Mathematical strategies and error quantification in coarse-graining of extended microscopic systems

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**Coarse-Graining (and reconstruction) of extended microscopic particle systems**


*Microscopics* $\mapsto$ **CG system** $\mapsto$ *Reconstructed Microscopics*

2. Stochastic lattice dynamics/ KMC

![Diagram](image-url)
Tschöp, Kremer, Batoulis, Bürger and Hahn *Acta Polymer.* '98.

L \equiv 100 \text{ Å} - 1000 \text{ Å}
\quad t \equiv O (1 \text{ sec})

L \equiv 10 \text{ Å} - 50 \text{ Å}
\quad t \equiv 10^{-8} \text{ sec} - 10^{-4} \text{ sec}

L \equiv 1 \text{ Å} - 3 \text{ Å}
\quad t \equiv 10^{-13} \text{ sec}
**Microscopics:** United Atom (UA) Model

- **Continuum model:** \( X \in (\mathbb{R}^3)^N \) – positions of \( N \) atoms on one macromolecule; \( m \) macromolecules.

- **Hamiltonian:**

\[
H_N(X) = H_b(X) + H_{nb}(X) + H_{Coul}(X) + H_{wall} + H_{kin}
\]

**Bonded Interactions:** Gaussian, FENE, etc. **short-range interactions**

\[
H_b(X) = \sum_i U_b(\theta_i, \phi_i, r_i)
\]

**Non-Bonded Interactions:** 12-6 Lennard Jones **long-range interactions.**

\[
H_{nb}(X) = \sum_{i,j} U_{nb}^{LJ}(|x_i - x_j|)
\]

- **Molecular Dynamics**
Equilibrium Gibbs measure at $\beta = \frac{1}{kT}$.

$$\mu(dX) = \frac{1}{Z} e^{-\beta H(X)} \prod dx_i$$

- UA is a typical set-up for CG in polymer science literature:
  
  
  Doi et. al. *J.Chem.Phys.* '02;
  
  Kremer et. al. *Macromolecules* '06, etc.
  
  Müller-Plathe *Chem.Phys.Chem* '00 (see P. Cummings' talk);
CG procedure, ”super-atoms”:

\[ T X = Q = (q_1, \ldots, q_m) \in Q, \text{ where } q_i \in \mathbb{R}^3. \]

**Exact coarse-grained Hamiltonian** \( \tilde{H}(Q) \):

1. **Microscopic equilibrium Gibbs measure** at \( \beta = \frac{1}{kT} \).

\[
\mu(dX) = \frac{1}{Z} e^{-\beta H(X)} \prod_i dx_i
\]

2. **Renormalization map** \( \mapsto \) **CG Hamiltonian**:

\[
\tilde{H}(Q) = -\frac{1}{\beta} \log \int_{\{X|TX=Q\}} e^{-\beta H(X)} dX
\]
Goal: Approximate the coarse-grained measure

\[ \mu^c(dQ) \sim e^{-\beta \bar{H}(Q)} dQ \]

Break-up of the computational task:

**Simplifying assumptions**

(i) \( \bar{H} \) decouples:

\[ \bar{H}(Q) = \bar{H}_b + \bar{H}_{nb} = \sum_{\text{CG var.}} \bar{U}_b + \bar{U}_{nb} \]

(ii) \( \bar{U}_b = \bar{U}_b^\theta + \bar{U}_b^\phi + \bar{U}_b^r \) where each term depends *only* on torsion angle \( \phi \), rotation angle \( \theta \) and distance \( r \) respectively between successive CG particles.

(iii) \( \bar{U}_{nb} \) depends *only* on two-body interactions between CG particles; *no multi-body interactions* included.
How to calculate the CG non-bonded interactions $\bar{U}_{nb}$: McCoy-Curro scheme, *Macromolecules* ’98.

For two isolated small molecules with centers of mass at $q_1, q_2$:

$$U_{nb}(|q_1 - q_2|) = -\frac{1}{\beta} \log \int_{\{X|TX=(q_1,q_2)\}} e^{-\beta H(X)} dX$$

- The computation is feasible but disregards multi-body interactions.
Difficulties in coarse-graining methods:

Often: wrong predictions in dynamics, phase transitions, melt structure near interfaces, etc. See for instance:

- CG in polymers:

- "classical" example: nearest neighbor Ising vs. Curie-Weiss (Mean Field)
Mathematics and Numerics of CG:

-Numerical accuracy of CG methods; the effect of randomness:

Compression of the measure rather than just $H = H(X)$:

$$e^{-\beta H(X)}dX \sim \mu_{\text{micro}}(dX) \mapsto \mu_{\text{cg}}(dQ) \sim e^{-\beta \bar{H}(Q)}dQ$$

-Assess the role of multi-body CG interaction terms

-"Reverse map"-reconstruct microscopic info from CG.
2. Stochastic lattice dynamics–Ising Systems

\[ \sigma(x) = 0 \text{ or } 1: \text{ site } x \text{ is resp. empty or occupied.} \]

**Hamiltonian:**
\[ H_N(\sigma) = -\frac{1}{2} \sum_{x \neq y} J(x, y)\sigma(x)\sigma(y) + h \sum_x \sigma(x) \]

- \( h \): external field
- \( J \): potential with interaction range \( L \),
\[ J(x - y) = \frac{1}{L} V\left(\frac{i - j}{L}\right), \quad x = i/N, \quad y = j/N \]

possibly short-/long-range interactions.
Canonical Gibbs measure: at the inverse temperature $\beta = \frac{1}{kT}$,

$$\mu_{\Lambda,\beta}(\sigma = \sigma_0) = \frac{1}{Z_{\Lambda,\beta}} \exp \left\{ - \beta H_N(\sigma_0) \right\} P_N(\sigma = \sigma_0)$$

[Probability of the configuration $\sigma_0$]

Prior distribution: $P_N(\sigma = \sigma_0) = \prod_{x \in \Lambda} P(\sigma(x) = \sigma_0(x))$

Dynamics: Continuous Time Markov Chains–detailed balance.
Arrhenius adsorption/desorption dynamics:

Adsoption/desorption dynamics: $\sigma(x) = 0$ or 1: site $x$ is resp. empty or occupied.

Generator: $L_X f(\sigma) = \sum_x c(x, \sigma, X)[f(\sigma^x) - f(\sigma)]$

Transition rate: $c(x, \sigma, X) = c_0 \exp[-\beta U(x)]$

$U(x)$: Energy barrier a particle has to overcome in jumping from a lattice site to the gas phase.

- Detailed Balance
- $U(x) = U(x, \sigma, X) = \sum_{z \neq x} J(x - z)\sigma(z) - h(X)$.
- strong interactions/low temperature $\rightarrow$ clustering/phase transitions
Why study this system?

0. Many-particle system, related to realistic models, KMC, etc.


   How CG performs in predicting phase transitions and various rare events?


   How CG performs in transient and long time regimes?

3. Numerous analytic benchmark solutions; a variety of mathematical physics tools.
Hierarchical coarse-graining of stochastic lattice dynamics
[ K., Majda, Vlachos, PNAS'03, JCompPhys'03; K. Vlachos J.Chem.Phys.'03]

Construct a \textbf{stochastic process} for a hierarchy of “mesoscopic” length or time scales that \textit{includes fluctuations} properly.

In general it is \textbf{non-markovian}

\textbf{Stochastic closures}: can we write a new \textit{approximating} Markov process for $\eta_t$?

\textbf{Ergodicity}: Are the long-time dynamics reproduced?
Microscopic Process

state 1  state 2  ...

CG state 2  CG state 1  CG state m...

state N-1  state N

Microscopic equilibria

Coarse-Grained Process

Lumping + error  Reconstruction +error

CG state 1  CG state 2

Lumping + error  Reconstruction +error

CG state m

CG equilibria

Error Estimates
Equilibrium

CG Hamiltonian–Renormalization Group Map (again):

\[
e^{-\beta H^c(\eta)} = \int e^{-\beta H_N(\sigma)} P_N(d\sigma \mid \eta) \equiv \mathbb{E}[e^{-\beta H_N} \mid \eta]
\]

with the conditional prior

\[
P_N(d\sigma \mid \eta) = \prod_{k \in \Lambda^c} \prod_{x \in C_k} \rho_k(d\sigma(x)), \quad \rho_k(\sigma(x) = 1) = \frac{\eta_k}{q}, \quad \rho_k(\sigma(x) = 0) = \frac{q - \eta_k}{q}
\]

The "exact" CG Gibbs measure on CG space

\[
\mu_{\Lambda^c, q, \beta}^\Lambda(d\eta) = \frac{1}{Z_{\Lambda^c, q, \beta}^\Lambda} e^{-\beta H^c(\eta)} P_{M, q}(d\eta)
\]

with coarse-grained prior

\[
P_{M, q}(d\eta) = \prod_{k \in \Lambda^c} \rho_q(d\eta(k)), \quad \rho_q(\eta(k) = \omega) = \frac{q!}{\omega!(q - \omega)!} \left(\frac{1}{2}\right)^q
\]
Building approximate CG Hamiltonian

**Step 1:** identify a base state (a base measure) and a “small” parameter $\epsilon$

*Example: Finite or Long-range potential of radius $L$*

$$\epsilon \equiv C\beta \frac{q}{L} |\nabla V|_{\infty}$$

**Step 2:** choose a suitable expansion and expand the approximation error in $\epsilon$

Expand $\mu^{c,M,q,\beta}$ around the approximate equilibrium measure rather than the product measure $P_N(d\sigma|\eta)$:

$$e^{-H^c} = e^{-\bar{H}^{(0)}} \mathbb{E}[e^{-(H_N-\bar{H}^{(0)})} | \eta]$$

or equivalently

$$H^c(\eta) = \bar{H}^{(0)} - \log \mathbb{E}[e^{-(H_N-\bar{H}^{(0)})} | \eta]$$

Q: A suitable choice $H^{(0)}$? What is the error?
Heuristics – Ordinary expansion

Step 1  Expansion of $e^{\Delta H}$

$$e^{\Delta H} = \left(1 + \Delta H + \frac{1}{2}(\Delta H)^2 + O((\Delta H)^3)\right)$$

$$\mathbb{E}[e^{\Delta H(\eta)} | \eta] = 1 + \mathbb{E} [\Delta H | \eta] + \frac{1}{2} \mathbb{E} [(\Delta H)^2 | \eta] \ldots$$

Step 2  Expansion of log

$$1 + \mathbb{E} [\Delta H | \eta] + \mathbb{E} [(\Delta H)^2 | \eta] - \mathbb{E} [\Delta H | \eta]^2 + O((\Delta H)^3)$$

Step 3  Estimate

$$\Delta H \equiv H_N - \bar{H}^{(0)} = N \cdot O(\epsilon)$$

and compute conditional expectations

Rigorous analysis – Cluster expansion

K., P. Plechac (U. of TN/ORNL), L. Rey-Bellet (UMass), D. Tsagkarogiannis (Max-Planck, Leipzig),

$M^2AN$, to appear; J.Non Newt. Fluid Mech., submitted
Q: A suitable choice $H^{(0)}$?

$$\mathbb{E} \left[ H_N - \bar{H}^{(0)} \mid \eta \right] = 0$$

Define two-body CG interaction:

$$\bar{J}(k,l)\eta(k)\eta(l) = \mathbb{E} \left[ \sum_{x \in C_k, y \in C_l} J(x - y) \sigma(x)\sigma(y) \mid \eta \right]$$

Where

$$\bar{J}(k,l) = \frac{1}{q^2} \sum_{x \in C_k} \sum_{y \in C_l, y \neq x} J(x - y),$$

$$\bar{J}(l,l) = \bar{J}(0,0) = \frac{1}{q(q - 1)} \sum_{x \in C_l} \sum_{y \in C_l, y \neq x} J(x - y)$$

• Analogy to McCoy-Curro scheme in polymers.
Approximate CG Hamiltonian

\[ \bar{H}^{(0)}(\eta) = -\frac{1}{2} \sum_{l \in \Lambda^c_M} \sum_{k \neq l} \bar{J}(k, l)\eta(k)\eta(l) - \frac{1}{2} \bar{J}(0, 0) \sum_{l \in \Lambda^c_M} \eta(l)(\eta(l) - 1) + \sum_{l \in \Lambda^c_M} \bar{h}(l)\eta(l) \]

Approximating Gibbs measure:

\[ \bar{\mu}_{M, q, \beta}^{(0)}(d\eta) = \frac{1}{Z_{M, q, \beta}} e^{-\beta \bar{H}^{(0)}(\eta)} P_{M, q}(d\eta), \]

Corrections to the Hamiltonian $\bar{H}^{(0)}$—Multi-body terms

- “$0^{th}$-order” approximation is $\bar{H}^{(0)}(\eta) = \sum_{k,l} \bar{J}(k-l)\eta(k)\eta(l)$

- “higher-order” — expand the blocking error
  
  $$e^{-\beta H^c(\eta)} = e^{-\beta H_{M}^{(0)}(\eta)} \mathbb{E}[e^{-\beta (H_{N}(\sigma) - \bar{H}_{M}^{(0)}(\eta))} | \eta]$$

  and calculate correction terms
  
  $$H^c(\eta) = H^{(0)}(\eta) + H^{(1)}(\eta) + O(\epsilon^2)$$

  $$\bar{H}^{(1,2)}(\eta) = \beta \sum_{k_1} \sum_{k_2 > k_1} \sum_{k_3 > k_2} [j_{k_1k_2k_3}^2 (-E_1(k_1)E_2(k_2)E_1(k_3) + ...)$$

  Notation: $\bar{H}^{(1)} = \bar{H}^{(1,1)} + \bar{H}^{(1,2)}$
\[ E_r(k) \equiv E_r(\eta(k)) = (2\eta(k)/q - 1)^r + o_q(1) \]

“Moments” of interaction potential \( J \):

\[
\begin{align*}
\hat{j}^1_{kl} &= \sum_{x \in C_k} \sum_{y \in C_l} (J(x - y) - \bar{J}(k, l))^2 \\
\hat{j}^2_{kl} &= \sum_{x \in C_k} \sum_{y, y' \in C_l} (J(x - y) - \bar{J}(k, l))(J(x - y') - \bar{J}(k, l)) \\
\hat{j}^2_{k_1 k_2 k_3} &= \sum_{x \in C_{k_1}} \sum_{y \in C_{k_2}} \sum_{z \in C_{k_3}} (J(x - y) - \bar{J}(k_1, k_2))(J(y - z) - \bar{J}(k_2, k_3))
\end{align*}
\]

**Computational complexity**

Evaluation of the Hamiltonian:

<table>
<thead>
<tr>
<th>Microscopic: ( H_N(\sigma) )</th>
<th>Count</th>
<th>Speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>CG1: ( \bar{H}^{(0)}_M )</td>
<td>( O(N L^d) )</td>
<td>1</td>
</tr>
<tr>
<td>CG2: ( \bar{H}^{(0)}_M + \bar{H}^{(1)}_M )</td>
<td>( O(M L^d/q^d) )</td>
<td>( O(q^2d) )</td>
</tr>
</tbody>
</table>

\( q, L \)
Demonstration: Rare events and metastability

Coverage in Time

- Microscopic $q=1$
- $q=10$
- $q=20$
- $q=50$
- Birth-Death
  - $\beta J_0=6$
- Nodes =1000
- Pot. Radius=100

Time (non-dim)
$\alpha = 1.5, N=1000, \beta J_0 = 6$
CG Arrhenius lattice dynamics

Switching Time PDFs/Autocorrelations-corrections

joint work with Sasanka Are (UMass)
Dynamics

**Birth-Death** type process, with interactions.

\[ L_{e} g(\eta) = \sum_{k \in \Lambda_{c}} c_{a}(k, \eta) \left[ g(\eta + \delta_{k}) - g(\eta) \right] + \]

\[ c_{d}(k, \eta) \left[ g(\eta - \delta_{k}) - g(\eta) \right]. \]

- **Coarse-grained** rates:

  **Adsorption rate** of a single particle in the \( k \)-coarse cell
  \[ c_{a}(k, \eta) = q - \eta(k) \]

  **Desorption rate** (approximate–error estimates)
  \[ c_{d}(k, \eta) = \eta(k) \exp \left[ -\beta \left( U_{0} + \bar{U}(k) \right) \right] \]

  \[ \bar{U}(l) = \sum_{\substack{k \in \Lambda_{c} \\ k \neq l}} \bar{J}(l, k) \eta(k) + \bar{J}(0, 0) \left( \eta(l) - 1 \right) - \bar{n}. \]

**Q:** Errors in finite and long times? Ergodicity?
Analysis and numerics: **Transient** and **long-time** comparisons

Error I–Loss of information during coarse-graining

- Specific relative entropy:

\[
\mathcal{R}(\mu \mid \nu) := \frac{1}{N} \sum_{\sigma} \log \left\{ \frac{\mu(\sigma)}{\nu(\sigma)} \right\} \mu(\sigma) \quad .\diamond
\]

**Idea:** Cluster expansions around the coarse Hamiltonian \( \bar{H} = \bar{H}^0 \)

- “higher-order” corrections – expand the blocking error

\[
e^{-\beta H'(\eta)} = e^{-\beta H_M^{(0)}(\eta)} \mathbb{E}[e^{-\beta (H_N(\sigma) - \bar{H}_M^{(0)}(\eta))} \mid \eta]
\]

and calculate **correction terms**

\[
H^c(\eta) = H^{(0)}(\eta) + H^{(1)}(\eta) + O(\epsilon^2)
\]
• Controlling the expansion: “high-temperature” cluster expansion techniques (Cammarota CMP 82, Procacci, De-Lima, Scoppola LMP 98)

• Related work: M. Suzuki et. al.’95, Cassandro/Presutti ’96, Bovier/Zahradnik ’97; cluster expansions around mean-field; focus on criticality.

**Theorem 1:** A priori error estimate

Define the “small” parameter \( \epsilon \equiv C\beta \frac{q}{L} \|V'\|_\infty \)

\[
\mathcal{R} \left( \bar{\mu}_{M,q,\beta}^{(\alpha)} | \mu_{N,\beta^0T^{-1}} \right) = O \left( \epsilon^{\alpha+2} \right).
\]

**Remark:** One order gain in ”compression” of the Gibbs states.
Error Estimates for observables – Dynamics


**Theorem 2:**

coarse grained observables/quantity of interest: $\psi$,

microscopic dynamics: $\sigma_t$,

course-grained dynamics: $\eta_t$

Then for any fixed time $0 < T < \infty$

$$|E\psi(T\sigma_T) - E\psi(\eta_T)| \leq C_T \epsilon^2,$$

- $T\sigma_t =$ **Projection** on coarse variables $= \sum_{y \in D_k} \sigma_t(y)$.

- Error accumulation as $T \to \infty$? 2nd order error estimates at **equilibrium**
Difficulty: $T\sigma_t(k) = \sum_{y \in D_k} \sigma_t(y)$ is not a Markov process.

Elements of the proof:

1. $\gamma_t$: Markovian reconstruction of the microscopic process $\sigma_t$ from the coarse process $\eta_t$ with controlled error:

   $$|E\phi(\sigma_T) - E\phi(\gamma_T)| \leq C_T \epsilon^2,$$

2. Stochastic averaging $\rightarrow$ cancellations and 2nd order accuracy.

3. Bernstein-type estimates to control discrete derivatives—here related to the number of jumps—extensive system!

Reverse CG map–Microscopic Reconstruction

[K., P. Plechac, A. Sopasakis, SIAM Num. Anal. ’06]

Main features:

a. Reverse the CG via the conditional prior $P_N(\sigma|\eta)$;

b. $P_N(\sigma|\eta)$ is a product measure $\implies$ ”local” reconstruction at each coarse-cell;

c. Reconstruction for equilibrium and dynamics;

d. Numerical error estimate for reconstructed microscopic dynamics $\gamma_t$:

$$|E\phi(\sigma_T) - E\phi(\gamma_T)| \leq C_T \epsilon^2,$$

- Improved strategies for reconstruction at equilibrium based on a relative entropy formulation + cluster expansions:

  J. Trashorras (Paris IX) and D. Tsagkarogiannis (Max-Planck, Leipzig)
A posteriori error expansion—Adaptive Coarse-Graining

[K., Plechac, Rey-Bellet, Tsagkarogiannis, JNNFM submitted, ’07]

1. Cluster expansions → sharp a posteriori estimates for the relative entropy.

The error indicator $R(.)$ is given by the terms $\bar{H}^{(1)}, \bar{H}^{(2)}$ and depends only on the coarse variable $\eta$:

$$\mathcal{R} \left( \mu_{m,q}^{(0)} \mid \mu_{N o T} \right) = E_{\bar{G}^{(0)}}[R(\eta)] + \log \left( E_{\mu^{(0)}}[e^{R(\eta)}] \right) + O(\epsilon^3)$$

2. A posteriori ”Quantity of interest” estimates.
A mathematical prototype: Competing short ($L_K = 1$) and long ($L_J = 64$) range

$$H_N = -K \sum_{|x-y|=1} \sigma(x)\sigma(y) - \frac{J}{2N} \sum_{x,y} \sigma(x)\sigma(y) + h \sum_x \sigma(x)$$

Exact solution in 1D (M. Kardar, PRB ’83)
Example: Adaptive computation of phase diagrams

Spatial adaptivity:
2. **CG in macromolecules**

joint work with: **P. Plecháč (U of TN, ORNL), V. Harmadaris (Max Planck Inst. Polymers)**

*Prototype problem*: Small molecules with internal DOF

![Ethane gas molecule](image-url)
Dimers

\[ H(X) = \sum_{i=1}^{N} U_b(|x_{2i} - x_{2i+1}|) + \sum_{i=1}^{2N} \sum_{j \neq i} U_{nb}(|x_i - x_j|) \]

Microscopic state space: \( X \in (\mathbb{R}^3)^{2N} \) – microscopic positions
Coarse-level state space: \( Q \in (\mathbb{R}^3)^N \) – center of mass of dimers
Coarse-graining operator: \( q_i \equiv (TX)(i) = \frac{1}{2}(x_{2i-1} + x_{2i}) \)

Equilibrium measure:

\[ \mu(dX) = \frac{1}{Z} e^{-\beta H(X)} \prod dx_i \]

**Goal:** approximate the coarse-grained measure

\[ \mu^c(dQ) \sim e^{-\beta H(Q)} dQ \]
Exact coarse-grained Hamiltonian:

\[ \bar{H}(Q) = -\frac{1}{\beta} \log \int_{\{X|TX=Q\}} e^{-\beta H(X)} dX \]

Prior distribution:

\[ P(dX) = \frac{1}{Z_b} e^{-\beta H_b(X)} dX \]

and factorize over diams

\[ P(dX) = \prod_{i=1}^{N} \frac{1}{Z_1} e^{-\beta U_b(|x_{2i}-x_{2i+1}|)} dx_{2i} dx_{2i+1} \]

Follow the lattice “recipe”:

1. Coarse-grain the prior: \[ \bar{P}(dQ) = \prod_{i=1}^{N} \bar{p}^{(1)}(dq_i) \]

\[ \bar{p}^{(1)}(dq_i) = \left[ \frac{2}{Z_1} \int e^{-\beta U_b(2|q_i-x_{2i}|)} dx_{2i} \right] dq_i = \rho^{(1)}(q_i) dq_i \]
2. Compute the conditional prior:

\[ p^{(1)}(dx_{2i}|q_k) = \frac{2}{Z_1} \frac{e^{-\beta U_b(2|q_i-x_{2i}|)}}{\rho^{(1)}(q_i)} dx_{2i} \]

3. Construct a coarse-grained approximation of the pair potential \( U_{nb} \):

\[ \bar{U}_{nb}(q_i, q_j) = \int \int U_{nb}(|x_{2i} - x_{2j}|) p^{(1)}(dx_{2i}|q_i)p^{(1)}(dx_{2j}|q_j) \]

4. Approximate non-bonded Hamiltonian

\[ \bar{H}^{(0)}(Q) = 4 \sum_{i=1}^{N} \sum_{j=1}^{N} \bar{U}_{nb}(q_i, q_j) \]
Pair distribution functions and CG non-bonded potentials

![Graphs showing pair distribution functions and CG non-bonded potentials](image)

- $U_L$, $4U_L$, $U_{NE}$ 260K, $-k_BT\ln(g(r))$, 260K
- $U_{nb}$, $U_L$, $4U_L$, $U_{NE}$ 260K, $-k_BT\ln(g(r))$, 260K

$r$ (Å) vs. $g(r)$

- $U_L$, $4U_L$, $U_{NE}$ 260K, $-k_BT\ln(g(r))$, 260K
- $U_{nb}$, $U_L$, $4U_L$, $U_{NE}$ 260K, $-k_BT\ln(g(r))$, 260K
Error estimation

Follow the same route as for lattice systems

\[ e^{-\beta \tilde{H}(Q)} = e^{-\beta \tilde{H}^0(Q)} \int e^{-\beta (H_{nb}(X) - \tilde{H}^0(Q))} \bar{p}(dX|Q) \]

*Cluster expansion* around \( H^0(Q) \).