II.2) Semi-dilute expansion.

Idea: dilute $\Rightarrow$ particles don't interact much

"Cluster expansion": $\left\{\begin{array}{l}\text{0th order} \to \text{pure solvent}\\ \text{1st order} \to \text{1-part contr.}\\ \text{2nd order} \to \text{2-part contr.}\\ \quad\text{etc.}\end{array}\right.$

A) CLUSTER EXPANSIONS

Definition. For set fct $F : 2^{\{1\dots n\}} \to \mathbb{R}$,

<u>cluster expansion</u> is
$$F(\{1\dots n\}) = F(\emptyset) + \sum_k \underbrace{\big(F(\{k\}) - F(\emptyset)\big)}_{=:\,\delta^k F(\emptyset)}$$
$$+ \sum_{k<l} \underbrace{F(\{k,l\}) - F(\{k\}) - F(\{l\}) + F(\emptyset)}_{=:\,\delta^{k,l} F(\emptyset) \,=\, \delta^k \delta^l F(\emptyset).}$$
$$+ \dots$$
$$= \sum_{m=0}^{n} \sum_{\substack{S\subset\{1\dots n\}\\ \# S = m}} \delta^S F(\emptyset).$$

"Taylor expansion" for set fcts.

Now corrector φ_e is fct of $\{I_n\}_{n\in\mathbb{N}}$

say $\varphi_e \equiv \varphi_e^{\mathbb{N}}$

& consider $S \mapsto \varphi_e^S$ corrector associated with $\{I_n\}_{n\in S}$

More precisely: $\forall$ finite S $\exists!\, \varphi_e^S \in \dot{H}^1$: $\left\{\begin{array}{ll} -\Delta \varphi_e^S = 0, & \left(\bigcup_{n\in S} I_n\right)^c = \mathcal{Y}_S^c\\ \nabla\varphi_e^S + e = 0, & \mathcal{Y}_S\\ \int_{\partial I_n} \partial_\nu \varphi_e^S = 0 & \forall n \in S\end{array}\right.$

(note $\varphi_e^\emptyset = 0$)

$\Rightarrow$ decompose $e\cdot\bar{B}e = \mathbb{E}\,|\nabla\varphi_e^{\mathbb{N}} + e|^2$
$$= |e|^2 + \underbrace{\mathbb{E}\sum_n \delta^n |\nabla\varphi_e^\emptyset + e|^2}_{e\cdot\bar{B}^{(1)}e} + \underbrace{\mathbb{E}\sum_{n<m} \delta^{nm} |\nabla\varphi_e^\emptyset + e|^2}_{e\cdot\bar{B}^{(2)}e} + \dots$$

$\delta^{nm}\varphi_e^\emptyset$ meaning how much $\varphi_e^{nm} \neq \varphi_e^n + \varphi_e^m$.

Difficulties:

- truncate this infinite series (OK / skip)
- each cluster term is itself divergent !!

$$\delta^n |\nabla \varphi_e^\emptyset + e|^2 = |\nabla \varphi_e^n + e|^2 - |e|^2$$

$$= 2e \cdot \nabla \varphi_e^n + |\nabla \varphi_e^n|^2$$

$$\lesssim \langle x_n \rangle^{-d}$$

exercise: deduce this decay from Green's representation formula

$$\nabla \varphi_e^n(x) = -\int_{\partial I_n} \left(\nabla G(x-y) - \fint_{I_n} \nabla G(x-\cdot) \right) \nu \cdot (\nabla \varphi_e^n + e)(y) \, \nu \, dS(y)$$

$$|\nabla \varphi_e^n(x)| \lesssim |x - x_n|^{-d} \underbrace{\left(\int_{I_n + B} |\nabla \varphi_e^n + e|^2 \right)^{1/2}}_{\lesssim 1} .$$

$$\Rightarrow \mathbb{E} \sum_n \left| \delta^n |\nabla \varphi_e^\emptyset + e|^2 \right| = \infty$$

no absolute convergence!

$\Rightarrow$ need renormalization ...

Approach:

- start from finite-volume approximation

$$\begin{cases} Q_L = \left(-\frac{L}{2}, \frac{L}{2}\right)^d \\ \mathcal{I}_L = \bigcup_n I_{nL} : \begin{cases} \mathcal{I}_L \ L\text{-periodic} \\ \mathcal{I}_L \cap Q_{L-1} = \mathcal{I} \cap Q_{L-1} \end{cases} \end{cases}$$

$$e \cdot \bar{B}_L e = \mathbb{E} \fint_{Q_L} |\nabla \varphi_{Le} + e|^2 \quad \text{where} \quad \begin{cases} -\Delta \varphi_{Le} = 0, & Q_L \setminus \mathcal{I}_L \\ \nabla \varphi_{Le} + e|_{\mathcal{I}_L} = 0 \\ \int_{\partial I_{nL}} \partial_\nu \varphi_{Le} = 0, & \varphi_{Le} \in H^1_{per}(Q_L) \end{cases}$$

$$\to e \cdot \bar{B} e \text{ as } L \uparrow \infty$$

- cluster expansion for $\bar{B}_L$ makes sense for fixed L (finite volume)

$$\leadsto \bar{B}_L = \mathrm{Id} + \bar{B}_L^{(1)} + \bar{B}_L^{(2)} + \cdots$$

- use hidden cancellations (= 'renormalization') to define $\bar{B}_L^{(k)} \xrightarrow{L \uparrow \infty} \bar{B}^{(k)}$.

Einstein's term

$$e\cdot \bar{B}_L^{(1)} e = \mathbb{E}\sum_n \fint_{Q_L} \delta^n |\nabla\varphi_{eL}^n + e|^2$$

$$= \underbrace{\mathbb{E}\sum_n \fint_{Q_L} \underbrace{|\nabla\varphi_{eL}^n|^2}_{\langle\cdot - x_{n,L}\rangle^{-2d}}}_{\text{unif. convergent}} + \cancel{2e\cdot\mathbb{E}\sum_n \underbrace{\fint_{Q_L}\nabla\varphi_{eL}^n}_{=0}}$$

$$\xrightarrow{L\uparrow\infty} \mathbb{E}\sum_n |\nabla\varphi_e^n|^2 < \infty \quad \ldots \quad \underline{\text{trivial renormalization!}}$$

Higher orders: no such simple cancellation was found

- only to 2nd order a trick was found by Batchelor-Green '72. (requiring a careful IBP and decomposition)
- for order ≥ 3: open problem in physics.

Here's the detail for 2nd-order Batchelor argument:

$$e\cdot \mathcal{B}_L^{(2)} e = \mathbb{E}\sum_{n<m}\fint_{Q_L} \delta^{nm} |\nabla\varphi_{eL}^{\circ} + e|^2$$

$$= \mathbb{E}\sum_{n<m}\fint_{Q_L}\left(|\nabla\varphi_{eL}^{nm}|^2 - |\nabla\varphi_{eL}^{n}|^2 - |\nabla\varphi_{eL}^{m}|^2\right)$$

$$= \iint dy\,dz\; f_2(y,z)\left(\underbrace{\fint_{Q_L}|\nabla\varphi_{eL}^{yz}|^2}\; - \underbrace{\fint_{Q_L}|\nabla\varphi_{eL}^{y}|^2}\; - \underbrace{\fint_{Q_L}|\nabla\varphi_{eL}^{z}|^2}\right)$$

$$L^{-d}\int_{\partial I_y} \overbrace{e\cdot(x-y)}^{-\varphi_y}\,\partial_\nu\varphi_{eL}^{yz} + \text{sym}$$

$$= L^{-d}\int_{I_y^c}\nabla\varphi_{eL}^{y}\cdot\nabla\varphi_{eL}^{yz} - \int_{\partial I_z}\varphi_{eL}^{y}\,\partial_\nu\varphi_{eL}^{yz} + \text{sym}$$

$$= -L^{-d}\int_{\partial I_y} e\cdot(x-y)\,\partial_\nu\varphi_{eL}^{y} - \int_{\partial I_z}\varphi_{eL}^{y}\,\partial_\nu\varphi_{eL}^{yz} + \text{sym}$$

$$= -2\iint dy\,dz\; f_2(y,z)\; L^{-d}\int_{\partial I_y}\varphi_{eL}^{z}\;\partial_\nu\varphi_{eL}^{yz}$$

$$= -2\iint dy\,dz\; f_2(y,z)\; L^{-d}\int_{\partial I_y}\varphi_{eL}^{z}\,\partial_\nu\varphi_{eL}^{y} \;-\; 2\iint dy\,dz\; f_2(y,z)\, L^{-d}\int_{\partial I_y}\varphi_{eL}^{z}\,\underbrace{\partial_\nu(\varphi_{eL}^{yz}-\varphi_{eL}^{y})}_{\sim\langle y-z\rangle^{-2d}}$$

note $\int dz\left(\int_{\partial I_y}\varphi_{eL}^{z}\,\partial_\nu\varphi_{eL}^{y}\right) = \left(\int\varphi^{\circ}\right)\int_{\partial I_y}\partial_\nu\varphi^{y} = 0!$

$$= -2\iint dy\,dz\;\underbrace{\left(f_2(y,z)-\lambda_1^2\right)}_{\equiv h_2(y,z)}\; L^{-d}\underbrace{\int_{\partial I_y}\varphi^{z}\partial_\nu\varphi^{y}}_{\sim\langle y-z\rangle^{-d}}$$

suffices $|h_2(y,z)| \lesssim \langle y-z\rangle^{-d-\gamma}$, $\gamma>0$.

correlation decay.

INGREDIENT:

- cancellation
- + correlation decay.

$\Longrightarrow \quad \bar{B}^{(2)}_L \xrightarrow{L\uparrow\infty} \bar{B}^{(2)}$ well-defined!

Need a simpler argument that generalizes to higher order...

New input: fine decomposition of multiparticle correctors to unravel cancellations

↪ use "method of reflections" (Smoluchowski 1900s)

(B) METHOD OF REFLECTIONS.

For
$$\begin{cases} -\Delta u_S = h, & \mathcal{I}_S^c \\ \nabla u_S = 0, & \mathcal{I}_S \\ \int_{\partial I_n} \partial_\nu u_S + \int_{I_n} h = 0, & \forall n \in S \end{cases}$$
recall
$$\begin{cases} u_S = \pi^S v \\ -\Delta v = h \mathbb{1}_{\mathcal{I}_S^c}, \quad \text{in } \mathbb{R}^d \\ \pi^S : \dot{H}^1 \to \{ z \in \dot{H}^1 : \nabla z|_{\mathcal{I}_S} = 0 \} \end{cases}$$

(& similarly $\varphi_e + e\cdot x = \pi(e\cdot x)$ for corrector – see later)

Method of reflection: decompose many-particle solution $\pi^S v$
in terms of 1-particle projections
by adding / subtracting "reflections"

Reflection operator $Q^n = 1 - \pi^n$
$$\begin{cases} -\Delta Q^n v = 0, & I_n^c \\ \nabla Q^n v = \nabla v, & I_n \\ \int_{\partial I_n} \partial_\nu Q^n v = 0 \end{cases}$$
(indeed correcting BC on I_n)

& note $\nabla Q^n v(x) \sim D^2 G(x - X_n) \fint_{I_n} \nabla v$.

(dipole form)

In those terms, expand for instance:

$$\pi^{nm} v = v - (Q^n v + Q^m v) + (Q^m Q^n v + Q^n Q^m v) - \cdots$$

In other words, the method of reflections amounts to:

$$\left|\begin{array}{l} \pi v \sim \lim_{k\uparrow\infty} (1-\mathcal{L})^k v, \quad \mathcal{L} = \sum_n Q^n. \\ \left(\text{note indeed } \operatorname{Ker}\mathcal{L} = \operatorname{Im}\pi \quad - \text{ if } \mathcal{L}v = 0 \Rightarrow \langle v, \mathcal{L}v\rangle = \sum_n \|Q^n v\|^2 = 0 \right. \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \left. \Rightarrow \pi^n v = v \quad \forall n\,!\right) \end{array}\right.$$

Theorem (Höfer '18)

$$\left[\begin{array}{l} \|\nabla\pi v - \nabla(1-\mathcal{L})^k v\|_{L^2} \le \left(C\, d_{min}^{-d}\right)^k, \quad k \ge 1 \\ \\ \text{where } d_{min} := \min_{n\neq m} |x_n - x_m| \end{array}\right.$$

$\Rightarrow$ super useful, explicit expansion when $d_{min} \gg 1$

BUT note $\lambda \lesssim d_{min}^{-d}$ $\to$ requires stronger info on dilution ($d_{min} \gg 1$ instead of just $\lambda \ll 1$)

Proof.

$\boxed{\text{Step 1}}$ $\left[\text{Suffices to prove } \mathcal{L} = (1+\hat\lambda T)Q, \quad Q = 1-\pi, \text{ for some } \left[\begin{array}{l} T: \operatorname{Im}Q \to \operatorname{Im}Q \\ \|T\| \le C \end{array}\right.\right.$

Indeed: then get
$$1 - \mathcal{L} - \pi = -\hat\lambda T Q$$
$$(1-\mathcal{L})^k - \pi = (-\hat\lambda T Q)^k, \quad k \ge 1. \qquad (\hat\lambda \equiv d_{min}^{-d})$$

$\boxed{\text{Step 2}}$ Conclusion.

As $\left\{\begin{array}{l} \operatorname{Ker}\mathcal{L} = \operatorname{Im}\pi = \ker Q, \\ \operatorname{Im}\mathcal{L} = \operatorname{Im}Q, \end{array}\right.$ get $\exists!\, T: \mathcal{L} = (1+\hat\lambda T)Q$.

Note: $\|\nabla Q v\|_{L^2} \approx \|\nabla v\|_{L^2(\mathcal{I})}$ $\Rightarrow$ remains to check: $\left[\ \|\nabla \overbrace{(1-\mathcal{L})Q}^{-\hat\lambda T Q} v\|_{L^2(\mathcal{I})} \lesssim \hat\lambda \|\nabla Q v\|_{L^2(\mathcal{I})}\right.$

We compute $\nabla(1-\mathcal{L})Qv = \nabla Qv - \sum_m \nabla Q_m Q v = -\sum_{m(\neq n)} Q v$ in I_n.

$$\hookrightarrow \|\nabla(1-\mathcal{L})Qv\|_{L^2(\mathcal{I})} = \Big(\sum_n \int_{I_n} \Big|\sum_{m(\neq n)} \underbrace{\nabla Q_m Q v}\Big|^2\Big)^{1/2} \overset{C-Z}{\lesssim} \hat\lambda \|\nabla Q v\|_{L^2(\mathcal{I})}$$

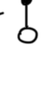
$\left[\begin{array}{l} \approx \nabla\nabla G(x_n - x_m) \int_{I_m} \nabla Q v \\ \hookrightarrow \text{argue by assuming this} \\ \quad - \text{or see details in Höfer '18!} \end{array}\right]$ $\square$

In particular, this can be applied to correctors:

$$\nabla\varphi_e^S + e = \nabla\pi^S(\overbrace{e\cdot x}^{\equiv E}) = \operatorname{argmin}\Big\{\int|\Psi - e|^2 : \Psi|_{\mathcal{I}_S} = 0, \ \& \ \nabla\times\Psi = 0\Big\}$$

$\hookrightarrow$ get e.g. $\nabla\delta^{nm}\varphi = (\nabla\varphi^{nm} + e) - (\nabla\varphi^n + e) - (\nabla\varphi^m + e) + e$

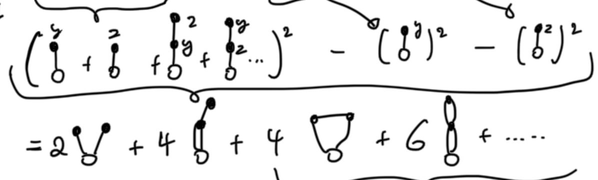
$$= \nabla\big(\cancel{1} - (\cancel{Q^n} + \cancel{Q^m}) + (Q^nQ^m + Q^mQ^n) - \dots\big)E$$
$$- \nabla(\cancel{1} - \cancel{Q^n})E - \nabla(\cancel{1} - \cancel{Q^m})E + \cancel{\nabla E}$$

$= 2$  $- 2$  $+ \dots$

c) RENORMALIZATION.

$$e \cdot \bar{B}_L^{(2)} e = \mathbb{E} \sum_{n<m} \fint_{Q_L} |\nabla \varphi_{Le}^{nm}|^2 - |\nabla \varphi_{Le}^{n}|^2 - |\nabla \varphi_{Le}^{m}|^2 .$$

$$= \iint_{Q_L \times Q_L} dy\, dz\, f_2(y,z) \fint_{Q_L} |\nabla \varphi_{Le}^{yz}|^2 - |\nabla \varphi_{Le}^{y}|^2 - |\nabla \varphi_{Le}^{z}|^2 .$$



a priori problematic

ok: each corresponds to summable integral

exercise: check for instance!

indeed get $\iint_{Q_L \times Q_L} dy\, dz\, f_2(y,z) \fint_{Q_L} dx \, \langle x-y\rangle^{-d} \langle y-z\rangle^{-d} \langle z-x\rangle^{-d} \lesssim \lambda_2$!

Magic: problematic terms have cancellations!
(in fact each leaf creates cancellation)

* $\rightarrow \iint_{Q_L \times Q_L} dy\, dz\, f_2(y,z) \fint_{Q_L} dx \, \underbrace{(\nabla Q_L^y E)(x)}_{(\nabla Q_L^0 E)(x-y)} \underbrace{(\nabla Q_L^z E)(x)}_{(\nabla Q_L^0 \cdots)(x-z)}$

where $\int_{Q_L} (\nabla Q_L^0 E) = 0$!

$$= \iint_{Q_L \times Q_L} dy\, dz\, \underbrace{\left(f_2(y,z) - \lambda_1^2\right)}_{\substack{h_2(y,z) \\ \text{2-point correlation}}} \fint_{Q_L} dx \, \underbrace{(\nabla Q_L^0 E)(x-y)}_{\langle x-y\rangle^{-d}} \underbrace{(\nabla Q_L^{0\sim})(x-z)}_{\langle x-z\rangle^{-d}}$$

is L-uniformly summable if $|h_2(y,z)| \lesssim \langle y-z\rangle^{-\alpha}$ for some $\alpha > 0$.
(algebraic correlation decay)

& allows for limit as $L \uparrow \infty$!

* exercise: corresponding cancellation for

indeed: $\iint_{Q_L \times Q_L} dy\, dz\, f_2(y,z) \fint_{Q_L} dx \, \underbrace{(\nabla Q_L^y E)(x) (\nabla Q_L^y Q_L^z E)(x)}_{(\nabla Q_L^0 E)(x-y)\, (\nabla Q_L^0 Q_L^{z-y} E)(x-y)}$

& $\int_{Q_L} (\dots)\, dz = 0$!

$$= \iint_{Q_L \times Q_L} dy\, dz\, \underbrace{h_2(y,z)}_{\substack{\langle y-z\rangle^{-\alpha} \\ \text{for some } \alpha>0}} \fint_{Q_L} dx \, \underbrace{(\nabla Q_L^0 E)(x-y) (\nabla Q_L^0 Q_L^{z-y} \cdots)(x-y)}_{\langle x-y\rangle^{-d} \langle x-y\rangle^{-d} \langle z-y\rangle^{-d}}$$

is again L-uniformly summable! ✓

Theorem. (MD- Gloria '22)

If correlation fcts have algebraic decay $\left(h_k(y_1 \cdots y_k) \lesssim \min_{i \neq j} |y_i - y_j|^{-\alpha} \right)$

Then $\bar{B} = Id + \bar{B}^{(1)} + \dots + \bar{B}^{(k)} + O(\lambda_{k+1} |\xi L|^k)$

where $\bar{B}^{(k)}$ given by renormalized cluster formula, $|\bar{B}^{(k)}| \lesssim \lambda_k |\xi L|^{k-1}$

& $|\bar{B}^{(k)}_L - \bar{B}^{(k)}| \lesssim L^{-\alpha \wedge 1} (\xi L)^{k-1}$

Rem: Don't use full reflection method: rather recombine parts with enough decay.

$\Rightarrow$ get finite expansion!

e.g. for 2 particles:

- $-\Delta \delta^{yz} \varphi = -\delta_{\partial I_y} \partial_\nu (\varphi^{yz} - \varphi^y) - \delta_{\partial I_z} \partial_\nu (\varphi^{yz} - \varphi^z)$ in $\mathbb{R}^d$

  $\Rightarrow \nabla \varphi^{yz} = \underbrace{-\int_{\partial I_y} \left(\nabla G(\cdot - u) - \fint_{I_y} \nabla G \right) \partial_\nu (\varphi^{yz} - \varphi^y)}_{\equiv \nabla \mathcal{Q}^y (\varphi^{yz} - \varphi^y)} + \text{sym}$

- similarly $\nabla(\varphi^{yz} - \varphi^y) = \nabla \mathcal{Q}^z_{(y)} \varphi^{yz}$ where $\mathcal{Q}^z_{(y)}$ is defined in terms of Green's fct $G_{(y)}$ in $\mathbb{R}^d \setminus I_y$ with $\nabla G_{(y)}|_{I_y} = 0$

$\leadsto$ get $\nabla \varphi^{yz} = \nabla \mathcal{Q}^y \mathcal{Q}^z_{(y)} \varphi^{yz} + \text{sym}$

$= \underbrace{\nabla \mathcal{Q}^y \mathcal{Q}^z_{(y)} \varphi^z}_{} + \underbrace{\nabla \mathcal{Q}^y \mathcal{Q}^z_{(y)} \mathcal{Q}^y_{(z)} \varphi^{yz}}_{\text{summarizes}} + \text{sym}$

summarizes

 + ...!

Rem: sedimentation problem $\Rightarrow$ even worse decay (longer range).

BUT can exploit correlations in a similar way!