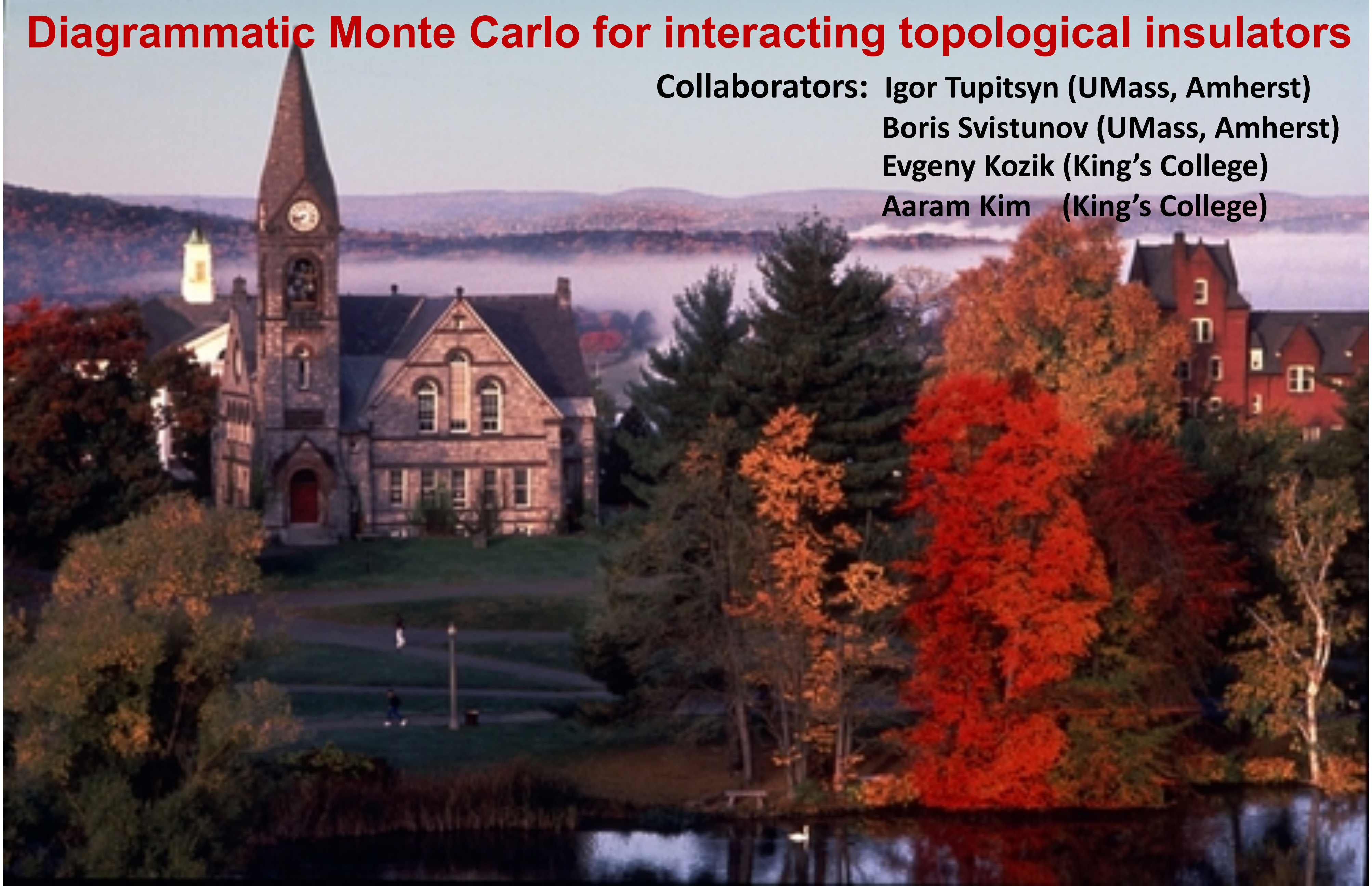
Diagrammatic Monte Carlo for interacting topological insulators

Collaborators: Igor Tupitsyn (UMass, Amherst)
Boris Svistunov (UMass, Amherst)
Evgeny Kozik (King's College)
Aaram Kim (King's College)



Aspen, March 9, 2020

SIMONS FOUNDATION
Advancing Research in Basic Science and Mathematics

AFOSR
MURI

National Science Foundation
WHERE DISCOVERIES BEGIN

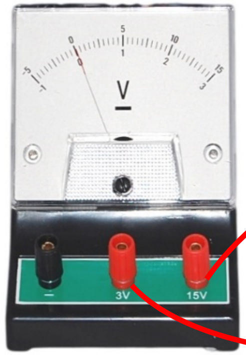
Diagrammatic Monte Carlo: where do we stand (homotopic action)

Application to Interacting TI: Phase diagram of the Haldane-Hubbard model

Diagrammatic Monte Carlo for connected Feynman diagrams solves the <u>computational complexity</u> problem for fermions

$$H_{Fermions} = \sum_{k\alpha} (\varepsilon(k,\alpha) - \mu_\alpha)\psi^\dagger_{k\alpha}\psi_{k\alpha} + \frac{1}{2}\sum_{rr'abcd} V_{abcd}(r-r')\psi^\dagger_{r'd}\psi^\dagger_{rc}\psi_{rb}\psi_{r'a} + \ldots$$

Voltmeter (or Martin Zwierlein):
What fermionic sign problem?



Fermions do not have a sign problem

A similar Hamiltonian with random parameters and unlimited range of support,

$$H = \sum_{kab} \varepsilon_{ab}(p)\psi^\dagger_{ka}\psi_{kb} - \sum_{ra} \mu_a(r)\psi^\dagger_{ra}\psi_{rb} + \frac{1}{2}\sum_{rr'abcd} V_{abcd}(r,r')\psi^\dagger_{r'd}\psi^\dagger_{rc}\psi_{rb}\psi_{r'a} + \ldots$$

covers the entire complexity of all known materials and structures in Nature!

There is no ambition to solve it in one shot, so …

We consider regular systems, one by one

Computational Complexity Problem (CCP)

[Revelent question: ***How easily can one improve the accuracy of computed answers?*****]**

Let Q and ε be the quantity of interest **in the thermodynamic limit (TL)** and its desired accuracy, respectively.

The numerical scheme is said to have CCP if the CPU time, t_Q ***, required to compute*** Q ***with accuracy*** ε ***diverges faster than any polynomial function of*** $\varepsilon^{-1} \to \infty$

The problem is considered to be solved if $\ln t_Q \propto \ln \varepsilon^{-1}$

Why thermodynamic limit? Because in finite size systems with $N = L^d$ particles the ultimate scaling of $t_Q(N)$ (if it can be reached in practice) is always subject to CLT with $t_Q(N) \propto \varepsilon^{-2}$

Diagrammatic MC

1. Use connected Feynman diagrams to express your answer directly in the **thermodynamic limit** as series of multi-dimensional integrals

2. Simulate the latter by Monte Carlo methods: $Q = \sum_{j=0}^{\infty} a_j g^j$ the expansion parameter

$$a_j = \iiint \underbrace{dX_1 dX_2 \mathrm{K}\; dX_j}_{\text{Internal variables}} \sum_{\text{£ =connected topologies, int. lines}} D(j, \text{£}\,; X_1, X_2 \mathrm{K}\; X_j)$$

Sing-problem does not apply here: no dependence on the particle number (therm. limit directly)

- Series convergence is only possible for fermions because different diagrams cancel each other = **sign blessing I**

- Fast summation of topologies with the help of determinants = **sign blessing II**

CCP and Diagrammatic MC

Define an approximation $Q_n = \sum_{j=0}^{n} a_j g^j$ **(truncated sum)**

For convergent series $\left|(Q - Q_n)/Q\right| \propto (g/g_C)^n$ **with** $g < g_C$ **, and accuracy** ε **is reached at**

$$n_\varepsilon \propto \ln \varepsilon / \ln(g/g_C)$$

All order-n contributions can be computed in time [R. Rossi PRL'17**]**

$$t_Q \propto e^{\# n_\varepsilon}$$

Talk by Michel Ferrero

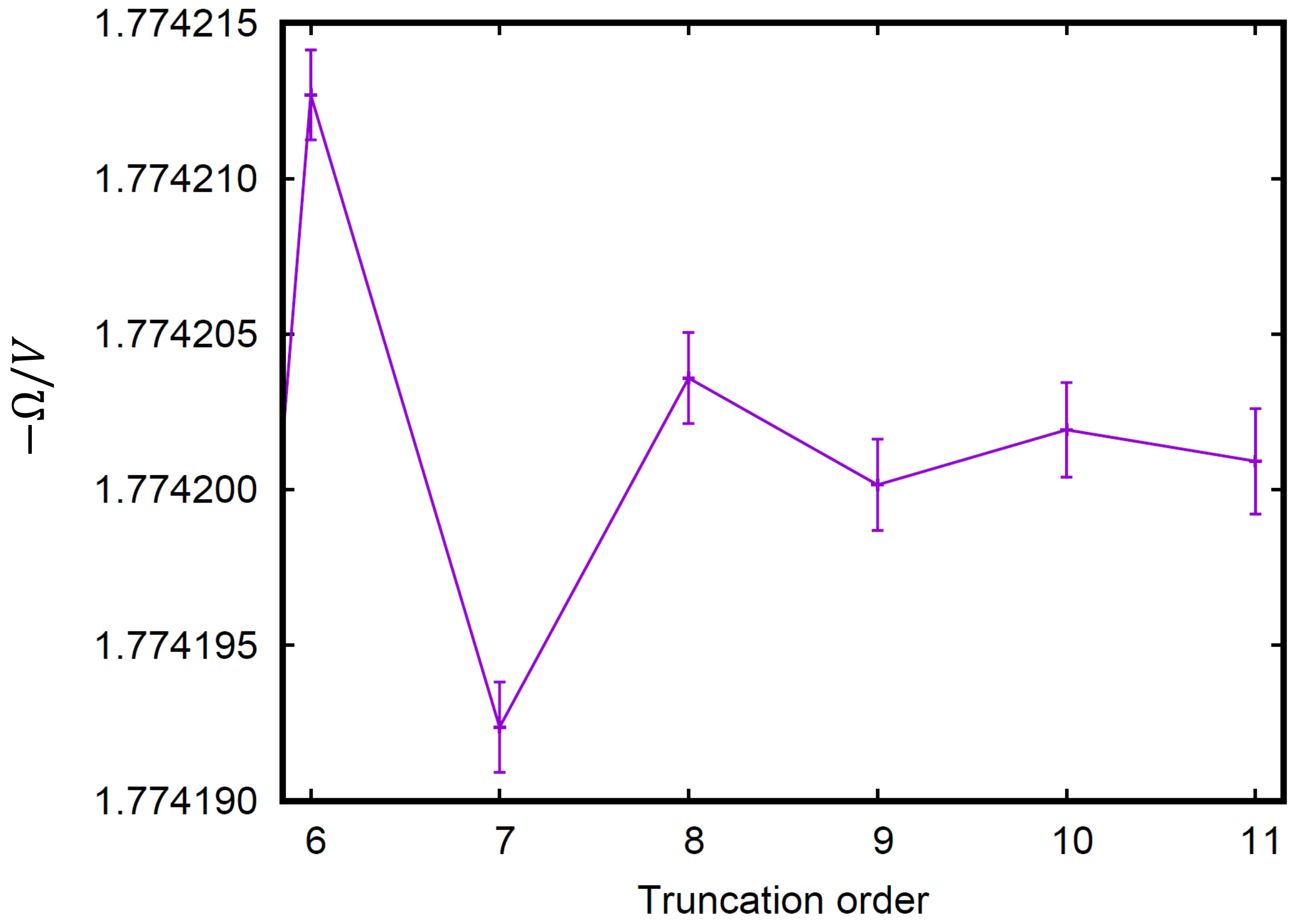
and CCP is solved: $\boxed{\ln t_Q \propto n_\varepsilon \propto \ln \varepsilon^{-1}}$

When series converge

2D Fermi-Hubbard model $H = -t \sum_{<ij>\sigma} \psi^{\dagger}_{j\sigma} \psi_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$

with $U/t = 2, \quad T/t = 0.125, \quad n = 0.87500(2)$

R. Rossi, PRL '17



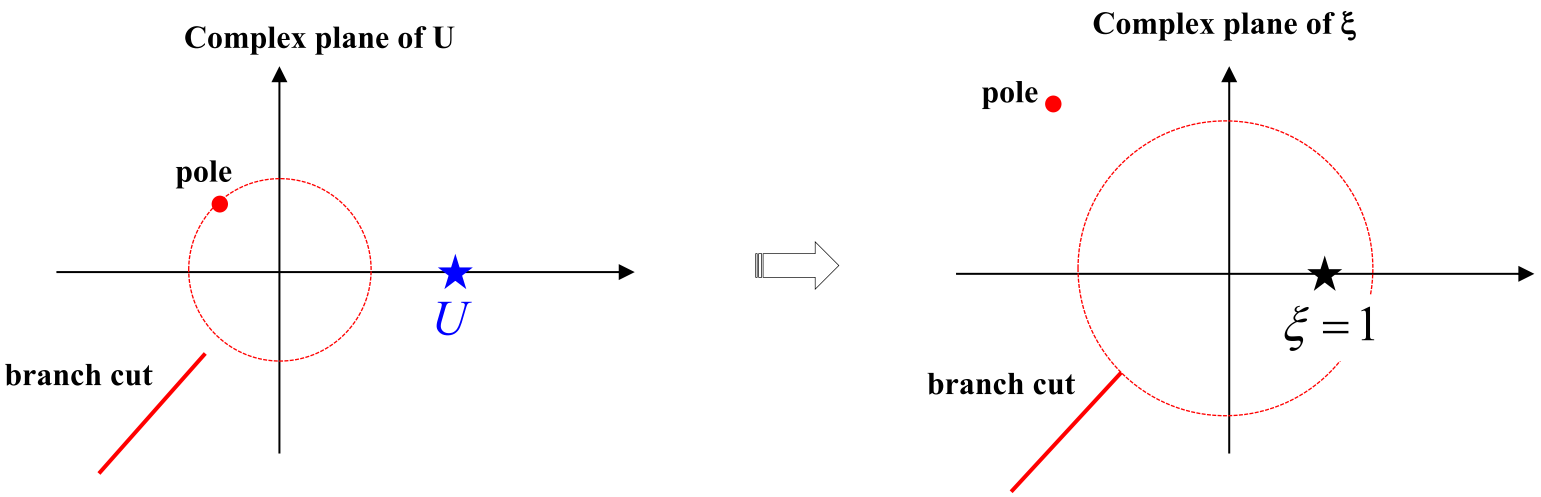
$E/N = 1.25992(6)$

Six to five digits (depending on quantity) accuracy for a finite-T answer away from n=1!

When series diverge or convergence is slow

Change the "origin of expansion" using shifted-action (renormalization) tools

R.Rossi, F. Werner, NP, and B. Svistunov, PRB '16



$$S[\psi] = \bar{\psi} G_0^{-1} \psi + S_{\text{int}}[\psi] \;\; \rightarrow \;\; S_\xi[\psi, \Lambda] = \bar{\psi} \tilde{G}_0^{-1} \psi + \bar{\psi}[\xi \Lambda_1 + \xi^2 \Lambda_2 + ..]\psi + \xi S_{\text{int}}[\psi]$$

Expand e^{-S_ξ} in powers of ξ

Equivalence of two setups:
One condition on any number of arbitrary functions $\;\; S_{\xi=1} = S \;$ if $\; \tilde{G}_0^{-1} + \sum_k \Lambda_k = G_0^{-1}$

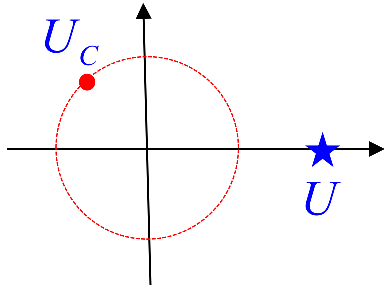
MF, DMFT, HF, GW, symmetry breaking, etc.

When series diverge or convergence is slow: past practice

Re-summation methods (for series with finite convergence radius)

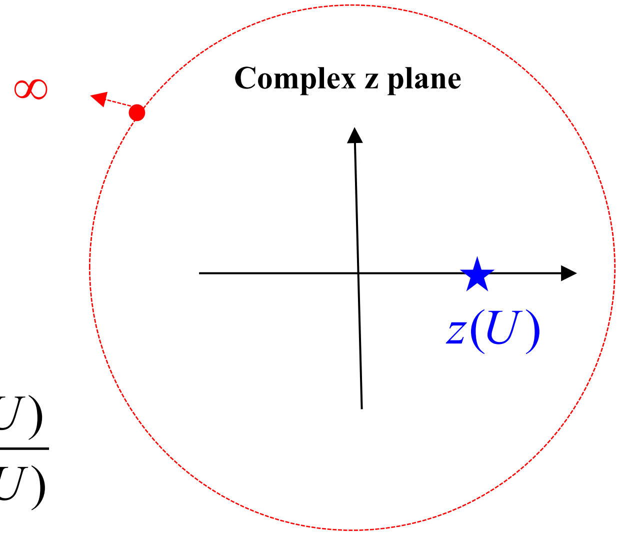
Complex U plane

Conformal mapping:

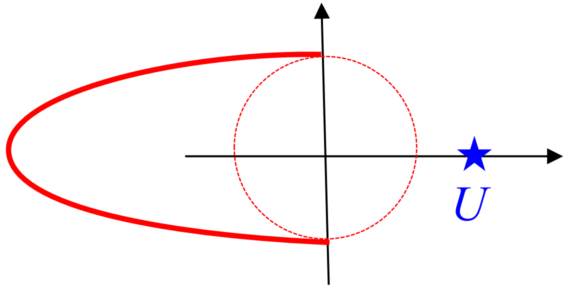


$$z = \frac{U}{U - U_C}$$

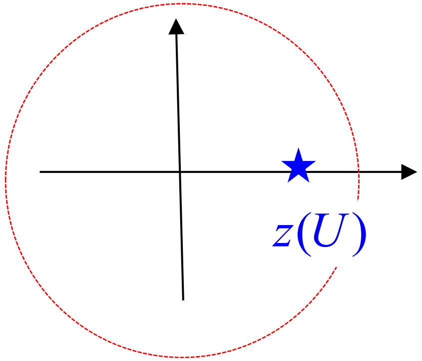
Complex z plane



Generalization = Pade $\quad z = \dfrac{P_k(U)}{P_m(U)}$



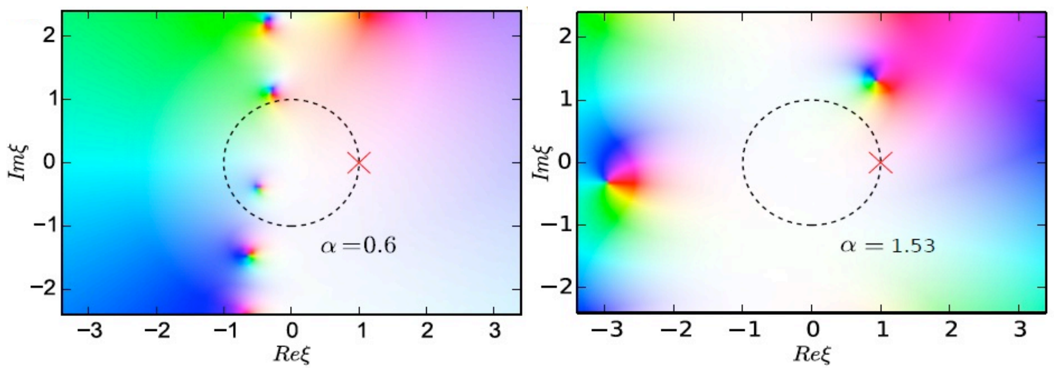
$$z = \frac{{}_pF_q(a,b,c,U)}{{}_sF_t(a',b',c',U)}$$



Hypergeometric functions

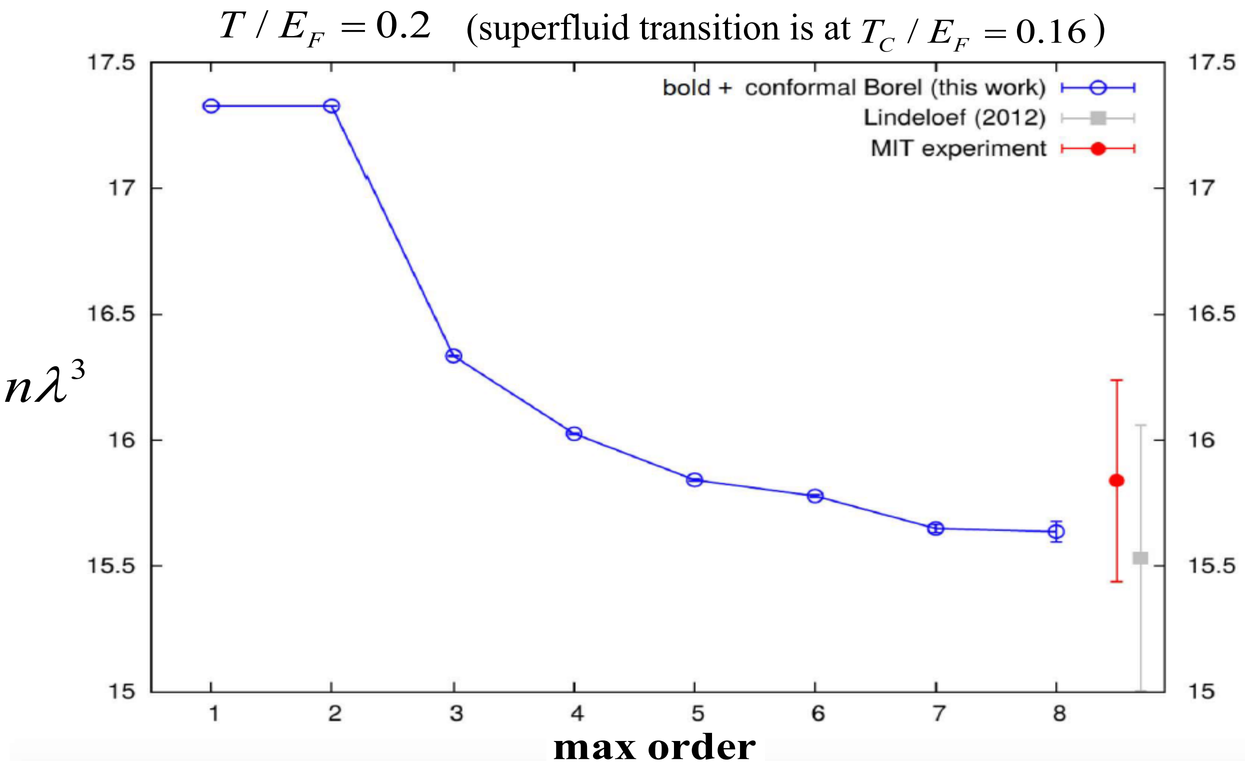
Borel, conformal Borel, Meijer-G, never-heard-of-method …

When series diverge or convergence is slow



This is how it works in practice for the Hubbard model

Talk by Michel Ferrero



and unitary Fermi gas (series with zero convergence radius)

R. Rossi, F. Werner, K. van Houcke '18

Homotopic action: when diagrammatic expansion converges (always!)

Homotopy: a continuous map from one function to another. What about many-body action?

$$S[\psi]=\bar{\psi}G_0^{-1}\psi \; + \; S_{\rm int}[\psi] \;\; \rightarrow \;\; S_\xi[\psi,\Lambda;\ldots]=\bar{\psi}\tilde{G}_0^{-1}\psi \; + \; \bar{\psi}\Lambda(\xi)\psi \; + \; S_{\rm int}[\psi,\xi] \; + \; \ldots$$

Hubbard-Stratonovich fields, if any

$\tilde{G}_0^{-1}$ **- design the best "starting point"**

$\Lambda(\xi)$ **- design to compensate for diagrams originating from** $S_{\rm int}[\psi,\xi]$

$S_{\rm int}[\psi,\xi]$ **- designe for best convergence**

The only restrictions are: $S_{\xi=1}\equiv S$

$\Lambda(\xi)$ **and** $S_{\rm int}[\psi,\xi]$ **can be expanded into Taylor series in** ξ **(convergent for** $\xi\le 1$)

$$S_\xi[\psi,\Lambda;\ldots]=\bar{\psi}\tilde{G}_0^{-1}\psi \; + \; \sum_{j=1}\xi^j\left\{\bar{\psi}\Lambda^{(j)}\psi + S_{\rm int}^{(j)}[\psi]\right\} \; + \; \ldots$$

Homotopic action: when diagrammatic expansion converges (always!)

$$S_\xi[\psi,\Lambda;\ldots]=\bar{\psi}G^{-1}\psi \;+\; \sum_{j=1}\xi^j\left\{\bar{\psi}\Lambda^{(j)}\psi+\,S_{\text{int}}^{(j)}[\psi]\right\}\;+\;\ldots$$

- includes all shifted action tools but is more flexible, transparent, intuitive, and easy to use

- “absorbs” resummation techniques – the series will converge automatically:

Suppose the series in powers of g for $S[\psi]=\bar{\psi}G_0^{-1}\psi \;+\; gS_{\text{int}}[\psi]$ diverge

Under conformal mapping, $g=f(\xi)=\sum_{k=1}c_k\xi^k$, the divergent series $\sum_{j=0}a_j g^j$ are transformed to convergent $\sum_{j=0}b_j\xi^j$ series

These series are automatically obtained by considering $S_\xi[\psi]=\bar{\psi}G^{-1}\psi \;+\; \sum_{j=1}\xi^j\underbrace{\frac{gc_j}{f(1)}S_{\text{int}}[\psi]}_{S_{\text{int}}^{(j)}[\psi]}$

Gains: reduced variance; iterative conformal maps without loss of accuracy

When we do not know yet what we do …

Shifted action with optimized perturbation theory[P. Stevenson '81] idea:

K. Chen & K. Haule, Nature communications '19

$$S[\psi]=\bar{\psi}G_0^{-1}\psi+S_{\text{int}}[\psi] \;\rightarrow\; \text{Hubbard-Stratanovich} \;\rightarrow\; S[\psi,\varphi]=\bar{\psi}G_0^{-1}\psi+\varphi^* D_0^{-1}\varphi+\varphi\bar{\psi}\psi$$

$$S[\psi,\varphi] \;\rightarrow\; S_\xi[\psi,\Lambda,\varphi,\Theta]$$

Final result must be independent of arbitrary shifts, so choose them such that

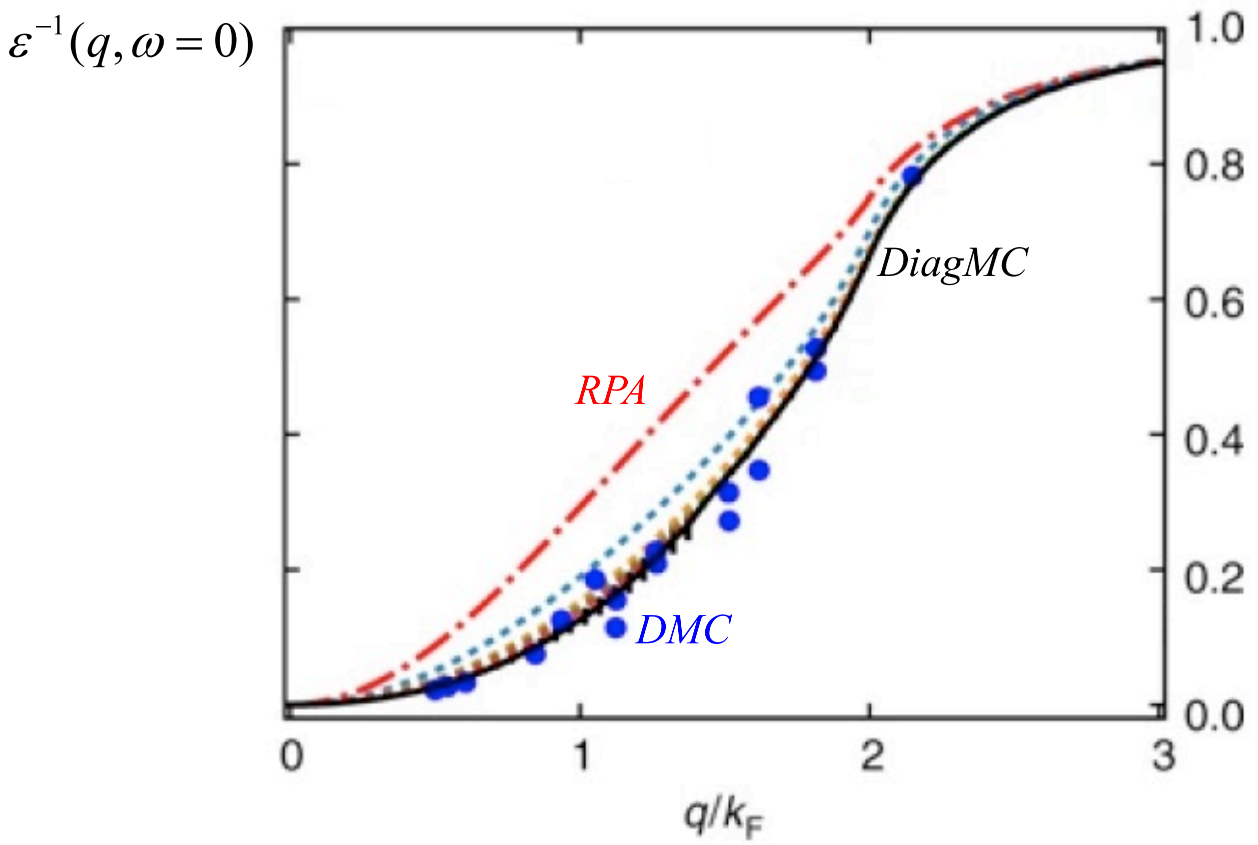
$$\partial Q_n/\partial\Lambda=0 \;\;,\;\; \partial Q_n/\partial\Theta=0$$

You loose Taylor series but convergence can be improved dramatically.

When we do not know yet what we do: jellium model

K. Chen & K. Haule, Nature communications ’19

$r_S = 4, \quad T / E_F = 0.04$



Interacting topological insulators: finite convergence radius even at T=0!

Kind of a trivial statement for a gapped system

Dirac fermions also have finite convergence radius!

(Fermi surface vs Fermi point)

Proved for graphene-type system

Alessandro Giuliani and Vieri Mastropietro '09

General Proof for interacting Weyl and Dirac semimetals

Johan Carlström and Emil J. Bergholtz '17

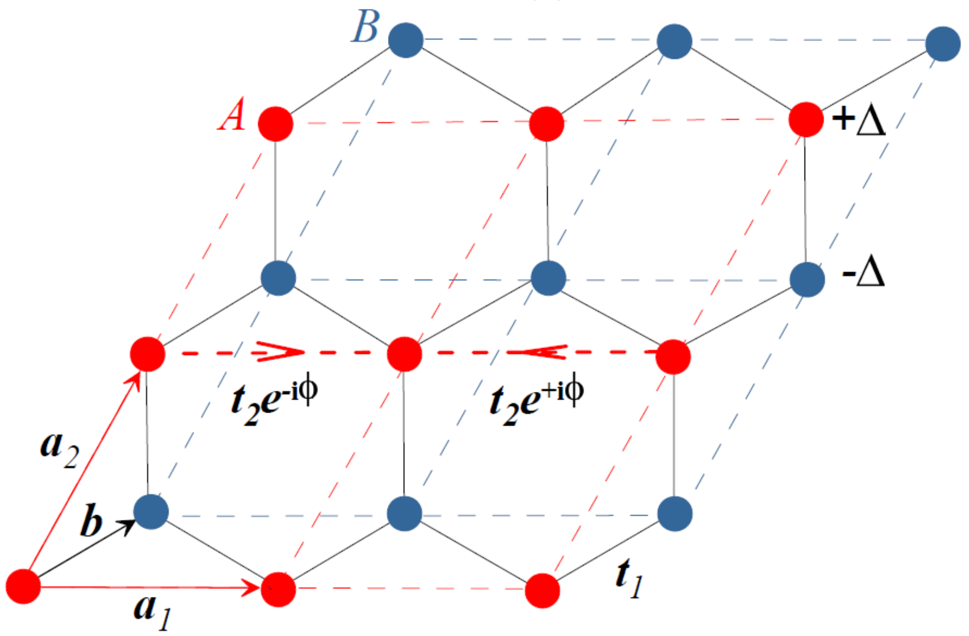
Haldane-Hubbard model

$$H_0 = -t_1 \sum_{<ij>\sigma} \left(a^\dagger_{i\sigma} b_{j\sigma} + h.c. \right) - \mu \sum_{i\sigma} n_{i\sigma}$$

$$-t_2 \sum_{<<kj>>\sigma} \left(e^{i\,\eta_{kj}\,\phi} (a^\dagger_{k\sigma} a_{j\sigma} + b^\dagger_{k\sigma} b_{j\sigma}) + h.c. \right)$$

$$+\Delta_{AB} \left(\sum_{i_A} n_{i_A} - \sum_{i_B} n_{i_B} \right)$$

(a)

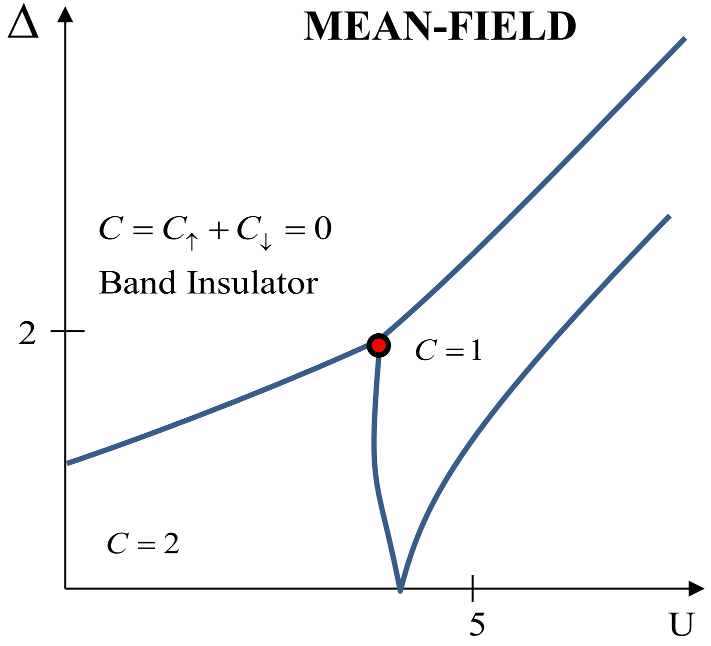


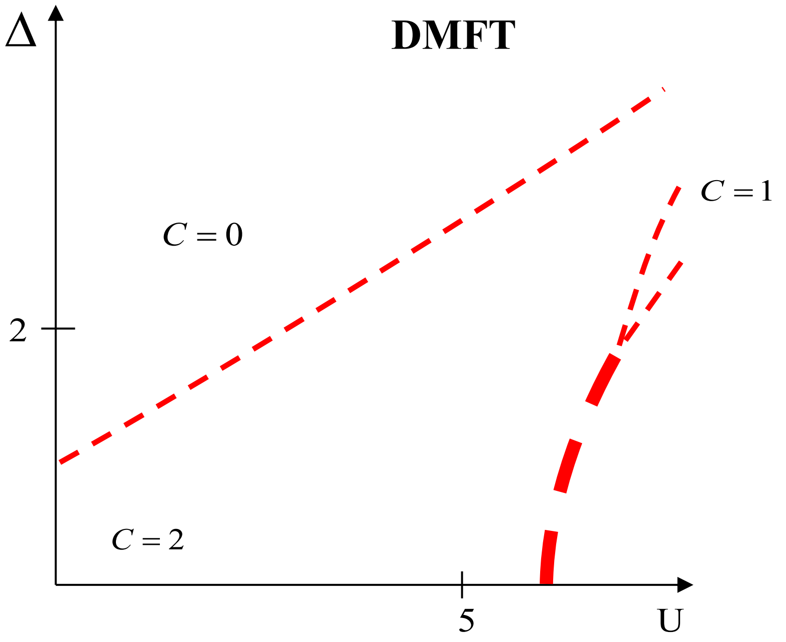
$\phi = \pi / 2$ (this talk)

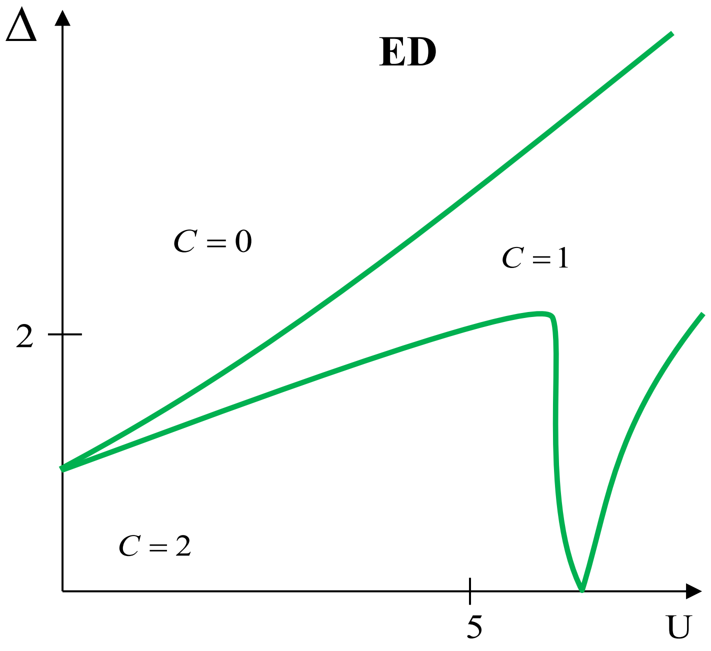
$$H_{\text{int}} = \frac{1}{2} \sum_{ij\sigma\sigma'} V_{\sigma\sigma'}(|\vec{r}_i - \vec{r}_j|) n_{i\sigma} n_{j\sigma'} \quad \rightarrow \quad \mathrm{U} \sum_i n_{i\uparrow} n_{i\downarrow}$$

T.I. Vanhala, T. Siro, L. Liang, M. Troyer, A. Harju, P. Torma '16 (for $t_2 = 0.2 t_1$)

T.I. Vanhala, T. Siro, L. Liang, M. Troyer, A. Harju, P. Torma ‘16





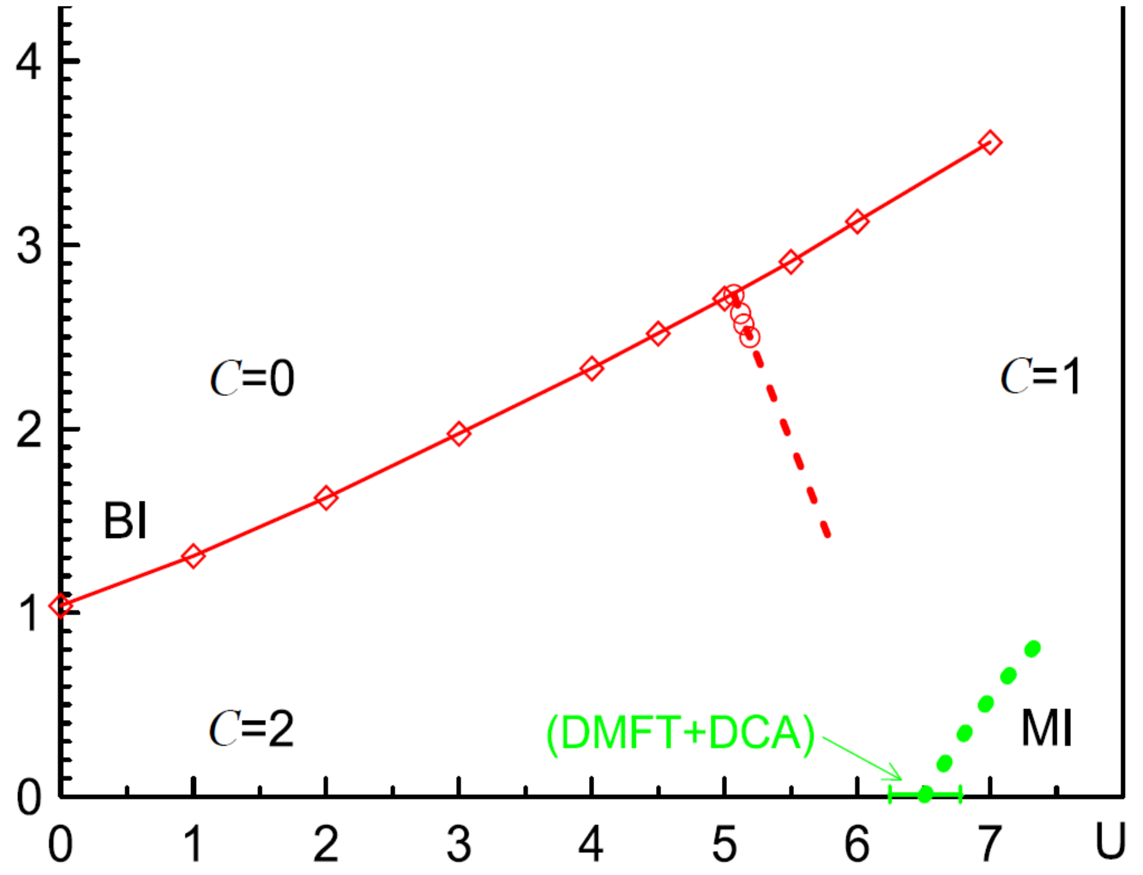


Some differences, even if only quantitative, are exceeding 300%

So, where is the junction point?

Skeleton DiagMC solution

(converged after 5-th order)



Conclusions:

Diagrammatic expansions for interacting fermions produce convergent results even in the strongly correlated regime – action design/optimization is vital!