Strictly correlated electrons in second quantization at finite temperature

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Setup

- Consider a fermionic Fock space $\mathcal{F}$ with p states defined by creation operators $a_1^\dagger, \ldots, a_p^\dagger$.
- $\hat{n}_i$ denote the corresponding number operators and $\hat{N} = \sum_i \hat{n}_i$ the total number operator.
- Free energy
$$\Omega = -\beta^{-1} \log \mathrm{Tr}(e^{-\beta \hat{H}}).$$
- Gibbs variational principle
$$\Omega = \inf_{\hat{P} \in \mathcal{D}} \left[\mathrm{Tr}(\hat{H}\hat{P}) + \beta^{-1} S(\hat{P}) \right].$$
Here $\mathcal{D}$ denotes density operators on the Fock space $\mathcal{F}$ and $S(\hat{P}) := \mathrm{Tr}[\hat{P} \log \hat{P}]$ is the von Neumann entropy.
- (Can imagine $\beta = \infty$ case if you want, until otherwise noted.)

Setup

- Fix particle number N:

$$\Omega = \inf_{\hat{P}\,:\,\mathrm{Tr}[\hat{N}\hat{P}]=N} \left[\mathrm{Tr}(\hat{H}\hat{P}) + \beta^{-1}S(\hat{P})\right].$$

- Consider Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_1,$$

  where $\hat{H}_0$ is the single-body part.
- Assume that many-body part $\hat{H}_1$ takes the following Coulomb-like form:

$$\hat{H}_1 = \lambda \sum_{ij} U_{ij}\hat{n}_i\hat{n}_j.$$

  WLOG $U_{ij} = U_{ji}$ and $U_{ii} = 0$.
- Motivated by the *strictly correlated* limit of $\lambda \to +\infty$. (From now on, omit λ from notation.)

"KS-SCE"

- For a density operator $\hat{P}$ on the Fock space, can define density $\rho \in [0,1]^p$ via

$$\rho_i := \mathrm{Tr}[\hat{n}_i \hat{P}].$$

- Now rewrite free energy and bound:

$$\begin{aligned}
\Omega &= \inf_{\rho\,:\,\mathbf{1}^\top\rho = N} \left\{ \inf_{\hat{P}\mapsto\rho} \left[\mathrm{Tr}(\hat{H}_0\hat{P}) + \mathrm{Tr}(\hat{H}_1\hat{P}) + \beta^{-1} S(\hat{P}) \right] \right\} \\
&\geq \inf_{\rho\,:\,\mathbf{1}^\top\rho = N} \left\{ \inf_{\hat{P}\mapsto\rho} \left[\mathrm{Tr}(\hat{H}_0\hat{P}) \right] + \inf_{\hat{P}\mapsto\rho} \left[\mathrm{Tr}(\hat{H}_1\hat{P}) + \beta^{-1} S(\hat{P}) \right] \right\} \\
&=: \inf_{\rho\,:\,\mathbf{1}^\top\rho = N} \left\{ \mathcal{F}_0[\rho] + \mathcal{F}_{\mathrm{SCE}}[\rho] \right\}.
\end{aligned}$$

- Looks like we just did the same thing as in first quantization, but actually no. In particular, we will get a multi-marginal OT problem where the *number of marginals is number p of sites,* **not** *the number N of electrons*!

"KS-SCE"

- In summary, want so solve

$$\Omega_{\mathrm{SCE}} := \inf_{\rho\,:\,\mathbf{1}^\top\rho = N} \left\{\mathcal{F}_0[\rho] + \mathcal{F}_{\mathrm{SCE}}[\rho]\right\},$$

  where

$$\mathcal{F}_0[\rho] := \inf_{\hat{P}\mapsto\rho} \left[\mathrm{Tr}(\hat{H}_0\hat{P})\right], \quad \mathcal{F}_{\mathrm{SCE}}[\rho] := \inf_{\hat{P}\mapsto\rho} \left[\mathrm{Tr}(\hat{H}_1\hat{P}) + \beta^{-1}S(\hat{P})\right].$$

- $\mathcal{F}_0$ is 'easy.' Infimizer is a noninteracting state. Concave conjugate is energy

$$\mathcal{F}_0^*(u) = \lambda_{\min}\left[\left(\hat{H}_0 + \sum_i u_i\hat{n}_i\right)\Big|_{\mathcal{F}_N}\right].$$

- $\mathcal{F}_0^*$ concave. Generically strictly concave but *not* smooth, so gradient injective but multi-valued at some points where eigenvalues cross (i.e., zero gap).
- This means gradient map of $\mathcal{F}_0$ (the inverse) is many-to-one, so it is well-posed to compute. Don't care that it's not injective.

Solving the model

- Recall

$$\Omega_{\mathrm{SCE}} = \inf_{\rho\,:\,\mathbf{1}^\top\rho = N} \left\{ \mathcal{F}_0[\rho] + \mathcal{F}_{\mathrm{SCE}}[\rho] \right\},$$

- First idea: want to solve $\nabla\mathcal{F}_{\mathrm{SCE}}[\rho] = -\nabla\mathcal{F}_0[\rho]$, i.e.,

$$\rho = \left((\nabla\mathcal{F}_0)^{-1} \circ (-\nabla\mathcal{F}_{\mathrm{SCE}}) \right)[\rho].$$

- Fixed-point iteration.
- Finite temperature *does* fix the problem with $\nabla\mathcal{F}_{\mathrm{SCE}}$.
- If zero gap, there is a problem via $(\nabla\mathcal{F}_0)^{-1}$.
- Could fix at least numerically by apportioning some entropy to the non-interacting part of the infimum.
- But gradient descent actually ok regardless because sum of two functional is differentiable, strongly convex (with parameter $\sim \beta^{-1}$).
- Remains to discuss the $\mathcal{F}_{\mathrm{SCE}}$ part and how to compute the gradient.

The SCE part

- Recall
$$\mathcal{F}_{\mathrm{SCE}}[\rho] := \inf_{\hat{P} \mapsto \rho} \left[\mathrm{Tr}(\hat{H}_1 \hat{P}) + \beta^{-1} S(\hat{P}) \right].$$
- Nothing really 'quantum' about $\hat{H}_1$ on its own since the $\hat{n}_i$ are all diagonalized by the occupation number basis.
- Can derive
$$\mathcal{F}_{\mathrm{SCE}}[\rho] = \inf_{\pi \in \Pi(\rho)} \left[\sum_{\mathbf{s} \in \{0,1\}^p} c(\mathbf{s}) \pi(\mathbf{s}) + \beta^{-1} S(\pi) \right].$$
Here $\Pi(\rho)$ is probability measures π on $\{0,1\}^p$ s.t. i-th marginal π_i of π is given by $\pi_i = (1-\rho_i)\delta_0 + \rho_i \delta_1$. S is (convex) Shannon entropy.
- Cost is $c(\mathbf{s}) := \sum_{i,j=1}^p U_{ij} s_i s_j$.
- Nothing but an entropically regularized multi-marginal OT problem (on binary hypercube). Gradient w.r.t. ρ is dual potential (modulo some sign convention).

SDP relaxation and the entropy

- As discussed in Lin's talk, can derive SDP relaxation of representable set of two-marginals. More details in Lexing Ying's talk later this week.
- But new difficulty: how to write $S(\pi)$ in terms of two-marginals?
- You can't, but consider Bethe approximation

$$S_{\mathrm{B}}(\{\pi_{ij}\}_{i \neq j}) := \sum_{i<j} S(\pi_{ij}) - (p-2) \sum_{i} S(\pi_i).$$

- Since 1-marginals are fixed, just contributes a convex term to the SDP from Lin's talk.
- Finite temperature formalism makes it clear that the OT problem is essentially doing some 'variational inference' for a classical spin system, with spin-interaction matrix determined by U_{ij}.
- Popular approach in graphical models literature: (loopy) belief propagation (BP).
- Our method is equivalent to *adding* the semidefinite constraint to the variational formulation of BP (cf. book by Mézard/Montanari).

Where is this going?

- SCE intriguing direction but extremely difficult to evaluate in practice.
- In first quantization, numerical approaches rely on space discretization; no way obvious way to make use of a more efficient basis.
- Here we have an ansatz and algorithmic approach that are going to yield *at least something* in a reasonable amount of time for models of physical interest, e.g., long-range Hubbard model.
- Is second-quantized KS-SCE a good model? Strictly speaking, probably not, but can it tell us useful things?
- Second quantization permits us to imagine hybrid approach with traditional correlated methods.
- Splitting $\hat{H}_0 + \hat{H}_1$ doesn't *have* to be between non-interacting and interacting parts. Just need to have some trust in ability to 'solve' $\hat{H}_0$. Then SCE part will yield effective potential contribution to $\hat{H}_0$ mimicking effect of the 'rest of the Hamiltonian.'
- Or could imagine separating out a long-range part via $\hat{H}_1$ to make use of forward model for $\hat{H}_0 + \hat{u}$ relying on short-range Hamiltonian.