Dual fermions

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Some references

Fermionic HS transformation

C. Bourbonnais, PhD thesis, Sherbrooke (1986)
S.K. Sarker, J. Phys. C **21**, L667 (1988).
S. Pairault, D. Senechal, A.-M.S. Tremblay
PRL **80**, 5389 (1998); EPJ (2000)

Dual fermions in quantum clusters

A.N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, and A. Georges
PRB **79**, 045133 2009

A fermionic Hubbard-Stratonovich transformation for strong coupling

$$h_i(c_{i\sigma}^\dagger, c_{i\sigma}) = U c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\downarrow} c_{i\uparrow} \qquad \mathcal{H}^1 = \sum_\sigma \sum_{ij} V_{ij} c_{i\sigma}^\dagger c_{j\sigma}$$

$$Z = \int [\mathrm{d}\gamma^\star \mathrm{d}\gamma] \exp - \int_0^\beta \mathrm{d}\tau \left\{ \sum_{i\sigma} \gamma_{i\sigma}^\star(\tau) \left(\frac{\partial}{\partial\tau} - \mu \right) \gamma_{i\sigma}(\tau) + \sum_i h_i(\gamma_{i\sigma}^\star(\tau), \gamma_{i\sigma}(\tau)) + \sum_{ij\sigma} V_{ij} \gamma_{i\sigma}^\star(\tau) \gamma_{j\sigma}(\tau) \right\} . \quad (5)$$

$$\int_0^\beta \mathrm{d}\tau \sum_{ij\sigma} V_{ij} \gamma_{i\sigma}^\star(\tau) \gamma_{j\sigma}(\tau) = \sum_{ab} V_{ab} \gamma_a^\star \gamma_b = \langle \gamma | V | \gamma \rangle$$

$$\int [\mathrm{d}\psi^\star \mathrm{d}\psi] \, \mathrm{e}^{\langle \psi | V^{-1} | \psi \rangle + \langle \psi | \gamma \rangle + \langle \gamma | \psi \rangle} = \det(V^{-1}) \, \mathrm{e}^{-\langle \gamma | V | \gamma \rangle}$$

$$Z = Z_0 \int [\mathrm{d}\psi^\star \mathrm{d}\psi] \, \mathrm{e}^{\langle \psi | V^{-1} | \psi \rangle} \left\langle \mathrm{e}^{\langle \psi | \gamma \rangle + \langle \gamma | \psi \rangle} \right\rangle_0$$

Exact diagonalization impurity solver

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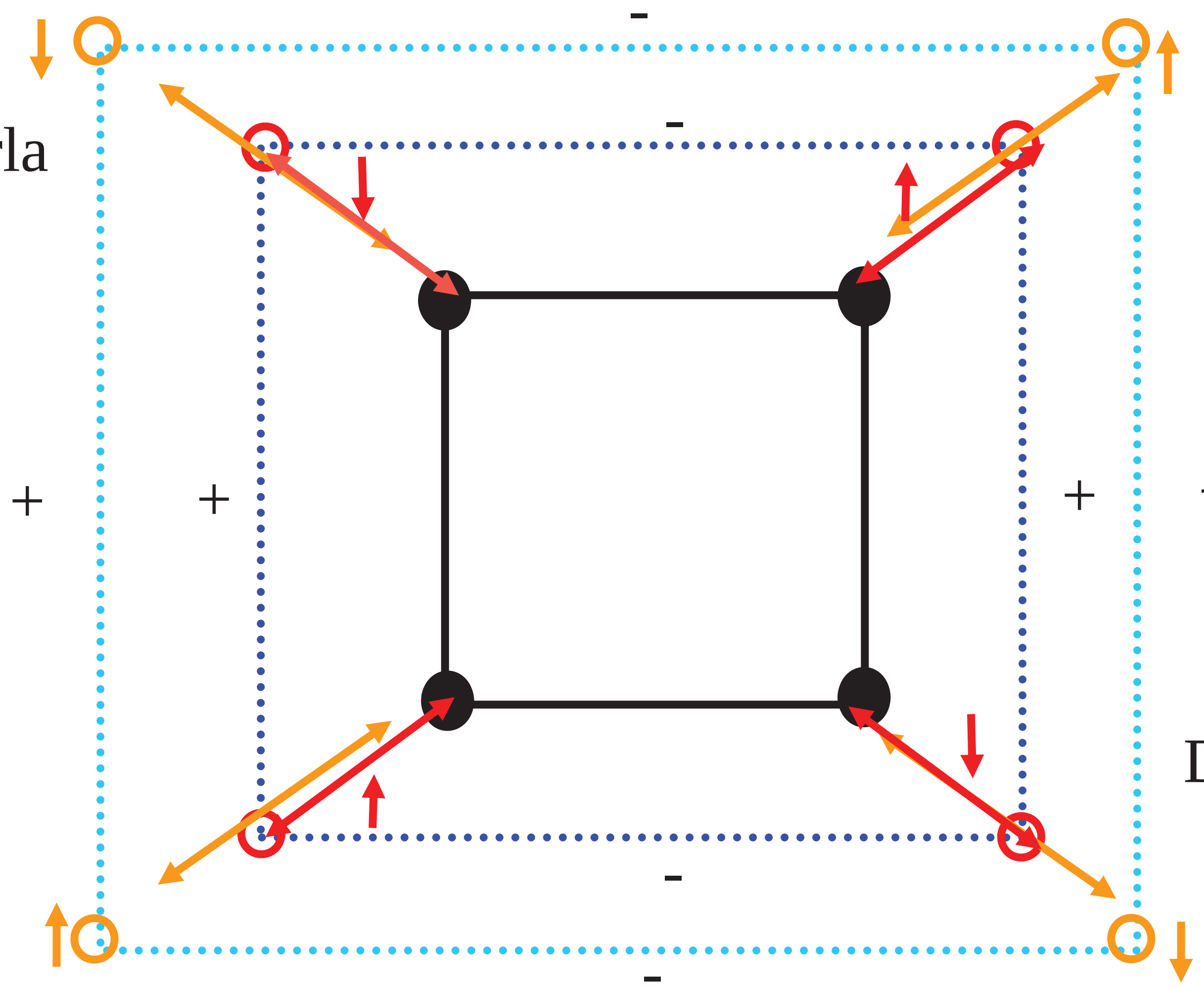
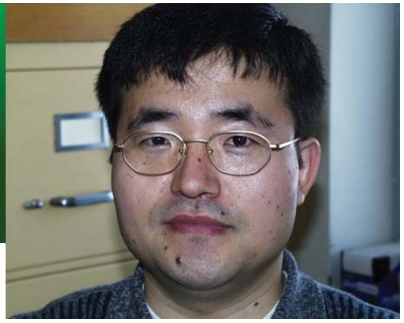
Parametrization of bath

S. Kancharla





B. Kyung

David Sénéchal

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Effect of finite bath

- Minimize a distance function to find bath parameters at iteration *i+1*:
  - Weight (cutoff) needed
  - Effective temperature

$$d = \sum_{\mu,\nu} \sum_{n} W(i\omega_n) \left| \Delta_{\mu,\nu}^{(i+1)}(i\omega_n) - \Delta_{\mu,\nu}^{(i)}(i\omega_n) \right|^2$$

Implementation issues (not trivial!)

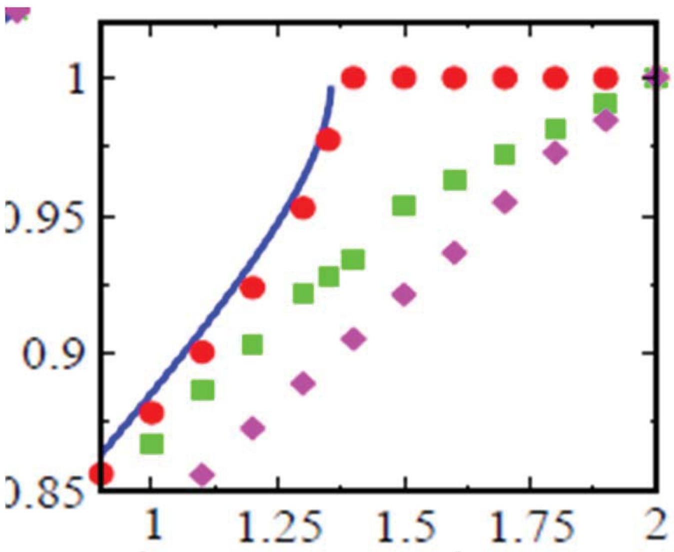
- Exact diagonalization code issues
  - Need Lanczos or band Lanczos or Arnoldi
  - Integrations are difficult (do them in imaginary plane in the cas of frequency)
  - Value of Lorentzian broadening for dynamics
- General bath difficult to converge
  - Start from known easy solutions and do small change on Hamiltonian parameters

Some references

M. Caffarel and W. Krauth, PRL, **72**, 1545 (1994).
E. Koch, G. Sangiovanni, and O. Gunnarsson, PRB , **78**, 115102 (2008).
A.Liebsch and N.-H. Tong, PRB, **80**, 165126 (2009).
David Sénéchal Phys. Rev. B **81**, 235125 (2010)
D. Sénéchal, “An introduction to quantum cluster methods,"
Lecture notes from the CIFAR - PITP
International Summer School on Numerical Methods
for Correlated Systems in Condensed Matter, Sherbrooke, Canada,
arXiv:0806.2690 (2008).

Benchmarks

ED solver

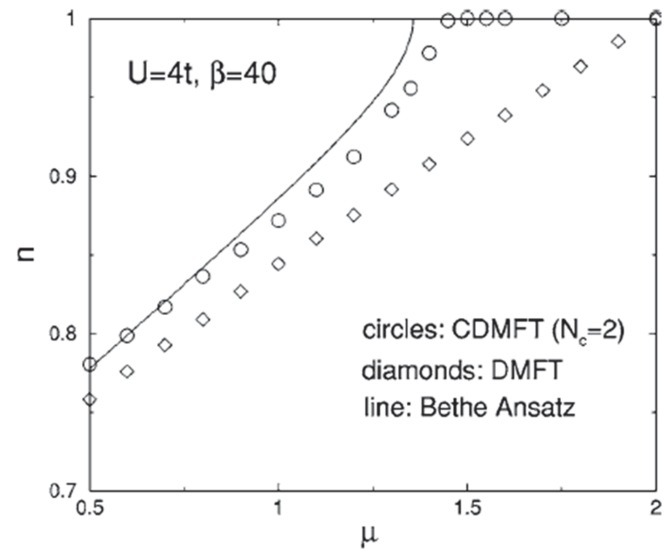


Red, $U/t = 4, N_c = 2, N_b = 8$

Solid line: Bethe ansatz

Capone, Civelli, *et al.*
PRB **69**, 195105 2004.

QMC solver



Kyung, Kotliar, AMST
PRB **73**, 205106 (2006)

CT-QMC impurity solver

Monte Carlo method

Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner,
Rev.Mod.Phys. **83**, 349 (2011)

$$Z = \int_{\mathcal{C}} d\mathbf{x}\, p(\mathbf{x}).$$

$$\langle A \rangle_p = \frac{1}{Z} \int_{\mathcal{C}} d\mathbf{x}\, \mathcal{A}(\mathbf{x}) p(\mathbf{x}).$$

$$\langle A \rangle_p \approx \langle A \rangle_{\mathrm{MC}} \equiv \frac{1}{M} \sum_{i=1}^{M} \mathcal{A}(\mathbf{x}_i).$$

$$\langle A \rangle = \frac{1}{Z} \int_{\mathcal{C}} d\mathbf{x}\, \mathcal{A}(\mathbf{x}) p(\mathbf{x}) = \frac{\int_{\mathcal{C}} d\mathbf{x}\, \mathcal{A}(\mathbf{x})[p(\mathbf{x})/\rho(\mathbf{x})]\rho(\mathbf{x})}{\int_{\mathcal{C}} d\mathbf{x}[p(\mathbf{x})/\rho(\mathbf{x})]\rho(\mathbf{x})} \equiv \frac{\langle A(p/\rho) \rangle_\rho}{\langle p/\rho \rangle_\rho}.$$

Monte Carlo: Markov chain

- Ergodicity
- Detailed balance

$$\frac{W_{\mathbf{xy}}}{W_{\mathbf{yx}}} = \frac{p(\mathbf{y})}{p(\mathbf{x})} \qquad W_{\mathbf{xy}} = W_{\mathbf{xy}}^{\mathrm{prop}} W_{\mathbf{xy}}^{\mathrm{acc}}$$

$$W_{\mathbf{xy}}^{\mathrm{acc}} = \min[1, R_{\mathbf{xy}}] \qquad R_{\mathbf{xy}} = \frac{p(\mathbf{y}) W_{\mathbf{yx}}^{\mathrm{prop}}}{p(\mathbf{x}) W_{\mathbf{xy}}^{\mathrm{prop}}}$$

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Reminder on perturbation theory

$$
\begin{aligned}
\exp(-\beta(H_a + H_b)) &= \exp(-\beta H_a)U(\beta) \\
\frac{\partial U(\beta)}{\partial \beta} &= -H_b(\beta)U(\beta) \\
U(\beta) &= 1 - \int_0^\beta d\tau H_b(\tau) + \int_0^\beta d\tau \int_0^\tau d\tau' H_b(\tau)H_b(\tau') + \ldots
\end{aligned}
$$

Partition function as sum over configurations

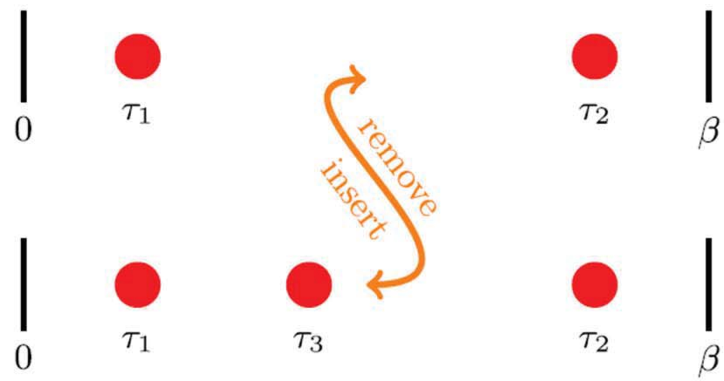
$$Z = \mathrm{Tr}[\exp(H_a + H_b)]$$

$$= \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \, \mathrm{Tr}[e^{-\beta H_a} H_b(\tau_k) \times H_b(\tau_{k-1}) \cdots H_b(\tau_1)].$$

$$Z = \sum_{k=0}^{\infty} \sum_{\gamma \in \Gamma_k} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k w(k, \gamma, \tau_1, \ldots, \tau_k)$$

$$\mathbf{x} = (k, \gamma, (\tau_1, \ldots, \tau_k)), \qquad p(\mathbf{x}) = w(k, \gamma, \tau_1, \ldots, \tau_k) d\tau_1 \cdots d\tau_k,$$

Updates



$$W^{\text{prop}}_{(k,\vec{\tau}),(k+1,\vec{\tau}')} = \frac{d\tau}{\beta}$$

$$W^{\text{prop}}_{(k+1,\vec{\tau}'),(k,\vec{\tau})} = \frac{1}{k+1}.$$

$$\begin{aligned} R_{(k,\vec{\tau}),(k+1,\vec{\tau}')} &= \frac{p((k+1,\vec{\tau}'))}{p((k,\vec{\tau}))} \frac{W^{\text{prop}}_{(k+1,\vec{\tau}'),(k,\vec{\tau})}}{W^{\text{prop}}_{(k,\vec{\tau}),(k+1,\vec{\tau}')}} \\ &= \frac{w(k+1)d\tau'_1 \cdots d\tau'_{k+1}}{w(k)d\tau_1 \cdots d\tau_k} \frac{1/(k+1)}{d\tau/\beta} \\ &= \frac{w(k+1)}{w(k)} \frac{\beta}{k+1}. \end{aligned}$$

Beard, B. B., and U.-J. Wiese, 1996, Phys. Rev. Lett. **77**, 5130.
Prokof'ev, N. V., B. V. Svistunov, and I. S. Tupitsyn, 1996, JETP Lett. **64**, 911.

Solving cluster in a bath problem

- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.

  - P. Werner, A. Comanac, L. de’ Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

  - K. Haule, Phys. Rev. B **75**, 155113 (2007).

Some Algorithmic details:
3 improvements

Continuous-time QMC : CT-HYB

$$H_{\text{imp}} = H_{\text{loc}}(d_i^\dagger, d_i) + \sum_{i\mu}(V_{\mu i} a_\mu^\dagger d_i + V_{\mu i}^* d_i^\dagger a_\mu)$$
$$+ \sum_\mu \epsilon_\mu a_\mu^\dagger a_\mu,$$

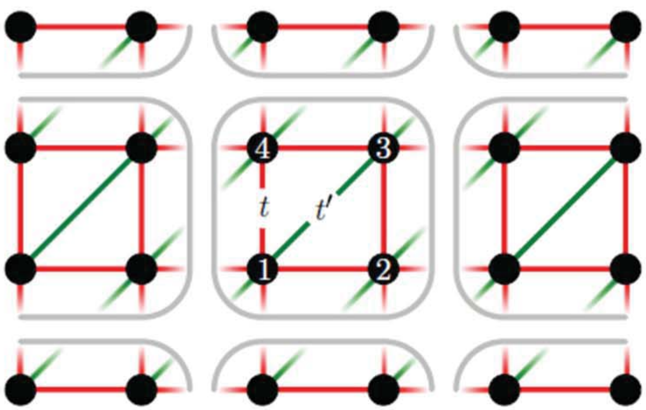
$$Z = \mathrm{Tr} T_\tau e^{-\beta H_0} e^{-\int_0^\beta d\tau (H_{\text{hyb}}(\tau) + H_{\text{hyb}}^\dagger(\tau))}$$
$$= \sum_{k \geq 0} \frac{1}{k!^2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau_1' \cdots d\tau_k' \mathrm{Tr} T_\tau e^{-\beta H_0}$$
$$\times H_{\text{hyb}}(\tau_1) H_{\text{hyb}}^\dagger(\tau_1') \cdots H_{\text{hyb}}(\tau_k) H_{\text{hyb}}^\dagger(\tau_k').$$

$$= \sum_{k \geqslant 0} \sum_{i_1 \cdots i_k} \sum_{i_1' \cdots i_k'} \frac{1}{k!^2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau_1' \cdots d\tau_k'$$
$$\times \mathrm{Tr} T_\tau e^{-\beta H_{\text{loc}}} d_{i_1}(\tau_1) d_{i_1'}^\dagger(\tau_1') \cdots d_{i_k}(\tau_k) d_{i_k'}^\dagger(\tau_k')$$
$$\times Z_{\text{bath}} \langle \hat{V}_{i_1}^\dagger(\tau_1) \hat{V}_{i_1'}(\tau_1') \cdots \hat{V}_{i_k}^\dagger(\tau_k) \hat{V}_{i_k'}(\tau_k') \rangle, \qquad \hat{V}_i = \sum_\mu V_{\mu i}^* a_\mu$$

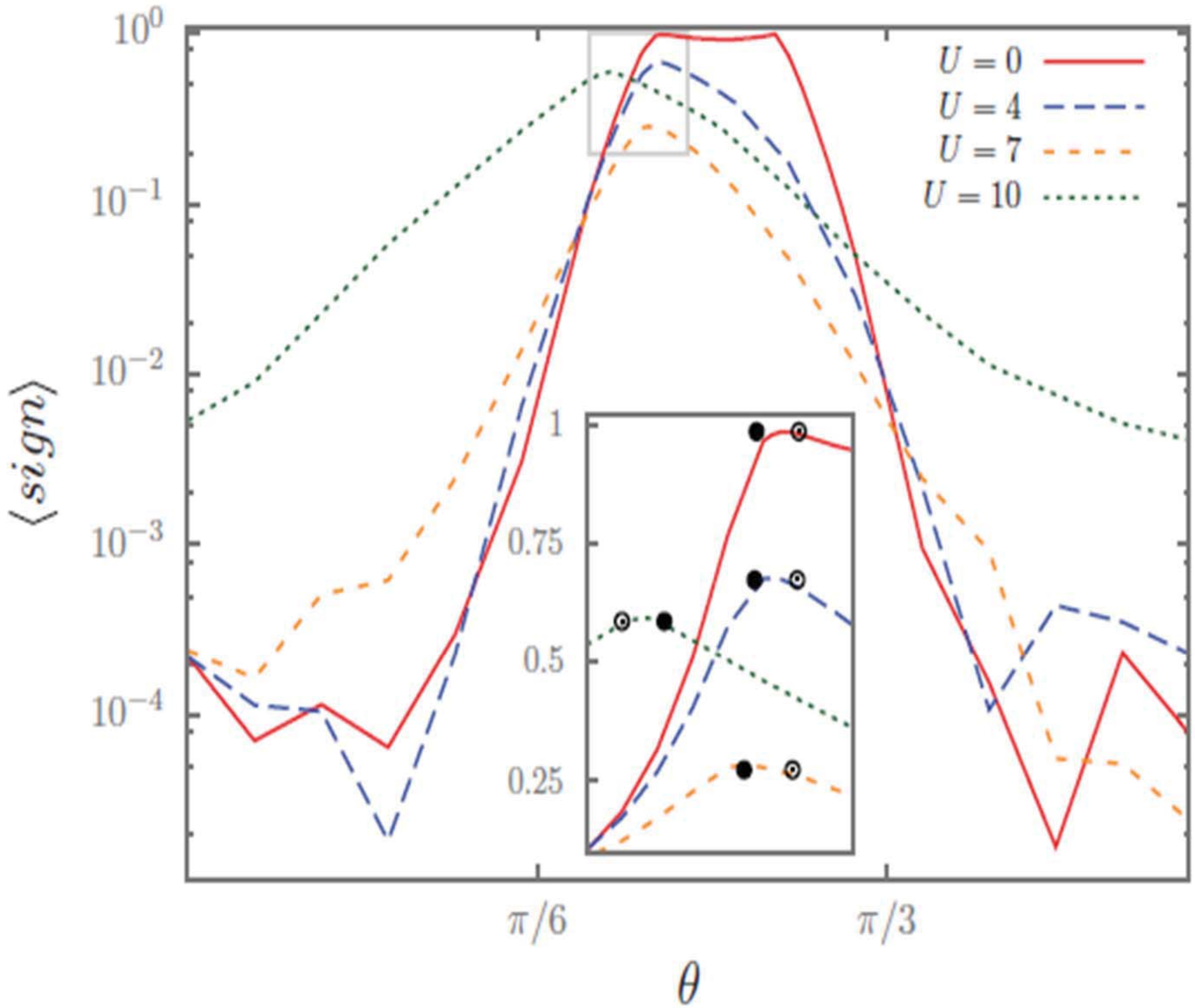
P. Sémon, G. Sordi, A.-M.S. Tremblay, Phys. Rev. B **89**, 165113 (2014)

Reducing the sign problem

$$\cos\theta c'_{A_1\sigma} - \sin\theta c_{A_1\sigma}, \quad \sin\theta c'_{A_1\sigma} + \cos\theta c_{A_1\sigma}$$



$t'/t = 0.8$



C_{2v}

$2A_1, B_1, B_2$

Ergodicity of the hybridization expansion with two operator updates and broken symmetry

$$H_{\mathrm{imp}} = H_{\mathrm{loc}}(d_i^\dagger, d_i) + \sum_{i\mu}(V_{\mu i} a_\mu^\dagger d_i + V_{\mu i}^* d_i^\dagger a_\mu) + \sum_\mu \epsilon_\mu a_\mu^\dagger a_\mu,$$

Patrick Sémon

$$Z = \mathrm{Tr} T_\tau e^{-\beta H_0} e^{-\int_0^\beta d\tau (H_{\mathrm{hyb}}(\tau) + H_{\mathrm{hyb}}^\dagger(\tau))}$$

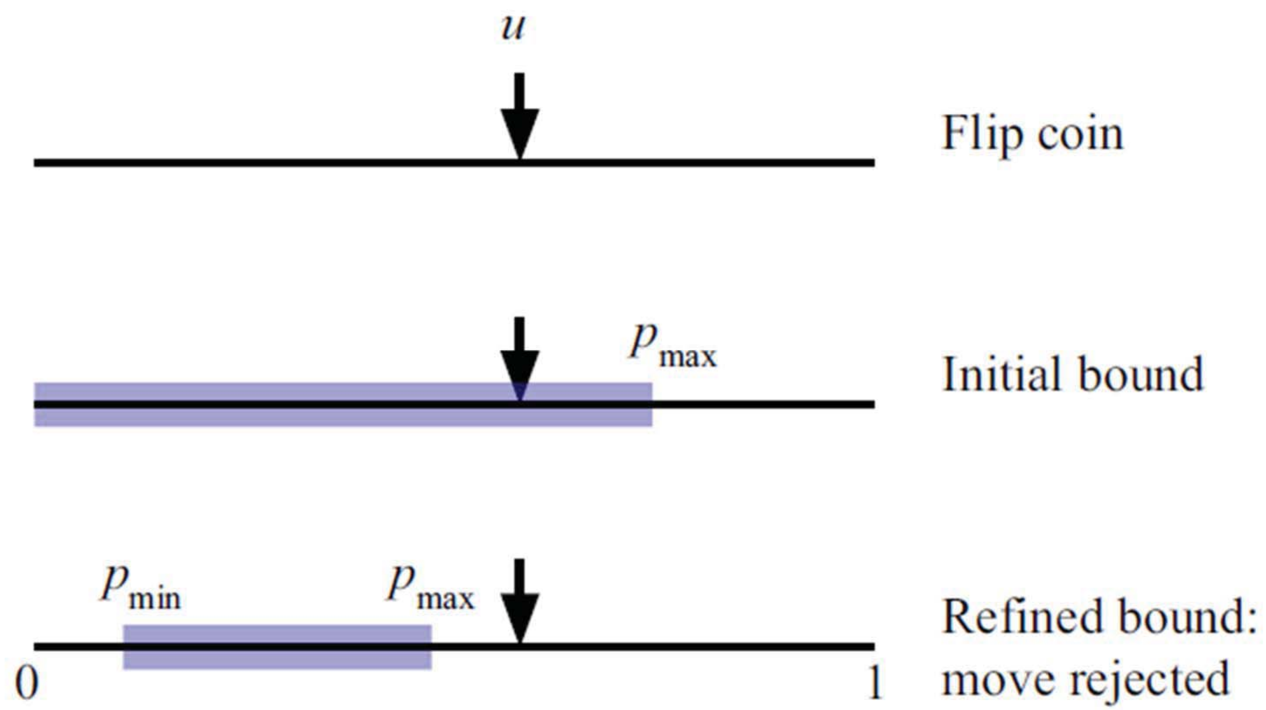
$$= \sum_{k \geq 0} \frac{1}{k!^2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau_1' \cdots d\tau_k' \mathrm{Tr} T_\tau e^{-\beta H_0} \times H_{\mathrm{hyb}}(\tau_1) H_{\mathrm{hyb}}^\dagger(\tau_1') \cdots H_{\mathrm{hyb}}(\tau_k) H_{\mathrm{hyb}}^\dagger(\tau_k').$$

$$\boxed{\mathrm{Tr}[d_{\uparrow(0,\pi)} d_{\downarrow(0,\pi)} d_{\downarrow(\pi,0)}^\dagger d_{\uparrow(\pi,0)}^\dagger] \times \Delta_{a\uparrow(0,\pi),\downarrow(0,\pi)} \Delta_{a\uparrow(\pi,0),\downarrow(\pi,0)}}$$

P. Sémon, G. Sordi, A.-M.S. Tremblay, Phys. Rev. B **89**, 165113 (2014)

Lazy Skip-List : 1 Lazy

Fast rejection algorithm : the lazy part



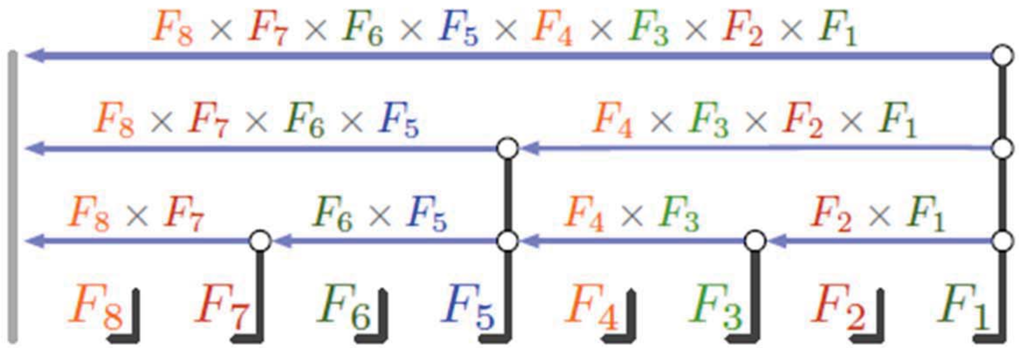
P. Sémon, Chuck-Hou Yee, K. Haule, A.-M.S. Tremblay, Phys. Rev. B **90**, 075149 (2014)

MC weights in CT-HYB some notation

$$w\{(i_1,\tau_1)\cdots(i_k',\tau_k')\} = \mathrm{Det}\,\boldsymbol{\Delta}\,\mathrm{Tr}_{\mathrm{loc}}\Big[\mathrm{T}_\tau e^{-\beta H_{\mathrm{loc}}} \times d_{i_k}(\tau_k)d^\dagger_{i_k'}(\tau_k')\cdots d_{i_1}(\tau_1)d^\dagger_{i_1'}(\tau_1')\Big]$$

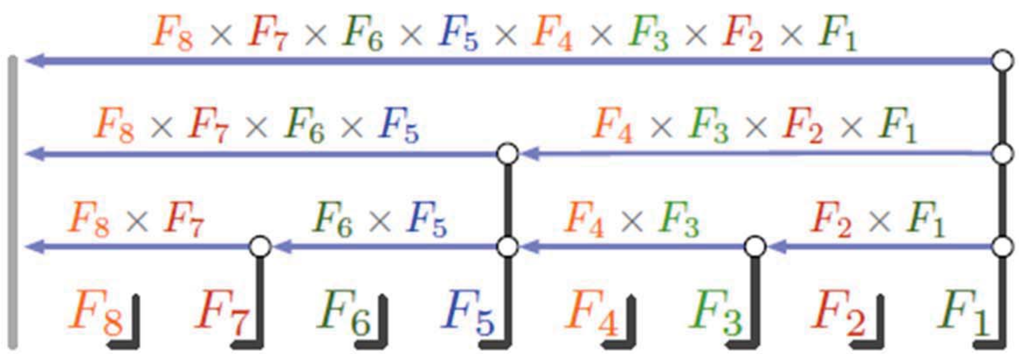
$$\mathrm{Tr}_{\mathrm{loc}}\, P_{\beta-\tau_k}\, F_{i_k}\, P_{\tau_k-\tau_k'}\, F^\dagger_{i_k'} \cdots F_{i_1}\, P_{\tau_1-\tau_1'}\, F^\dagger_{i_1'}\, P_{\tau_1'}$$

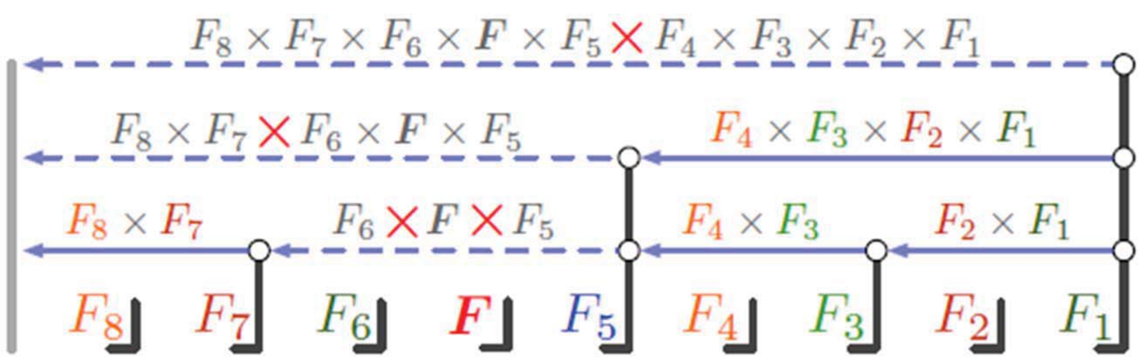
Lazy Skip List : Skip List



Tree structure : E. Gull, ETH thesis

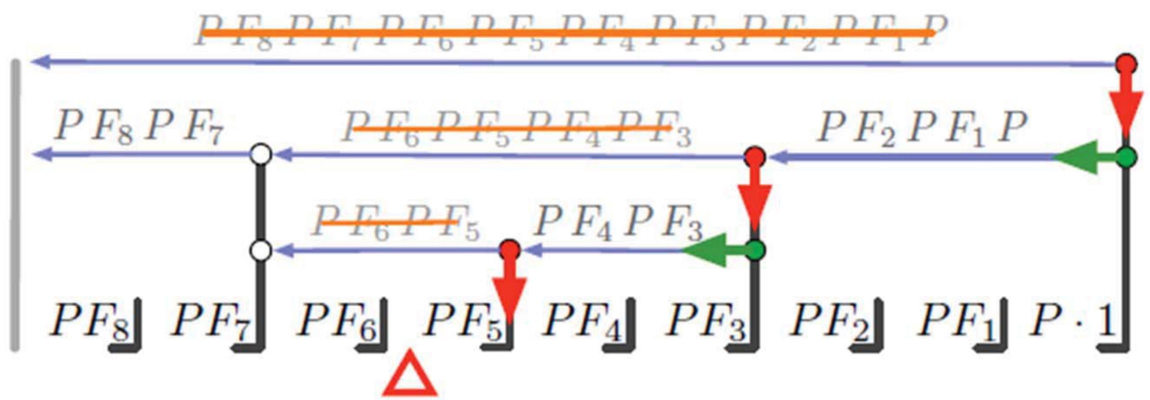
Lazy Skip List : Skip List





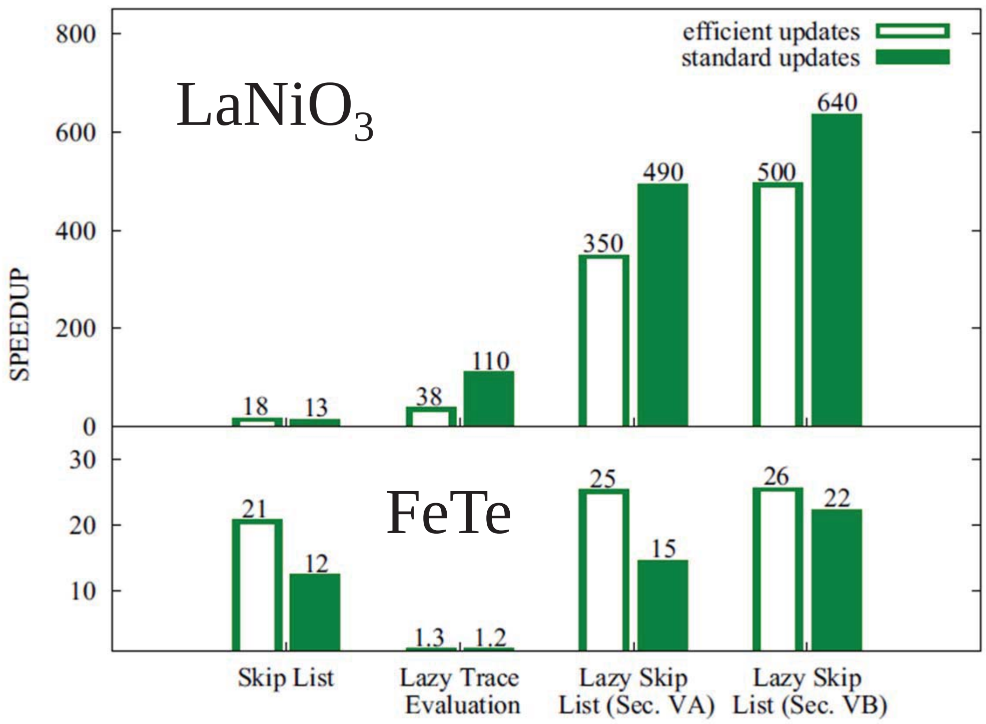
Tree structure : E. Gull, ETH thesis

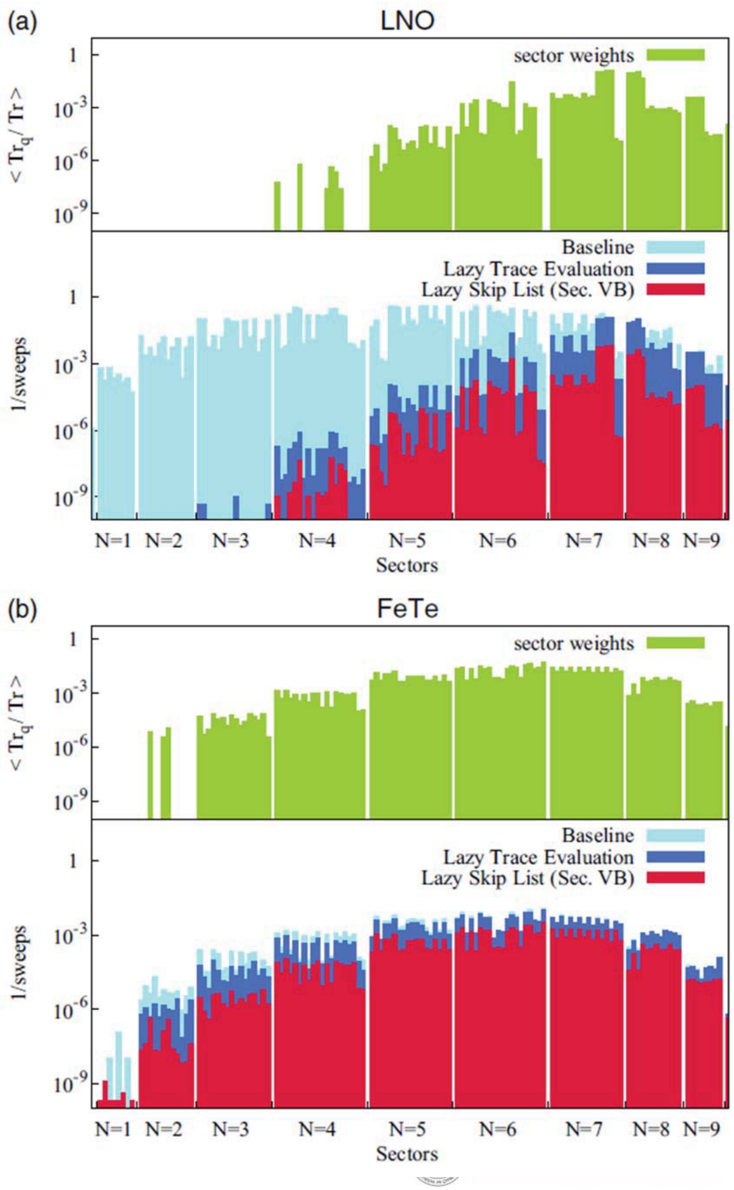
Some more details



Subproducts stored in blue arrows are emptied
if tail coincides with red arrow

Lazy Skip-List: Speedup (beat Moore)





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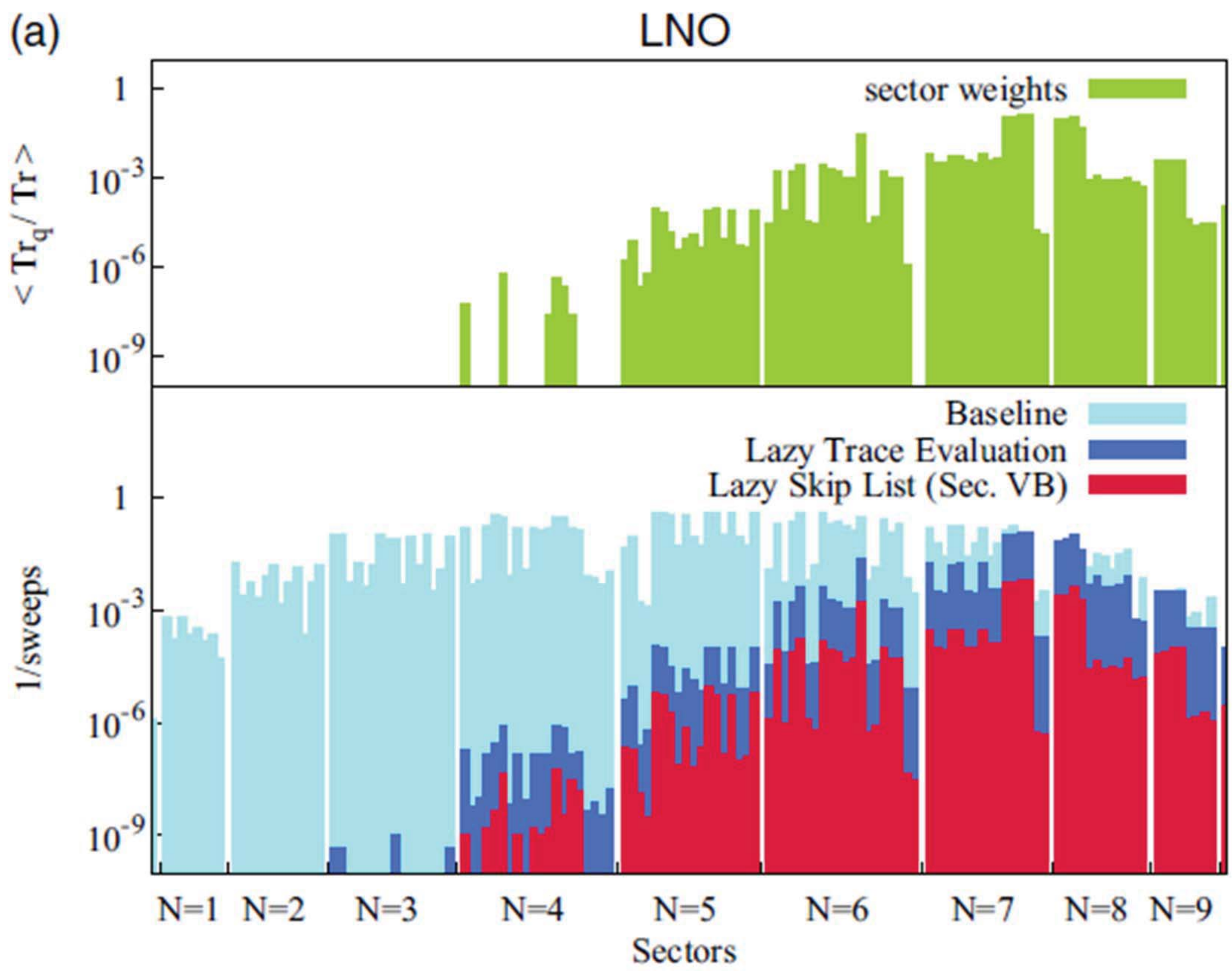

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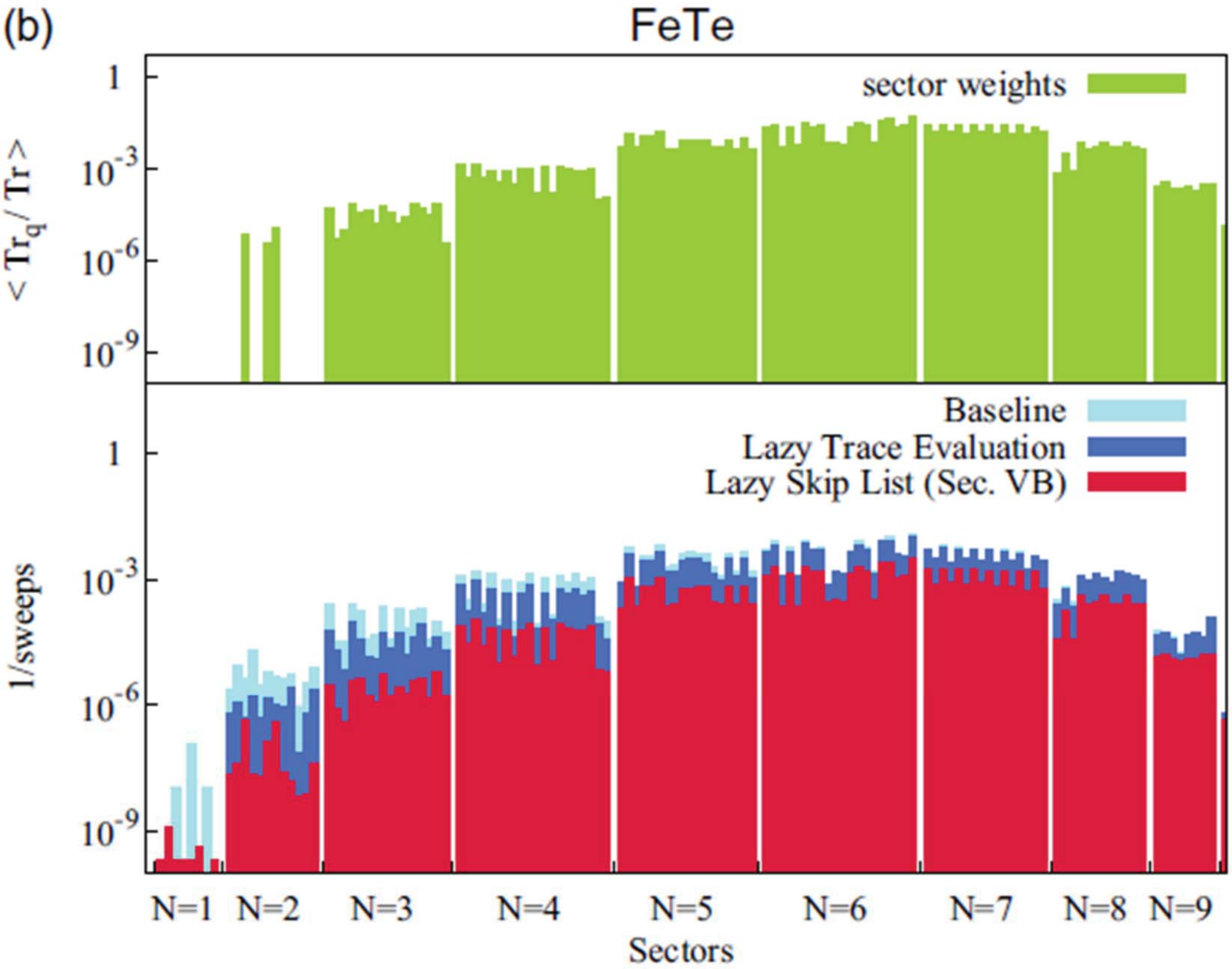

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Maximum Entropy analytical continuation

Look for cond-mat soon

D. Bergeron, A.-M.S. Tremblay

A new maximum entropy approach and a user friendly software for analytic continuation of numerical data

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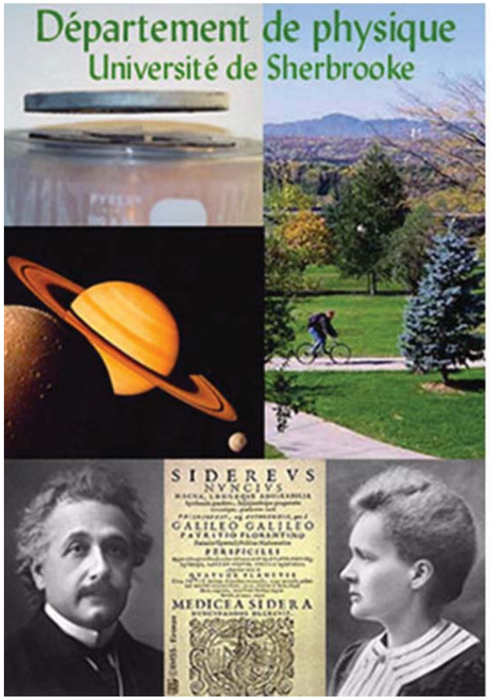

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