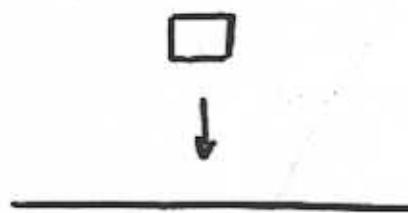


Closed functions and exact functions in interacting particle systems

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Molecular Beam Epitaxy

Deposition



Surface diffusion



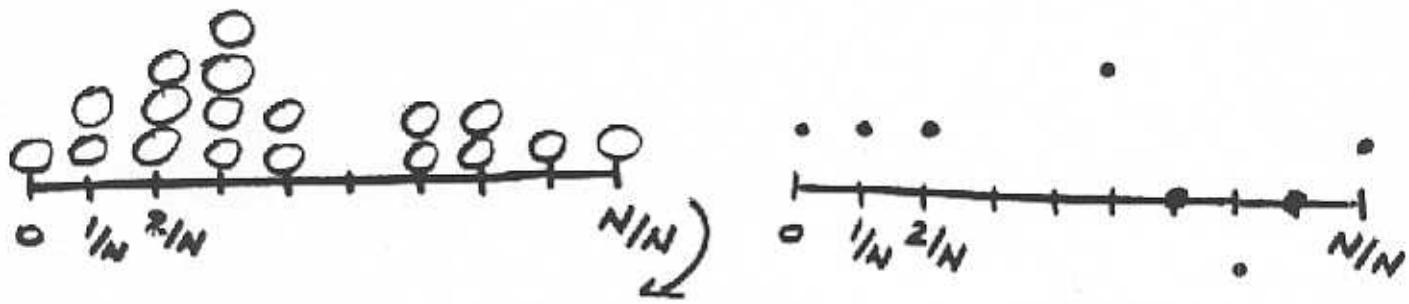
Desorption



Solid on solid model

$h:$

$s:$



h_i^N - the height of the surface at site $\frac{i}{N}$

$s_i^N = h_{i+1}^N - h_i^N$ - the slope of the surface at site $\frac{i}{N}$

$$s_N^N = h_1^N - h_N^N$$

$$h_{i+1}^N = s_i^N + s_{i-1}^N + \dots + s_1^N + h_1^N$$

Configurations: $h = (h_1^N, h_2^N, \dots, h_N^N) \in \mathbb{Z}^N$

$$s = (s_1^N, s_2^N, \dots, s_N^N) \in \mathbb{Z}^N$$

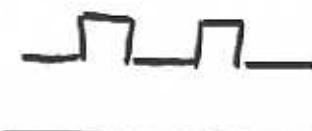
Energy of a configuration: $H(h) = \sum_{i=1}^N V(h_{i+1} - h_i)$



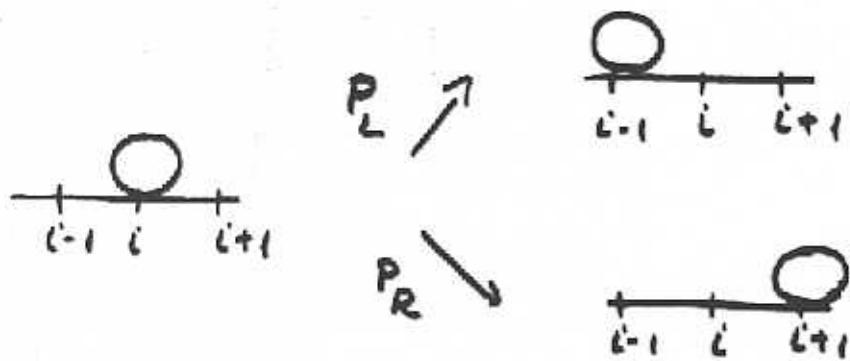
$t=0$



$t=1$

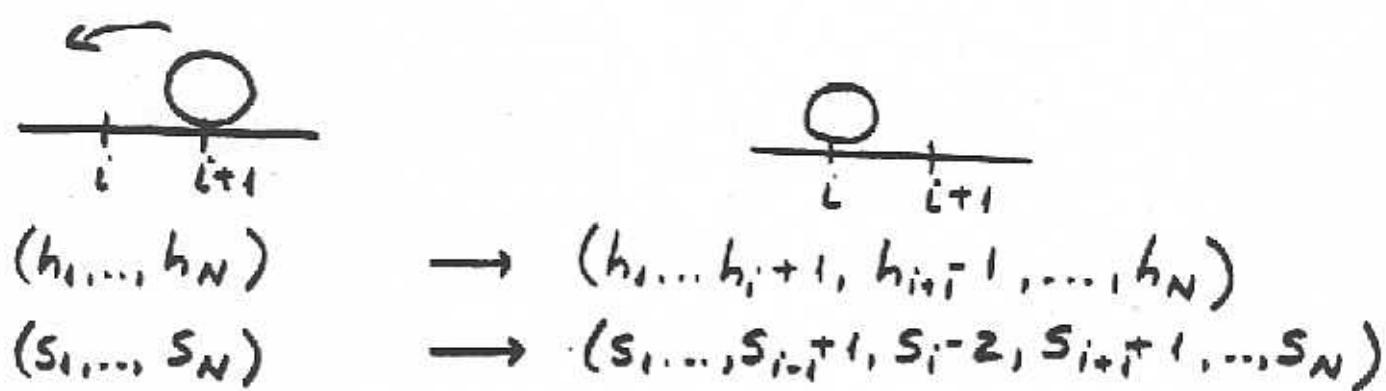
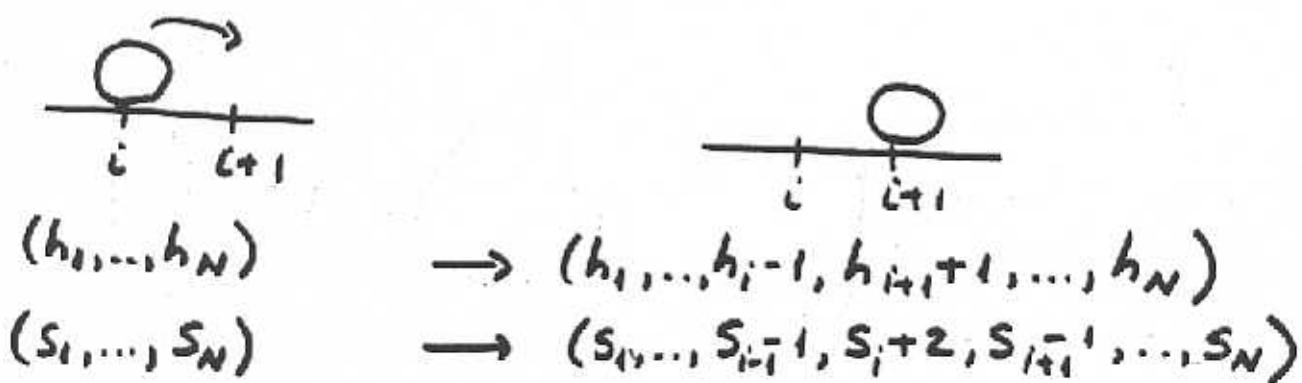


Dynamics



Time \sim exponential distribution with intensity $\lambda(h)$

At rate $1 + e^{H(h) - H(h_{\text{new}})} = \lambda(h) \cdot p(h, h_{\text{new}})$



Dynamics:

$$\{S^n(t)\}_{t \geq 0} = \{ (S_1^n(t), \dots, S_N^n(t)) \}_{t \geq 0}$$

(the slope process)

- right-continuous time-homogeneous Markov process
- jump process
- preserves $\sum_{i=1}^N S_i^n$
- $\nu_\lambda(s) = \frac{e^{\lambda \sum s_i} - H(s)}{Z} ds_1 \dots ds_N$ are equilibrium measures
- reversible wrt ν_λ .
- ergodic on $\sum_{i=1}^N S_i^n = C$

$\{S^n(t, s)\}_{t \geq 0}$ - possible evolution of the system

Generator:

$$(Lf)(s) = \sum_{s_{\text{new}}} (1 + e^{H(s) - H(s_{\text{new}})}) (f(s_{\text{new}}) - f(s))$$

Empirical distribution:

$$\mu^N(t) = \frac{1}{N} \sum_{i=1}^N S_i^N(N^t \epsilon) \cdot \delta_{\frac{i}{N}}$$

• random measure on $[0,1]$

$$\mu^N(t) = \frac{1}{N} \sum_{i=1}^N S_i^N(N^t \epsilon, \omega) \delta_{\frac{i}{N}} \quad \epsilon \text{ all } [0,1]$$

$$\langle \mu^N(t), \varphi \rangle = \frac{1}{N} \sum_{i=1}^N S_i^N(N^t \epsilon) \cdot \varphi\left(\frac{i}{N}\right)$$

φ - test function

Def $\{\mu^N(t)\}_{N \geq 0}$ corresponds to the profile
 $s(t, u)$ if :

$$\lim_{N \rightarrow \infty} P \left(\left| \frac{1}{N} \sum_{i=1}^N S_i^N(N^t \epsilon, \omega) \varphi\left(\frac{i}{N}\right) - \int s(t, u) \varphi(u) du \right| > \varepsilon \right) = 0$$

$\forall \varepsilon > 0$, $\forall \varphi$ - test function

$$= 0$$

(i.e. $\mu^N(t) \rightarrow s(t, u) du$ weakly in probability)

$$\begin{array}{ccc}
 \mu^N(0) & \longrightarrow & \mu^N(t) \\
 \downarrow & & \downarrow ? \\
 s_0(u)du & \dashrightarrow ? \rightarrow s(t,u)du & = \frac{1}{N} \rightarrow 0
 \end{array}$$

distance
between
particles

the time goes by

What is the relation between $s_0(u)$ and $s(t,u)$?

- $\{s(t,u)\}_{t \geq 0}$ is the solution of a deterministic equation started at $s_0(u)$

What is the form of this equation?

- equation = hydrodynamic scaling limit of the model

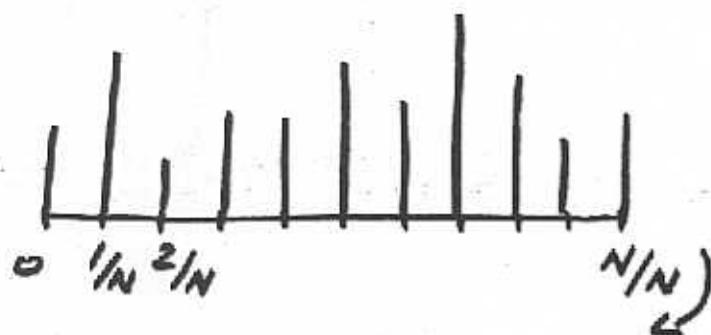
the law of large numbers
at time $t=0$



the law of large numbers
at a later time t

This result is not trivial because
 $\{S_1^N(t), \dots, S_N^N(t)\}$ are not independent

Ginzburg-Landau model



h_i^N - height of the surface at site $\frac{i}{N}$

$$s_i^N = h_{i+1}^N - h_i^N, \quad s_N^N = h_1^N - h_N^N$$

- slope of the surface at site $\frac{i}{N}$

$$h_{i+1}^N = s_i^N + s_{i-1}^N + \dots + s_1^N + h_1^N$$

Configurations: $h = (h_1^N, \dots, h_N^N) \in \mathbb{R}^N$

$$s = (s_1^N, \dots, s_N^N) \in \mathbb{R}^N$$

Energy of a configuration: $H(h) = \sum_{i=1}^N \frac{(h_{i+1}^N - h_i^N)^2}{2}$

Dynamics:

$$\{s^N(t)\}_{t \geq 0} = \{(s_1^N(t), \dots, s_N^N(t))\}_{t \geq 0}$$

(the slope process)

- continuous, time-homogeneous Markov process
- diffusion process
- preserves $\sum_{i=1}^N s_i^N$
- $\vartheta_\lambda(s) = \frac{e^{\lambda \sum s_i - H(s)}}{Z} ds_1 \dots ds_N$ are equilibrium measures
- reversible wrt ϑ_λ
- ergodic on $\sum_{i=1}^N s_i^N = C$

Generator:

$$\langle (-L_N)f, f \rangle_{\vartheta_\lambda} = \frac{1}{2} \sum_{i=1}^N \int_{\mathbb{R}^N} a_i (X_i f)^2(s) d\vartheta_\lambda(s)$$

$$X_i = \partial_{i-1} - 2\partial_i + \partial_{i+1}$$

$$a_i = \alpha(x_{i-1}, x_i, x_{i+1})$$

Hydrodynamic scaling limit of GL-model

Assume the slope process starts in some non-equilibrium measure so that $\{\mu^N(0)\}_{N \geq 0}$ corresponds to some initial profile $s_0(u)$.

Let \mathcal{Q}_T^N be the law of the measure-valued process $\{\mu^N(t)\}_{t \in T}$. Then:

$$\mathcal{Q}_T^N \xrightarrow[N \rightarrow \infty]{} \delta_{\{s(t, u) \text{ def of } s\}_{0 \leq t \leq T}} \text{ weakly}$$

where $\{s(t, u)\}_{0 \leq t \leq T}$ is the weak solution of:

$$\begin{cases} \partial_t s = - \partial_u^2 (\hat{a}(s) \partial_u^2 s) \\ s(0, u) = s_0(u) \end{cases}$$

Uniqueness of the Cauchy problem $\Rightarrow \{\mu^N(t)\}_{N \geq 0}$ corresponds to the profile $s(t, u)$.

Transport coefficient:

$$\hat{a}(\lambda) = \inf_g E_{\tilde{\nu}_\lambda} \left[a \left(1 - (z_1 - 2z_0 - z_1) \left(\sum_{i \in Z} z_i g_i \right) \right)^2 \right]$$

g - cylinder function

z - shift.

Stochastic differential system:

$$\{ ds_i^N(t) = \frac{1}{2} (\psi_{i-1} - 2\psi_i + \psi_{i+1}) dt + dM_i^N(t)$$

$$1 \leq i \leq N$$

$$M_i^N(t) = \sqrt{\alpha_{i-1}} dB_{i-1}(t) - 2\sqrt{\alpha_i} dB_i(t) + \sqrt{\alpha_{i+1}} dB_{i+1}(t).$$

$\{ M_i^N(t) \}_{t \geq 0}$ is a martingale

$$\psi_i = X_i(a_i) - a_i(s_{i-1} - 2s_i + s_{i+1})$$

$$\text{if } a_i = C \Rightarrow \psi_i = -C(s_{i-1} - 2s_i + s_{i+1}) = -C \Delta_i s$$

\Rightarrow "gradient model"

if $a_i \neq C \Rightarrow$ "non-gradient model"

Sketch proof for the HSL of the Ginzburg-Landau model

- we look for a microscopic version of the limiting PDE
- the infinitesimal change in the empirical distribution is

$$d\langle \mu^N(t), \varphi \rangle = \frac{N^2}{2N} \sum_{i=1}^N w_i \varphi''\left(\frac{i}{N}\right) dt + dM^N(t)$$

S.R.S. Varadhan's idea to find HSL of nongradient models is to prove the fluctuation-dissipation equation

$$w_i \sim \hat{a}(s_i) (s_{i+1} - 2s_i + s_{i-1}) + L(\varepsilon, g)$$

- $d\langle \mu^N(t), \varphi \rangle = -\frac{1}{2} \langle \mu^N(t), (\hat{a}(s_i) \varphi''\left(\frac{i}{N}\right))'' \rangle dt$
+ "negligible terms"

- if $\lim_{N \rightarrow \infty} \mu^N(t) = S(t, u) du$ then

$$\partial_t S(t, u) = -\frac{1}{2} \partial_u^2 (\hat{a}(s) \partial_u^2 S(t, u))$$

Fluctuation dissipation equation:

$$s_i = \hat{a}(s) (s_{i-1} - 2s_i + s_{i+1}) + Lg_i$$

current = \hat{a} . laplacian of the + rapid slope field fluctuations

- control $\frac{1}{N^2} \int_0^{N^2 T} f(s^N(t)) dt$ by the central limit theorem variance $2 \langle f, (-L)^{-1} f \rangle$

Functional CLT: (Kipnis, Varadhan, 1986)

Let $\{y(t)\}_{t \geq 0}$ be a Markov process, reversible with respect to $\bar{\pi}$, stationary and ergodic.

Let $f \in L_2(\bar{\pi})$ and $E_{\bar{\pi}}[f] = 0$. Then:

$$\left\{ \frac{1}{\sqrt{\lambda}} \int_0^{\lambda t} f(y(s)) ds \right\}_{t \geq 0} \xrightarrow{\lambda \rightarrow \infty} \{ \sigma \beta_t \}_{t \geq 0}$$

where:

$$\sigma^2 = 2 \langle f, (-L)^{-1} f \rangle_{\bar{\pi}}$$

Subspaces of $L^2(\mathbb{R}^{\mathbb{Z}}, \mu = \bigotimes_{i \in \mathbb{Z}} \frac{1}{\sqrt{2\pi}} e^{-\frac{x_i^2}{2} dx_i})$

Let $D_0 = \sum_{i=-k}^k a_i \partial_i$ be a vector field with constant coefficients and $D_j = \sum_{i=-k}^k a_i \partial_{i+j}$ the translations of D_0 .

Let $(\zeta f)(z) = f(\zeta z)$ be the shift action on function and ζ^m be the m-fold composition of ζ .

The space of closed functions:

$$\mathcal{H}_{c, D} = \{f \in L^2(\mathbb{R}^{\mathbb{Z}}, \mu) \mid D_i \zeta_j f = D_j \zeta_i f\}$$

The space of exact functions:

$$\mathcal{H}_{e, D} = \left\{ f \in L^2(\mathbb{R}^{\mathbb{Z}}, \mu) \mid f = D_0 \left(\sum_{i \in \mathbb{Z}} c_i g_i \right) \right\}$$

g -cylinder function

Why do we call them closed functions?

$$v = \sum_{i=-\infty}^{\infty} w_i dx_i$$

$$dv = \sum_{i=-\infty}^{\infty} \left(\sum_{j=-\infty}^{\infty} D_j(w_i) dx_j \right) \wedge dx_i$$

$w = \sum_{i=-\infty}^{\infty} \tau_i f dx_i$ is closed (i.e. $dv=0$) iff.

$$D_j(\tau_i f) = D_i(\tau_j f) \quad \forall j \in \mathbb{Z}$$

(i.e. f is closed)

Question: What is the codimension of $\mathcal{H}_{C,D}$
inside $\mathcal{H}_{C,D}$

Theorem 1. *The following decomposition results hold:*

a) *Glauber case*

if $D_0 = Z_0 = \partial_0$ then $\mathcal{H}_{c,Z} = \mathcal{H}_{e,Z}$;

b) *Kawasaki case (S.R.S. Varadhan 1990)*

if $D_0 = Y_0 = \partial_1 - \partial_0$ then $\mathcal{H}_{c,Y} = \mathbb{R}1 \oplus \mathcal{H}_{e,Y}$;

c) *Fourth order Ginzburg-Landau field*

if $D_0 = X_0 = \partial_1 - 2\partial_0 + \partial_{-1}$ then

$\mathcal{H}_{c,X} = \mathbb{R}1 \oplus \mathcal{H}_{e,X}$.

Examples: $x_n + x_{-n} - 2x_0$ *is X_0 -exact. x_0 is not X_0 -exact but can be approximated with exact functions.*

Symmetric Fock space of $l^2(\mathbb{Z})$

is the Hilbert space of states of a system with indefinite number of particles. "Births" and "deaths" of particles take place in the system.

$$\begin{aligned} L^2(\mathbb{R}^{\mathbb{Z}}, \mu) &\cong \Gamma_s(l^2(\mathbb{Z})) \\ \bigoplus_{N \geq 0} \mathcal{H}_N &\cong \bigoplus_{N \geq 0} l^2(\mathbb{Z})^{\odot N} \end{aligned}$$

An orthogonal basis of $L^2(\mathbb{R}^{\mathbb{Z}}, \mu)$ is $\{H_I\}_I$ where I is a multi-index with finitely many non-zero entries.

$$I = \{i_n\}_{n \in \mathbb{Z}} \implies H_I(x) = \prod_{n \in \mathbb{Z}} H_{i_n}(x_n)$$

$$\mathcal{H}_N = \text{Span}\{H_I \mid |I| = \sum_{n \in \mathbb{Z}} i_n = N\}$$

\mathcal{H}_N is the N -particle space

$$\mathcal{H}_1 = \text{Span}\{x_n \mid n \in \mathbb{Z}\}$$

Basic states:

one particle $\rightarrow \mathbb{Z} = \{\dots, -n, \dots, -1, 0, 1, \dots, n, \dots\}$

N particles $\rightarrow \mathbb{Z}^N / S^N = \{\dots, (n_1, \dots, n_N), \dots\}$

Note : There is a bijective correspondence between:

$$\{I \mid |I| = N\} \longrightarrow \mathbb{Z}^N / S^N$$

$$I = \{\dots, i_{-1}, i_0, i_1, \dots\}$$

$$z_I = (\dots, \underbrace{-1, \dots, -1}_{i_1}, \underbrace{0, \dots, 0}_{i_0}, \underbrace{1, \dots, 1}_{i_1}, \dots)$$

Note: There is a bijective correspondence between:

$$\begin{array}{ccc} l^2(\mathbb{Z})^{\odot N} & \longrightarrow & L^2(\mathbb{Z}^N / S^N, \mathbb{R}) \\ \mathcal{H}_N & \longrightarrow & \end{array}$$

$$f \in \mathcal{H}_N \longrightarrow \hat{f} \in L^2(\mathbb{Z}^N / S^N, \mathbb{R})$$

$$f = \sum_{|I|=N} \hat{f}_I H_I \longrightarrow \hat{f}(z) = \hat{f}(z_I)$$

$$c_1 \|\hat{f}\|_2 \leq \|f\|_2 \leq c_2 \|\hat{f}\|_2$$

Proposition: A function is D_0 -closed if and only if the projections $P_{\mathcal{H}_N}f$ are D_0 -closed for all $N \geq 0$.

Note: $P_{\mathcal{H}_0}f = c1$

Note: The decomposition theorem is true if we can approximate any $f \in \mathcal{H}_N$, f D_0 -closed with D_0 -exact functions. ($\text{N} \geq 1$)

$$\sum_{i \in \mathbb{Z}} D_0(\tau_i g_k) \xrightarrow{L^2} f \quad ?$$

$N \geq 1$

S^N - the group of transformations generated by

$$\tau_{ij} : \mathbb{R}^N \rightarrow \mathbb{Z}^N$$

$$\tau_{ij}(z_1, \dots, z_N) = (z_1, \dots, \hat{z_j}, \dots, z_i, \dots, z_N)$$

\tilde{S}^N . the group of transformations generated by

$$\tau_{ij}$$
 and $\tau_L : \mathbb{Z}^N \rightarrow \mathbb{Z}^N$

$$\tau_L(z_1, \dots, z_N) = (-z_1, z_2 - z_1, \dots, z_N - z_1)$$

$$\text{Let } f \in \mathcal{H}_N, f = \sum_{\underline{z} \in \mathbb{Z}^N / S^N} \hat{f}(\underline{z}) H_{\underline{z}}$$

f is closed iff there is a \tilde{S}^N -invariant function c so that:

$$(Ac)(z) = c(z+e) - 2c(z) + c(z-e) = \hat{f}(z)$$

$$e = (1, \dots, 1)$$

f is exact iff there is a \tilde{S}^N -invariant function c with compact support so that:

$$(Ac)(z) = c(z+e) - 2c(z) + c(z-e) = \tilde{f}(z)$$

Reformulation of the problem (Nz1)

$$A: \mathcal{F}(\mathbb{Z}^N/\tilde{S}^N, \mathbb{R}) \longrightarrow \mathcal{F}(\mathbb{Z}^N/S^N, \mathbb{R})$$

$$(Ac)(z) = c(z+e) - 2c(z) + c(z-e)$$

$$e = (1, 1, \dots, 1)$$

Suppose $\hat{f} \in L^2(\mathbb{Z}^N/S^N, \mathbb{R})$, $\hat{f} = Ac$

can we find a sequence of compactly supported functions $c_k \in \mathcal{F}(\mathbb{Z}^N/\tilde{S}^N, \mathbb{R})$

so that

$$\begin{array}{ccc} Ac_k & \xrightarrow{L^2} & \hat{f} \\ & k \rightarrow \infty & \end{array}$$

Construction of the approximation

Assumption: $\hat{f} \in L^2(\mathbb{Z}^N/S^N, \mathbb{R})$, $\hat{f} = Ac$, $N \geq 1$

Step 1. We solve for \tilde{S}^N - invariant function c , $Ac = \hat{f}$. c is unique up to a constant and can be normalized to have zero mean inside a region Ω_k of the lattice. Call this normalization c^k .

Step 2. We choose a cut-off function ϕ_k that is \tilde{S}^N - invariant. ϕ_k is an average of characteristic functions of regions invariant under the action of \tilde{S}^N .

$$\phi_k = \frac{1}{k} \sum_{i=k+1}^{2k} \frac{1}{i} \sum_{j=i+1}^{2i} 1_{H_j}$$

Step 3. We show

$$A(c^k \phi_k) \xrightarrow{L^2} \hat{f}$$

by estimating the error terms in $A(c^k \phi_k)$. The main inequality used to bound the error term is the spectral gap of a graph.

Cheeger inequality

Assume $G = (V, E)$ is a finite graph such that all vertices have degree less than k . The quadratic form:

$$q_G(f) = \sum_{i \simeq j} (f(i) - f(j))^2$$

defines a unique symmetric operator with eigenvalues $0 = \lambda_1 < \lambda_2 < \dots < \lambda_N$. The spectral gap of this operator is bounded from below by the Cheeger constant

$$C = \frac{1}{2k} \inf \frac{|\partial A|}{|A|} \leq \lambda_2.$$

If f is a zero mean function defined on the vertices of the graph then:

$$C \sum_{i \in V} f(i)^2 < \sum_{i \simeq j} (f(i) - f(j))^2.$$