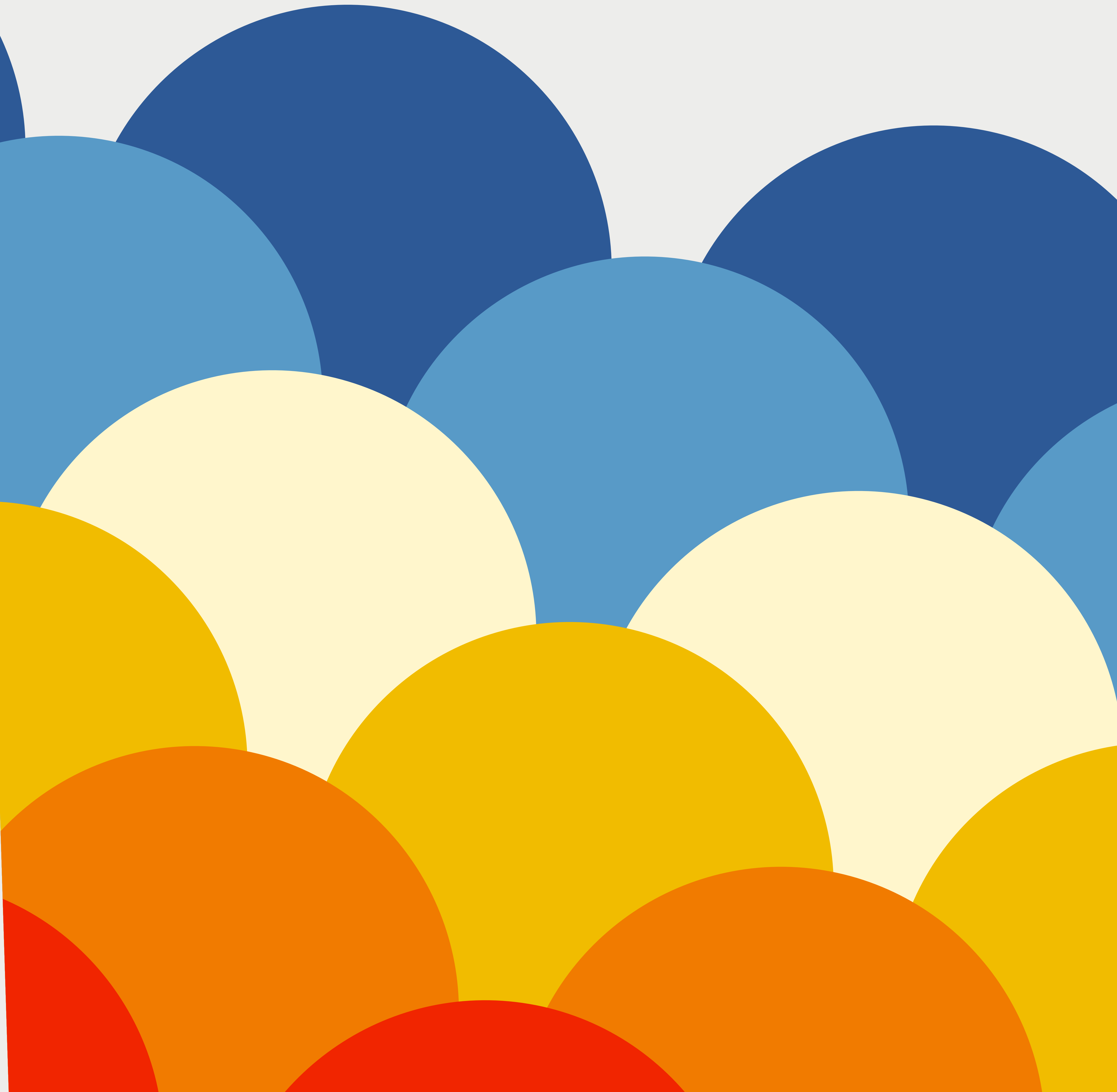
Short Takes 331

Toward QMC: Trotter-Suzuki factorization



Toward finite-temperature Quantum Monte Carlo (QMC):

The Trotter-Suzuki factorization.

Fundamental object in equilibrium thermodynamics

$\mathcal{Z}$: partition function (grand canonical) $= \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]$

β: $\frac{1}{T}$, T: temperature

μ: chemical potential

$\hat{H}$: Hamiltonian $= \hat{T} + \hat{V}$

$\hat{T}$: free part (kinetic energy)

$\hat{V}$: interaction

$\hat{N}$: particle number op.

- Usually, $[\hat{H},\hat{N}]=0$ (i.e. $\hat{N}$ represents a conserved quantity), so we can simplify

$$\exp(-\beta(\hat{H}-\mu\hat{N})) = e^{-\beta\hat{H}}\, e^{\beta\mu\hat{N}}.$$

Moreover, then,

$$\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] = \sum_{N=0}^{\infty} z^N Q_N \quad , \quad z = e^{\beta\mu}$$

$$Q_N = \mathrm{Tr}_N\left[e^{-\beta\hat{H}}\right]$$

"canonical partition function".

- The main difficulty in dealing with $\mathcal{Z}$ is that $e^{-\beta\hat{H}}$ is essentially impossible to compute.

Why? Mostly because of $\hat{V}$ and because $[\hat{T},\hat{V}]\neq 0$.

For that reason,

$$e^{-\beta\hat{H}} \neq e^{-\beta\hat{T}}\, e^{-\beta\hat{V}}$$

- The Trotter-Suzuki factorization is the generic name for a family of approximations where...

① $e^{-\beta\hat{H}} = \left(e^{-\tau\hat{H}}\right)^{N_\tau}$ (exact)

$$\beta = \tau \cdot N_\tau$$

$N_\tau \gg 1$ ← in this sense, τ is "small".

② $e^{-\tau\hat{H}} \to e^{-\tau\hat{T}}\, e^{-\tau\hat{V}}$ ← error starts at order τ^2

or

$e^{-\tau\frac{\hat{T}}{2}}\, e^{-\tau\hat{V}}\, e^{-\tau\frac{\hat{T}}{2}}$ ← error starts at order τ^3

or

⋮

Note: $e^{-\tau\hat{H}} = 1 - \tau\hat{H} + \frac{\tau^2}{2}\hat{H}^2 + \ldots$

whereas

$$e^{-\tau\hat{T}}\, e^{-\tau\hat{V}} = 1 - \tau(\hat{T}+\hat{V}) + \tau^2\underbrace{\left(\frac{\hat{T}^2}{2} + \frac{\hat{V}^2}{2} + \hat{T}\hat{V}\right)}_{\neq\ \frac{\hat{H}^2}{2}} + \ldots$$

while

$$e^{-\tau\frac{\hat{T}}{2}}\, e^{-\tau\hat{V}}\, e^{-\tau\frac{\hat{T}}{2}} = 1 - \tau(\hat{T}+\hat{V}) + \tau^2\underbrace{\left(\frac{\hat{T}^2}{2} + \frac{\hat{V}^2}{2} + \frac{1}{2}(\hat{T}\hat{V}+\hat{V}\hat{T})\right)}_{=\ \hat{H}^2/2} + \ldots$$

So... Different flavors of the decomposition feature varying levels of correctness & complexity, usually competing against each other.

This factorization is essential all over many-body physics, even in some classical applications, but notably in quantum computing applications.

It remains an area of research.

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