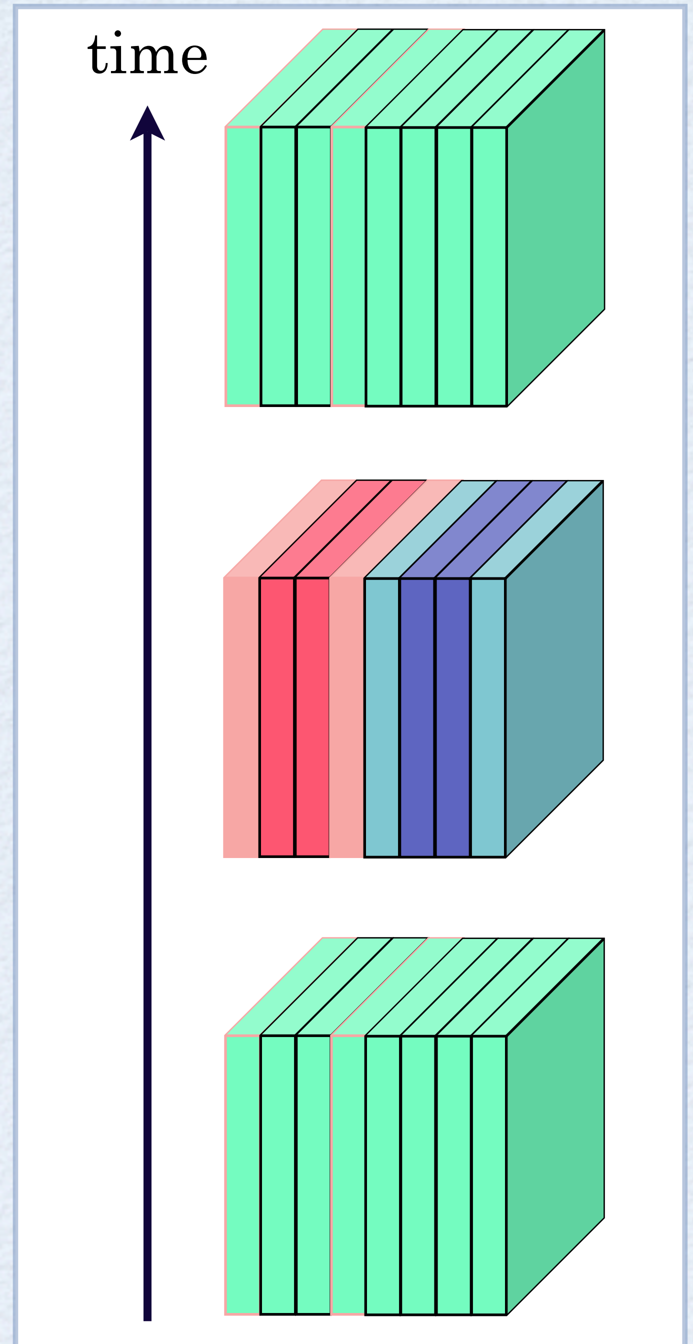
Thermal conductivity: MD methods

Reverse molecular dynamics



$$\lambda = \frac{\Delta E}{2 S t_{\mathrm{sim}} \langle \frac{\Delta T}{\Delta x} \rangle}$$

F. Müller-Plathe,
J. Chem. Phys. 106, 6082 (1997).



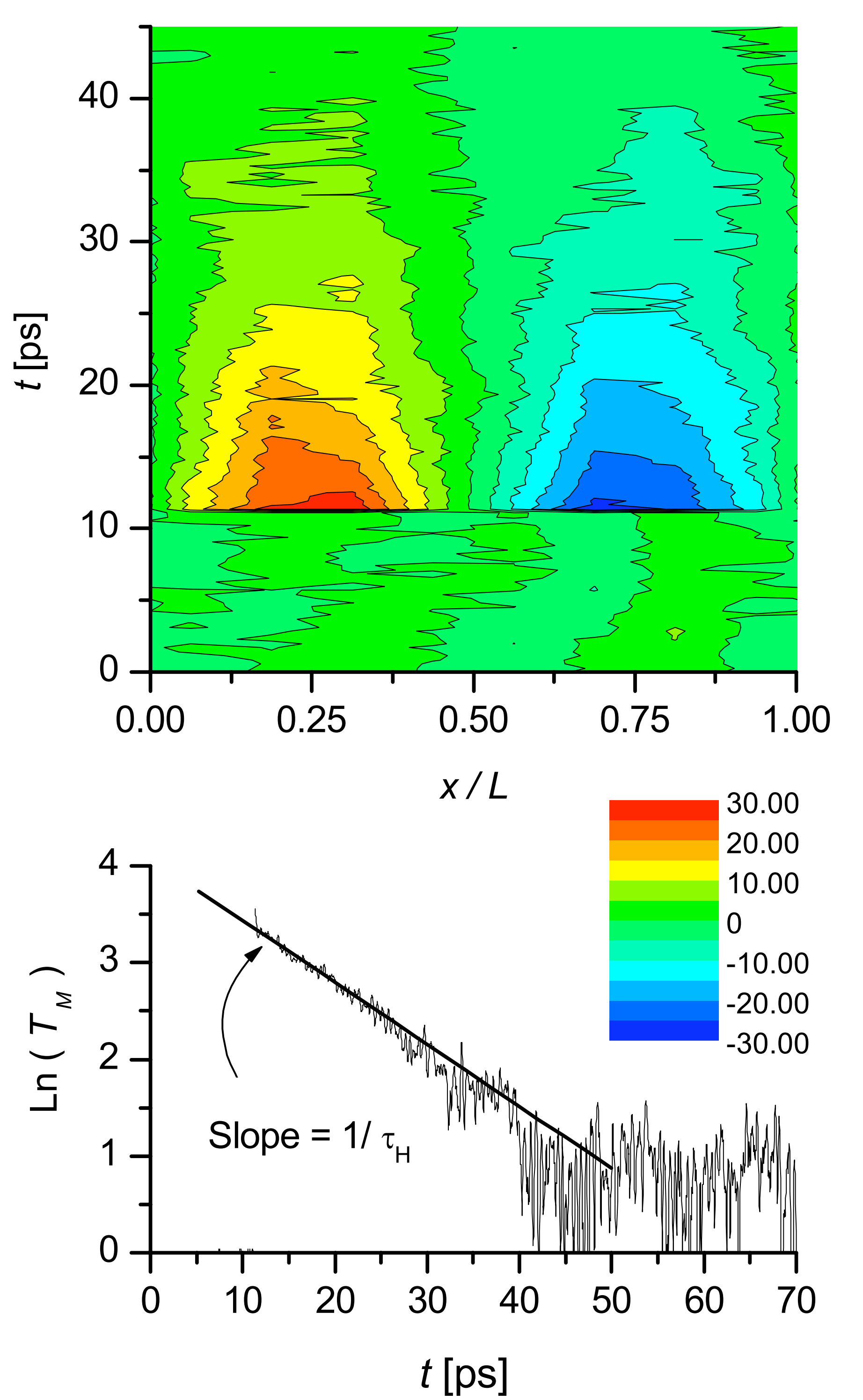
Spatial temperature modulation

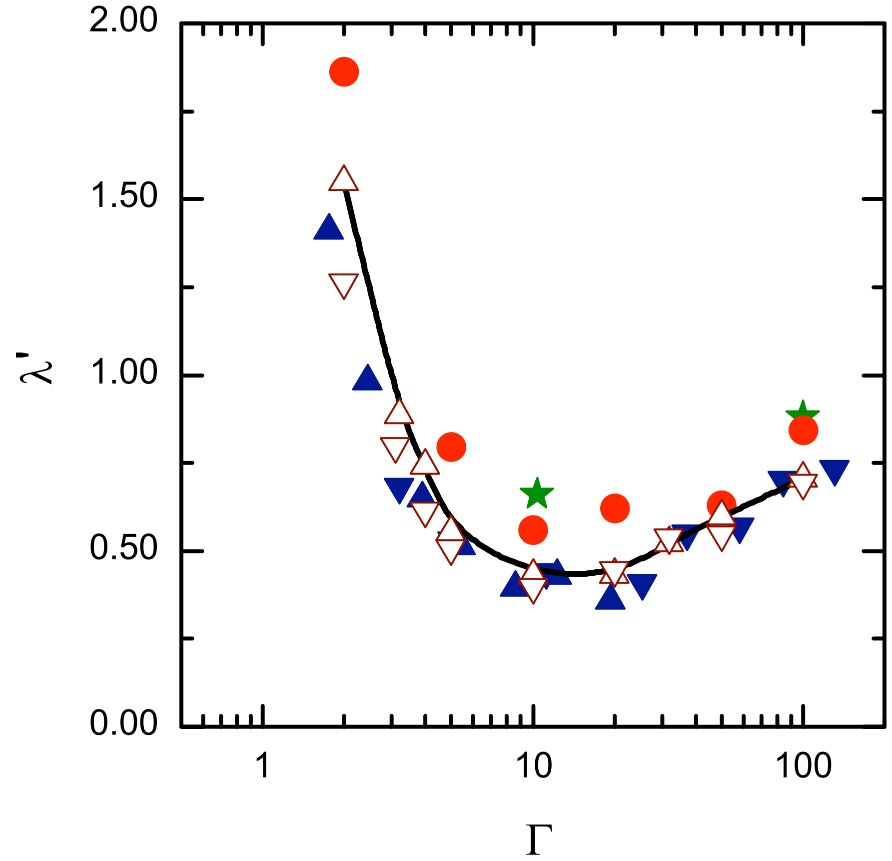
$$\frac{\partial T}{\partial t} = \frac{\lambda}{c\rho} \frac{\partial^2 T}{\partial x^2}$$

$$\lambda = \frac{c\rho}{\tau_{\mathrm{H}}} \left(\frac{L}{2\pi} \right)^2$$

Z. Donkó, B. Nyíri, L. Szalai, and S. Holló,
Phys. Rev. Lett. 81, 1622 (1998).

Thermal conductivity of 3D Coulomb liquids





$$\lambda' = \frac{\lambda}{nk\omega_{\mathrm{p}}a^2}$$

★ B. Bernu, P. Vieillefosse, and J. P. Hansen, Phys. Lett. 63A, 301 (1977);
B. Bernu and P. Vieillefosse Phys. Rev. A , 2345 (1978)

Z. Donko, B. Nyiri, L. Szalai and S. Hollo, Phys. Rev. Lett. 81, 1622 (1998);
Z. Donko and B. Nyiri, Phys. Plasmas , 45 (2000) 8192
▲ N=8192
▼ N=1024

● G. Salin and J.-M. Caillol, Phys. Rev. Lett. 88, 065002 (2002);
G. Salin and J.-M. Caillol, Phys. Plasmas 10, 1220 (2003)
N=128 ... 864, κ = 0.01

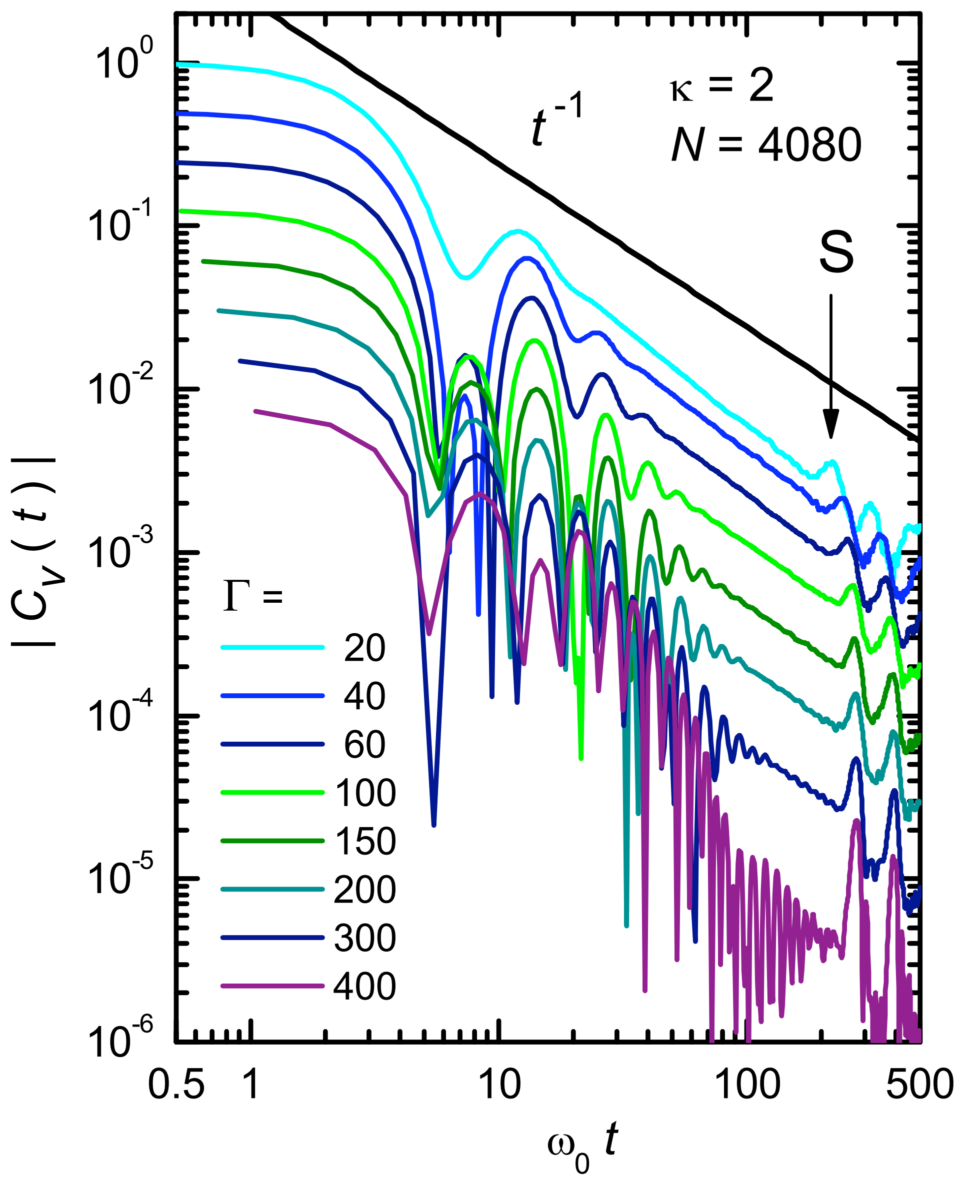
Z. Donko and P. Hartmann, Phys. Rev. E 69, 016405 (2004).
—△— N=6400, κ = 0.1
▽ N=1600, κ = 0.1

Transport in 2 dimensional Yukawa liquids

$D = \frac{1}{2}\int_0^\infty C_v \mathrm{d}t$	$C_v \equiv \langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle$	VACF
$\eta = \frac{1}{VkT}\int_0^\infty C_\eta \mathrm{d}t$	$C_\eta \equiv \langle P_{xy}(t)P_{xy}(0)\rangle$	SACF
$\lambda = \frac{1}{VkT^2}\int_0^\infty C_\lambda \mathrm{d}t$	$C_\lambda \equiv \langle J_{Qx}(t)J_{Qx}(0)\rangle$	EACF

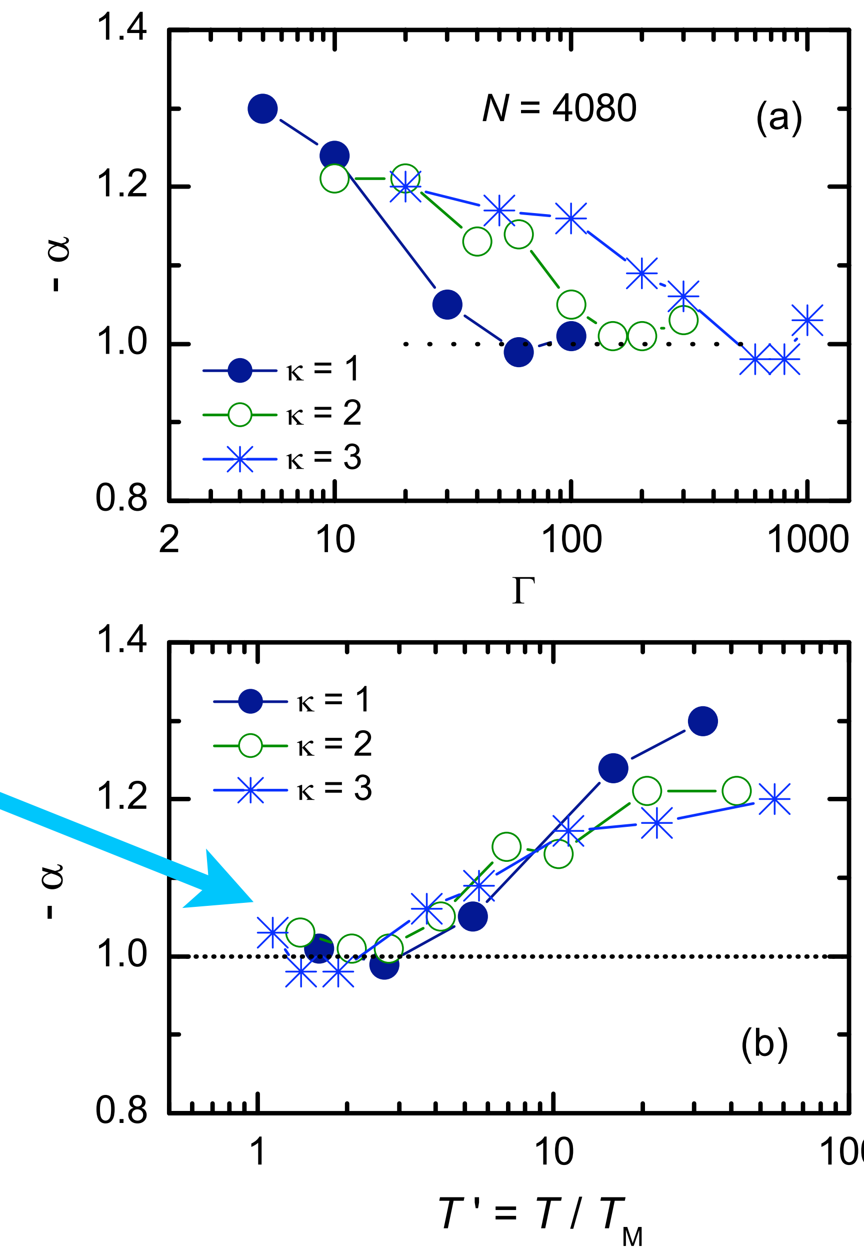
- Motivation: experiments on 2D systems - indicate superdiffusion
- Alder and Wainwright [Phys. Rev. A 1, 18 (1970)] observed t^{-1} decay of the VACF in computer simulations of 2D hard disk system.
- Ernst, Hauge, and van Leeuwen [Phys. Rev. Lett. 25, 1254 (1970)] have shown that the kinetic contributions to the autocorrelation functions of shear stress and energy current exhibit the same behavior.
- This implies that the transport coefficients do not exist in 2D..... BUT : Isobe [Phys. Rev. E 2008] → large scale simulation of hard disk fluid: the decay of the VACF is *slightly* faster than 1/t for a range parameters of the system!
- DO UNIQUE TRANSPORT COEFFICIENTS EXIST FOR 2D YUKAWA LIQUIDS ???

Diffusion: Velocity autocorrelation function (2D)



Need big system especially at high Γ and low κ

SUPERDIFFUSION at low temperature

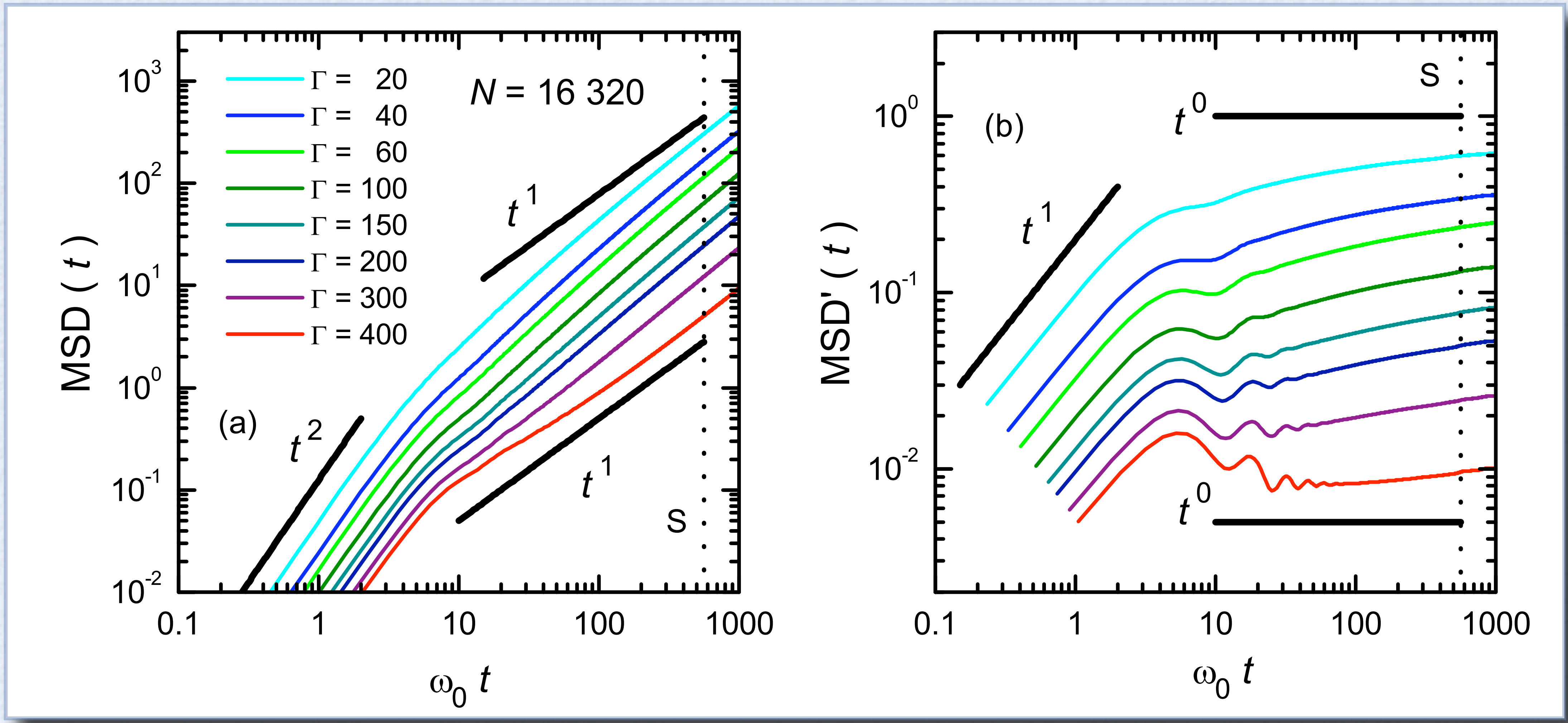


Features: initial oscillations (caging) + smooth decay + sound peaks ("S")

Z. Donkó, J. Goree, P. Hartmann, and Bin Liu, Phys. Rev. E 79, 026401 (2009)

2D Transport: mean squared displacement

$$\mathrm{MSD}(t) = \langle\ |\mathbf{r}(t) - \mathbf{r}(0)|^2\ \rangle \qquad D = \frac{1}{2N_d\ t}\langle\ |\mathbf{r}(t) - \mathbf{r}(0)|^2\ \rangle$$



Z. Donkó, J. Goree, P. Hartmann, Bin Liu, Phys. Rev. E 79, 026401 (2009)

Conclusion (2009):

- looks to be superdiffusion within time limit
- longer time: “ who knows ...?? ”

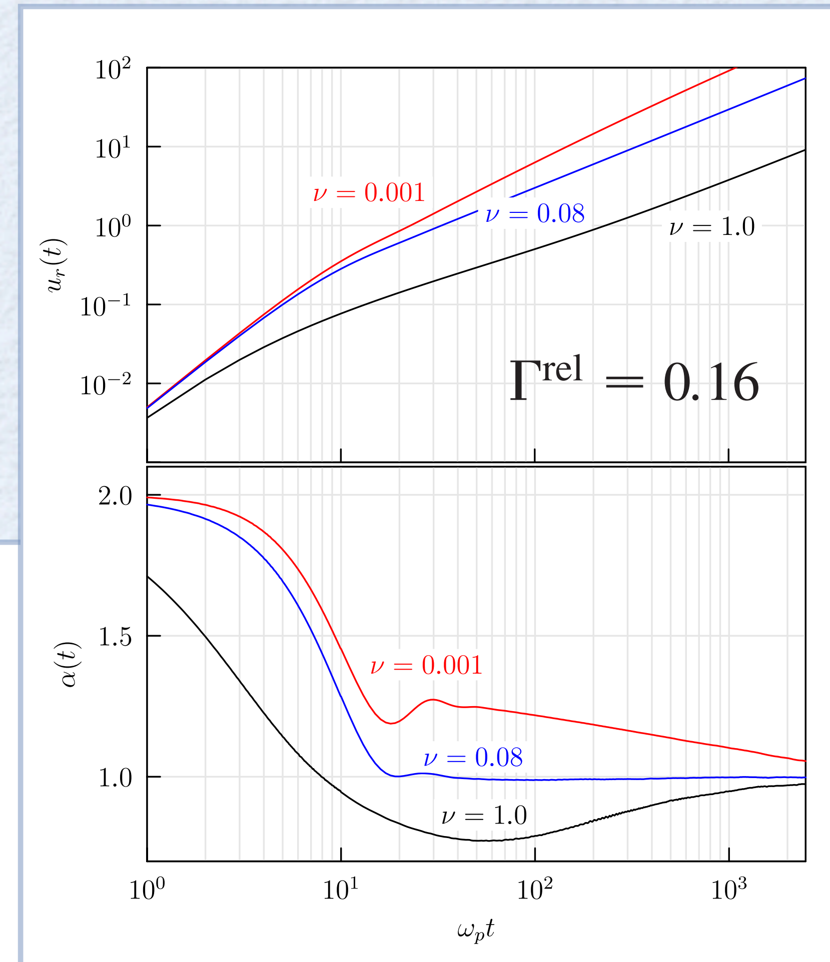
2D diffusion: latest news

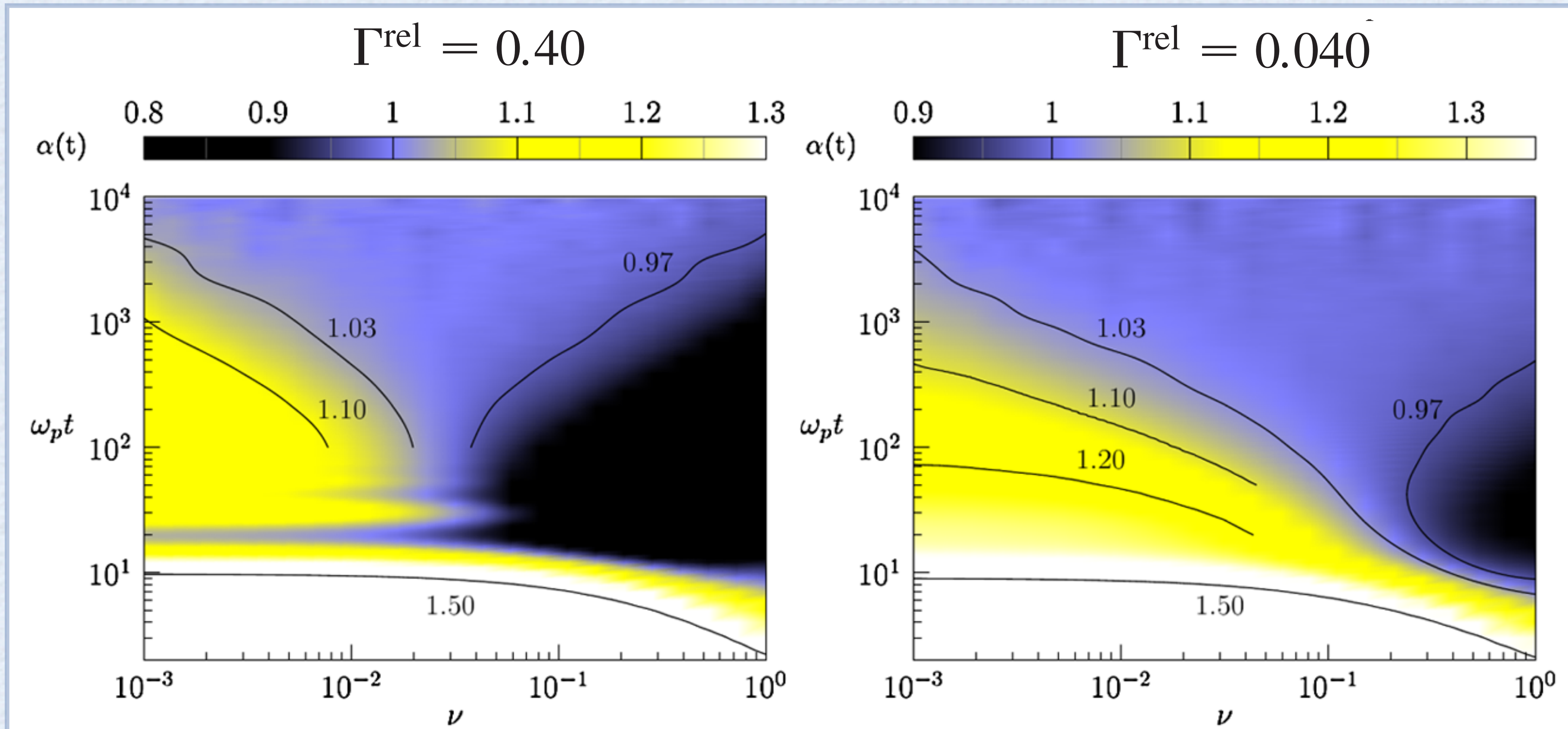
PRL **103,** 195001 (2009) PHYSICAL REVIEW LETTERS week ending 6 NOVEMBER 2009

Is Diffusion Anomalous in Two-Dimensional Yukawa Liquids?

T. Ott and M. Bonitz

- Tendency towards normal diffusion at long times
- Relation to dusty plasma experiments (timescale, equilibrium)
- *Accuracy of MD at long times???*

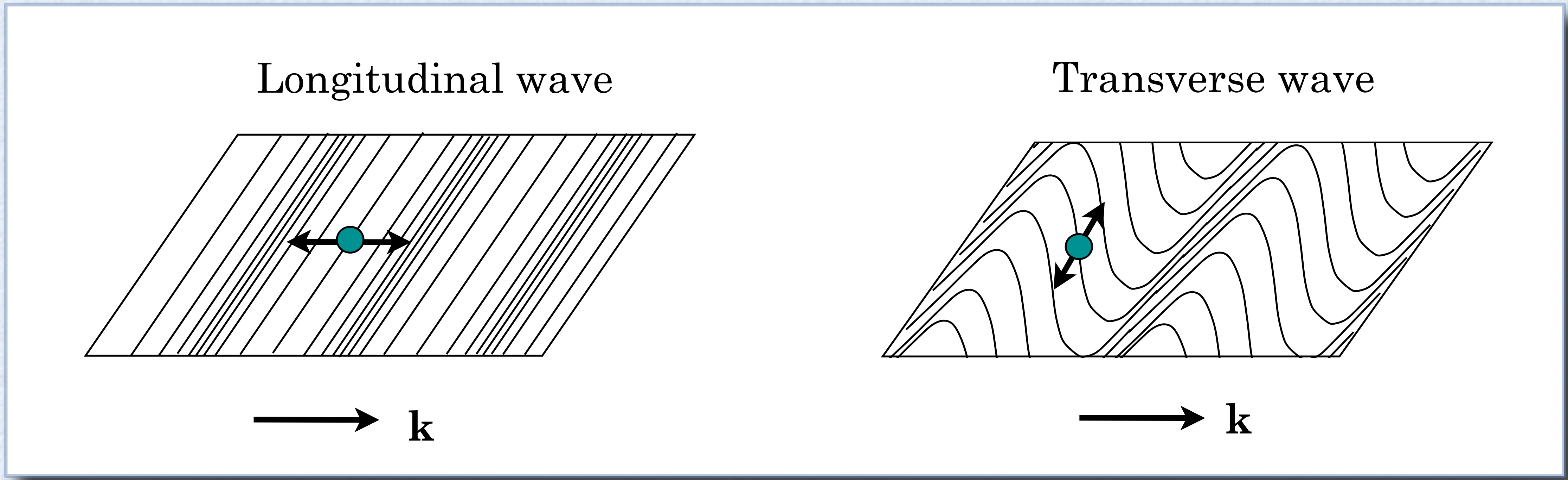




$$\Gamma^{\mathrm{rel}} = \Gamma/\Gamma_c$$

Collective excitations

Collective excitations in 3D liquids



Microscopic density fluctuations: → Dynamical structure function:

$$\rho(k,t) = \sum_{j=1}^{N} \exp\left[ikx_j(t)\right]$$

$$S(k,\omega) = \frac{1}{2\pi N} \lim_{\Delta T \to \infty} \frac{1}{\Delta T} |\rho(k,\omega)|^2 \qquad \rho(k,\omega) = \mathcal{F}\left[\rho(k,t)\right]$$

Microscopic current fluctuations: → Longitudinal and transverse current-current fluctuation spectra

$$\lambda(k,t) = \sum_{j=1}^{N} v_{jx}(t) \exp\left[ikx_j(t)\right]$$

$$\tau(k,t) = \sum_{j=1}^{N} v_{jy}(t) \exp\left[ikx_j(t)\right]$$

$$L(k,\omega) \qquad T(k,\omega)$$

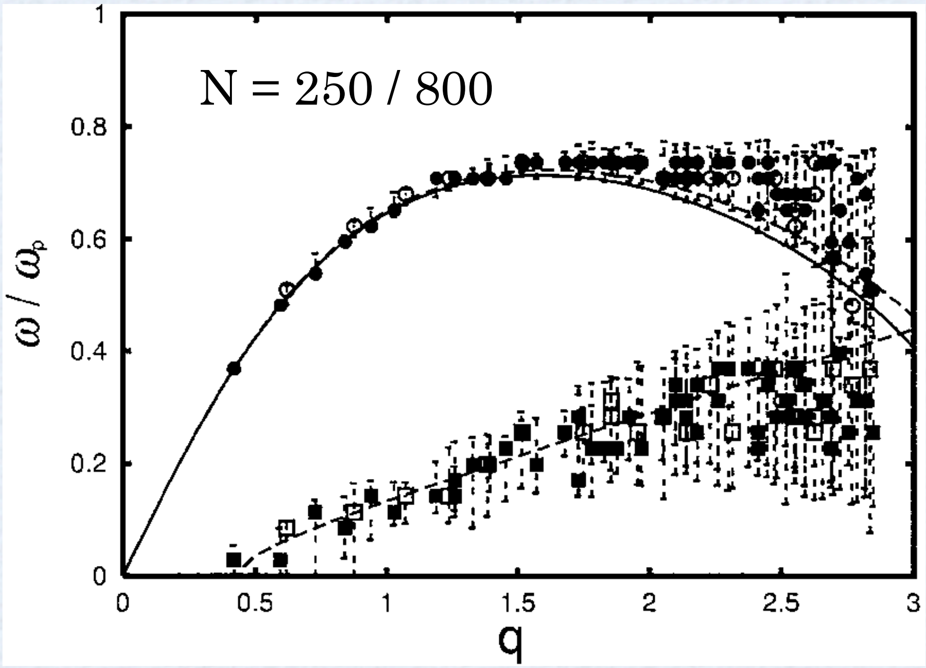
Collective excitations in 3D liquids

QLCA theory:

G. Kalman, M. Rosenberg, and H. E. DeWitt, Phys. Rev. Lett. 84, 6030 - 6033 (2000)

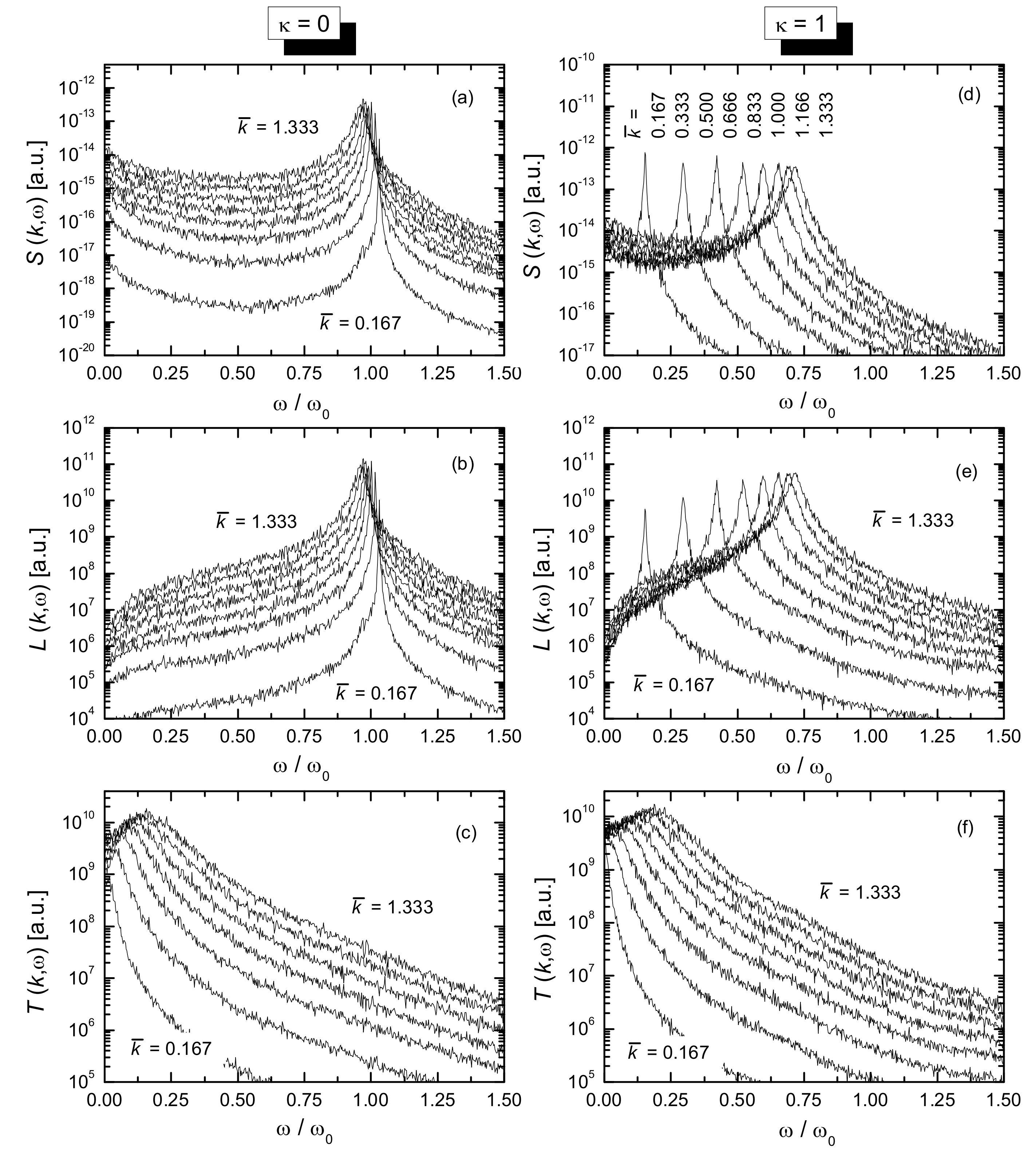
First MD simulations

H. Ohta & S. Hamaguchi, Phys. Rev. Lett. 84, 6026 (2000)

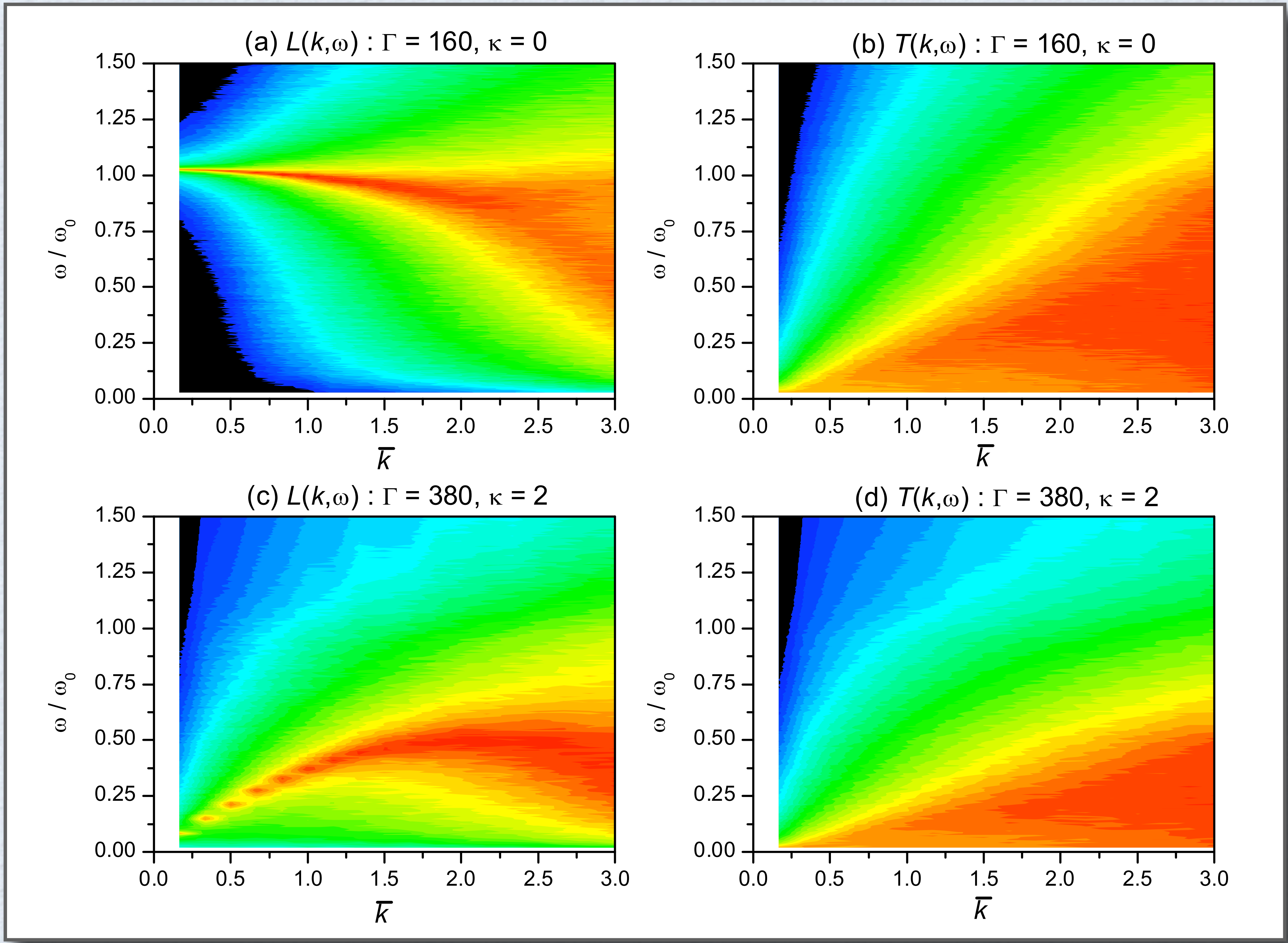


Z. Donkó, G. J. Kalman & P. Hartmann, J. Phys. Cond. Matter 20, 413101 (2008)

$N = 12800$



Collective excitations in 3D liquids



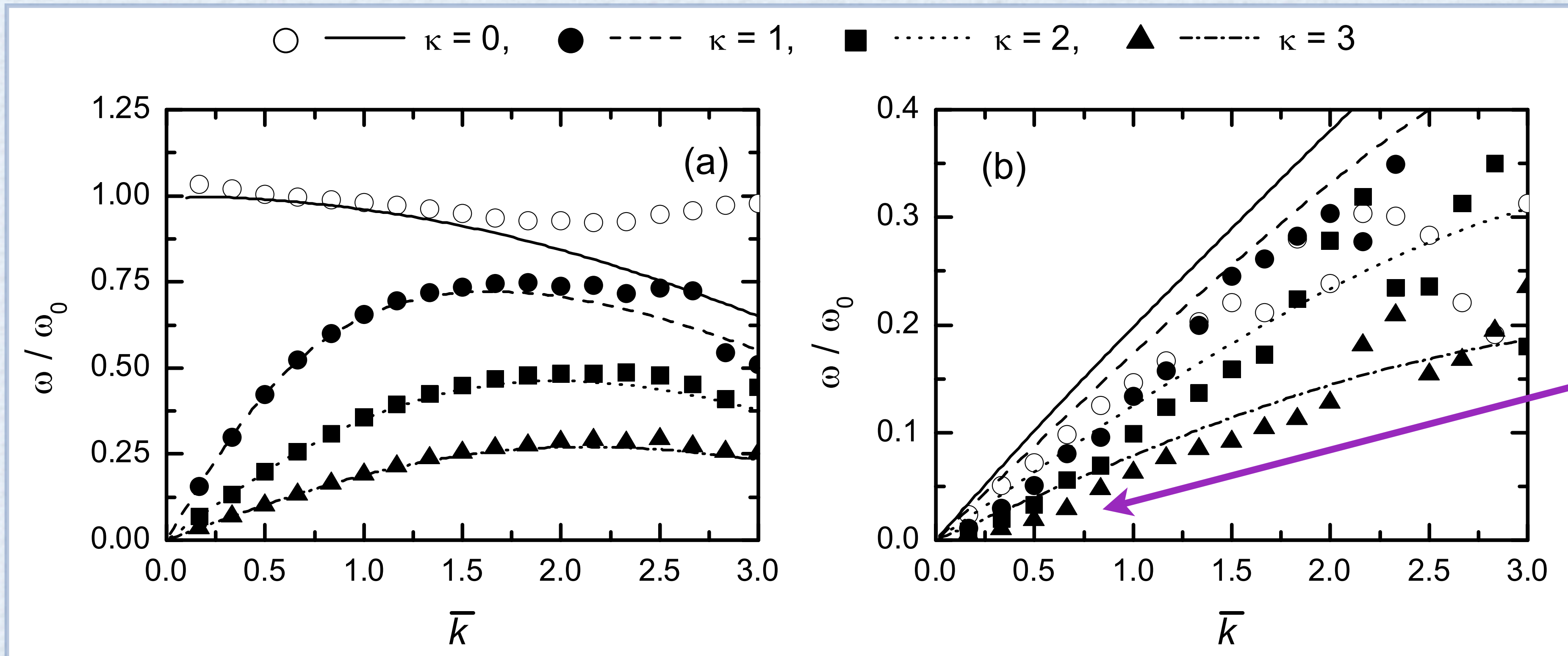
Coulomb:

L : const. freq.
T : acoustic

Yukawa:

L : quasi-acoustic
T : acoustic

Collective excitations in 3D liquids: MD vs. theory



Cutoff of T-mode at finite k: liquid

M.S. Murillo Phys. Rev. Lett. 85, 2514 (2000)

EXP: J. Goree

QLCA theory:

$$\Omega_{\rm L}^2(\mathbf{k}) = \Omega_0^2(\mathbf{k}) + \omega_{0,\rm 3D}^2 \frac{\bar{k}^2}{2} \int_0^\infty \Lambda^{\rm 3D}\left(\bar{k}\bar{r}, \kappa\bar{r}\right) h(\bar{r}) {\rm d}\bar{r} \qquad \Omega_0^2(\mathbf{k}) = \omega_{0,\rm 3D}^2 \frac{\bar{k}^2}{\bar{k}^2+\kappa^2}$$

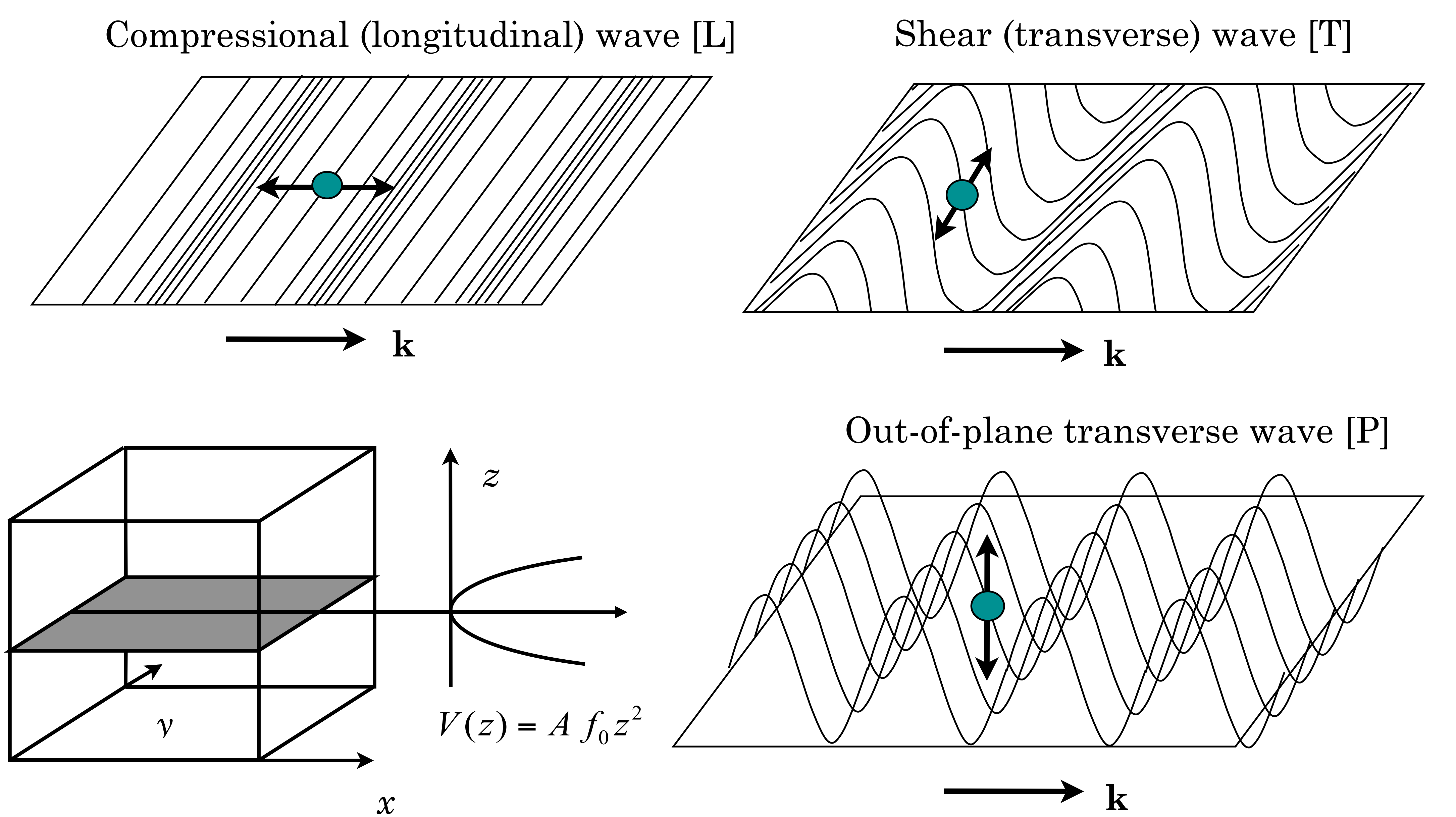
$$\Omega_{\rm T}^2(\mathbf{k}) = \omega_{0,\rm 3D}^2 \frac{\bar{k}^2}{2} \int_0^\infty \Theta^{\rm 3D}\left(\bar{k}\bar{r}, \kappa\bar{r}\right) h(\bar{r}) {\rm d}\bar{r}$$

$$\Lambda^{\rm 3D}(x,y) = -2\frac{{\rm e}^{-y}}{x}\left[\left(1+y+y^2\right)\left(\frac{\sin(x)}{x} + 3\frac{\cos(x)}{x^2} - 3\frac{\sin(x)}{x^3}\right) - \frac{y^2}{6}\left(1 + 3\frac{\sin(x)}{x} + 12\frac{\cos(x)}{x^2} - 12\frac{\sin(x)}{x^3}\right)\right]$$

$$\Theta^{\rm 3D}(x,y) = \frac{1}{2}\left[\frac{{\rm e}^{-y}}{x} y^2 \left(1 - \frac{\sin(x)}{x}\right) - \Lambda^{\rm 3D}(x,y)\right]$$

Z. Donkó, G. J. Kalman & P. Hartmann, J. Phys. Cond. Matter 20, 413101 (2008)

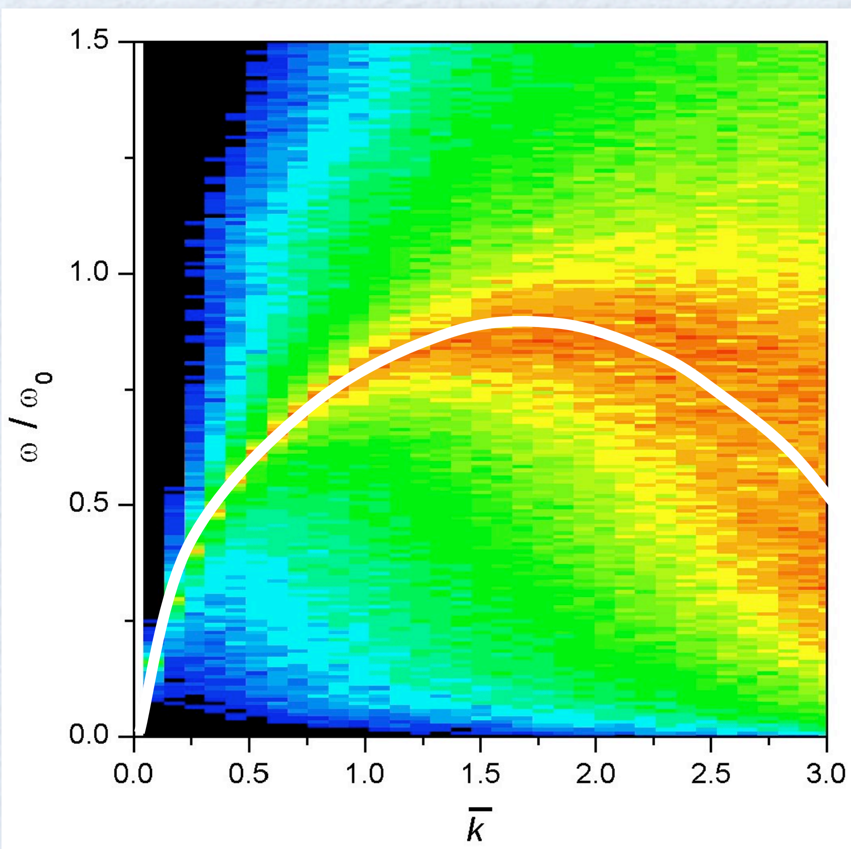
Collective excitations in a quasi-2D liquid



Collective excitations in a quasi-2D liquid

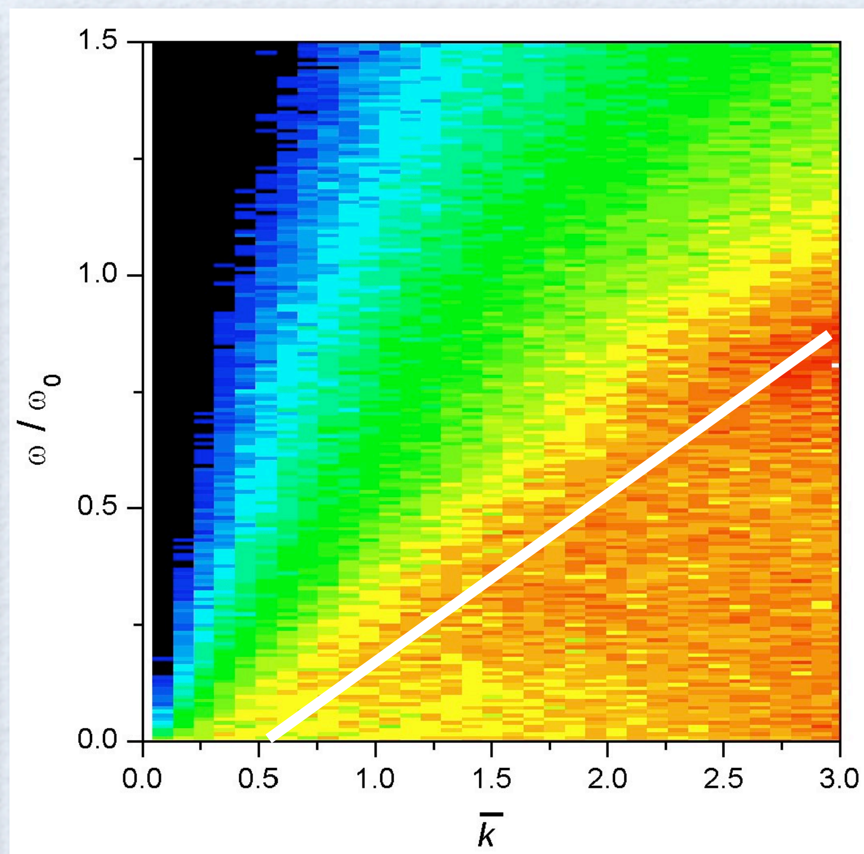
Γ= 100,   κ = 0.27

Longitudinal mode



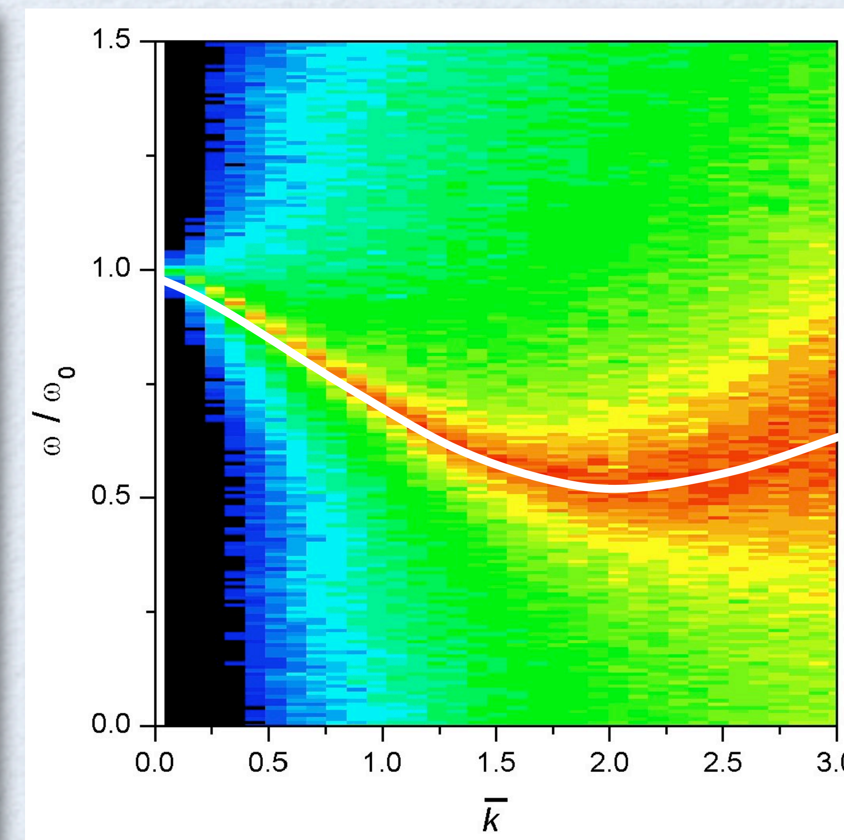
L : quasi-acoustic

In-plane transverse mode



T : acoustic

Out-of-plane transverse mode



P : optical

Z. Donkó, P. Hartmann, G. J. Kalman, M. Rosenberg, Contrib. Plasma Phys. 43, 282-284 (2003).
G. J. Kalman, P. Hartmann, Z. Donkó, M. Rosenberg, Phys. Rev. Lett. 92, 065001 (2004).

Summary

- Simulation studies aid the understanding of theoretical and experimental results
- Simulations are suitable for a wide variety of strongly coupled many-particle systems
- Equilibrium / non-equilibrium Molecular Dynamics simulations can be used to study
  - structural & thermodynamical properties
  - collective excitations
  - localization and transport
  - ... and numerous other physical phenomena

THANK YOU FOR YOUR ATTENTION