# Dynamics in random fields of hard and soft spheres

Kay Kirkpatrick
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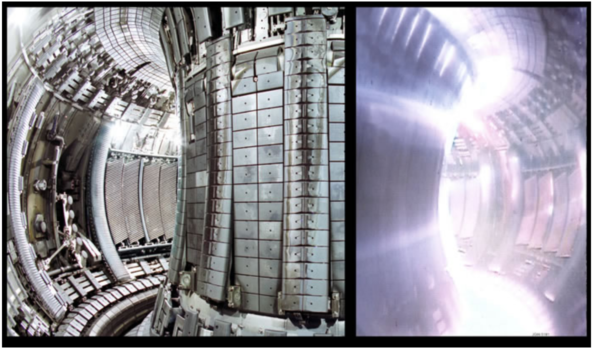

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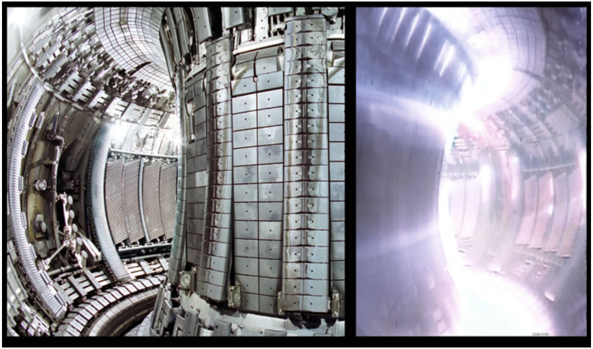

Joint work in progress with Fraydoun Rezakhanlou (Berkeley).

# Motivation

Boltzmann (1890s): Predicted the equation for dilute (ideal) gas.

Landau (1954): Predicted the equation for plasma (ionized gas).

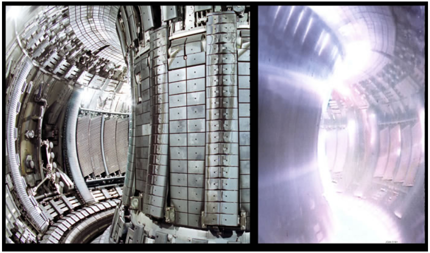

Figure: Fusion reactor empty and running. (Courtesy of EFDA-JET)

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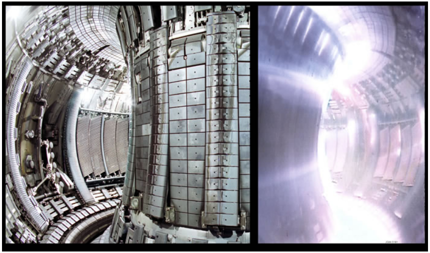

Figure: Fusion reactor empty and running. (Courtesy of EFDA-JET)

JET (Joint European Torus) produced 16 MW for under a second.
ITER may produce 500 MW for up to 1,000 seconds in 2018.

# Outline

- One particle in a random field of hard spheres $\rightsquigarrow$ Boltzmann equation (dilute gas)
- A tagged particle in the full hard-sphere model

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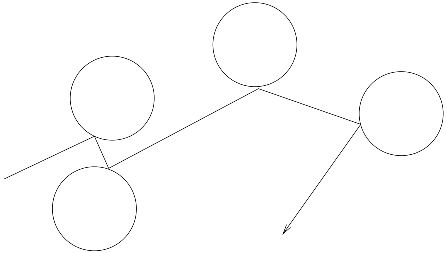
- One particle in a random field of hard spheres $\rightsquigarrow$ Boltzmann equation (dilute gas)
- A tagged particle in the full hard-sphere model
- One particle in a random field of soft spheres $\rightsquigarrow$ Landau equation (plasma)
- Outlook: the full soft-sphere model and plasma-surface interactions

# The one-particle microscopic models

A point particle moves through a field of identical, stationary, randomly distributed hard spheres of radius $\varepsilon$ going to 0.



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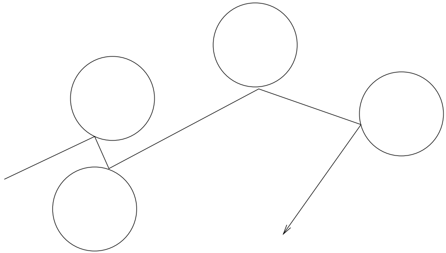

Another motivation: Drude-Lorentz model of electrons in metals. Collisions between electrons and metallic atoms are significant, but electron-electron collisions are neglected.

# The main difficulties

The conceptual difficulty is the apparent disparity between the microscopic reversibility and determinism, and the macroscopic irreversibility and randomness.

- Average over all allowable configurations of obstacles.
- Many microscopic degrees of freedom are integrated out.

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- Take a low-density limit in the hard-sphere model.
- Preview of soft spheres: Make each collision almost imperceptible (the weak coupling limit).

# The reduced hard-sphere model of a dilute gas

The microscopic equations of motion are Newtonian:

$$\begin{cases} \dot{x}^\varepsilon = v^\varepsilon, & x^\varepsilon(0) = x, \\ \dot{v}^\varepsilon = -\sum_{i=1}^{\infty} \nabla V^\varepsilon(x^\varepsilon(t) - r_i), & v^\varepsilon(0) = v. \end{cases}$$

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- $\varepsilon$ is the radius of the obstacles (and will go to zero)
- $\omega = \{r_i\}_{i=1}^{\infty}$ is a Poisson point process with density $\mu_\varepsilon = \mu\varepsilon^{1-d}$. In the tube of radius $\varepsilon$ that the particle sweeps out in one unit of time, there are about $\varepsilon^{1-d} \cdot \varepsilon^d = \varepsilon$ obstacles (low density).
- The rescaled potential is:

$$V^\varepsilon(x - r_i) = V\left(\frac{|x - r_i|}{\varepsilon}\right) := \begin{cases} \infty & \text{if } |x - r_i| \leq \varepsilon, \\ 0 & \text{else.} \end{cases}$$

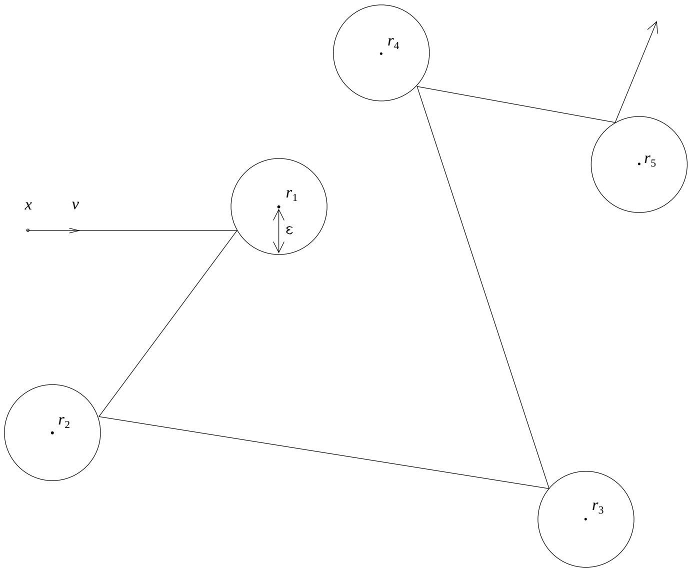


Figure: A trajectory for the microscopic hard-sphere model.

# The Boltzmann-Grad limit

Gallavotti (1973): If $(x^\varepsilon(t), v^\varepsilon(t))$ is the family of solutions to the microscopic model with initial conditions $(x, v)$, and $f_0$ is a suitable distribution of starting points $x$ and velocities $v$, then in the Boltzmann-Grad limit:

$$\mathbb{E}^\omega f_0(x^\varepsilon(t), v^\varepsilon(t)) \xrightarrow{\varepsilon \to 0} f(x, v, t),$$

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$$\begin{cases} \partial_t f + v \cdot \nabla_x f = \int_{S^1} [v \cdot \theta]^+ [f(x, R_\theta(v), t) - f(x, v, t)] d\theta \\ \qquad f(x, v, 0) = f_0(x, v). \end{cases}$$

Here $R_\theta(v) := v - 2(v \cdot \theta)\theta$ is rotation by angle $\theta$.

# Stronger results for the Boltzmann-Grad limit

Spohn (1977-78): The family of processes $(x^\varepsilon(t), v^\varepsilon(t))$ converges in law as $\varepsilon \to 0$ to a Markov process $(\overline{x}(t), \overline{v}(t))$ that has the infinitesimal generator:

$$\mathcal{L}f(x,v) = -v \cdot \nabla_x f + \int_{S^1} [v \cdot \theta]^+ [f(x, R_\theta(v)) - f(x,v)] d\theta.$$

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Boldrighini, Bunimovich, and Sinai (1983): improved the mode of convergence to almost everywhere.

# The limiting process

The Markov process $(\overline{x}(t), \overline{v}(t))$ looks like a random walk with random step lengths $\ell_i$ (distributed exponentially) and random direction changes $\theta_i$.

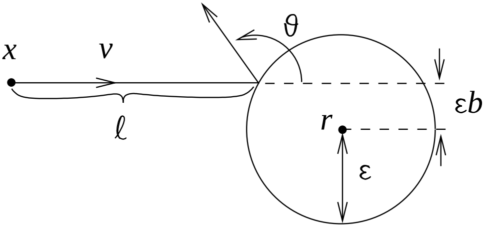



Figure: Change of variables from angle $\theta$ to impact parameter $b$.

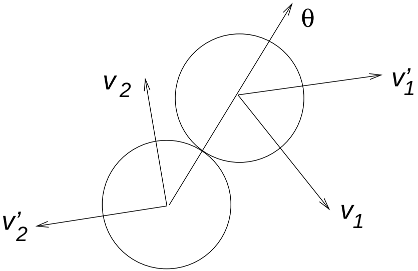
The impact parameter $b_i$ is distributed uniformly.

# The full hard-sphere model

Consider a model with all the hard spheres moving.

# The full hard-sphere model

We have a fluid of $N$ particles with diameter $\varepsilon$, with centers at $x_1, \ldots, x_N$ in $\mathbb{T}^d$ and velocities $v_1, \ldots, v_N$ in $\mathbb{R}^d$, that collide when $|x_i - x_j| = \varepsilon$:




Outgoing velocities: $v_i' = v_i - [\theta \cdot (v_i - v_j)]\theta, \quad \theta := \dfrac{x_i - x_j}{|x_i - x_j|}$.

# States and their distribution functions

States $\omega := (x_1, v_1, \ldots, x_N, v_N)$ in the allowable configuration space,

$$\Omega_N := \{\omega \in (\mathbb{T}^d \times \mathbb{R}^d)^N : |x_i - x_j| \geq \varepsilon \text{ for } i \neq j\}.$$

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Invariant measure for dynamics:

$$\mu_N(d\omega) = \frac{1}{Z_N} \prod_{i \neq j} \mathbb{1}(|x_i - x_j| \geq \varepsilon) \prod_i \underbrace{\frac{\exp\left(-\frac{|v_i|^2}{2\beta}\right)}{(2\pi\beta)^{d/2}}}_{h_\beta(v_i)} dx_i dv_i.$$

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Initial distribution function $F^{(N)}(\omega)\mu_N(d\omega)$.

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Too many degrees of freedom, so look at **k-particle dist. fns**:

$$F_k^{(N)}(x_1, v_1, ..., x_k, v_k, t) :=$$

$$\int F^{(N)}(\omega, t) \prod_{\substack{i \neq j,\ i \geq 1 \\ j \geq k+1}} \mathbb{1}(|x_i - x_j| \geq \varepsilon) \prod_{j \geq k+1} h_\beta(v_j) dx_j dv_j.$$

# The BBGKY hierarchy and its limit

The $k$-particle distribution functions satisfy the BBGKY hierarchy:

$$\partial_t F_k^{(N)}(x_1, v_1, ..., x_k, v_k, t) + \mathbf{v}_k \cdot \nabla_{\mathbf{x}_k} F_k^{(N)}(x_1, v_1, ..., x_k, v_k, t) =$$

$$(N-k)\varepsilon^{d-1} \sum_{j=1}^{k} \int_{\mathbb{R}^d} \int_S d\theta dv_{k+1} [\theta \cdot (v_j - v_{k+1})]$$

$$\times F_{k+1}^{(N)}(x_1, ..., v_k, x_j - \varepsilon\theta, v_{k+1}, t).$$

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Boltzmann-Grad limit, $\varepsilon^{1-d} = N \to \infty$, the Boltzmann hierarchy:

$$\partial_t g_k(x_1, v_1, ..., x_k, v_k, t) + \mathbf{v}_k \cdot \nabla_{\mathbf{x}_k} g_k(x_1, v_1, ..., x_k, v_k, t) =$$

$$\sum_{j=1}^{k} \int_{\mathbb{R}^d} \int_S d\theta dv_{k+1} [\theta \cdot (v_j - v_{k+1})]^+$$

$$\times [g_{k+1}(x_1, ..., v_j', ..., x_j, v_{k+1}', t) - g_{k+1}(x_1, ..., v_j, ..., x_j, v_{k+1}, t)].$$

# Results for the full hard-sphere model

Lanford (1975): For short times, and for initial states that aren't highly correlated, we have convergence to the solution of the Boltzmann hierarchy:

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Illner-Pulvirenti (1987): Same for all time with small initial data.

van Beijeren-Lanford-Lebowitz-Spohn (1979): Imagine tagging a particle–painting it red and following it. Then its distribution function converges to a Markov process corresponding to the Boltzmann equation.

# Tagging a particle in the full hard-sphere model

K.-Rezakhanlou (New proof of vBLLS, 2009): Suppose that $\omega$ has initial distribution $F^{(N)}(\omega)\mu_N(d\omega) = g^0(x_1, v_1)\mu_N(d\omega)$. Then the tagged (first) particle has a distribution function that converges:

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$$F_1^{(N)}(x_1, v_1, t) \xrightarrow{N\to\infty} g(x_1, v_1, t)h_\beta(v_1)dx_1dv_1.$$

And the macroscopic dynamics are governed by the Boltzmann equation:

$$\begin{aligned}\partial_t g + v\partial_{x_1} g = \int_{\mathbb{R}^d}\int_S & d\theta dv_2[\theta\cdot(v_1 - v_2)]^+ h_\beta(v_1) \\ & \times [g(x_1, v_1', t) - g(x_1, v_1, t)],\end{aligned}$$

$$g(x_1, v_1, 0) = g^0(x_1, v_1).$$

# The main novelties of our proof

We need only the first three of the $k$-particle distribution functions, and the first two equations of the BBGKY hierarchy.

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The challenge in these proofs is always to prove Boltzmann's Stosszahlansatz: that particles are uncorrelated just before collision (the hardest part of these proofs).

For the Stosszahlansatz, we use velocity averaging: the flow term, $\partial_t + v \cdot \nabla_x$, has a smoothing effect, once we take a weighted average in $v$.

# Outline

- Those were the hard-sphere models, reduced and full
- Reduced soft-sphere models and the Landau equation
- Outlook: full soft-sphere model and plasma-surface interactions

# The intractable plasma model

Landau's full model, with all the particles moving and interacting according to Coulomb repulsion, has resisted rigorous analysis.

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Instead of the full Coulomb potential, look at a bump-function potential (or a truncated Coulomb potential, Desvillettes-Pulvirenti '99).

# The reduced soft-sphere model of a plasma

The equations of motion for a particle among soft spheres:

$$\begin{cases} \dot{x}_\alpha^\varepsilon = v_\alpha^\varepsilon, & x_\alpha^\varepsilon(0) = x, \\ \dot{v}_\alpha^\varepsilon = -\sum_{i=1}^{\infty} \nabla V_\alpha^\varepsilon(x_\alpha^\varepsilon(t) - r_i), & v_\alpha^\varepsilon(0) = v. \end{cases}$$

- Parameter $\alpha \in (0, 1/2]$: $\alpha = 0$ corresponds to hard spheres, small $\alpha$ to high density of steep obstacles, large $\alpha$ to very high density of slight ones.
- $\omega = \{r_i\}_{i=1}^{\infty}$ is PPP with higher density: $\mu_\varepsilon = \mu\varepsilon^{1-d-2\alpha}$
- The potential $V \geq 0$ is a radial bump function, and the rescaled potential is:
$$V_\alpha^\varepsilon(x - r_i) = \varepsilon^\alpha V\left(\frac{|x - r_i|}{\varepsilon}\right).$$

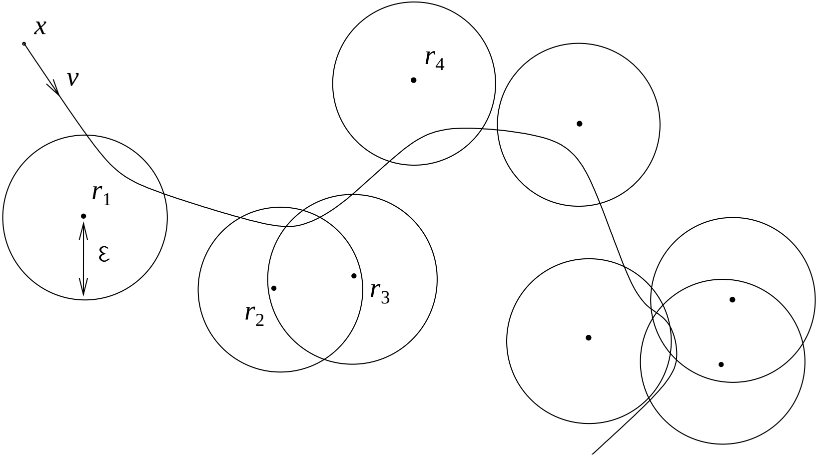


Figure: A trajectory for the microscopic soft-sphere model

# The weak coupling limit: $\alpha = 1/2$

Kesten-Papanicolaou (1980): If $\alpha = 1/2$, $d \geq 3$, then

$$(x^{\varepsilon}_{1/2}(t), v^{\varepsilon}_{1/2}(t)) \to (\overline{x}(t), \overline{v}(t))$$

in distribution, where $(\overline{v}(t))$ is a diffusion process with infinitesimal generator $\zeta\Delta_v$. Really a random field $F$ instead of $F = -\sum \nabla V$.

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The result in two dimensions is harder because of recurrence.

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Komorowski-Ryzhik (2005): $\alpha = 1/2$, $d = 2$, random field $F$.

For $\alpha < 1/2$, the difficulty is that each obstacle has more effect.

# The weak coupling limit: $\alpha$ small

Desvillettes and Ricci (2001): If $\alpha \in (0, 1/8)$, $d = 2$, and $f_0$ is an initial distribution, then

$$\mathbb{E} f_0(x_\alpha^\varepsilon(t), v_\alpha^\varepsilon(t)) \xrightarrow{\varepsilon \to 0} f(x, v, t).$$

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And $f$ is the solution of the linear Landau equation,

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**Theorem** (K., 2007): This can be extended to $\alpha \in [1/8, 1/4)$. But above $1/4$, there are too many clusters of obstacles.

# The weak coupling limit: unifying stronger result

**Theorem** (K., 2007): If $\alpha \in (0, 1/2)$, $d = 2$, then

$$(x_\alpha^\varepsilon(t), v_\alpha^\varepsilon(t)) \xrightarrow{\varepsilon \to 0} (\overline{x}(t), \overline{v}(t)) \quad \text{in law,}$$

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where $(\overline{v}(t))$ is a diffusion with infinitesimal generator $\zeta \Delta_v$.

In particular, for an initial distribution $f_0$, we have:

$$\mathbb{E} f_0(x^\varepsilon_\alpha(t), v^\varepsilon_\alpha(t)) \to f(x, v, t),$$

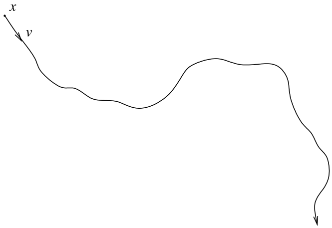
with the macroscopic dynamics given by the linear Landau equation:

$$\begin{cases} \partial_t f - v \cdot \nabla_x f = \zeta \Delta_v f \\ f(x, v, 0) = f_0(x, v). \end{cases}$$

# The weak coupling limit: universality result

**Theorem** (K., 2007): Moreover, the diffusion coefficient $\zeta$ is independent of $\alpha \in (0, 1/2]$:

$$\zeta = \frac{\mu}{2} \int_{-1}^{1} \left( \int_{b}^{1} V'\left(\frac{|b|}{u}\right) \frac{b\,du}{u\sqrt{1-u^2}} \right)^2 db.$$




The velocity diffusion for all $\alpha$. Microscopic distinctions between obstacle steepness and density all disappear in the scaling limit.

# The memory effects in the weak coupling case

Key idea: Only some kinds of recurrence are bad–and they're rare.

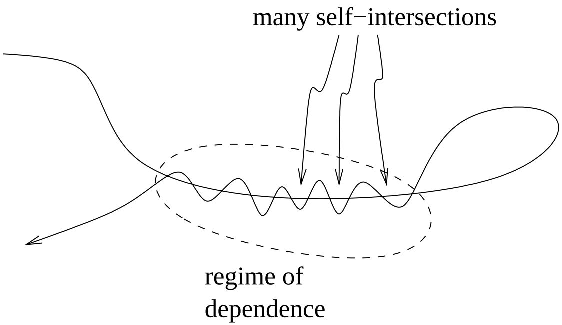



Figure: Correlation with past due to many self-intersections.

# The memory effects in the weak coupling case, cont.

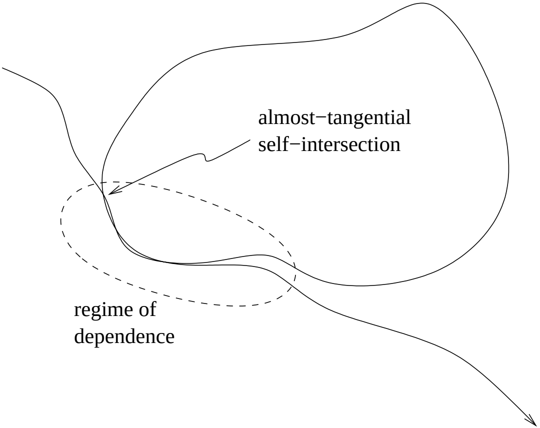



Figure: Correlation with past due to a small-angle self-intersection.

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- Show that such bad behavior is negligible in the limit (almost-tangential and repeated self-intersections), and cut them off.
- Show that the family of stopped processes is tight.
  **Key:** Better estimates on clusters of overlapping obstacles and the amount of time spent interacting with each cluster.

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- Show that the family of stopped processes is tight.
  **Key:** Better estimates on clusters of overlapping obstacles and the amount of time spent interacting with each cluster.
- Identify the infinitesimal generator of the limiting process as $\zeta\Delta_v$ via the Stroock-Varadhan martingale characterization.

# The main novelties of the proofs

- Show that such bad behavior is negligible in the limit (almost-tangential and repeated self-intersections), and cut them off.
- Show that the family of stopped processes is tight.
  **Key:** Better estimates on clusters of overlapping obstacles and the amount of time spent interacting with each cluster.
- Identify the infinitesimal generator of the limiting process as $\zeta\Delta_v$ via the Stroock-Varadhan martingale characterization.
- Show that the diffusion constant $\zeta$ is independent of $\alpha$.
  **Key:** A slick change of variables and good estimates, to identify it with the Fourier-space form from the SV MG char.

# Outline

- Hard-sphere models
- Those were the reduced soft-sphere models

- Outlook: full soft-sphere model and plasma-surface interactions

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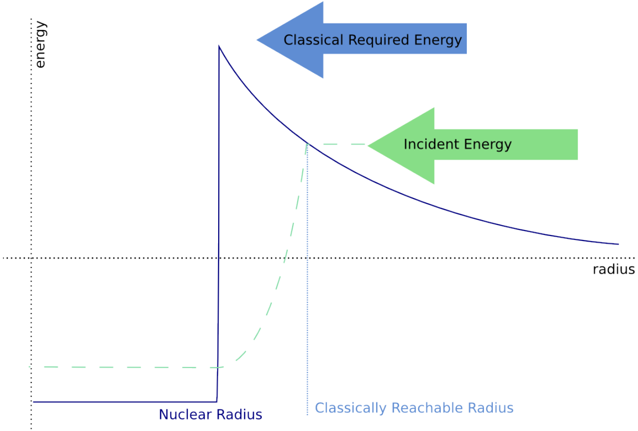
Holy grail: the full model with Coulomb interactions.

Even better: quantum many-body systems with long-scale Coulomb and short-scale strong-force interactions.

# Application to fusion

In order to get nuclei to fuse, one must raise their energies into the plasma regime ($10^8$ K) to overcome electrostatic repulsion.




Energy curve for fusion. (Courtesy of C. Deaconu)

# Plasma-surface interactions: the challenge

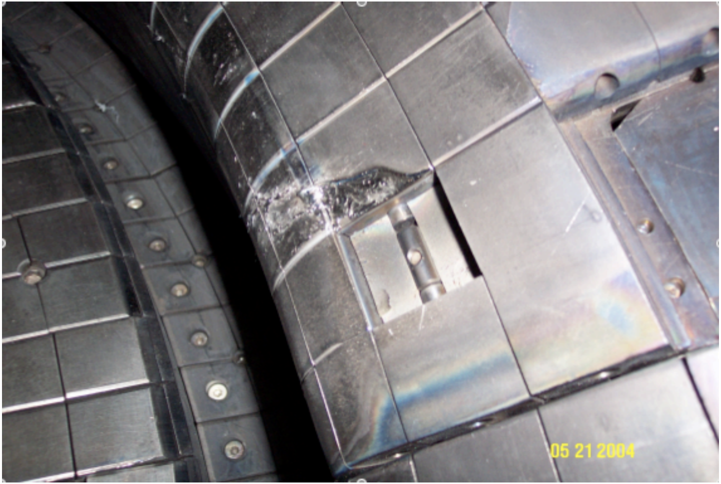
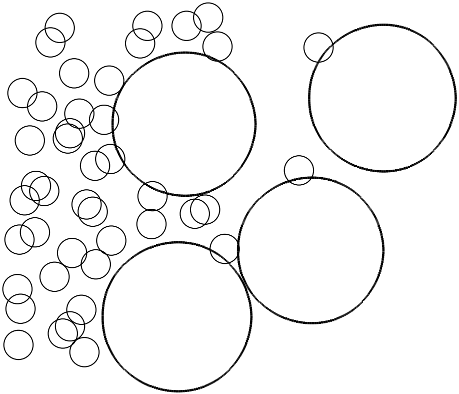


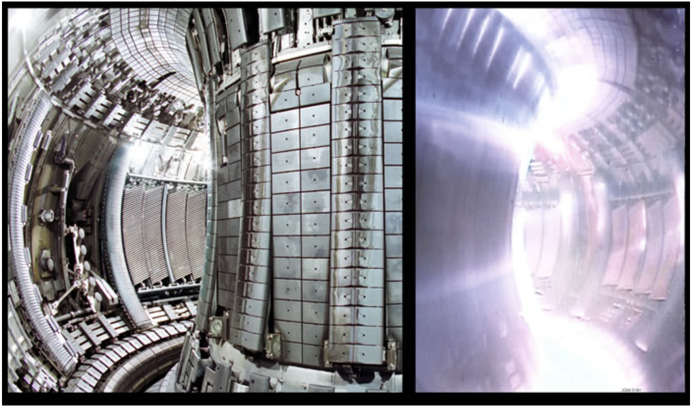

Figure: Plasma-damaged molybdenum tiles. (Courtesy of MIT's PSFC)

# Plasma-surface interactions: an impressionistic picture



Moving small plasma particles and fixed heavy metal atoms.

# Thank you



arXiv:0905.0649; forthcoming