Fluctuations of current in non-stationary diffusive lattice gases

Baruch Meerson Hebrew University of Jerusalem

Pavel Sasorov (IAM, Moscow) and Arkady Vilenkin (Hebrew U)

BSF United States - Israel Binational Science Foundation

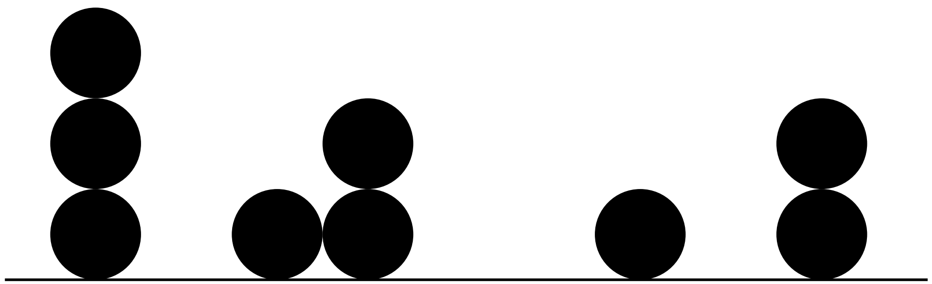
Non-equilibrium Statistical Physics, ICTS,
Bangalore, 2015

Plan

- ✓ Diffusive lattice gases and Macroscopic Fluctuation Theory
- ✓ Statistics of current on an infinite line
- ✓ Perturbative approaches: typical (small) fluctuations and very large fluctuations
- ✓ "Elliptic gases" and "hyperbolic gases"
- ✓ Some results for the SSEP and KMP models
- ✓ Summary

Diffusive lattice gases

SSEP: simple symmetric exclusion process



RWs, ZRP: $\alpha=\alpha(n_i)$ random walkers; zero-range process

KMP (Kipnis, Marchioro and Presutti 1982): random exchange of energy among neighbors

Large-scale behavior: fluctuating hydrodynamics

$$\partial_t \rho = \nabla \cdot \left[D(\rho)\nabla\rho + \sqrt{\sigma(\rho)}\,\xi(\mathbf{x},t) \right],$$

ξ: Gaussian noise, delta-correlated in $\mathbf{x}$ and t

Spohn 1991

Diffusive lattice gases are fully characterized, at large scales, by the diffusivity $D(\rho)$ and mobility $\sigma(\rho)$

$$\partial_t \rho = \nabla \cdot \left[D(\rho) \nabla \rho + \sqrt{\sigma(\rho)} \boldsymbol{\xi}(\mathbf{x}, t) \right]$$

$D(\rho)$ and $\sigma(\rho)$ are related to the equilibrium free energy density $F(\rho)$:

$$\frac{d^2 F(\rho)}{d\rho^2} = \frac{2D(\rho)}{\sigma(\rho)}$$

Einstein-Kubo relation

When noise is ignored: diffusion equation $\partial_t \rho = \nabla \cdot \left[D(\rho) \nabla \rho \right]$

Simple examples of diffusive lattice gases

Model	$D(r)$	$\sigma(r)$	$F(r)$
RWs	1	$2r$	$r \ln r - r$
SSEP	1	$2r(1-r)$	$r \ln r + (1-r) \ln(1-r)$
KMP	1	$4r^2$	$-(1/2) \ln r$
ZRP	$\alpha'(r)$	$2\alpha(r)$	$\int^r du \, \ln \alpha(u)$

$\alpha'(r)>0$

Macroscopic Fluctuation Theory (MFT)

Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim (2001, … 2014)

Large parameter: number of particles in relevant region of space. Extends the weak-noise WKB theory of Freidlin and Wentzel to fields

MFT can be derived from Fluctuating Hydrodynamics via saddle-point expansion of the proper path integral (Tailleur, Kurchan, Lecomte 2007). This leads to a minimization problem which can be cast into a classical Hamiltonian field theory for the particle density q(x,t) and conjugate "momentum" density p(x,t):

$$\partial_t q = \nabla \cdot [D(q)\nabla q - \sigma(q)\nabla p]$$

$$\partial_t p = -D(q)\,\nabla^2 p - \frac{1}{2}\sigma'(q)(\nabla p)^2$$

$$\partial_t q = \delta H / \delta p,$$

$$\partial_t p = -\delta H / \delta q,$$

$$H[q(\mathbf{x},t), p(\mathbf{x},t)] = \int d\mathbf{x}\, \mathcal{H},$$

$$\mathcal{H} = -D(q)\nabla q \cdot \nabla p + \frac{1}{2}\sigma(q)(\nabla p)^2$$

$$\partial_t q = \nabla \cdot [D(q)\nabla q - \sigma(q)\nabla p)]$$

$$\partial_t p = -D(q)\, \nabla^2 p - \frac{1}{2}\sigma'(q)(\nabla p)^2$$

Boundary conditions, in **x** and t, are problem-dependent

Deterministic limit: p(**x**,t)=0: downhill trajectories

$$\partial_t q = \nabla \cdot \left[D(q)\nabla q\right]$$

Fluctuations: p(**x**,t)≠0: uphill trajectories, the optimal density history

The probability density of a large deviation is given by the mechanical action along a proper uphill trajectory:

$$-\ln \mathscr{P} \cong S = \int d\mathbf{x} \int_0^T dt \left[p(\mathbf{x},t)\partial_t q(\mathbf{x},t) - \mathscr{H}\right]$$

$$= \frac{1}{2}\int d\mathbf{x} \int_0^T dt\, \sigma(q)(\nabla p)^2$$

If the initial condition is random, one should also find the optimal *initial* density profile and add to S the Boltzmann-Gibbs free energy "cost" of creating it

MFT emerged in the context of

non-equilibrium steady states of lattice gases

Expected density profile solves the steady-state mean-field problem

$$D(\bar{\rho})\, d\bar{\rho}\,/\,dx = \text{const}$$

$$\bar{\rho}(\mathrm{x}=0) = \rho_{-} \qquad \bar{\rho}(\mathrm{x}=\mathrm{L}) = \rho_{+}$$

Density fluctuations $\mathscr{P}[\rho(x)] \sim \exp\{-LF[\rho(x/L)]\} \quad L >> 1$

$F[\rho(x/L)]$ large deviation functional

Optimal path

Reviews: Derrida 2007, Jona-Lasinio 2010, Bertini et al 2015

MFT emerged in the context of

non-equilibrium steady states of lattice gases

Average current $\langle J \rangle = \frac{A(\rho_-, \rho_+)}{L}$

Fluctuations of current $\mathscr{P}(J) \sim \exp[-LS(J, \rho_-, \rho_+)], \quad L >> 1$

$S(J, \rho_-, \rho_+)$ large deviation function

Is the optimal path stationary for any J?

Reviews: Derrida 2007, Jona-Lasinio 2010, Bertini et al. 2015

MFT emerged in the context of

non-equilibrium steady states of lattice gases

• Long range correlations

• Uphill trajectory is different from time-reversed downhill trajectory

• Non-smooth parameter dependence of large deviation function/functional: phase transitions (Bunin, Kafri and Podolsky 2012)

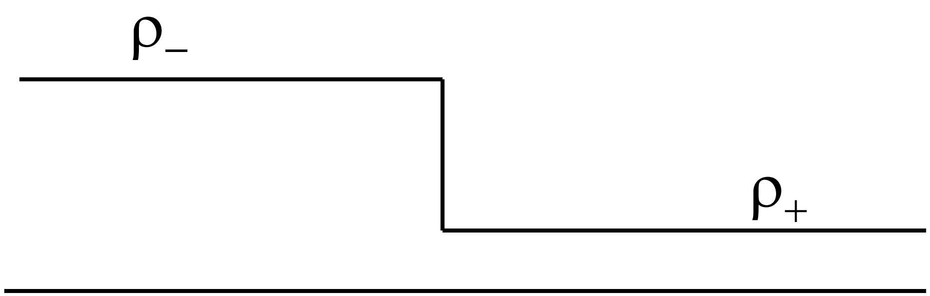
Reviews: Derrida 2007, Jona-Lasinio 2010, Bertini et al. 2014

Non-stationary settings are also interesting

Today: Fluctuations of mass/energy transfer through a point on an infinite line

Derrida and Gerschenfeld 2009, Sethuraman and Varadhan 2011, Krapivsky and M 2012,

M and Sasorov 2013, 2014, Vilenkin, M and Sasorov 2014



$$J = \int_0^\infty [\rho(x,T) - \rho(x,0)]\, dx$$

Deterministic profile

$$\langle J \rangle = \frac{\rho_- - \rho_+}{\sqrt{\pi}} \sqrt{T}$$

for Random Walkers (RWs), SSEP and KMP

$$\mathcal{P}(J) \sim \exp\left[-\sqrt{T}\, S\left(\frac{J}{\sqrt{T}}, \rho_-, \rho_+\right)\right]$$

Large deviation function $S\left(\frac{J}{\sqrt{T}}, \rho_-, \rho_+\right) = ?$ Even $\rho_- = \rho_+$ is nontrivial

What is optimal path of the system conditioned on J?

MFT formulation of the problem: Derrida and Gerschenfeld 2009

$$\partial_t q = \partial_x [D(q)\partial_x q - \sigma(q)\partial_x p)]$$

$$\partial_t p = -D(q)\, \partial_x{}^2 p - \frac{1}{2}\sigma'(q)(\partial_x p)^2$$

Deterministic step-like initial condition: $q(x,t=0) = \rho_- \theta(-x) + \rho_+ \theta(x)$

The integral constraint $J = \int_0^\infty [q(x,T) - q(x,0)]\, dx$ calls for a Lagrange multiplier

and leads to boundary condition

$$p(x,t=T) = \lambda\theta(x)$$

λ is ultimately fixed by J

$$q(x \to -\infty, t) = \rho_-, \quad q(x \to \infty, t) = \rho_+,$$
$$p(x \to \pm\infty, t) = 0.$$

Exact solution is not available except for Random Walkers

Numerical solutions for particular lattice gases:

Iteration algorithm of Chernykh and Stepanov (2001)

Krapivsky and M 2012, Vilenkin, M and Sasorov 2014

Today: Perturbative approaches based on additional small parameters:

1. Small J, hence small λ. Expansion in powers of λ. Krapivsky and M (2012)

2. Very large J: diffusion terms in the MFT equations are very small

   M and Sasorov 2013, 2014; Vilenkin, M and Sasorov 2014

Small J: small-λ expansion

$$q(x,t) = q_0(x,t) + \lambda q_1(x,t) + \lambda^2 q_2(x,t) + \dots$$
$$p(x,t) = \qquad\qquad \lambda p_1(x,t) + \lambda^2 p_2(x,t) + \dots$$

For D=1 $\quad q_0(x,t) = \rho(x,t) = \frac{\rho_- + \rho_+}{2} + \frac{\rho_+ - \rho_-}{2}\,\mathrm{erf}\left(\frac{x}{\sqrt{4t}}\right)$

In the 1st order we obtain

$$(\partial_t - \partial_{xx})q_1 = -\partial_x[\sigma(\rho)\partial_x p_1],$$
$$\partial_t p_1 = -\partial_{xx} p_1,$$
$$q_1(x,0) = 0, \quad p_1(x,T) = \theta(x).$$

The 1st-order solution yields the variance of $\mathcal{P}(J)$ for all lattice gases with D=const:

$$< J^2 >_c = V(\rho_-, \rho_+, \sigma)\,\sqrt{T},$$

Krapivsky and M 2012

$$V(\rho_-, \rho_+, \sigma) = \int_0^1 \frac{dt}{4\pi t} \int_{-\infty}^{\infty} dx\, \sigma[\rho(x, 1-t)]\, e^{-x^2/2t}$$

Higher orders would give higher cumulants of $\mathcal{P}(J)$

Very large J: What if we neglect the diffusion terms?

$$\partial_t q + \partial_x [\sigma(q) v] = 0,$$
$$\partial_t v + \frac{1}{2}\partial_x \left[\sigma'(q) v^2\right] = 0,$$

$$v(x,t) = \partial_x p(x,t).$$

Inviscid equations:
Euler hydrodynamics

The boundary condition at t=T becomes $v(x, t=T) = \lambda\,\delta(x)$

Hodograph transformation: from q(x,t) and v(x,t) to t(q,v) and x(q,v)

This leads to a linear 2nd order PDE for t(q,v):

$$\sigma(q)\partial_q^{\,2} t - \frac{1}{2}\sigma''(q) v^2 \partial_v^{\,2} t + 2\sigma'(q)\partial_q t - 2\sigma''(q) v \partial_v t = 0.$$

This equation can be of elliptic, hyperbolic or parabolic type, leading to three classes of lattice gases:

$\sigma''(q) > 0$ hyperbolic class
$\sigma''(q) < 0$ elliptic class
$\sigma''(q) = 0$ (RWs) parabolic class

SSEP is elliptic, KMP is hyperbolic

M and Sasorov 2013, 2014,
Vilenkin, M and Sasorov 2014

Elliptic class: the singularity $v(x, t=T) = \lambda\delta(x)$ can *develop* at t=T, see e.g. B. A. Trubnikov and S. K. Zhdanov, Phys. Rep. **155**, 137 (1987), a review of "quasi-Chaplygin gases".

Hyperbolic class: a delta-function singularity of v would have to be present *at all times* $0 \le t \le T$ *which is not allowed*

Therefore, the inviscid limit yields a well-posed problem for the "elliptic gases", and an ill-posed problem for the "hyperbolic gases".

Two different strategies of solution at large J:

"Elliptic gases": Drop the diffusion terms and solve the inviscid hodograph equation. Implemented for the SSEP with $\rho_-=\rho_+$

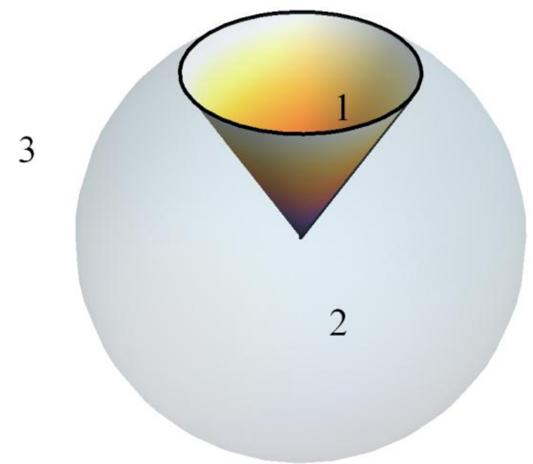
M and Sasorov 2014, Vilenkin, M and Sasorov 2014

"Hyperbolic gases": Take diffusion into account to regularize pulse-like singularities of q and v at 0<t<T. Use the inviscid equations in the "outer" regions, and match the inner and outer solutions. Implemented for the KMP M and Sasorov 2013

Very large J, SSEP, $\rho_-=\rho_+=n_0$

$$q(1-q)\partial_q{}^2 t + v^2\partial_v{}^2 t + 2(1-2q)\partial_q t + 4v\partial_v t = 0$$

The hodograph equation is separable. Further, it can be transformed into Laplace's equation in 3d. Flat initial condition corresponds to geometry of a cone. Problem soluble analytically



The initial density n_0 determines the cone angle. For $n_0=1/2$ the cone becomes a disk, and the solution can be expressed in elementary functions

Vilenkin, M and Sasorov 2014,

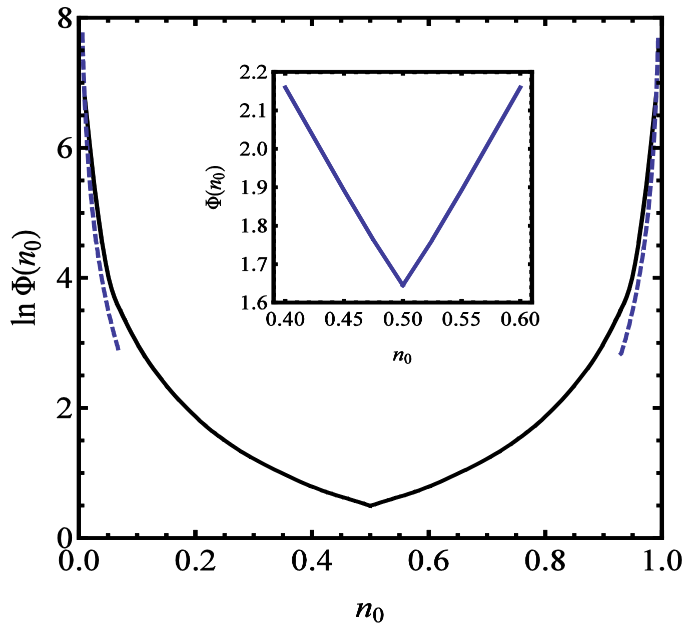
M and Sasorov 2014

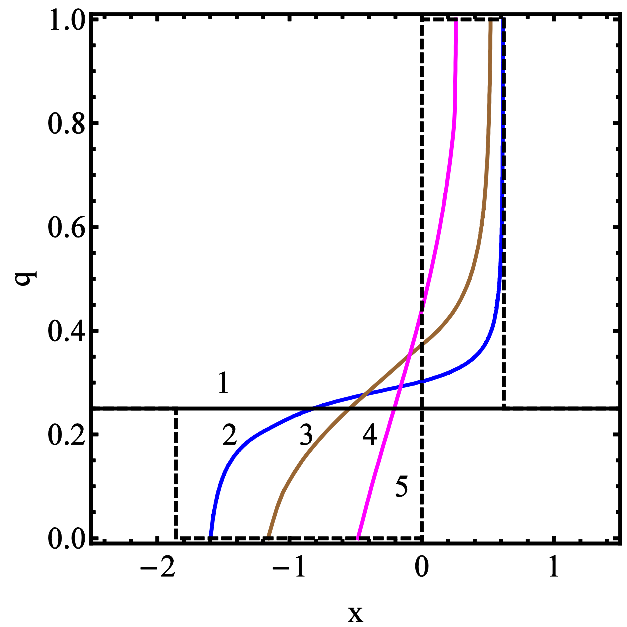
Very large J, SSEP, $\rho_- = \rho_+ = n_0$

$$\mathscr{P}(J) \sim \exp[-\sqrt{T}\, S(j, n_0)], \quad j = J/\sqrt{T}$$

$$S(j \to \infty, n_0) = \Phi(n_0)\, j^3.$$

The function $\Phi(n_0)$ and the optimal path determined analytically





Full solution includes non-hodograph regions, shocks

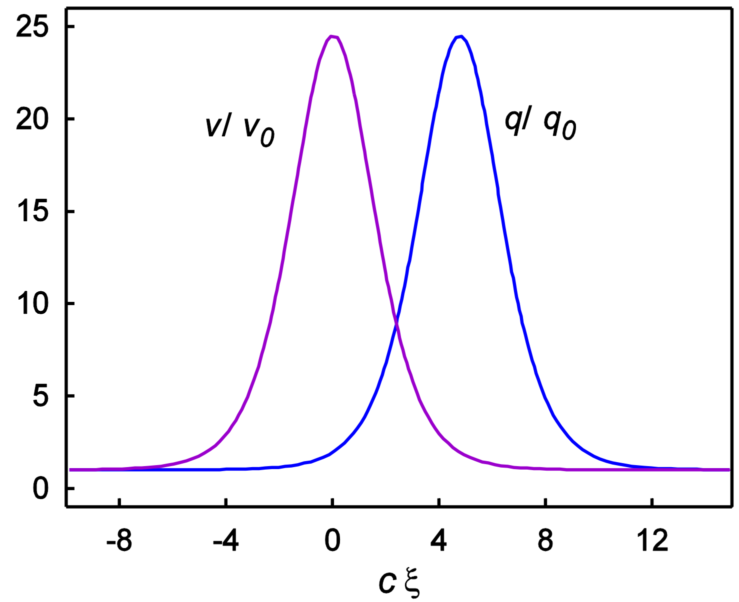
M and Sasorov 2013, 2014, Vilenkin, M and Sasorov 2014

The $S \sim j^3$ scaling was predicted by Derrida and Gershenfeld (2009)

Very large J, KMP model

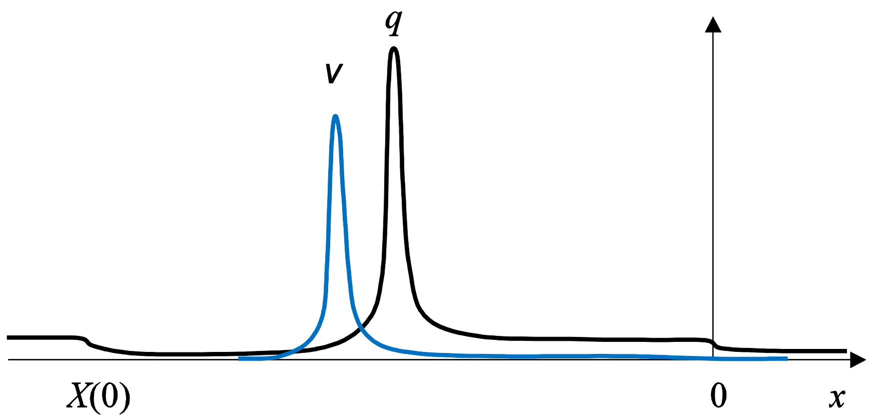
Building blocks: exact soliton-like solutions of MFT equations

$$q(x,t) = q(x-ct), \quad v(x,t) = v(x-ct),$$
$$v(x,t) = \partial_x p(x,t)$$



M and Sasorov 2013

Very large J, KMP model



Optimal path: Coupled large-amplitude solitary pulses, of q and v. They propagate with a constant speed, but their amplitudes slowly grow with time, as the q-pulse collects most of the available energy on its way to x=0. The action mostly comes from the pulses

$$\mathscr{P}(J) \sim \exp[-\sqrt{T}\, S(j,\rho_-,\rho_+)],$$

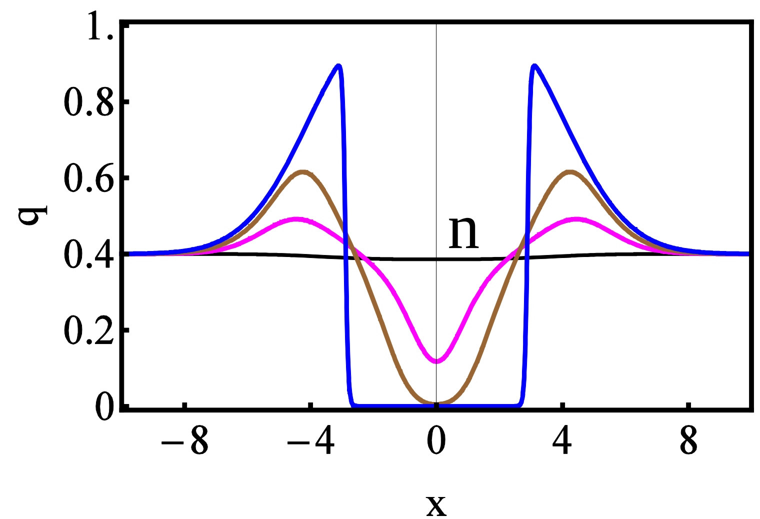
$$S(j\to\infty,\rho_-,\rho_+) = j\left[2\ln j + \ln(2\ln j) + \frac{\ln(2\ln j)}{2\ln j} + \ldots\right],$$

$$j = \frac{J}{\rho_-\sqrt{T}}.$$

M and Sasorov 2013

Another non-stationary setting: formation of void at time T

Krapivsky, M and Sasorov 2012



$$\mathscr{P}(L,T) \sim \exp[-T^{d/2} S_d(\frac{L}{\sqrt{T}}, n)], \quad T >> 1, L >> 1$$

d: dimension of space

$S_d(\frac{L}{\sqrt{T}}, n)$ large deviation function

Optimal path...

Other non-stationary settings analyzed with MFT:

Statistics of integrated current on a ring (Bertini et al 2005, Bodineau and Derrida 2005, Hurtado and Garrido 2011): the first system where breakdown of the additivity principle was discovered

Statistics of particle absorption by a target (M and Redner 2014, M, Vilenkin and Krapivsky 2014). Everlasting role of initial conditions in 1d

Statistics of the position of a tagged particle in a single-file diffusion in 1d (Krapivsky, Mallick and Sadhu 2014,2015) Everlasting role of initial conditions in 1d

Melting of an Ising quadrant at zero temperature (Krapivsky, Mallick and Sadhu 2014) Mappable to the SSEP, very similar to the problem we have discussed in this talk

Summary

Complete statistics of fluctuations of integrated current is still unknown, except for RWs

MFT yields the *variance* for D=const, or for any D(ρ) but flat initial density profile

MFT yields *far tails* of the distribution, for the SSEP and KMP models which exemplify the elliptic and hyperbolic universality classes, respectively

The perturbative approaches are also useful for other MFT settings

Each new solved example improves our understanding of large deviations far from equilibrium, and develops intuition

Thank you