Fluctuations, Large Deviations and Rigidity for Coulomb Systems and other Non-Gibbsian Measures

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LDF for Equilibrium Systems with Integrable Interactions

The Boltzmann-Gibbs-Einstein relation for the probability that the number of particles N_{Λ} , in a macroscopic region Λ inside a much larger box V, $V >> \Lambda$ ($V = \mathbb{R}^d / \mathbb{Z}^d$), with $< N_{\Lambda} >= \rho |\Lambda|$ will have a value $n|\Lambda|$, $n \neq \rho$, is given by

Probability
$$(N_{\Lambda} = n|\Lambda|) \sim \text{Exp}\{-|\Lambda|[f(n)] - f(\rho) - \lambda(n - \rho)]\}$$

where $f(\rho)$ is the usual Helmholtz free enrgy per unit volume and $\lambda = \frac{\partial f(\rho)}{\partial \rho}$ is the chemical potential.

To get "typical" fluctuations we set, $n = \rho + \frac{\xi}{\sqrt{|\Lambda|}}$ and expand the LDF around $n = \rho$. This yields

$$\mathsf{Prob}(u) = \mathsf{Exp}[-rac{1}{2}rac{u^2}{\sigma}]$$

where $\sigma = (\frac{\partial^2 f}{\partial \rho^2})^{-1}$ is the compressibility.

According to Ginibre's Theorem (with some generalization), $\sigma \ge \sigma_0 > 0$ for systems with integrable potentials (the proof actually requires a lot more). At critical points σ is infinite. Coulomb potentials are however very far from being integrable and the LDF as well as fluctuations require a separate study. I shall do that first then consider some very simple non-equilibrium systems for which the LDF can be computed explicitly not only for N_{Λ} but also for a density profile $\rho(x)$.

The properties of macroscopic matter are almost entirely determined by the Coulomb interactions between electrons and nuclei, satisfying appropriate quantum statistics.

While the real world is 3 dimensional it is useful to consider such systems also in other dimensions and as classical systems. The Coulomb interaction between charges e_i, e_j at positions $\mathbf{r}_i, \mathbf{r}_j$ in \mathbb{R}^d is, with $r = |\mathbf{r}_i - \mathbf{r}_j|$,

$$v_{d}(r) = \begin{cases} -e_{i}e_{j}r & d = 1\\ -e_{i}e_{j}\log(r) & d = 2\\ +e_{i}e_{j}r^{2-d} & d \ge 3 \end{cases}$$
(1)

I shall also consider the Jellium or one-component-plasma (OCP) model (introduced by Wigner) in which particles with a positive charge *e* move in a uniform background of negative charge with density $-\rho e$. The background produces an external potential proportional to ρer_i^2 ; r_i the distance from the center of rotational symmetry.

My concern here will be primarily with effects due to the long range nature of the Coulomb potential. When necessary, we can think of the charges as being smeared out in little balls or having hard cores to take care of the singular contact interactions in $d \ge 2$.

To fluctuate is normal and in most cases fluctuations are themselves normal, by which I mean that in a region Λ with volume $|\Lambda|$, they grow like the square root of $|\Lambda|$ as in a Poisson process (or faster as at critical points). There are however many very interesting cases where the fluctuations are subnormal. This includes local charge fluctuations in globally neutral macroscopic systems, the case I shall now discuss. To get a feeling for what such fluctuations might look like we note that in many situations, such as those involving fluids at low and moderate temperatures, we usually consider macroscopic systems as made up of neutral atoms or molecules interacting via effective short range Lennard-Jones type potentials. In such cases, the fluctuations in the net charge Q_{Λ} in a region Λ will be due entirely to the surface of Λ cutting these entities in a "random" way. $\langle Q_{\Lambda}^2 \rangle$ may then be expected to be proportional to the surface area of Λ .

The question naturally arises as to whether this type of behavior is indeed a consequence, in some or all situations, of the true Coulomb interactions. In particular, is it true for charge fluctuations in plasmas, molten salts, metals, etc., where bare Coulomb interactions are part of the effective Hamiltonian? The question naturally arises as to whether this type of behavior is indeed a consequence, in some or all situations, of the true Coulomb interactions. In particular, is it true for charge fluctuations in plasmas, molten salts, metals, etc., where bare Coulomb interactions are part of the effective Hamiltonian?

To simplify matters I shall consider the classical OCP (with e = 1) whose structure is of interest also in other contexts, such as the distribution of eigenvalues of random matrices. I will indicate the difference with multi-component systems when relevant.

Now, while for systems with short range interactions one can prove (Ginibre) that the variance in particle number N_{Λ} in a region $\Lambda \subset \mathbb{R}^d$ grows at least as fast as the volume $|\Lambda|$

$$\mathcal{V}_{\Lambda} = \langle (N_{\Lambda} - \langle N_{\Lambda} \rangle)^2 \rangle \geq c |\Lambda|, \quad c > 0,$$
 (2)

this does not hold for Coulomb interactions. Fluctuations in the charge Q_{Λ} , which for the OCP is the same as fluctuations in N_{Λ} with $\langle N_{\Lambda} \rangle = \rho |\Lambda|$, will, as already noted, only grow as the surface area $\langle Q_{\Lambda}^2 \rangle \sim |\partial \Lambda|$. This is in fact what one can prove, under reasonable assumptions on clustering.

To see how this comes about we note that the variance \mathcal{V}_{Λ} is expressible in terms of the pair correlation function of the infinite system. For a translation invariant system we have,

$$\begin{split} \mathcal{V}_{\Lambda} &= \int_{\Lambda} \int_{\Lambda} \mathrm{d}\mathbf{r}_{1} \mathrm{d}\mathbf{r}_{2} \, G(\mathbf{r}_{1} - \mathbf{r}_{2}) \\ &= |\Lambda| \int_{\mathbb{R}^{d}} G(\mathbf{r}) \mathrm{d}\mathbf{r} - \int_{\mathbb{R}^{d}} G(\mathbf{r}) \alpha_{\Lambda}(\mathbf{r}) \mathrm{d}\mathbf{r}, \end{split}$$

where

$$\begin{split} \mathcal{G}(\mathbf{r}_1 - \mathbf{r}_2) &= \left\langle \sum_{i,j} \delta(\mathbf{r}_1 - \mathbf{x}_i) \delta(\mathbf{r}_2 - \mathbf{x}_j) \right\rangle - \rho^2, \\ &= \rho \delta(\mathbf{r}_1 - \mathbf{r}_2) + \rho_2(\mathbf{r}_1 - \mathbf{r}_2) - \rho^2, \\ \alpha_{\Lambda}(\mathbf{r}) &= \int \chi_{\Lambda}(\mathbf{r} + \mathbf{r}_1) [1 - \chi_{\Lambda}(\mathbf{r}_1)] \mathrm{d}\mathbf{r}_1 \\ \chi_{\Lambda}(\mathbf{y}) &= \begin{cases} 1 & \mathbf{y} \in \Lambda \\ 0 & \mathbf{y} \notin \Lambda \end{cases} \end{split}$$

This is modified in a simple way for a periodic system. For charge fluctuations in multi-charge systems $G(\mathbf{r})$ corresponds to the charge-charge correlations. When $\Lambda \uparrow \mathbb{R}^d$ in a self similar way α_{Λ} will grow like the surface area $|\partial \Lambda| \sim |\Lambda|^{(d-1)/d}$ with $|\partial \Lambda| = 2$ for d = 1. Averaging $\alpha_{\Lambda}(\mathbf{r})/|\partial \Lambda|$ over rotations we obtain

$$\lim_{|\Lambda|\to\infty}\frac{\alpha_{\Lambda}(\mathbf{r})}{|\partial\Lambda|}=\alpha_d \ |\mathbf{r}|,$$

where

$$\alpha_d = \begin{cases} 1/2 & d = 1\\ 1/\pi & d = 2\\ \dots & \end{cases}$$

In Coulomb systems

$$\lim \frac{1}{|\Lambda|} \mathcal{V}_{\Lambda} = \int_{\mathbb{R}^d} G(\mathbf{r}) \mathrm{d}\mathbf{r} = 0, \qquad (3)$$

due to Debye screening. This is known as the "first sum rule". Systems satisfying (3) are also known as superhomogeneous.

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$$\frac{\mathcal{V}_{\Lambda}}{|\partial\Lambda|} \to -\alpha_d \int_0^\infty r^d G(r) dr, \qquad (4)$$

where we have sphericalized G. Equation (4) is called the Stillinger-Lovett relation. When (3) holds but (4) is infinite the variance will grow faster than the surface area but slower than the volume.

Question Can the variance grow slower than $|\partial \Lambda|$. The answer by J. Beck is "no" if the distribution is rotational invariant (or Λ is a sphere). It is still an open question how small this variance can be and whether it attains its minimum value for a regular lattice. Going beyond the variance, we also have that for Coulomb systems in $d \ge 2$ the charge fluctuation satisfy a central limit theorem : deviation from the average divided by the square root of the variance gives

$$\frac{(N_{\Lambda} - \langle N_{\Lambda} \rangle)}{\sqrt{\mathcal{V}_{\Lambda}}} \to \xi,$$

a standard Gaussian random variable. This was proven by Martin-Yalcin.

In fact the following is true: let \mathbb{R}^2 (generally \mathbb{R}^d) be divided into squares Γ_i of area L^2 whose centers are located $L\mathbb{Z}^2$. Setting

$$\xi_j = Q(\Gamma_j)/\sigma(\Gamma_j), \quad \sigma(\Gamma_j) = KL^{1/2}$$

we find that the joint distribution of the $\{\xi_j\}$ approaches as $L \to \infty$ a Gaussian measure with covariance

$$C_{j,k} = \left[\delta_{j,k} - \frac{1}{4}\sum_{e}\delta_{j-k,e}\right] = \frac{1}{4}\left[-\Delta\right]_{j,k},\qquad (*)$$

where e is the unit lattice vector and Δ is the discrete Laplacian.

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where *e* is the unit lattice vector and Δ is the discrete Laplacian. This means that the charge fluctuations in $\Gamma_{j,L}$ are compensated by the opposite charges in neighboring (cubes). This is exactly what one would expect when the charges are bound together in neutral molecules.

The same holds for d > 2. In d = 1, $|\partial \Lambda| = 2$ and as shown by M-Y the charge (particle in OCP) fluctuations are bounded and have a well-defined non Gaussian distribution as $|\Lambda| \to \infty$.

As might be expected from the reduction of fluctuations, the probability of large deviations from charge neutrality, for multi-component or OCP system, will be smaller for Coulomb systems than those for systems with short range interactions. This problem was studied by Jancovici, L., and Manificat (JLM) in (1993), using electrostatic type arguments. They found that this is indeed the case in all dimensions and all β .

For the 2*d* OCP with density $\rho = 1$, the probability of having n(R) particles in a disc of radius *R*, corresponding to a charge $|Q| = |n(R) - \pi R^2|$, behaves as

$$\mathsf{Prob}\left\{ |\mathit{n}(\mathsf{R}) - \pi \mathsf{R}^2| > \mathsf{R}^lpha
ight\} \sim \exp\left[- \mathit{c}_lpha \mathsf{R}^{\phi(lpha)}
ight],$$

with

$$\phi(\alpha) = \begin{cases} 2\alpha - 1 & , \quad \frac{1}{2} < \alpha \le 1 \\ 3\alpha - 2 & , \quad 1 \le \alpha \le 2 \\ 2\alpha & , \quad \alpha \ge 2 \end{cases}$$

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This probability is much smaller than the large deviations for systems with short range interactions where, e.g. for $\alpha = 2$ one would get e^{-cR^2} instead of e^{-cR^4} . As usual the symbol \sim means that taking the logarithm of both sides and dividing by $R^{\phi(\alpha)}$ we get a finite limit when $R \to \infty$.

These "macroscopic" results can be checked and confirmed at $\beta = 2$ where we have explicit solutions for the correlation functions. We can get then additional information such as the charge density outside the disc of radius R conditioned on there being no particles inside. In particular the density at $r = R^+$ is given by $\rho(R^+) \sim \frac{1}{2}\pi\rho^2 R$

It turns out that the large deviation function we obtained is of the same form, in its dependence on α as that of a point process generated by the zeroes of a Gaussian Entire Function, $f = \sum \frac{\xi^k}{\sqrt{k!}} z^k$, with the ξ_k i.i.d standard complex Gaussians (Nazarov, Sodin, Volberg).

The Jancovici–Lebowitz–Manificat Law for Large Fluctuations of Random Complex Zeroes

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Abstract: Consider a Gaussian Entire Function

$$f(z) = \sum_{k=0}^{\infty} \zeta_k \frac{z^k}{\sqrt{k!}},$$

where ζ_0, ζ_1, \ldots are Gaussian i.i.d. complex random variables. The zero set of this function is distribution invariant with respect to the isometries of the complex plane. Let n(R)be the number of zeroes of f in the disk of radius R. It is easy to see that $\mathbb{E}n(R) = R^2$, and it is known that the variance of n(R) grows linearly with R (Forrester and Honner). We prove that, for every $\alpha > 1/2$, the tail probability $\mathbb{P}\left\{ |n(R) - R^2| > R^{\alpha} \right\}$ behaves as $\exp\left[-R^{\varphi(\alpha)}\right]$ with some explicit piecewise linear function $\varphi(\alpha)$. For some special values of the parameter α , this law was found earlier by Sodin and Tsirelson, and by Krishnapur.

In the context of charge fluctuations of a one-component Coulomb system of particles of one sign embedded into a uniform background of another sign, a similar law was discovered some time ago by Jancovici, Lebowitz and Manificat. For d = 1, we have, as already noted, the probability of having the charge going to infinity in any interval of length L goes to zero independent of how $L \to \infty$, i.e., the $\phi(\alpha)$ is infinite for $\alpha > 0$. (It may be interesting to note here that this fact is not a consequence of having bounded variance in any interval as can be shown by a counter-example (Goldstein, Lebowitz, Speer).) The situation in d = 3 is similar to that in d = 2 although the details differ. So far we have discussed fluctuations and large deviations of the charge in a region Λ without saying anything about the configuration of particles/charges outside Λ , i.e. in $\Lambda^c = \mathbb{R}^d \setminus \Lambda$. We ask now: what can we say about the distribution of points (charge) inside Λ given the configuration in Λ^c , i.e., we want the conditional probability $\mu_{\Lambda}(dX_{\Lambda}|X_{\Lambda^c})$ of a configuration in dX_{Λ} given X_{Λ^c} .

For equilibrium Gibbs measures of systems with short range interactions the answer to this is given by the DLR (Dobrushin, Lanford, Ruelle) equations.

$$\mu_{\Lambda}\left(\mathbf{x}_{1},\ldots\mathbf{x}_{N}|X_{\Lambda^{c}}\right) = \frac{\exp\left[-\beta U(X_{\Lambda}|X_{\Lambda^{c}})\right]}{\int e^{-\beta U(X_{\Lambda}|X_{\Lambda^{c}})}dX_{\Lambda}}$$
(5)

where $U(X_{\Lambda}|X_{\Lambda^c})$ is the potential energy of a configuration in Λ given the configuration in $\Lambda^c = \mathbb{R}^d \setminus \Lambda$.

This equation involving $U(X_{\Lambda}|X_{\Lambda^c})$ holds for all infinite volume Gibbs measures whether these are obtained as limits of finite volume micro-canonical, canonical or grand-canonical ensembles (with the appropriate β and z for the first two). It does not however work for systems with long range Coulomb interactions, where $U(X_{\Lambda}|X_{\Lambda^c})$ may be infinite for many configurations.

Aizenman and Martin (AM 1981), using earlier work by Lenard, gave a characterization of these measures in d = 1 via the electric field E(x).

Using this description AM proved that the charge in an interval $[a, b] = \Lambda$, which corresponds for the OCP to the number of particles in Λ , is uniquely specified by the configuration X_{Λ^c} for all typical configurations with respect to infinite volume measure μ . (The set of atypical configurations has measure zero).

This "number rigidity" property, i.e, $N_{\Lambda} = f(X_{\Lambda^c})$, was recently proven by Ghosh and Peres (GP2012) to hold for the OCP in d = 2, at $\beta = 2$. It was also proven by Ghosh (G2012) to hold at $\beta = 2$ for the d = 1 Dyson log gas, i.e, for charged particles in one dimension interacting via a 2*d* logarithmic Coulomb potential in a uniform background. The variance of particle number in an interval [a, b] in this system grows like $\log(b - a)$ which is slower than $|\Lambda|$ but greater than $|\partial\Lambda|$. This "number rigidity" property, i.e, $N_{\Lambda} = f(X_{\Lambda^c})$, was recently proven by Ghosh and Peres (GP2012) to hold for the OCP in d = 2, at $\beta = 2$. It was also proven by Ghosh (G2012) to hold at $\beta = 2$ for the d = 1 Dyson log gas, i.e, for charged particles in one dimension interacting via a 2*d* logarithmic Coulomb potential in a uniform background. The variance of particle number in an interval [a, b] in this system grows like $\log(b - a)$ which is slower than $|\Lambda|$ but greater than $|\partial\Lambda|$.

GP also showed that while N_{Λ} is fixed by X_{Λ^c} the distribution of points inside Λ is not rigid: it is in fact absolutely continuous with respect to the Lebesgue measure. The same is true for the 1*d* Coulomb system studied by MA.

The 2*d* and 1*d* cases studied by GP correspond (as is well known) respectively to the distribution of the bulk eigenvalues of the random matrices chosen from the Ginibre ensemble and of the Gaussian Unitary Ensemble (GUE or GCE). In the Ginibre ensemble each of the entries in a $N \times N$ marix are iid complex Gaussian random variables while the GUE consists of random Gaussian Hermitian matrices whose eigenvalues are real. The infinite volume measure μ is obtained by letting $N \to \infty$ and scaling to make the density ρ uniform.

The 2d and 1d cases studied by GP correspond (as is well known) respectively to the distribution of the bulk eigenvalues of the random matrices chosen from the Ginibre ensemble and of the Gaussian Unitary Ensemble (GUE or GCE). In the Ginibre ensemble each of the entries in a $N \times N$ marix are iid complex Gaussian random variables while the GUE consists of random Gaussian Hermitian matrices whose eigenvalues are real. The infinite volume measure μ is obtained by letting $N \to \infty$ and scaling to make the density ρ uniform. In both cases the eigenvalue distribution is known to be a determinantal process. It was these processes that were the focus of GP. Their proof of rigidity looks very different from that of AM. However from a physical point of view the GP systems are just examples of Coulomb systems. Their rigidity should therefore follow from charge screening in Coulomb systems.

In recent work with Aizenman and Ghosh we were indeed able to prove rigidity for systems (point processes) d = 1 and 2 in which $\frac{\mathcal{V}}{|\Lambda|} \rightarrow 0$, i.e, the variance in the particle number (or charge) grows slower than the volume. These are called superhomogeneous processes. We require in addition that the truncated pair correlation function decays at least as fast as r^{-2} in d = 1 and as $r^{-(4+\epsilon)}$ in d = 2. This includes all the cases mentioned before as well as the 1d log gas for $\beta < 2$, the 2d two component Coulomb system in d = 2for $\beta < 2$ using results of Samai, and the 2*d* OCP for small β . I believe in fact that this is the case for all β in d = 1 and 2 but should not hold in d > 3.

Rigidity-Non rigidity transition in d = 3

Consider a point process obtained by displacing each point $x \in \mathbb{Z}^d$ by Y_x , i.i.d. random variables with distribution w(y)dy. Then the point process is rigid in \mathbb{Z}^1 if Y_x has a finite first moment, in \mathbb{Z}^2 if Y_x has a finite second moment, in \mathbb{Z}^d , $d \ge 3$ there is for w(y) a Gaussian with variance σ a "phase transition". The process is rigid if $\sigma < \sigma_c$ and not rigid if $\sigma > \sigma_c$. (Y.peres and A.Sly on arXiv).

Simple Exclusion Process

In d = 1, with nearest neighbor jumps

$$\tau = \{\tau_i\} \quad \tau_i = \{0, 1\}, \quad i \in \mathbf{Z}$$

Particles attempt to jump to the neighboring site on right with rate 1 and to the left with rate $q \leq 1$: they succeed if site on which they attmept to jump is empty, otherwise nothing happens. All stationary translation invariant measures on Z are (superpositions) of Bernoulli or product measures with density $r \in [0, 1]$, prob $\{\tau_i = 1\} = r$.

Also true for Z^d , d > 1, and more general jumps.

For M particles on L sites, with periodic bc, all $\begin{pmatrix} L \\ M \end{pmatrix}$ configurations have equal weight in the stationary state.

For q = 1, SSEP, the dynamics satisfies *detailed balance* with respect to the stationary measure.

For q < 1, ASEP, the dynamics doesn't satisfy detailed balance with respect to stationary measure.

Hydrodynamical Scaling of SEP

 $i \to x/\epsilon$, $s = t/\epsilon^{\alpha}$, x and t are macroscopic space and time scales, while $i \in \mathbf{Z}$ and s is the microscopic time variables.

Starting with an initial configuration (or measure) on a system with *L* sites, whose density profile converges to $\rho_0(x)$

$$\frac{1}{(b-a)L}\sum_{i=aL}^{bL}\tau_i \to \int_a^b \rho_0(x)dx, \quad L=\epsilon^{-1}$$

The density profile $\rho(x,t)$ will then evolve in time according to a deterministic macroscopic equation:

$$\frac{\partial \rho(x,t)}{\partial t} = F(\{\rho\}), \quad \rho(x,0) = \rho_0(x)$$

i.e.

$$\frac{1}{(b-a)L}\sum_{i=aL}^{b}\tau_i(t/\epsilon^{\alpha})\to \int_a^b\rho(x,t)dx$$

Also true for \mathbb{Z}^d .

For q < 1 ASEP: set $\alpha = 1$, then

$$\frac{\partial \rho(x,t)}{\partial t} + (1-q)\frac{\partial}{\partial x}[\rho(1-\rho)] = 0$$

Burger's Equation.

For q = 1, SSEP Case, "nothing" happens "on macroscopic scale" for times of order $\epsilon^{-1}t$. If, however, one waits for times of order $\epsilon^{-2}t$ one gets diffusive behavior

 $\frac{\partial \rho}{\partial t} = \frac{1}{2} \frac{\partial}{\partial x} [D(\rho) \frac{\partial \rho}{\partial x}]; \quad D = 1 \quad \text{for} \quad \text{SSEP}$ For $q = 1 - \lambda \epsilon$, WASEP, and $\alpha = 2$, one gets viscous Burger's equation

$$\frac{\partial \rho(x,t)}{\partial t} + \lambda \frac{\partial}{\partial x} \rho(1-\rho) = \frac{\partial^2 \rho}{\partial x^2}$$

SEP in Contact with Particle Reservoirs

In the bulk the dynamics are as before. At the boundary there are reservoirs which supply/absorb particles at rates (α, γ) and (β, δ) . These reservoirs have densities ρ_{α} and ρ_{β} , where

$$\rho_a = \frac{\alpha}{\alpha + \gamma}, \quad \rho_b = \frac{\delta}{\delta + \beta}, \quad \text{for SSEP}$$

The macroscopic profiles of open system with x = i/L in [0, 1] satisfies for SSEP and WASEP the same equation as before with *boundary* conditions $\rho(0) = \rho_a, \rho(1) = \rho_b$

This yields for the stationary state a typical density profile $\bar{\rho}(x)$ which is linear for the SSEP:

$$\overline{\rho}(x) = \rho_a + x(\rho_b - \rho_a), \quad x \in [0, 1]$$

and has a (hyperbolic) tangent shape in the WASEP.

We don't have a hydrodynamic equation for the open ASEP but its stationary typical profile can be computed. (Recent work of Bahadoran gives an equation for the ASEP. Rather complicated boundary conditions.) When $\rho_a = \rho_b = r$, the stationary state of this system will be that of equilibrium, i.e. the measure will be a product measure with density r,

$$\mu(\tau) = \prod_{i=1}^{L} [r\tau_i + (1-r)(1-\tau_i)] = \nu_L^{(r)}(\tau)$$

To get the stationary nonequilibrium measure when $\rho_a \neq \rho_b$, we have to use the matrix method of Derrida et al. (see book by Liggett). This gives

$$\bar{\mu}_L(\tau) = \frac{\langle W | \Pi_{i=1}^L(\tau_i D + (1 - \tau_i) E) | V \rangle}{\langle W | (D + E)^L | V \rangle}$$

The "matrices" D and E and the vectors $|V\rangle$ and $\langle W|$ satisfy

$$DE - qED = D + E$$

 $(\beta D - \delta E)|V\rangle = |V\rangle, \quad \langle W|(\alpha E - \gamma D) = \langle W|.$

Large Deviations for the Open SSEP

We are interested in the probability in the NESS, described by $\overline{\mu}_L$, of finding a profile $\rho(x)$ on the macroscopic scale, i.e. we want the probability of all configurations $(\tau_1, ..., \tau_L)$ such that

$$|rac{1}{L}\sum_{i=aL}^{bL} au_i - \int_a^b
ho(x)dx| < \delta_L$$

with $\delta_L \rightarrow 0$ as $L \rightarrow \infty$. The optimal profile would be the one with the overwhelmingly largest probability.

We expect and get in fact a "large deviation" result

$$P_L(\{\rho(x)\}) \simeq \exp[-L\mathcal{F}(\{\rho\})]$$

 \mathcal{F} is the large deviation functional (LDF), $\mathcal{F}(\{\rho\}) \geq 0$, with equality only for $\rho(x) = \overline{\rho}(x)$. Any other profile will have $\mathcal{F}(\{\rho\}) > 0$ and thus, for large L, exponentially small probability.

For the SSEP the LDF is given by

$$\mathcal{F}(\{\rho\}) = \sup \int_0^1 dx \{\rho(x) \log \left(\frac{\rho(x)}{F(x)}\right)$$

$$+(1-\rho(x))\log(\frac{1-\rho(x)}{1-F(x)})+\log(\frac{F'(x)}{\rho_a-\rho_b})\},$$

The sup is over all monotone F, satisfying the boundary conditions

$$F(0) = \rho_a, \quad F(1) = \rho_b, \quad \rho_a \ge \rho_b.$$

It is the unique non-increasing solution of the differential equation

$$\rho(x) = F(x) + \frac{F(x)[1 - F(x)]F''(x)}{F'(x)^2}.$$

Note that $\mathcal{F}(\{\rho\}) \geq \mathcal{F}_{eq}(\{\rho\})$ which would correspond to $F(x) = \overline{\rho}(x)$ so deviations from typical profile, $\overline{\rho}(x)$, are suppressed in this NESS.

Fluctuations from the LDF for the SSEP

Writing

$$\rho(x) \sim \bar{\rho}(x) + \frac{u(x)}{\sqrt{L}}$$

we obtain

$$\mathcal{F} \sim \int \int u(x) C^{-1}(x, x') u(x') dx dx'$$
$$C(x, x') = \bar{\rho}(x) [1 - \bar{\rho}(x)] \delta(x - x') + F_2(x, x')$$

such long range correlations are predicted by fluctuating hydrodynamics (Procaccia, ...), experiment (Sengers, ...). Spohn (1983) proved this for this system.

Kipnis, Marchioro, Presutti (KMP) Model of Heat Conduction

At each site of the lattice, i = 1, ..., L there is a harmonic oscillator (q_i, p_i) The oscillators share their energy $\xi_i = \frac{1}{2}(p_i^2 + q_j^2)$ at random times, $0 \le \xi_i$,

$$\xi_i' = p(\xi_i + \xi_{i+1})$$

 $\xi'_{i+1} = (1-p)(\xi_i + \xi_{i+1}), \quad i = 1, ..., L-1$

p randomly distributed in [0, 1]

$$\xi'_1 = r, \quad \text{with } w_a(r) = \beta_a e^{-\beta_a r}, \quad \beta_a = T_a^{-1}$$
$$\xi'_L = r, \quad \text{with } w_b(r) = \beta_b e^{-\beta_b r}, \quad \beta_b = T_b^{-1}$$

In scaling limit the temperature profile $\theta(x,t)$

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2}$$

$$\theta(0,t) = T_a, \quad \theta(1,t) = T_b$$

When $T_a = T_b = \beta^{-1}$ stationary state is equilibrium.

When $T_a \neq T_b$, NESS measure $\bar{\mu}(d\xi)$ is unknown. We know, however, the LDF for a profile $\theta(x)$,

 $Prob(\{\theta(x)\}) \sim e^{-L\mathcal{F}(\{\theta\})}$ $\mathcal{F}_{\mathsf{K}}(\{\theta\}) = \inf_{F} \int_{0}^{1} dx \left[\frac{\theta(x)}{F(x)} - 1\right]$ $-\log \frac{\theta(x)}{F(x)} - \log \frac{\theta'(x)}{T_{a} - T_{b}}$

F(x) satisfies the equation

 $F^{2}[F''/(F')^{3}] + \theta(x) = F(x), F(0) = T_{a}, F(1) = T_{b}$

Comparing with \mathcal{F} for the SSEP, we see both strong similarities and also important differences: \mathcal{F}_K involves an inf rather than sup. Consequently \mathcal{F}_K is not convex. Also $\mathcal{F}_K \leq \mathcal{F}_{eq}$ so fluctuations are enhanced.

0.01