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DIFFUSIVE SCALING IN ENERGY GINZBURG-LANDAU DYNAMICS

CARLANGELLO LIVERANI, STEFANO OLLA, AND MAKIKO SASADA

ABSTRACT. Ginzburg-Landau energy models arise as autonomous stochastic dynamics for the energies in coupled systems after a weak coupling limit (cf. [3, 6]). We prove here that, under certain conditions, the energy fluctuations of these stochastic dynamics are driven by the heat equation, under a diffusive space time scaling.

1. INTRODUCTION

Heat equation describes the macroscopic evolution of energy, after a coarse-graining limit, in system that have finite thermal conductivity. In a pinned chain of anharmonic oscillators or other coupled system conserving total energy, we expect that after a diffusive rescaling of space and time the space distribution of the energy converges to the solution of the corresponding heat equation. This is a very difficult open problem, even at the level of equilibrium fluctuations, that should converge to the solution of the corresponding linearized heat equation.

In recent years some mathematical progress have been obtained for weakly coupled very time mixing systems, in particular in [3] for deterministic dynamics in negative curvature manifolds, and in [6] for an-harmonic oscillators with stochastic perturbations that conserve kinetic energy of each oscillator. In these weak coupling limit, an autonomous stochastic dynamics of the energies of each system arise. These energies dynamics satisfy a system of stochastic differential equations conservative of the total energy and where the instantaneous energy exchange currents are related to the equilibrium fluctuation variance of the corresponding currents in the microscopic dynamics. These stochastic differential equations define a Markov process on the energies configurations, and are formally similar to the (non-gradient) Ginzburg-Landau dynamics considered by Varadhan in [9]. The

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main differences with respect to the dynamics in [9] are that the dynamics is here confined to positive values of the energies, and that the families of stationary (reversible) probability distributions correspond to potential growing linearly for large values of the energy (since they are derived from the energies marginals of the canonical Gibbs measures of the microscopic dynamics).

We obtain here the linearized heat equation for the behaviour of the energy fluctuations in equilibrium under a diffusive space-time scaling, for the energy Ginzburg-Landau dynamics. We use the non-gradient approach of Varadhan used in [9], properly adapted. Consequently this result is conditioned to the existence of a lower bound for the spectral gap of the generator of the corresponding finite dynamics. This gap bound is proven in [7] for the Ginzburg-Landau dynamics arising from the anharmonic oscillators with stochastic perturbations considered in [6]. For the GL arising in the deterministic case considered by [3] it remains an open problem, and in this moment we are not sure about the validity of such bound.

The present result imply a proof of the validity of the heat equation in two step: first the weak-coupling limit ([3, 6]), then the hydrodynamic diffusive space-time limit (at least in the linearized sense). A straight limit from the microscopic dynamics, without passing through the weak-coupling, has been performed in [7] in a special situation with a stochastic perturbation of the hamiltonian dynamics that involves directly also the positions.

The difficulties we encounter already in the two step are certainly instructive about the more difficult problem of the direct limit from the microscopic dynamics.

2. THE DYNAMICS

We consider the dynamics for the infinite system, and, in order to keep notation as simple as possible, in one dimension. The configuration space is given by: $\mathcal{E} = \{\mathcal{E}_x, x \in \mathbb{Z}\} \in (\mathbb{R}_+)^{\mathbb{Z}}$.

The dynamics is defined by the solution of the stochastic differential equations:

$$\begin{aligned} d\mathcal{E}_x(t) &= dJ_{x-1,x}(t) - dJ_{x+1,x}(t) \\ dJ_{x+1,x}(t) &= \alpha(\mathcal{E}_x(t), \mathcal{E}_{x+1}(t))dt + \sqrt{2}\gamma(\mathcal{E}_x(t), \mathcal{E}_{x+1}(t))dB_{x,x+1} \end{aligned} \quad (2.1)$$

The coefficients are related by the equations

$$\alpha(\mathcal{E}_0, \mathcal{E}_1) = e^{\mathcal{U}(\mathcal{E})} (\partial_{\mathcal{E}_1} - \partial_{\mathcal{E}_0}) (e^{-\mathcal{U}(\mathcal{E})} \gamma^2(\mathcal{E}_0, \mathcal{E}_1)) \quad (2.2)$$

with $\mathcal{U}(\mathcal{E}) = \sum_x U(\mathcal{E}_x)$, and we are interested in $U(a) \sim \log a$ for $a \rightarrow 0$ and $a \rightarrow \infty$. We will specify further conditions on γ^2 . Sometimes we will use the notation $\alpha_{x,x+1} = \alpha(\mathcal{E}_x, \mathcal{E}_{x+1})$, and similarly for $\gamma_{x,x+1}$.

The corresponding generator can be formally written as

$$L = \sum_x L_{x,x+1} \quad (2.3)$$

$$L_{x,x+1} = e^{\mathcal{U}(\mathcal{E})} (\partial_{\mathcal{E}_{x+1}} - \partial_{\mathcal{E}_x}) e^{-\mathcal{U}(\mathcal{E})} \gamma_{x,x+1}^2 (\partial_{\mathcal{E}_{x+1}} - \partial_{\mathcal{E}_x})$$

We will use also the finite dimensional generators

$$L_k = \sum_{x=-k}^{k-1} L_{x,x+1}. \quad (2.4)$$

There is a family of invariant measures given by

$$d\mu_\beta = \prod_x \frac{e^{-U(\mathcal{E}_x) - \beta \mathcal{E}_x}}{M(\beta)} d\mathcal{E}_x, \quad \beta > 0. \quad (2.5)$$

These probability measure are reversible and the corresponding dirichlet form are

$$\mathcal{D}(f) = \sum_x \mathcal{D}_{x,x+1}(f), \quad \mathcal{D}_{x,x+1}(f) = \int \gamma_{x,x+1}^2 (\partial_{\mathcal{E}_{x+1}} f - \partial_{\mathcal{E}_x} f)^2 d\mu_\beta \quad (2.6)$$

$$\mathcal{D}_k(f) = \sum_{x=-k}^{k-1} \mathcal{D}_{x,x+1}(f).$$

In this article we will consider only the dynamics in equilibrium, starting with initial configuration distributed by μ_β for a given $\beta > 0$. From standard arguments it follows, under reasonable conditions on α , the existence of the solution of the equilibrium dynamics, and that local smooth functions form a core for the domain of the generator L . We will not worry here about these issues and we assume that all these objects are well defined. We denote with \mathbb{P} the measure on $\mathcal{C}^0(\mathbb{R}_+, \mathbb{R}_+^{\mathbb{Z}})$ for the equilibrium dynamics determined by equation (2.1) and by \mathbb{E} the corresponding expectation. We will also use the notation $\mathbb{E}(f) = \langle f \rangle$.

3. EQUILIBRIUM FLUCTUATIONS

Our main goal is to prove the following theorem:

Theorem 1. *Let $G(y), F(y)$ smooth function with compact support on \mathbb{R} . Then*

$$\lim_{\varepsilon \rightarrow 0} \varepsilon \sum_{x,z} G(\varepsilon x) F(\varepsilon z) [\langle \mathcal{E}_x(\varepsilon^{-2}t) \mathcal{E}_z(0) \rangle - \langle \mathcal{E}_0 \rangle^2]$$

$$= \chi \iint G(y) F(y') \frac{e^{-(y-y')^2/2tD}}{\sqrt{2\pi tD}} dy dy' \quad (3.1)$$

Where $\chi = \langle \mathcal{E}_0^2 \rangle - \langle \mathcal{E}_0 \rangle^2 = \text{var}(\mathcal{E}_0)$. The diffusivity D is given by the usual Green Kubo formula, but will appear in the proof as a variational formula.

We specify here the assumption under which we are able to prove this theorem:

- γ is such the following spectral gap bound is satisfied:

$$\langle f^2 | \bar{\mathcal{E}}_k \rangle \leq C k^2 \mathcal{D}_k(f) \quad (3.2)$$

for any local function f such that $\langle f^2 | \bar{\mathcal{E}}_k \rangle = 0$, where $\langle \cdot | \bar{\mathcal{E}}_k \rangle$ denotes the microcanonical conditional expectation on the corresponding energy surface $\bar{\mathcal{E}}_k = \frac{1}{2k+1} \sum_{|x| \leq k} \mathcal{E}_x$. The constant C is independent of k but can depend on \mathcal{E}_k .

- For some $a \geq 1$ there exists $\tilde{\gamma}(\mathcal{E})$ such that:

$$a^{-1} \tilde{\gamma}(\mathcal{E}_0) \tilde{\gamma}(\mathcal{E}_1) \leq \gamma(\mathcal{E}_0, \mathcal{E}_1) \leq a \tilde{\gamma}(\mathcal{E}_0) \tilde{\gamma}(\mathcal{E}_1). \quad (3.3)$$

The function γ arising in [6] satisfies these conditions (in particular the spectral gap bound is proven in [7] with a constant C independent of the energy). It is an open problem at the moment if the γ function arising in [3] satisfies such conditions.

4. TIME VARIANCE

We start with computing the time evolution of the left hand side of (3.1) before the limit.

$$\begin{aligned} & \varepsilon \sum_{x,z} G(\varepsilon x) F(\varepsilon z) \left\{ \left[\langle \mathcal{E}_x(\varepsilon^{-2}t) \mathcal{E}_z(0) \rangle - \langle \mathcal{E}_0 \rangle^2 \right] - \left[\langle \mathcal{E}_x(0) \mathcal{E}_z(0) \rangle - \langle \mathcal{E}_0 \rangle^2 \right] \right\} \\ &= \varepsilon \sum_{x,z} G(\varepsilon x) F(\varepsilon z) \langle (\mathcal{E}_x(\varepsilon^{-2}t) - \mathcal{E}_x(0)) (\mathcal{E}_z(0) - \bar{e}) \rangle \\ &= \int_0^t \sum_{x,z} \left[G'(\varepsilon x) + \frac{1}{2} G''(\varepsilon x) \varepsilon \right] F(\varepsilon z) \langle \alpha_{x,x+1}(\varepsilon^{-2}s) (\mathcal{E}_z(0) - \bar{e}) \rangle ds + \mathcal{O}(\varepsilon), \end{aligned}$$

where, in the last line, we have used Schwarz inequality, stationarity, and, since $\alpha_{x,x+1} \in L^2$,

$$\left\| \sum_x G'''(\varepsilon z) \alpha_{x,x+1} \right\|_{L^2} \leq C_{\#} \varepsilon^{-1/2}$$

$$\left\| \sum_z F(\varepsilon z) (\mathcal{E}_z - \bar{e}) \right\|_{L^2} \leq C_{\#} \varepsilon^{-1/2}$$

Note that the term with the second derivative of G has exactly the same form as the one with G' . Thus, given the arbitrariness of G , it suffice to show that the term in G' has limit in order to prove that the one with G'' vanishes. Next choose local smooth functions $f(\mathcal{E})$ (with $\langle f \rangle = 0$) and set

$$\begin{aligned} \phi_f &= \alpha(\mathcal{E}_1, \mathcal{E}_0) - \kappa(U'(\mathcal{E}_1) - U'(\mathcal{E}_0)) - Lf \\ &= \alpha(\mathcal{E}_1, \mathcal{E}_0) - \kappa([U'(\mathcal{E}_1) - \beta] - [U'(\mathcal{E}_0) - \beta]) - Lf \end{aligned}$$

We will choose later the constant $\kappa = \chi D$ (this is also called thermal conductivity). We can then continue our computation:

$$= \int_0^t \varepsilon \sum_{x,z} G''(\varepsilon x) F(\varepsilon z) \kappa \langle [U'(\mathcal{E}_x(\varepsilon^{-2}s)) - \beta](\mathcal{E}_z(0) - \bar{e}) \rangle ds \quad (4.1)$$

$$+ \int_0^t \sum_{x,z} G'(\varepsilon x) F(\varepsilon z) \langle L\tau_x f(\varepsilon^{-2}s)(\mathcal{E}_z(0) - \bar{e}) \rangle ds \quad (4.2)$$

$$+ \int_0^t \sum_{x,z} G'(\varepsilon x) F(\varepsilon z) \langle \tau_x \phi_f(\varepsilon^{-2}s)(\mathcal{E}_z(0) - \bar{e}) \rangle ds + o(\varepsilon) \quad (4.3)$$

About line (4.1), we prove in section 8 that

$$\lim_{\varepsilon \rightarrow 0} \left\langle \left(\int_0^t \varepsilon^{1/2} \sum_z G''(\varepsilon z) [U'(\mathcal{E}_x(\varepsilon^{-2}s)) - \beta - \chi^{-1}(\mathcal{E}_x(\varepsilon^{-2}s) - \bar{e})] ds \right)^2 \right\rangle = 0 \quad (4.4)$$

Since $D = \kappa/\chi$,

$$\begin{aligned} & \left| \int_0^t \varepsilon \sum_{x,z} G''(\varepsilon x) F(\varepsilon z) \langle \{ \kappa [U'(\mathcal{E}_x(\varepsilon^{-2}s)) - \beta] - D[(\mathcal{E}_x(\varepsilon^{-2}s)) - \bar{e}] \} (\mathcal{E}_z(0) - \bar{e}) \rangle ds \right|^2 \\ & \leq \left\langle \left(\varepsilon^{1/2} \sum_z F(\varepsilon z) (\mathcal{E}_z(0) - \bar{e}) \right)^2 \right\rangle \\ & \cdot \left\langle \left(\int_0^t \varepsilon^{1/2} \sum_z G''(\varepsilon z) \kappa [U'(\mathcal{E}_x(\varepsilon^{-2}s)) - \beta - \chi^{-1}(\mathcal{E}_x(\varepsilon^{-2}s) - \bar{e})] ds \right)^2 \right\rangle \end{aligned}$$

This will close our equation if we prove that (4.2) and (4.3) lines will converge to 0 after the limit as $\varepsilon \rightarrow 0$ and minimization on the local function f .

Second term is easy:

$$\begin{aligned} & \left| \int_0^t \varepsilon^2 \sum_{x,z} G'(\varepsilon x) F(\varepsilon z) \langle \varepsilon^{-2} L\tau_x f(\varepsilon^{-2}s)(\mathcal{E}_z(0) - \bar{e}) \rangle ds \right|^2 \\ & = \left| (\mathcal{E}_z(0) - \bar{e}) \varepsilon^2 \sum_{x,z} G'(\varepsilon x) F(\varepsilon z) \langle (\tau_x f(\varepsilon^{-2}t) - \tau_x f(0))(\mathcal{E}_z(0) - \bar{e}) \rangle \right|^2 \\ & \leq \varepsilon^2 \left\langle \left(\varepsilon^{1/2} \sum_z F(\varepsilon z) (\mathcal{E}_z(0) - \bar{e}) \right)^2 \right\rangle \left\langle \left(\varepsilon^{1/2} \sum_x G'(\varepsilon x) (\tau_x f(\varepsilon^{-2}t) - \tau_x f(0)) \right)^2 \right\rangle \end{aligned}$$

since

$$\left\langle \left(\varepsilon^{1/2} \sum_z F(\varepsilon z) (\mathcal{E}_z(0) - \bar{e}) \right)^2 \right\rangle = \varepsilon \sum_z F(\varepsilon z)^2 \chi \leq \chi \|F\|_2^2$$

and similarly

$$\left\langle \left(\varepsilon^{1/2} \sum_x G'(\varepsilon x) (\tau_x f(\varepsilon^{-2}t) - \tau_x f(0)) \right)^2 \right\rangle \leq C \|G'\|^2 \sum_x \langle \tau_x f, f \rangle < \infty$$

since f is local and of null average.

About the third term, using again Schwarz inequality, the square is bounded by

$$\chi \|F\|_2^2 \left\langle \left(\int_0^t \varepsilon^{-1/2} \sum_x G'(\varepsilon x) \tau_x \phi_f(\varepsilon^{-2}s) ds \right)^2 \right\rangle$$

The rest of the work is in order to prove that

$$\inf_f \lim_{\varepsilon \rightarrow 0} \left\langle \left(\int_0^t \varepsilon^{-1/2} \sum_x G'(\varepsilon x) \tau_x \phi_f(\varepsilon^{-2}s) ds \right)^2 \right\rangle = 0$$

By the time variance estimate for a stationary markov process (see (4.1) in [7] or in chapter 2 of [5]):

$$\begin{aligned} & \left\langle \left(\int_0^t \varepsilon^{-1/2} \sum_x G'(\varepsilon x) \tau_x \phi_f(\varepsilon^{-2}s) ds \right)^2 \right\rangle \\ & \leq 16t \left\langle \left(\varepsilon^{1/2} \sum_x G'(\varepsilon x) \tau_x \phi_f \right) (-\varepsilon^{-2}L)^{-1} \left(\varepsilon^{1/2} \sum_x G'(\varepsilon x) \tau_x \phi_f \right) \right\rangle \\ & = 16t \sup_g \left\langle \varepsilon^{1/2} \sum_x G'(\varepsilon x) \langle \tau_x \phi_f g \rangle - \varepsilon^{-2} \mathcal{D}(g) \right\rangle \end{aligned}$$

After some steps (see proof of theorem 2 in [7]) we obtain that, for $k \ll \varepsilon^{-1}$ this is bounded by

$$Ct\varepsilon \sum_x G'(\varepsilon x)^2 (2k+1) \langle Av_{k'}(\phi_f), (-L_k)^{-1} Av_{k'}(\phi_f) \rangle - C_G O(\varepsilon k)$$

where $Av_k(\phi) = \frac{1}{2k+1} \sum_{j=-k}^k \tau_j \phi$, and $k' < k$ such that $Av_k(\phi)$ is localized between $(-k, \dots, k)$.

Now comes the hard work. Define the vector fields

$$\partial_{x,x+1} = \gamma_{x,x+1} (\partial_{\varepsilon_{x+1}} - \partial_{\varepsilon_x})$$

and

$$\partial_{x,x+1}^* = e^{\mathcal{U}} (\partial_{\varepsilon_{x+1}} - \partial_{\varepsilon_x}) e^{-\mathcal{U}} \gamma_{x,x+1}$$

its adjoint with respect to $d\mu$. Then we can write $L_{x,x+1} = \partial_{x,x+1}^* \partial_{x,x+1}$.

For any $k \in \mathbb{N}_*$, define the microcanonical expectation $\mathcal{M}_k \phi = \langle \phi | \bar{\mathcal{E}}_k \rangle$ where $\bar{\mathcal{E}}_k = (2k+1)^{-1} \sum_{|x| \leq k} \mathcal{E}_x$. Define the space of functions on $\mathbb{R}_+^{\mathbb{Z}}$

$$\mathcal{C}_0 = \{ \phi \in L^2(\mu) \text{ local} : \mathcal{M}_{k_0} \phi = 0 \text{ for a finite } k_0 \} \quad (4.5)$$

Since L_{k_0} , on each microcanonical surface, has a spectral gap bounded below by k_0^{-2} uniformly in the energy¹, we can invert $u_{k_0} = (-L_{k_0})^{-1}\phi$, for $\phi \in \mathcal{C}_0$ and we have

$$\mathcal{D}_{k_0}(u_{k_0}) = \langle u_{k_0}, \phi \rangle \leq \langle u_{k_0}^2 \rangle^{1/2} \langle \phi^2 \rangle^{1/2} \leq C^{1/2} k_0 \mathcal{D}_{k_0}(u_{k_0})^{1/2} \langle \phi^2 \rangle^{1/2}$$

and consequently

$$\mathcal{D}_{k_0}(u_{k_0}) \leq C k_0^2 \langle \phi^2 \rangle \quad (4.6)$$

In particular for any smooth local function h :

$$\langle \phi, h \rangle = \sum_{i=-k_0}^{k_0-1} \langle (\partial_{i,i+1} u_{k_0}), (\partial_{i,i+1} h) \rangle \leq C^{1/2} k_0 \langle \phi^2 \rangle^{1/2} \mathcal{D}_{k_0}(h)^{1/2} \quad (4.7)$$

For a local function $\phi \in \mathcal{C}_0$, we will show that the following limit exists

$$\lim_{k \rightarrow \infty} (2k+1) \langle Av_{k'}(\phi), (-L_k)^{-1} Av_{k'}(\phi) \rangle = \|\phi\|_{-1}^2 \quad (4.8)$$

we will compute such norm and to conclude the proof we need to show that

$$\inf_f \|\phi_f\|_{-1} = 0. \quad (4.9)$$

5. VARIATIONAL FORMULA FOR THE LIMIT SPACE-TIME VARIANCE

Let us compute the limit (4.8). For simplicity of notations, assume that $k_0 = 0$, i.e. $\phi = \partial_{0,1}^* F$, with $F = X_{0,1} u_0$ (following strictly the notation of the previous section). The general case, $k_0 < \infty$, follows easily by linearity.

$$\begin{aligned} & (2k+1) \langle Av_{k'}(\phi), (-L_k)^{-1} Av_{k'}(\phi) \rangle \\ &= \sup_h \left\{ 2 \left\langle \phi, \frac{1}{2k+1} \sum_{|j| \leq k'} \tau_j h \right\rangle - \frac{1}{2k+1} \mathcal{D}_k(h) \right\} \\ &= \sup_h \left\{ 2 \left\langle F, \partial_{0,1} \left(\frac{1}{2k+1} \sum_{|j| \leq k'} \tau_j h \right) \right\rangle - \frac{1}{2k+1} \mathcal{D}_k(h) \right\} \end{aligned}$$

Call $\xi^k(h) = \partial_{0,1} \left(\frac{1}{2k+1} \sum_{|j| \leq k'} \tau_j h \right)$, and observe that

$$\langle F, \xi^k(h) \rangle \leq \frac{C \|F\|_2}{2k} \mathcal{D}_k(h)^{1/2}$$

and that by Schwarz inequality

$$\langle \xi^k(h) \rangle^2 \leq \frac{1}{2k+1} \sum_{|j| \leq k'} \langle (\partial_{0,1} \tau_j h)^2 \rangle \leq \frac{1}{2k} \mathcal{D}_k(h)$$

¹Notice that it is not necessary here a uniform bound, since k_0 is fixed.

So we obtain the upper bound

$$(2k+1) \left\langle Av_{k'}(\phi), (-L_k)^{-1} Av_{k'}(\phi) \right\rangle \leq \sup_h \left\{ 2 \langle F, \xi^k(h) \rangle - \langle \xi^k(h)^2 \rangle \right\}$$

Since we can restrict the supremum on functions h such that $\langle \xi^k(h)^2 \rangle \leq \langle F^2 \rangle$, for any of such function h we can extract convergent subsequences in $L^2(d\mu)$.

Observe that

$$\partial_{z,z+1} \tau_x \xi^k(h) = \partial_{x,x+1} \tau_z \xi^k(h) \quad (5.1)$$

as long as $|x|$ and $|z|$ are small with respect to k and $|x-z| \geq 2$, (for $|x-z| < 2$ there are some relations that we will have to take into account). So any limit $\xi(h)$ for $k \rightarrow \infty$ enjoy of this property for any $x, z \in \mathbb{Z}$. We call *closed forms* (or germs of closed forms) all functions that satisfy property (5.1), and we denote the closed subset of such functions in $L^2(\mu)$ by \mathfrak{h}_c . So we have proved that, for $\phi = \partial_{0,1}^* F$, with $F = X_{0,1} u_0$:

$$\lim_{k \rightarrow \infty} (2k+1) \left\langle Av_{k'}(\phi), (-L_k)^{-1} Av_{k'}(\phi) \right\rangle \leq \sup_{\xi \in \mathfrak{h}_c} \left\{ 2 \langle F, \xi \rangle - \langle \xi^2 \rangle \right\} \quad (5.2)$$

Let us now study a lower bound. Observe that $L_k \sum_{|x| \leq k} x \mathcal{E}_x = \sum_{x=-k}^{k-1} \tau_x \alpha_{0,1}$. Computing we have:

$$(2k+1) \left\langle Av_k \alpha_{0,1}, (-L_k)^{-1} Av_k \phi \right\rangle \xrightarrow{k \rightarrow \infty} - \langle \gamma_{0,1} F \rangle \quad (5.3)$$

For a local smooth function f

$$(2k+1) \left\langle Av_{k'} Lf, (-L_k)^{-1} Av_{k'} \phi \right\rangle \xrightarrow{k \rightarrow \infty} - \sum_x \langle \phi \tau_x f \rangle = - \langle F \partial_{0,1} \Gamma_f \rangle \quad (5.4)$$

where we have defined the formal sum $\Gamma_f = \sum_x \tau_x f$ (since f is local, $\partial_{0,1} \Gamma_f$ is well define finite sum). Similarly:

$$(2k+1) \left\langle Av_{k'} Lf, (-L_k)^{-1} Av_{k'} Lf \right\rangle \xrightarrow{k \rightarrow \infty} \langle (\partial_{0,1} \Gamma_f)^2 \rangle \quad (5.5)$$

and all together, for any $a \in \mathbb{R}$:

$$(2k+1) \left\langle Av_{k'}(a\alpha_{0,1} + Lf), (-L_k)^{-1} Av_{k'}(a\alpha_{0,1} + Lf) \right\rangle \xrightarrow{k \rightarrow \infty} \langle (a\gamma_{0,1} + \partial_{0,1} \Gamma_f)^2 \rangle \quad (5.6)$$

Then for any $a \in \mathbb{R}$ and local f :

$$\begin{aligned} & (2k+1) \left\langle Av_{k'}(\phi), (-L_k)^{-1} Av_{k'}(\phi) \right\rangle \\ & \geq 2(2k+1) \left\langle Av_{k'}(\phi), (-L_k)^{-1} Av_{k'}(a\alpha_{0,1} + Lf) \right\rangle \\ & \quad - (2k+1) \left\langle Av_{k'}(a\alpha_{0,1} + Lf), (-L_k)^{-1} Av_{k'}(a\alpha_{0,1} + Lf) \right\rangle \\ & \xrightarrow{k \rightarrow \infty} 2a \langle \gamma_{0,1} F \rangle + 2 \langle F \partial_{0,1} \Gamma_f \rangle - \langle (a\gamma_{0,1} + \partial_{0,1} \Gamma_f)^2 \rangle \end{aligned}$$

So we have obtained

$$\|\phi\|_{-1}^2 \geq \sup_{a,f} \{2 \langle F, a\gamma_{0,1} + \partial_{0,1}\Gamma_f \rangle - \langle (a\gamma_{0,1} + \partial_{0,1}\Gamma_f)^2 \rangle\} \quad (5.7)$$

In order to show equality in this formula, we have to put together the upper and lower bound, i.e. to prove that every *closed form* $\xi \in \mathfrak{h}_c$ can be approximated in $L^2(\mu)$ by functions of the type $a\gamma_{0,1} + \partial_{0,1}\Gamma_f$, with local f , that we call *exact forms*. This is usually the hardest part of the proof, where a uniform bound on the spectral gap is needed. We prove this in section section 7.

The general case, for $k_0 > 0$ is obtained in the same way and for $\phi = -L_{k_0}u_{k_0}$ we have

$$\|\phi\|_{-1}^2 = \sup_{a,f} \left\{ 2 \sum_{i=-k_0}^{k_0} \langle \partial_{i,i+1}u_{k_0}, \tau_i (a\gamma_{0,1} + \partial_{0,1}\Gamma_f) \rangle - \langle (a\gamma_{0,1} + \partial_{0,1}\Gamma_f)^2 \rangle \right\} \quad (5.8)$$

6. HILBERT SPACE OF FLUCTUATIONS

By polarizing the $\|\cdot\|_{-1}$ norm, we can define a scalar product that we denote by $\langle\langle \cdot, \cdot \rangle\rangle_{-1}$, and the corresponding Hilbert Space by \mathcal{H}_{-1} . It is also clear, from the results of the previous section that

$$\langle\langle \phi, \psi \rangle\rangle_{-1} = \lim_{k \rightarrow \infty} (2k+1) \langle Av_{k'}(\phi), (-L_k)^{-1} Av_{k'}(\psi) \rangle \quad (6.1)$$

Straightforward calculations show that, denoting $\nabla_{0,1}U' = U'(\mathcal{E}_1) - U'(\mathcal{E}_0)$,

$$\langle\langle \nabla_{0,1}U', Lf \rangle\rangle_{-1} = 0 \quad (6.2)$$

and we have computed already, for $\phi = \partial_{0,1}^*F$:

$$\begin{aligned} \langle\langle \alpha_{0,1}, \psi \rangle\rangle_{-1} &= - \langle \gamma_{0,1}F \rangle \\ \langle\langle Lf, \psi \rangle\rangle_{-1} &= - \langle \partial_{0,1}\Gamma_f, F \rangle \end{aligned} \quad (6.3)$$

in particular

$$\langle\langle \alpha_{0,1}, \nabla_{0,1}U' \rangle\rangle_{-1} = -1 \quad (6.4)$$

and

$$\|\alpha_{0,1}\|_{-1}^2 = \langle \gamma_{0,1}^2 \rangle \quad (6.5)$$

Proposition 6.1.

$$\mathcal{H}_{-1} = \text{Clos}\{Lf, f \text{ local smooth}\} + \{a\alpha_{0,1}, a \in \mathbb{R}\} \quad (6.6)$$

$$\mathcal{H}_{-1} = \text{Clos}\{Lf, f \text{ local smooth}\} \oplus \{a\nabla_{0,1}U', a \in \mathbb{R}\} \quad (6.7)$$

This proposition assure that $\inf_f \|\phi_f\|_{-1} = 0$.

Proof. Consider first $\phi = \partial_{0,1}^* F$. Then as consequence of all above we have the variational formula:

$$\|\phi\|_{-1}^2 = \sup_{a \in \mathbb{R}, g \text{ loc}} \left\{ 2 \langle F, a\gamma_{0,1} + \partial_{0,1}\Gamma_g \rangle - \langle (a\gamma_{0,1} + \partial_{0,1}\Gamma_g)^2 \rangle \right\}.$$

In particular for ϕ_f we have $F = \gamma_{0,1} - \kappa\gamma_{0,1}^{-1} + \partial_{0,1}\Gamma_f$.

Observe that $\langle \gamma_{0,1}^{-1}, \partial_{0,1}\Gamma_g \rangle = 0$. So we have

$$\begin{aligned} \|\phi_f\|_{-1}^2 &= \sup_{a \in \mathbb{R}, g \text{ loc}} \left\{ -2a\kappa + 2 \langle \gamma_{0,1} + \partial_{0,1}\Gamma_f, a\gamma_{0,1} + \partial_{0,1}\Gamma_g \rangle - \langle (a\gamma_{0,1} + \partial_{0,1}\Gamma_g)^2 \rangle \right\} \\ &= \sup_{a \in \mathbb{R}, g \text{ loc}} \left\{ -2a\kappa + 2a \langle \gamma_{0,1} + \partial_{0,1}\Gamma_f, \gamma_{0,1} + \partial_{0,1}\Gamma_g \rangle - a^2 \langle (\gamma_{0,1} + \partial_{0,1}\Gamma_g)^2 \rangle \right\} \\ &= \sup_{a \in \mathbb{R}} \left\{ -2a\kappa + (2a - a^2) \langle (\gamma_{0,1} + \partial_{0,1}\Gamma_f)^2 \rangle \right\} \\ &= \frac{\langle (\gamma_{0,1} + \partial_{0,1}\Gamma_f)^2 \rangle - \kappa}{\langle (\gamma_{0,1} + \partial_{0,1}\Gamma_f)^2 \rangle}. \end{aligned}$$

Defining

$$\kappa = \inf_f \langle (\gamma_{0,1} + \partial_{0,1}\Gamma_f)^2 \rangle \quad (6.8)$$

we obtain the result. \square

7. CLOSED FORMS

Recall $\mathfrak{h}_c \subset L^2(\mu)$ is the space of the function ξ such that

$$\begin{aligned} \partial_{x,x+1}\tau_y\xi &= \partial_{y,y+1}\tau_x\xi, & |x-y| &\geq 2 \\ \partial_{x,x+1}\tau_{x+1}\xi &= \partial_{x+1,x+2}\tau_x\xi + (\partial_{x,x+1}\log\gamma_{x+1,x+2})\tau_{x+1}\xi - (\partial_{x+1,x+2}\log\gamma_{x,x+1})\tau_x\xi \end{aligned} \quad (7.1)$$

For any local smooth f, we call *exact forms* functions of the type

$$\partial_{0,1}\Gamma_f \quad (7.2)$$

Remark that satisfy (7.1) (i.e. they are closed).

Also the function $\xi = \gamma_{0,1}$ satisfy (7.1). More generally we call *exact* the function of the form $a\gamma_{0,1} + \partial_{0,1}\Gamma_f$. We want to prove that \mathfrak{h}_c is the closure in L^2 of such exact functions.

Strategy:

We take $\xi \in \mathfrak{h}_c$ and define for $y = -k, \dots, k$,

$$\xi_y^{(k)} = \mathbb{E}(\tau_y\xi | \mathcal{F}_k) \varphi(\bar{\mathcal{E}}_k), \quad \mathcal{F}_k = \sigma(\mathcal{E}_x, |x| \leq k)$$

where φ is a smooth function on \mathbb{R}_+ with compact support, such that $\varphi(E(\beta)) = 1$ and it is bounded by 1. This is a cutoff function that we need in order to make uniform bounds later.

Now we are in the classical finite dimensional situation, and on each microcanonical surface ($\bar{\mathcal{E}}_k = e$ fixed) $\{\xi_y^{(k)}, y = -k, \dots, k\}$ is a closed form

(in a weak sense), i.e. exact, so it can be integrated. Let $u_k(\mathcal{E}_x, |x| \leq k, \bar{\mathcal{E}}_k)$ such that $\partial_{y,y+1} u_k = \xi_y^{(k)}$ for $y = -k, \dots, k-1$. This derivative should be intended in the distributional sense. We can always recenter u_k in such a way that $\mathbb{E}(u_k | \mathcal{E}_x, |x| \leq k) = 0$.

By condition (3.3), we can directly assume that $\gamma(\mathcal{E}_0, \mathcal{E}_1) = \tilde{\gamma}(\mathcal{E}_0) \tilde{\gamma}(\mathcal{E}_1)$, since the corresponding dirichlet forms are equivalent, and consequently all approximations done in the corresponding Hilbert spaces.

Then we define

$$u_{k,l} = \frac{1}{2(k+l) \langle \gamma^2 \rangle} \mathbb{E} \left(\tilde{\gamma}_{k+l+1}^2 \tilde{\gamma}_{-k-l-1}^2 u_{2k} | \mathcal{F}_{k+l} \right)$$

$$\widehat{u}^{(k)} = \frac{4}{k} \sum_{l=k/2}^{3k/4} u_{k,l}$$

Now we compute

$$\partial_{0,1} \Gamma_{\widehat{u}^{(k)}} = \partial_{0,1} \sum_{x=-\infty}^{+\infty} \tau_x \widehat{u}^{(k)}$$

In the calculation there are *interior* terms that depends on

$$\partial_{x,x+1} \widehat{u}^{(k)}$$

that converges in $L^2(\mu)$ to $\tau_x \xi$.

Then there are boundary terms more tricky to control that, for x enough small, will converge to $a \tilde{\gamma}_0 \tilde{\gamma}_1$ for some $a \in \mathbb{R}$.

One of the boundary terms is given by

$$\begin{aligned} & \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l) \langle \gamma^2 \rangle} \tau_{-k-l} \left\{ \tilde{\gamma}_{k+l} \tilde{\gamma}_{k+l+1} \mathbb{E} \left(\tilde{\gamma}_{k+l+1}^2 \tilde{\gamma}_{-k-l-1}^2 \partial_{\mathcal{E}_{k+l}} u_{2k} | \mathcal{F}_{k+l} \right) \right\} \\ &= -\frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l) \langle \gamma^2 \rangle} \tilde{\gamma}_1 \tau_{-k-l} \mathbb{E} \left(\tilde{\gamma}_{-k-l-1}^2 \tilde{\gamma}_{k+l+1} \partial_{k+l+1, k+l} u_{2k} | \mathcal{F}_{k+l} \right) \quad (7.3) \\ &+ \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l) \langle \gamma^2 \rangle} \tilde{\gamma}_1 \tau_{-k-l} \mathbb{E} \left(\tilde{\gamma}_{k+l} \tilde{\gamma}_{k+l+1}^2 \tilde{\gamma}_{-k-l-1}^2 \partial_{\mathcal{E}_{k+l+1}} u_{2k} | \mathcal{F}_{k+l} \right) \end{aligned}$$

the other boundary terms are similar and will be treated in the same way. The first term of the rhs of (7.3) converges to 0 in L^2 , because $\partial_{k+l+1, k+l} u_{2k}$ are uniformly bounded in L^2 . The second term of the rhs of (7.3), after an integration by part, became

$$\begin{aligned} & \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l) \langle \gamma^2 \rangle} \tilde{\gamma}_1 \tilde{\gamma}_0 \tau_{-k-l} \mathbb{E} \left((\partial_{\mathcal{E}_{k+l+1}}^* \tilde{\gamma}_{k+l+1}^2) \tilde{\gamma}_{-k-l-1}^2 u_{2k} | \mathcal{F}_{k+l} \right) \quad (7.4) \\ &= \tilde{\gamma}_0 \tilde{\gamma}_1 h_k(\mathcal{E}_0, \mathcal{E}_{-1}, \dots, \mathcal{E}_{-7k/2}) \end{aligned}$$

where

$$\partial_{\mathcal{E}_{k+l+1}}^* \tilde{\gamma}_{k+l+1}^2 = -\partial_{\mathcal{E}_{k+l+1}} \tilde{\gamma}_{k+l,k+l+1}^2 + U'(\mathcal{E}_{k+l+1}) \tilde{\gamma}_{k+l,k+l+1}^2$$

We rewrite h_k as

$$\begin{aligned} \langle \tilde{\gamma}^2 \rangle h_k &= \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l)} \tau_{-k-l} \mathbb{E} \left((\partial_{\mathcal{E}_{k+l+1}}^* \tilde{\gamma}_{k+l+1}^2) \tilde{\gamma}_{-k-l-1}^2 u_{2k} | \mathcal{F}_{k+l} \right) \\ &= \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l)} \tau_{-k-l} \left[\mathbb{E} \left((\partial_{\mathcal{E}_{k+l+1}}^* \tilde{\gamma}_{k+l+1}^2) \tilde{\gamma}_{-k-l-1}^2 u_{2k} | \mathcal{F}_{k+l} \right) \right] \\ &= \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l)} \tau_{-k-l} \mathbb{E} \left((\partial_{\mathcal{E}_{k+l+1}}^* \tilde{\gamma}_{k+l+1}^2) \tilde{\gamma}_{-k-l-1}^2 u_{2k} | \mathcal{F}_{k+l} \right) \\ &= \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l)} \tau_{-k-l} \mathbb{E} \left(\frac{\tilde{\gamma}_{-k-l-1}^2}{k-l} \sum_{j=k+l+1}^{2k} \partial_{\mathcal{E}_j}^* \tilde{\gamma}_j^2 (u_{2k} \circ \pi^{j,k+l+1}) | \mathcal{F}_{k+l} \right) \\ &= \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l)} \tau_{-k-l} \mathbb{E} \left(u_{2k} \frac{\tilde{\gamma}_{-k-l-1}^2}{k-l} \sum_{j=k+l+1}^{2k} \partial_{\mathcal{E}_j}^* \tilde{\gamma}_j^2 | \mathcal{F}_{k+l} \right) \\ &+ \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{2(k+l)} \tau_{-k-l} \mathbb{E} \left(\frac{\tilde{\gamma}_{-k-l-1}^2}{k-l} \sum_{j=k+l+1}^{2k} \partial_{\mathcal{E}_j}^* \tilde{\gamma}_j^2 (u_{2k} \circ \pi^{j,k+l+1} - u_{2k}) | \mathcal{F}_{k+l} \right) \end{aligned} \quad (7.5)$$

Let us estimate the first expression of the rhs, by Schwarz inequality and the cutoff introduced, its square is bounded by

$$\begin{aligned} &\tau_{-k-l} \mathbb{E} \left(u_{2k}^2 \frac{4}{k} \sum_{l=k/2}^{3k/4} \tilde{\gamma}_{-k-l-1}^2 | \mathcal{F}_{k+l} \right) \left(\frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{\tilde{\gamma}_{-k-l-1}^2}{4(k+l)^2} \tau_{-k-l} \mathbb{E} \left(\left[\frac{1}{k-l} \sum_{j=k+l+1}^{2k} \partial_{\mathcal{E}_j}^* \tilde{\gamma}_j \right]^2 | \mathcal{F}_{k+l} \right) \right) \\ &= \tau_{-k-l} \mathbb{E} \left(u_{2k}^2 \frac{4}{k} \sum_{l=k/2}^{3k/4} \tilde{\gamma}_{-k-l-1}^2 | \mathcal{F}_{k+l} \right) \left(\frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{\tilde{\gamma}_{-k-l-1}^2}{4(k+l)^2} \frac{1}{(k-l)^2} \sum_{j=k+l+1}^{2k} \tau_{-k-l} \mathbb{E} \left((\partial_{\mathcal{E}_j}^* \tilde{\gamma}_j)^2 | \mathcal{F}_{k+l} \right) \right) \\ &\leq C \tau_{-k-l} \mathbb{E} \left(u_{2k}^2 | \mathcal{F}_{k+l} \right) \left(\frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{\tilde{\gamma}_{-k-l-1}^2}{4(k+l)^2 (k-l)} \right) \leq \frac{C'}{k^3} \tau_{-k-l} \mathbb{E} \left(u_{2k}^2 | \mathcal{F}_{k+l} \right) \end{aligned}$$

Since by the spectral gap $\langle u_{2k}^2 \rangle \leq Ck^3$ the μ expectation of this term is bounded in k .

Also the estimate of the second term follows as in [7]. The expectation of the square of the second term of (7.5) is bounded by

$$\begin{aligned}
& \left\langle \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{4(k+l)^2} \tilde{\gamma}_{-2k-2l-1}^4 \right\rangle \left\langle \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{(k-l)^2} \tau_{-k-l} \mathbb{E} \left(\sum_{j=k+l+1}^{2k} \partial_{\mathcal{E}_j}^* \tilde{\gamma}_j^2 (u_{2k} \circ \pi^{j,k+l+1} - u_{2k}) \middle| \mathcal{F}_{k+l} \right) \right\rangle^2 \\
& \leq \frac{C}{k^2} \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{(k-l)^2} \left\langle \left(\sum_{j=k+l+1}^{2k} \partial_{\mathcal{E}_j}^* \tilde{\gamma}_j^2 (u_{2k} \circ \pi^{j,k+l+1} - u_{2k}) \right)^2 \right\rangle \\
& \leq \frac{C}{k^2} \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{k-l} \sum_{j=k+l+1}^{2k} \left\langle (u_{2k} \circ \pi^{j,k+l+1} - u_{2k})^2 \right\rangle \\
& = \frac{C}{k^2} \frac{4}{k} \sum_{l=k/2}^{3k/4} \frac{1}{k-l} \sum_{j=k+l+1}^{2k} \sum_{i=j}^{k+l} (k+l-j) \left\langle (u_{2k} \circ \pi^{i,i+1} - u_{2k})^2 \right\rangle
\end{aligned}$$

Then we can bound

$$\left\langle (u_{2k} \circ \pi^{i,i+1} - u_{2k})^2 \right\rangle \leq \mathcal{D}_i(u_{2k})$$

following the same argument as in [7], concluding the proof.

8. PROOF OF BOLTZMANN-GIBBS PRINCIPLE

We prove here (4.4).

Let us denote

$$\phi_x = U'(\mathcal{E}_x) - \beta - \chi^{-1}(\mathcal{E}_x - \bar{e})$$

Notice that this function is not in \mathcal{C}_0 . But it has the following property. Define the microcanonical expectation $\Gamma_k \phi_0 = \langle \phi_0 | \bar{\mathcal{E}}_k \rangle$ where $\bar{\mathcal{E}}_k = (2k+1)^{-1} \sum_{|x| \leq k} \mathcal{E}_x$.

This actually can be explicitly computed and is gives

$$\langle U'(\mathcal{E}_0) | \bar{\mathcal{E}}_k \rangle = \beta + \frac{1}{2k+1} \partial_e \log f_k(\bar{\mathcal{E}}_k) \quad (8.1)$$

where $f_k(e)$ is the probability density of $\bar{\mathcal{E}}_k$ under $d\mu_\beta$. Using using theorem 1.4.1 of my large deviation course (consequence of the local CLT) we have that

$$\log f_k(e) = I(e) + \log g_k(e')$$

where g_k has order \sqrt{k} . Since $\partial_e I(e) = \chi(e - \bar{e}) + O(e - \bar{e})^2$, we have that

$$\Gamma_k(\phi_0)(\bar{\mathcal{E}}_k) = O(\bar{\mathcal{E}}_k - \bar{e})^2 + O(k^{-1})$$

Since $\langle (\bar{\mathcal{E}}_k - \bar{e})^4 \rangle = O(k^{-2})$ we have consequently:

Lemma 8.1.

$$k^2 \langle (\Gamma_k \phi_0)^2 \rangle \leq C \quad (8.2)$$

This is true because of the *first order* correction in ϕ_0 , one can see easily that for the function $\mathcal{E}_0 - \bar{e}$ this is false.

Define now $\tilde{\phi}_x = \phi_x - \tau_x \Gamma_k \phi_0 = \tau_x \tilde{\phi}_0$. Then

$$\begin{aligned} & \left\langle \left(\int_0^t \varepsilon^{1/2} \sum_z G''(\varepsilon z) \phi_z(\varepsilon^{-2}s) ds \right)^2 \right\rangle \\ & \leq 2 \left\langle \left(\int_0^t \varepsilon^{1/2} \sum_z G''(\varepsilon z) \tilde{\phi}_z(\varepsilon^{-2}s) ds \right)^2 \right\rangle \\ & \quad + 2t^2 \left\langle \left(\varepsilon^{1/2} \sum_z G''(\varepsilon z) \tau_z \Gamma_k \phi_0 \right)^2 \right\rangle \end{aligned}$$

Since $\tilde{\phi}_0$ is centered in every microcanonical, we can solve the equation $L_k u_k = \tilde{\phi}_0$, i.e. $\tilde{\phi} \in \mathcal{C}_0$ and the first term goes to 0 as $\varepsilon \rightarrow 0$ by the same estimates used in section 5.

Computing the last term we have:

$$\begin{aligned} & 2t^2 \varepsilon \sum_{z,x} G''(\varepsilon z) G''(\varepsilon x) \langle \tau_{z-x} \Gamma_k \phi_0, \Gamma_k \phi_0 \rangle \\ & \leq t^2 \varepsilon \sum_{z,x} (G''(\varepsilon z)^2 + G''(\varepsilon x)^2) \langle \tau_{z-x} \Gamma_k \phi_0, \Gamma_k \phi_0 \rangle \\ & = 2t^2 \varepsilon \sum_z G''(\varepsilon z)^2 \sum_x \langle \tau_x \Gamma_k \phi_0, \Gamma_k \phi_0 \rangle \\ & \leq Ct^2 \varepsilon \sum_z G''(\varepsilon z)^2 k \langle (\Gamma_k \phi_0)^2 \rangle \leq Ct^2 \|G''\|_2^2 k \langle (\Gamma_k \phi_0)^2 \rangle \end{aligned}$$

that goes to 0 as $k \rightarrow \infty$.

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CARLANGELLO LIVERANI, DIPARTIMENTO DI MATEMATICA, II UNIVERSITÀ DI ROMA (TOR VERGATA), VIA DELLA RICERCA SCIENTIFICA, 00133 ROMA, ITALY.

E-mail address: liverani@mat.uniroma2.it

STEFANO OLLA, CEREMADE, UMR CNRS 7534, UNIVERSITÉ PARIS-DAUPHINE, 75775 PARIS-CEDEX 16, FRANCE,

E-mail address: olla@ceremade.dauphine.fr

MAKIKO SASADA, UNIVERSITY OF TOKYO, TOKYO, JAPAN.

E-mail address: sasada@ms.u-tokyo.ac.jp