

VARIATIONAL DIAGRAMMATIC MONTE CARLO METHOD TO SOLVE THE ELECTRONIC STRUCTURE PROBLEM

Inventor of VDMC:

Kun Chen



Funding:

Simons Collaboration on the
Many Electron Problem

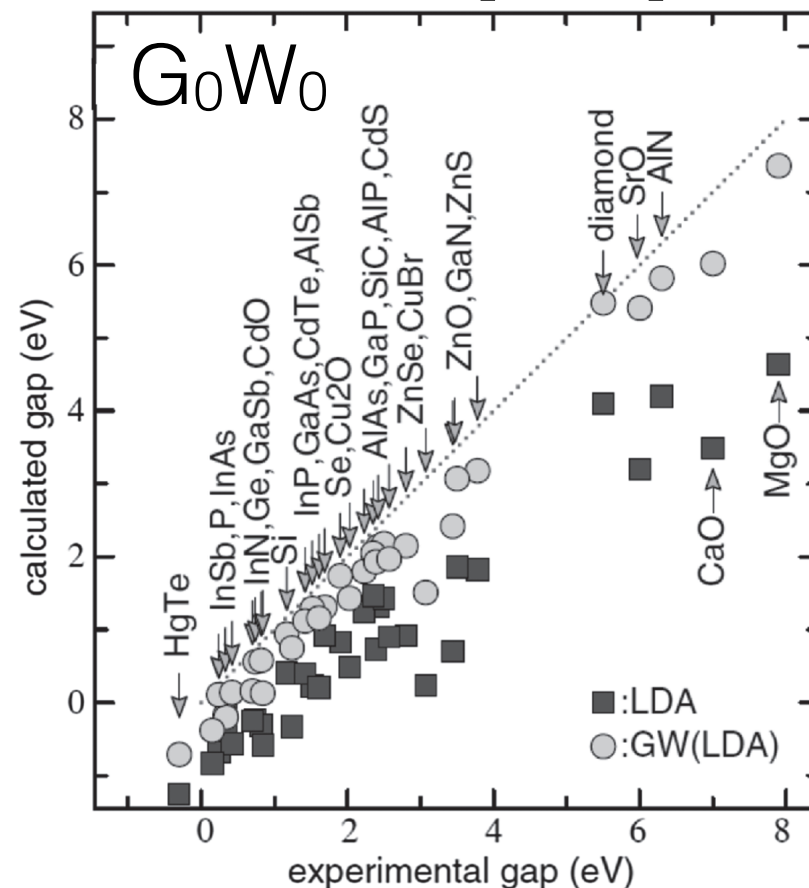
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Kristjan Haule



Material science: Are there any systematic methods?

- First order perturbation theory in the screened Coulomb interactions [GW] obtains very good gaps in semiconductors [Hedin].



from Richard Martin et.al., Interacting electrons

- While G_0W_0 comes close to experimental gaps in semiconductors, we do not know the error-bar of the calculation.
- In many metals and correlated solids DFT/GW fail, but we know only because of experiment.
- The self-consistent GW tends to produce way too large gaps as compared to experiment (need the estimation of error-bar).
- These methods are not BK conserving, and not functional derivable, and hence not stationary and robust with respect to small changes (discretization errors).

$$\Sigma = \text{---} \overset{W}{\text{---}} \overset{G_0}{\text{---}} \text{---}$$

$$W_q^{-1} = V_q^{-1} - \text{---} \overset{G_0}{\text{---}} \text{---}$$

There is a need to go beyond GW in a systematic way (estimating error-bar)

Systematic improvements beyond DMFT

DMFT is very successful, but extensions are very expansive or uncontrolled

A. Georges and G.Kotliar (1992)

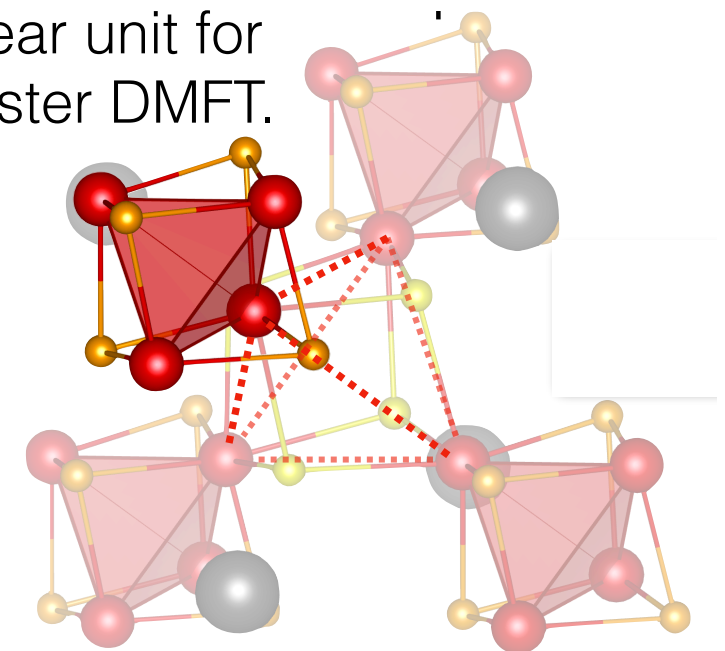
The controlled extension is the cluster-DMFT:

- Cellular DMFT (real space cluster) (Gabi Kotliar)
- DCA (momentum space cluster) (M. Jarrel, T. Mayer)

But complexity scales exponentially with cluster size.

Not clear how to treat long range Coulomb repulsion
(beyond boson bath approximation).

Clear unit for
cluster DMFT.



Also diagrammatic expansions beyond DMFT(see RMP **90**, 025003 (2018)):

- GW+DMFT
- D Γ A
- Trilex
- Quadrilex
- Dual Fermions
- Dual Bosons

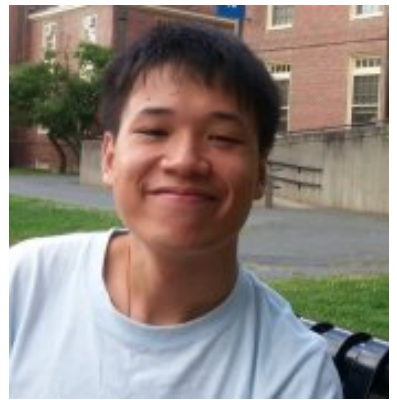
Complicated when extended beyond lowest order, i.e., require 6 leg vertex, 8 leg vertex (can not store such object).

Or uncontrolled (GW+DMFT, Trilex, Quadrilex)

Not clear how to treat long range Coulomb repulsion

Variational Diagrammatic Monte Carlo

Kun Chen & K. Haule, [arXiv:1809.04651](https://arxiv.org/abs/1809.04651)



Kun Chen

- *variational principle to determine best starting point* for perturbative expansion (such as screening by Yukawa form)
- leverage *sign blessing**: exact summation of diagrams that largely cancel (such as the conserving Baym-Kadanoff group of Hugenholtz diagrams)

* N. Prokof'ev, B. Svistunov, PRL 81, 2514 (1998)
N. Prokof'ev, B. Svistunov, PRB 77, 020408 (2008)

Alternative type of combining diagrams using determinants:

Riccardo Rossi, Rossi, PRL 119, 045701 (2017)

Variational Perturbation Theory

PHYSICAL REVIEW
LETTERS

Started with *Kleinert & Feynman*
Later improved by *Kleinert & Janke*

VOLUME 75

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NUMBER 15

Convergent Strong-Coupling Expansions from Divergent Weak-Coupling Perturbation Theory

W. Janke^{1,2} and H. Kleinert²

¹*Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany*

²*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany*

Anharmonic oscillator: $V(x) = \frac{1}{2}\omega^2 x^2 + gx^4$

Weak coupling series is diverging at small ω : $E_0 = \frac{\omega}{2} + g\frac{3}{4\omega^2} - g^2\frac{21}{8\omega^5} + g^3\frac{333}{16\omega^8} + \dots$

Rearrange perturbation: $V(x) = \frac{1}{2}\Omega^2 x^2 + \xi(gx^4 + \frac{1}{2}(\omega^2 - \Omega^2)x^2)$

Ω variational
parameter

counter-term

$\xi = 1$ set to unity at the end

Perform expansion: $E^{(1)}[\Omega], E^{(2)}[\Omega], \dots$

Principle of minimum sensitivity: $\frac{dE^n[\Omega]}{d\Omega} = 0 \rightarrow \Omega_{optimal}^n$

Final expansion: $E^{(1)}[\Omega_{optimal}^1], E^{(2)}[\Omega_{optimal}^2], \dots$

Variational Perturbation Theory

Check first order:

$$H = H_0 + \xi(gx^4 + \frac{1}{2}(\omega^2 - \Omega^2)x^2)$$

Expansion:

$$E^{(1)} = \langle \psi_0 | H | \psi_0 \rangle = \frac{\Omega}{2} + \xi \left(g \frac{3}{4\Omega^2} + \frac{1}{2} \frac{\omega^2 - \Omega^2}{2\Omega} \right) \xrightarrow{\xi=1} \frac{\Omega}{4} + \frac{1}{4} \frac{\omega^2}{\Omega} + g \frac{3}{4\Omega^2}$$

perturbative
correction

Notice $\omega = 0$ is fine.

Principle of minimum sensitivity: $\frac{dE^{(1)}}{d\Omega} = \frac{1}{4} - \frac{\omega^2}{4\Omega^2} - g \frac{3}{2\Omega^3} = 0$

$$\Omega^3 - \omega^2\Omega - 6g = 0$$

$$\text{At } \omega = 0 \quad \Omega_{optimal}^{(1)} = (6g)^{1/3}$$

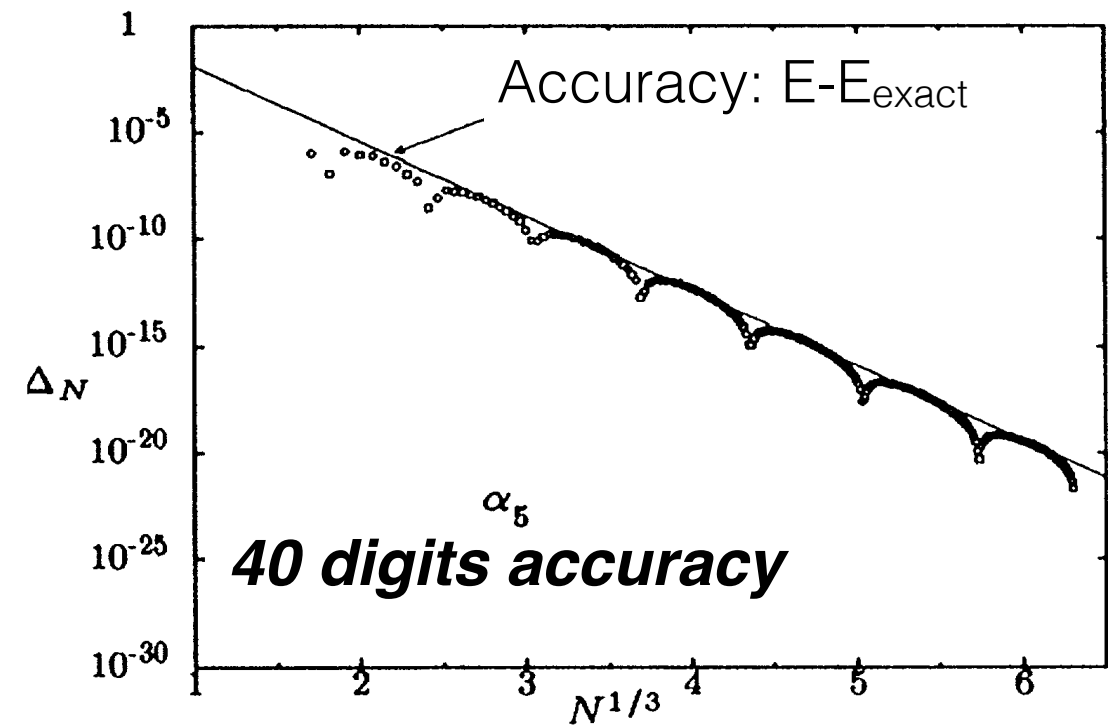
$$\text{Final first order: } E^{(1)}[\Omega_{optimal}^{(1)}] = g^{1/3} \frac{3}{8} 6^{1/3} \approx g^{1/3} 0.68142$$

$$\text{Exact result: } E^{exact} = g^{1/3} 0.66798$$

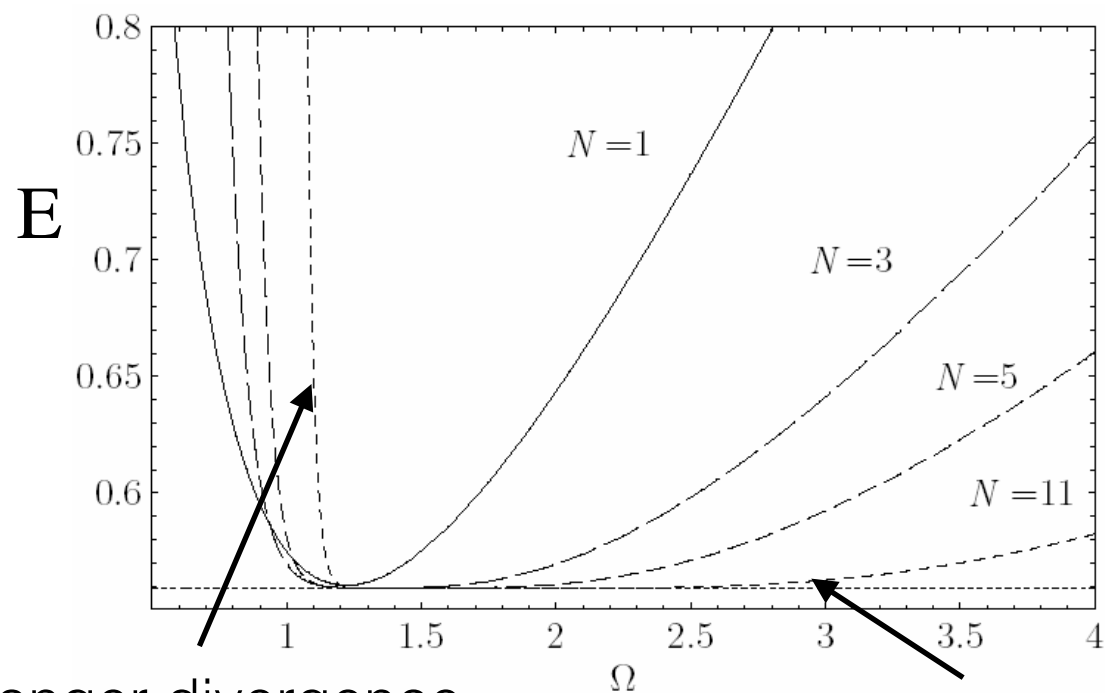
Turned diverging series into fast converging series

Variational Perturbation Theory

Higher order terms are well behaved
and rapidly converging

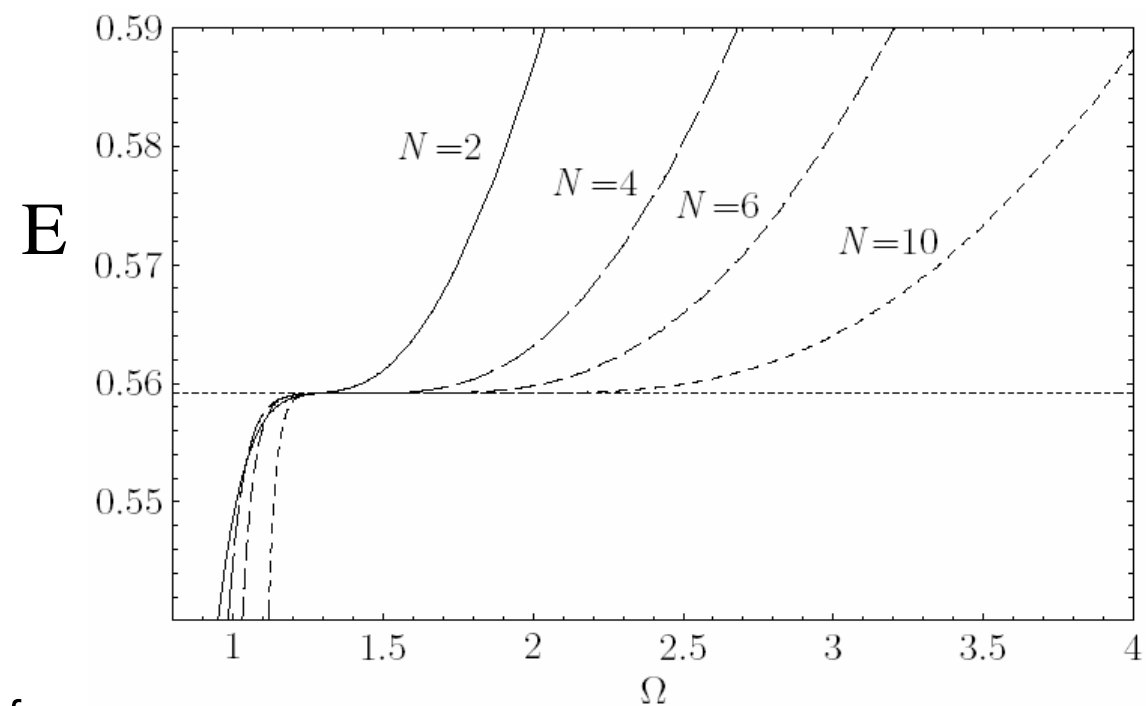


Even odd term optimization:



stronger divergence
at small w

larger plateau of
optimal value



Variational Diagrammatic Monte Carlo

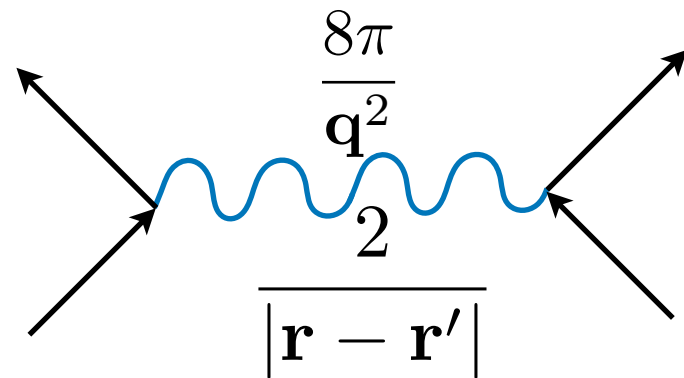
Lagrangian + counter-terms:

$$L = L_0 + \Delta L(\xi)$$

- 1) choose a good reference system (L_0), which allows for *emergent property*. We want to leverage the locality of correlations (*as known from success of LDA and DMFT*) to achieve fast convergence : screened short-range interaction in solids or DFT+DMFT solution the problem.
- 2) Optimize parameters in ΔL with principal of the minimal sensitivity, or renormalized condition. ΔL makes L exact, hence ΔL is not just the interaction, but more complicated Lagrangian with counter-terms.
- 3) Use *Diagrammatic Monte Carlo* to evaluate Feynman expansion to high order until convergence (use *sign blessed groups* to avoid sign problem)

Uniform Electron gas as testbed for method development

$$L = \sum_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma}^\dagger \left(\frac{\partial}{\partial \tau} - \mu - \frac{\hbar^2 \nabla^2}{2m} \right) \psi_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\mathbf{q} \neq 0} \rho_{\mathbf{q}} \frac{8\pi}{\mathbf{q}^2} \rho_{-\mathbf{q}} \quad \frac{2}{|\mathbf{r} - \mathbf{r}'|} \xrightarrow{\text{FT}} \frac{8\pi}{\mathbf{q}^2}$$



Coulomb interaction long ranged
bad sign problem for diagMC

with Hubbard-Stratonovich can be transformed to

$$L = \sum_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma}^\dagger \left(\frac{\partial}{\partial \tau} - \mu - \frac{\hbar^2 \nabla^2}{2m} \right) \psi_{\mathbf{k}\sigma} + \sum_{\mathbf{q} \neq 0} \Phi_{\mathbf{q}}^\dagger \frac{q^2}{8\pi} \Phi_{\mathbf{q}} + \frac{i}{\sqrt{2V}} \sum_{\mathbf{q} \neq 0} \rho_{\mathbf{q}} \Phi_{\mathbf{q}}^\dagger + \rho_{-\mathbf{q}} \Phi_{\mathbf{q}}$$

$\phi_{\mathbf{q}}(\mathbf{r})$

boson that mediates the interaction

$\psi_{\mathbf{k}\sigma}(\mathbf{r})$

electron operator

Uniform Electron gas, a testbed for method development

$$L = L_0 + \Delta L(\xi)$$

$$L_0 = \sum_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma}^\dagger \left(\frac{\partial}{\partial \tau} - \mu - \frac{\hbar^2 \nabla^2}{2m} \right) \psi_{\mathbf{k}\sigma} + \sum_{\mathbf{q} \neq 0} \Phi_{\mathbf{q}}^\dagger \frac{q^2}{8\pi} \Phi_{\mathbf{q}}$$

$$\Delta L = \frac{i}{\sqrt{2V}} \sum_{\mathbf{q} \neq 0} \rho_{\mathbf{q}} \Phi_{\mathbf{q}}^\dagger + \rho_{-\mathbf{q}} \Phi_{\mathbf{q}}$$

$$\phi_{\mathbf{q}}(\mathbf{r})$$

boson that mediates the interaction

$$\psi_{\mathbf{k}\sigma}(\mathbf{r})$$

electron operator

VDMC for electron gas



Kun Chen

$$L = L_0 + \Delta L(\xi)$$

$$L_0 = \sum_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma}^\dagger \left(\frac{\partial}{\partial \tau} - \mu - \frac{\hbar^2 \nabla^2}{2m} + v_{\mathbf{k}}(\xi = 1) \right) \psi_{\mathbf{k}\sigma} + \sum_{\mathbf{q} \neq 0} \Phi_{\mathbf{q}}^\dagger \frac{q^2 + \lambda_{\mathbf{q}}}{8\pi} \Phi_{\mathbf{q}}$$

$$\Delta L = - \sum_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma}^\dagger v_{\mathbf{k}}(\xi) \psi_{\mathbf{k}\sigma} - \xi \sum_{\mathbf{q} \neq 0} \Phi_{\mathbf{q}}^\dagger \frac{\lambda_{\mathbf{q}}}{8\pi} \Phi_{\mathbf{q}} + \sqrt{\xi} \frac{i}{\sqrt{2V}} \sum_{\mathbf{q} \neq 0} \rho_{\mathbf{q}} \Phi_{\mathbf{q}}^\dagger + \rho_{-\mathbf{q}} \Phi_{\mathbf{q}}$$

$$\phi_{\mathbf{q}}(\mathbf{r})$$

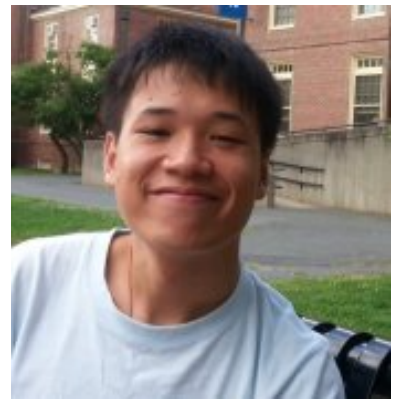
boson that mediates the interaction

$$\psi_{\mathbf{k}\sigma}(\mathbf{r})$$

electron operator

original problem at
 $\xi = 1$.

VDMC for electron gas



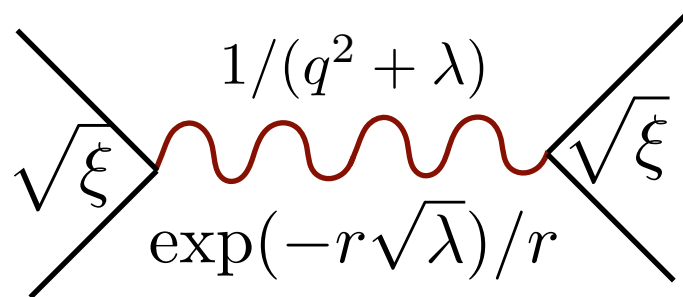
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$$L = L_0 + \Delta L(\xi)$$

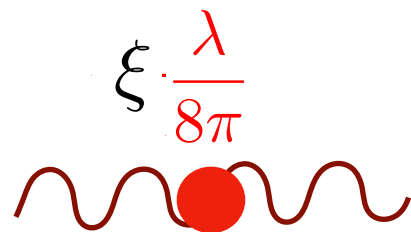
$$L_0 = \sum_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma}^\dagger \left(\frac{\partial}{\partial \tau} - \mu - \frac{\hbar^2 \nabla^2}{2m} + v_{\mathbf{k}}(\xi = 1) \right) \psi_{\mathbf{k}\sigma} + \sum_{\mathbf{q} \neq 0} \Phi_{\mathbf{q}}^\dagger \frac{q^2 + \lambda_{\mathbf{q}}}{8\pi} \Phi_{\mathbf{q}}$$

$$\Delta L = - \sum_{\mathbf{k}\sigma} \psi_{\mathbf{k}\sigma}^\dagger v_{\mathbf{k}}(\xi) \psi_{\mathbf{k}\sigma} - \xi \sum_{\mathbf{q} \neq 0} \Phi_{\mathbf{q}}^\dagger \frac{\lambda_{\mathbf{q}}}{8\pi} \Phi_{\mathbf{q}} + \sqrt{\xi} \frac{i}{\sqrt{2V}} \sum_{\mathbf{q} \neq 0} \rho_{\mathbf{q}} \Phi_{\mathbf{q}}^\dagger + \rho_{-\mathbf{q}} \Phi_{\mathbf{q}}$$

original problem at $\xi = 1$.



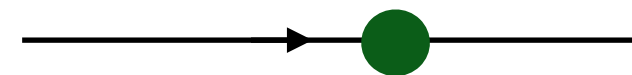
Coulomb interaction



Counter terms make sure that we get the exact answer at large order for any λ

$$G_{\mathbf{k}}^0(i\omega) = \frac{1}{i\omega + \mu - \frac{k^2}{2m} - v_{\mathbf{k}}}$$

electron propagator is optimized
(DFT KS-potential or DMFT self-energy, etc)



Counter-term makes sure that the exact answer is obtained for any $v_{\mathbf{k}}$ at large p.o.

What did we achieve?

$$\frac{1}{q^2 + \lambda}$$
$$\sqrt{\xi}$$
$$\exp(-r\sqrt{\lambda})/r$$

Coulomb is static
and short ranged with counter-term.

$$G_{\mathbf{k}}^0(i\omega) = \frac{1}{i\omega + \mu - \frac{k^2}{2m} - v_{\mathbf{k}}}$$

Electron propagator has “optimized
potential” (DFT-KS or DMFT self-energy)
+counter-term

Advantages:

- No need to deal with dynamic screening effects.
- No need to deal with long range Coulomb repulsion ("mother nature is usually local")
- Screening by λ regularizes the weight of Feynman diagrams at small q , and considerably improves the DiagMC efficiency
- We can start with “the best” single particle propagator (DFT,DMFT,..)

Open questions:

- How to determine parameters λ and $v_{\mathbf{k}}$

Single particle potential

For UEG $v_{\mathbf{k}}$ is chosen so that zero-th order is the screened Hartree-Fock, and we preserve Luttinger's theorem in G_0 and G at each order

$$v_{\mathbf{k}}(\xi) = \xi \Sigma_{\mathbf{k}}^x + \sum_{n=1}^{\infty} \xi^n \Delta\mu^{(n)}$$

where $\Delta\mu^{(n)}$ are numbers which take care of the shift of the chemical potential due to interaction

In solids, a better choice is probably:

$$v_{\mathbf{k}}(\xi = 1) = v_{LDA}^{KS} + \Delta\mu$$

$$v_{\mathbf{k}}(\xi = 1) = \Sigma_{LDA+DMFT} + \Delta\mu$$

For DMFT, expansion in powers of interaction exist, which can be used to expand the counter-term:

$$v_{\mathbf{k}}(\xi) = \sum_{n=1}^{\infty} \xi^n (\Sigma_{LDA+DMFT}^{(n)} + \Delta\mu^{(n)})$$

where $\Sigma_{LDA+DMFT} = \sum_{n=1}^{\infty} \Sigma_{LDA+DMFT}^{(n)}$

$$\xrightarrow{G^{LDA+DMFT}(\mathbf{k}, \omega)}$$

$$\xrightarrow{\xi^n (\Sigma_{LDA+DMFT}^{(n)} + \Delta\mu^{(n)})}$$


Screening length

Average perturbation order: $\langle N \rangle = \text{Tr}(\lambda W_{\mathbf{q}}) = \frac{\lambda}{q^2/(8\pi) - \tilde{\Pi}_{\mathbf{q}}} < \frac{\lambda}{-\tilde{\Pi}_{\mathbf{q}=0, \omega=0}}$

Possible choices for λ :

1) $\lambda = -\tilde{\Pi}_{\mathbf{q}=0, \omega=0}$

Makes sure that average p. order < 1
renormalized condition,
borrowed from renormalized perturbation theory

2) $\frac{\lambda}{8\pi} = -\tilde{\Pi}_{\mathbf{q}=0, \omega=0}^{N=1}$

Exact cancelation of bubbles+c.t. at low energy
i.e., self-consistent determination of screening

3) $\frac{d\tilde{\Pi}_{\mathbf{q}\omega=0}}{d\lambda} = 0 \rightarrow \lambda$

The principle of smallest sensitivity.
(borrowed from variational perturbation theory)

- 1) Poor convergence and rapid oscillations with orders (approx. 5-times too small)
- 2) To converge we need to go to order $25=8\pi$! (approx. 5 times too large)
- 3) The best choice is due to variational perturbation theory, i.e., still quite small perturbation order, but quite monotonic convergence to exact answer.

Example: expansion for polarization



Kun Chen

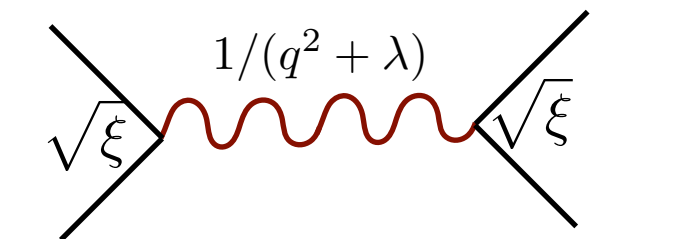
First order is the standard RPA:

$$W_{\mathbf{q}} = (v_{\mathbf{q}}^{-1} - \Pi_{\mathbf{q}})^{-1} = \left(\frac{q^2 + \lambda}{8\pi} - \xi \frac{\lambda}{8\pi} - \xi P_{\mathbf{q}}^0 - O(\xi^2) \dots \right)^{-1}$$

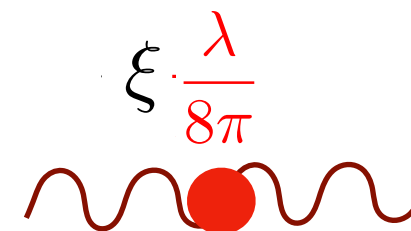
$$P = \text{[Diagram: bubble with shaded rectangle]} = \xi \text{[Diagram: empty bubble]}$$

Screened RPA

$$\begin{aligned}
 &+ \xi^2 (\text{[Diagram: bubble with vertical wavy line]} + \text{[Diagram: bubble with horizontal wavy line]} + \text{[Diagram: bubble with green dot]} \dots) + \quad \text{2n order correction} \\
 &+ \xi^3 (\text{[Diagram: bubble with internal loop]} + \text{[Diagram: bubble with two wavy lines]} + \text{[Diagram: bubble with red dot]} \dots) + \dots \quad \text{3rd order correction}
 \end{aligned}$$

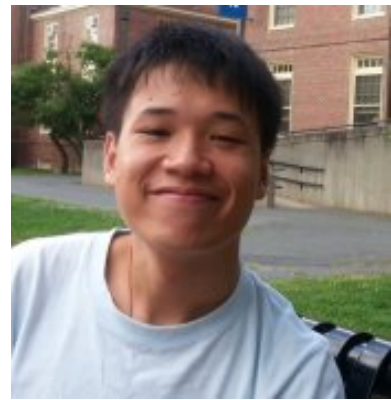


$$G_{\mathbf{k}}^0(i\omega) = \frac{1}{i\omega + \mu - \frac{k^2}{2m} - v_{\mathbf{k}}}$$



$$v_{\mathbf{k}}(\xi) = \xi(\Sigma_{\mathbf{k}}^x - \Sigma_{k_F}^x) + \xi^2 s_2 + \xi^3 s_3 + \dots$$

From sign problem to sign blessing



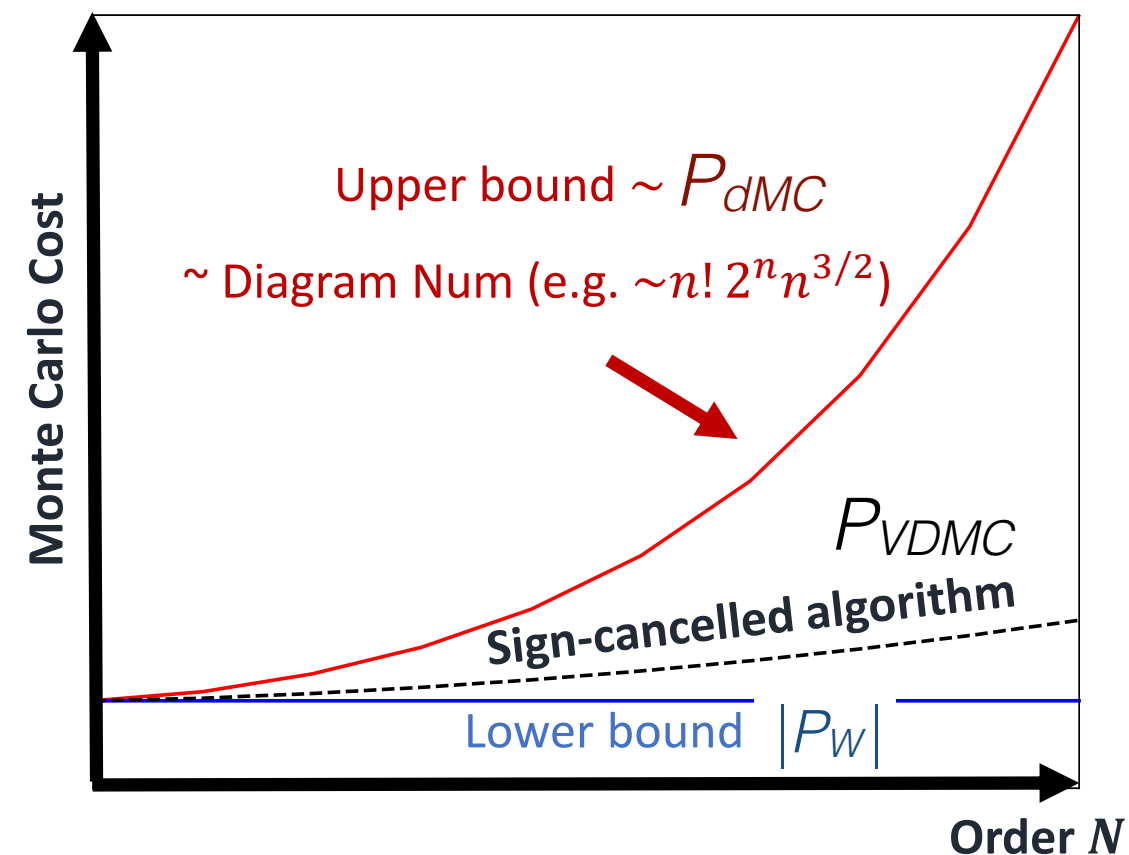
We want to calculate $\int [dx]^N \sum_{diag} W_{diag} \ll \int [dx]^N \sum_{diag} |W_{diag}|$

sign problem in MC!

Physical weight: $|P_W| = \left| \int [dx]^N \sum_{diag} W_{diag} \right|$

Weight in diagMC: $P_{dMC} = \int [dx]^N \sum_{diag} |W_{diag}|$

Weight in VDMC: $P_{VDMC} = \int [dx]^N \left| \sum_{diag} W_{diag} \right|$



Important observation: VDMC weight strongly depends on the internal variable arrangement:

in MC: $\int_{-1}^1 \int_{-1}^1 (w_1(k_1, k_2) + w_2(k_1, k_2)) dk_1 dk_2 \neq \int_{-1}^1 \int_{-1}^1 (w_1(k_1, k_2) + w_2(k_2, k_1)) dk_1 dk_2$

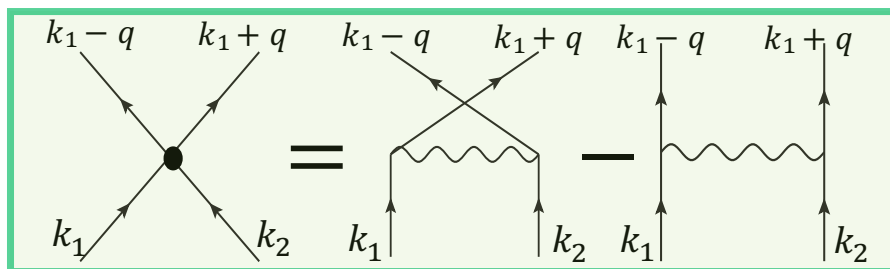
From sign problem to sign blessing

How to group diagrams to sign-blessed groups?

Symmetry preserved in each group:

Crossing symmetry, spin rotational symmetry,...

At the lowest order leads to “Hugenholtz diagrams”



Ward identity (each MC step is conserving):

Baym-Kadanoff algorithm is used to construct groups of diagrams with consistent internal variables (preserve particle number, energy, momentum **in each MC step**).

$$S[\psi^\dagger, \psi; U] = S[\psi^\dagger, \psi] - \int d1d2 \psi^\dagger(1)U(1,2)\psi(2)$$

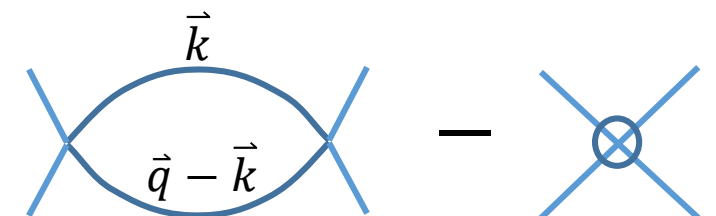
$$Z[U] = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^\dagger, \psi; U]}$$

$$G(1, 1') = \left. \frac{\delta \ln Z[U]}{\delta U(1', 1)} \right|_{U \rightarrow 0}$$

$$\chi(1, 2) = \left. \frac{\delta G(2, 2^+; U)}{\delta U(1^+, 1)} \right|_{U \rightarrow 0}$$

Vertex renormalization:

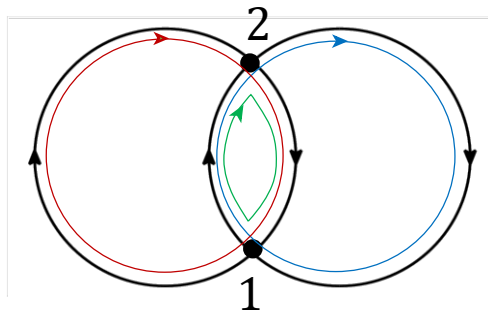
Make sure to combine diagram with the corresponding counter-term that cancels the high-energy contributions



Example of 3rd order polarization diagrams

Step 1:

Start with Hugenholtz diagram for the free energy functional $\log Z$. Choose momentum loops (shortest path) and time indices.

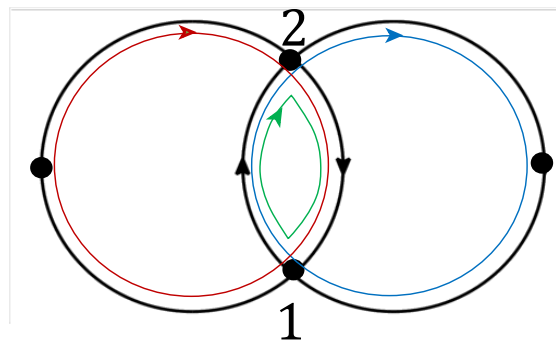


Step 2:

Attach two external vertices in all possible ways

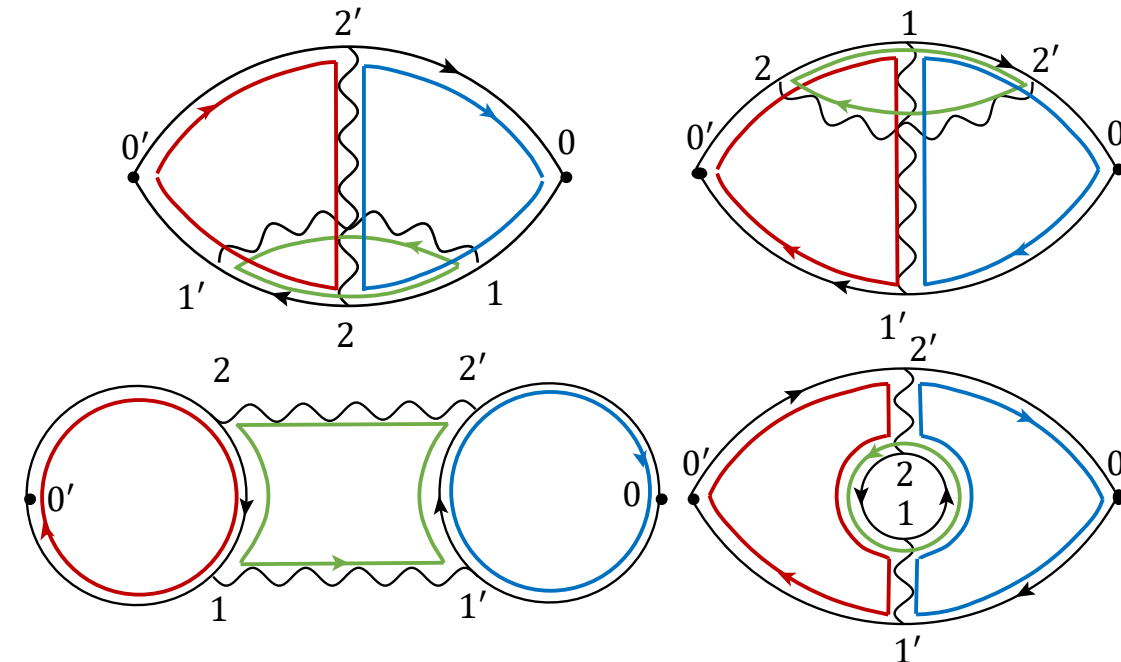
$$\frac{\delta^2 \log Z}{\delta U^2}$$

(creates a Baym-Kadanoff conserving group)

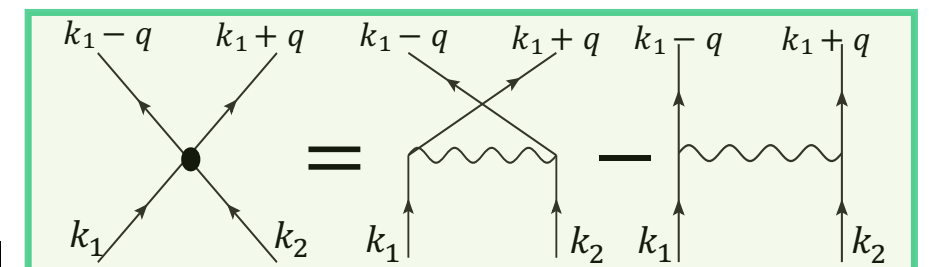


Step 3:

Expand each vertex in Hugenholtz diagrams, to generate normal Feynman diagrams. Keep all momenta and time indices equal to those in $\log Z$ diagram.



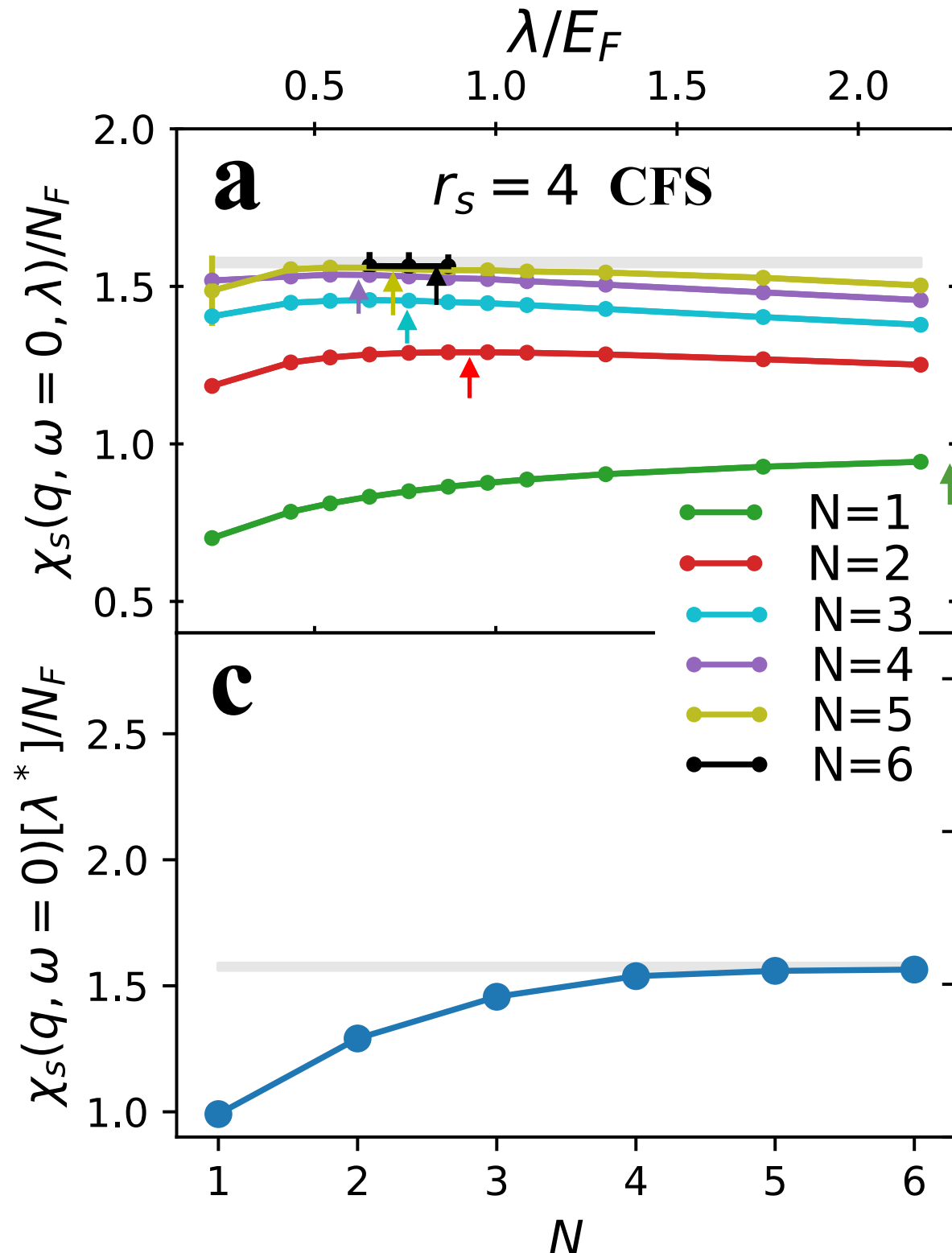
Notice that 2^N diagrams are evaluated at once by Hugenholtz trick : $GGG (V_1 - V_2) (V_1 - V_2) \dots$



Spin-susceptibility at $r_s=4$ ($\frac{1}{n} = \frac{4\pi r_s^3}{3}$)

spin susceptibility at $q=0, \omega=0$

see: Feynman & Kleinert, PRA 34, 5080 (1986)



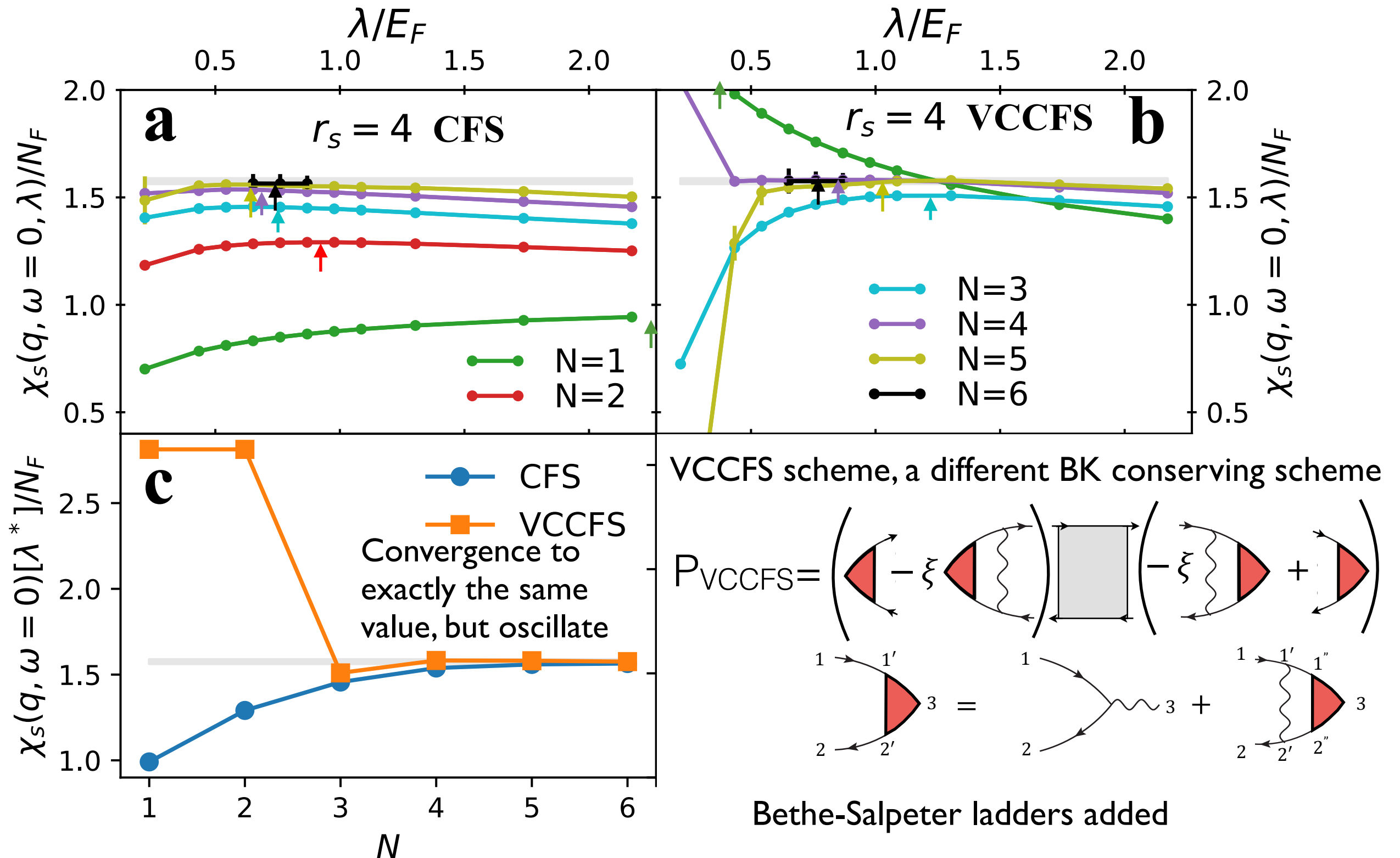
Scan in λ reveals the speed of convergence.

broad plateau in λ at large order $\Rightarrow$ converged value in the plateau.

Values at the optimum (principle of minimal sensitivity) converge very fast

Spin-susceptibility at $r_s=4$ ($\frac{1}{n} = \frac{4\pi r_s^3}{3}$)

spin susceptibility at $q=0, \omega=0$



Spin-susceptibility at $r_s=4$ ($\frac{1}{n} = \frac{4\pi r_s^3}{3}$)

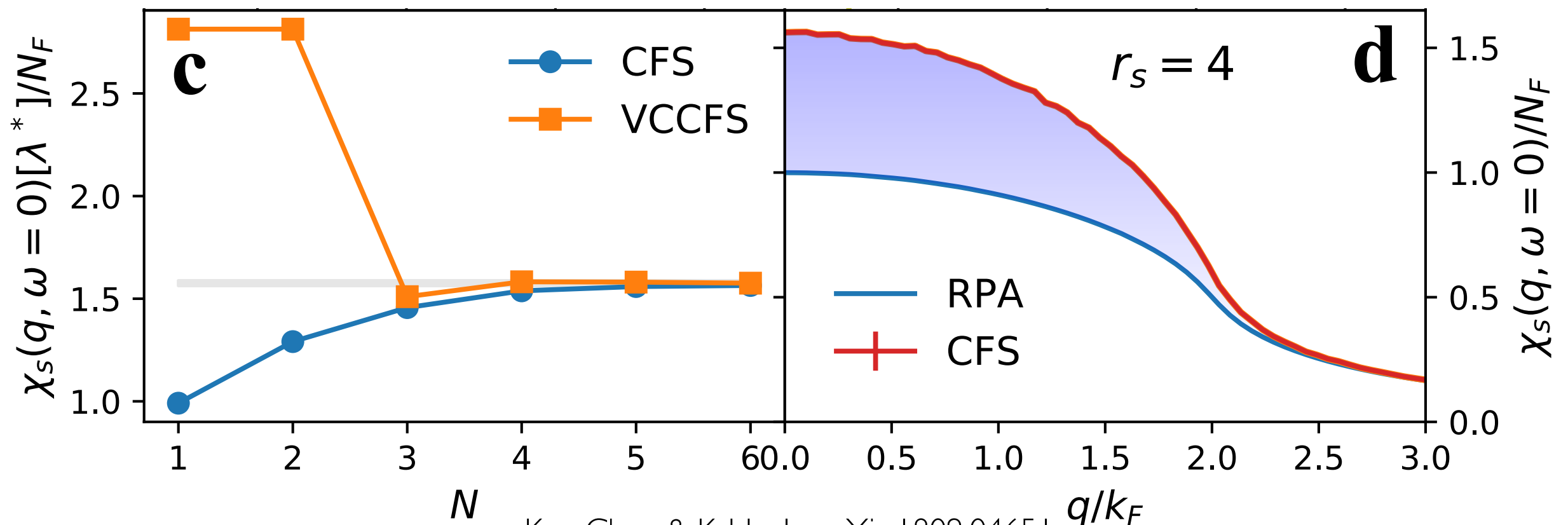
Calculated values at different densities.

VDMC get four significant digits at order $N=6$.

Consistent with literature, but significantly more precise.

r_s	χ_s/N_F	literature
1	1.152(2)	1.15-1.16
2	1.296(6)	1.27-1.31
3	1.438(9)	1.39-1.46
4	1.576(9)	1.51-1.62

spin susceptibility for different momenta.
RPA 57% underestimates.



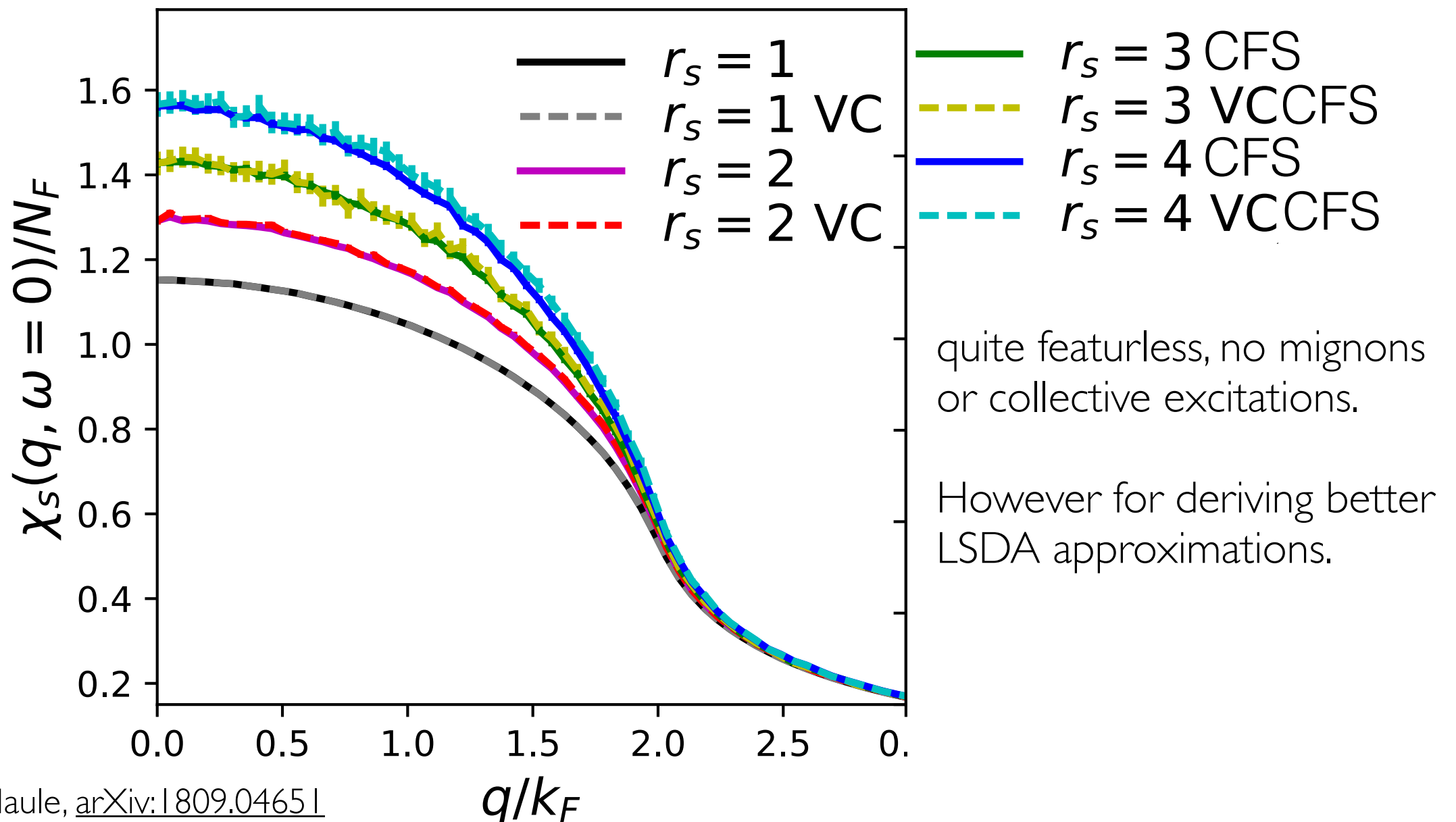
Spin-susceptibility

Spin susceptibility with and without vertex are almost indistinguishable at order N=6. Converged result for all momenta (at zero frequency)

dashed : vertex corrected

full line: without vertex corrections

RPA=1, is very wrong

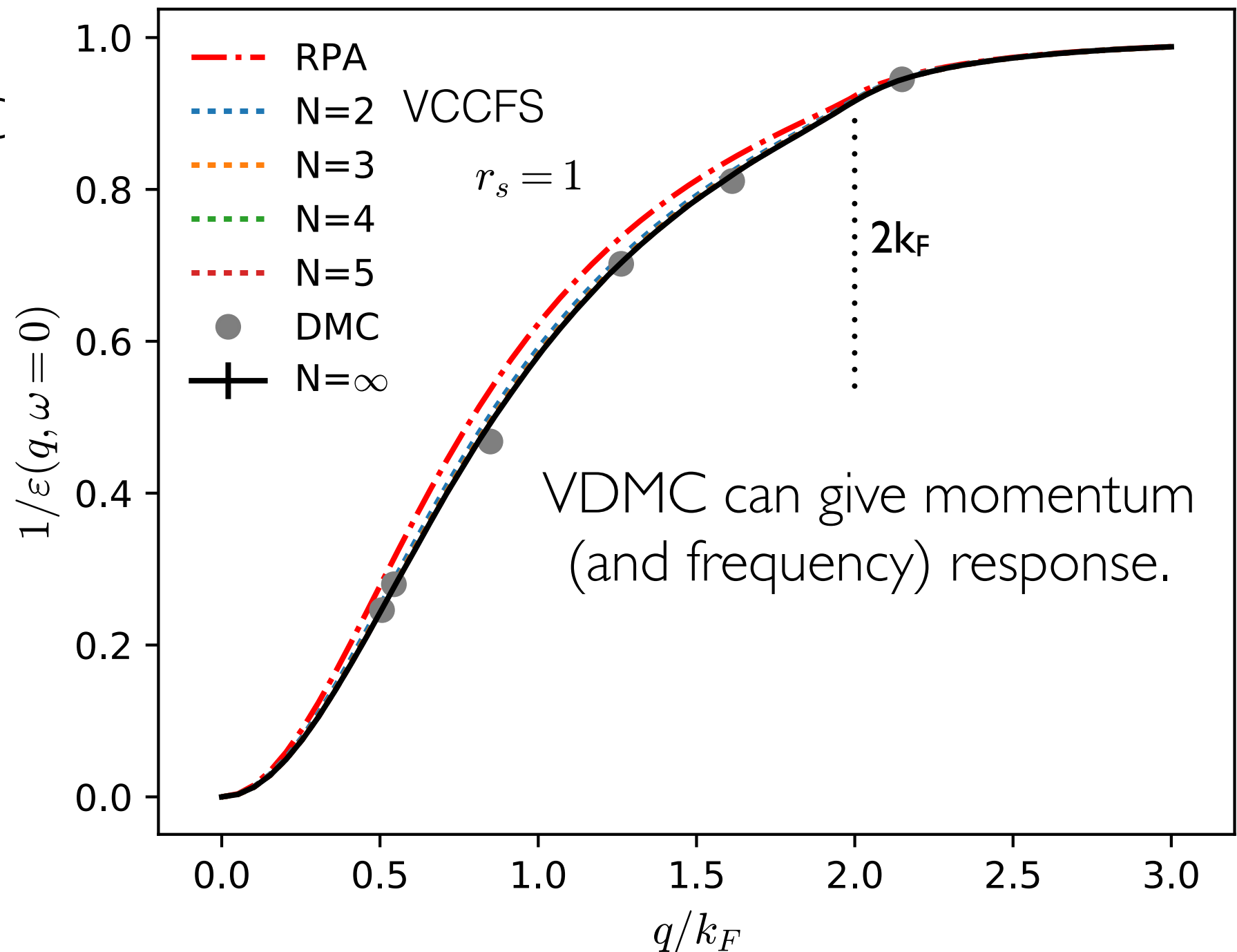


dielectric constant-direct comparison to DMC

Momentum dependence
challenging for DMC
because they treat
finite system.

Can beat DMC
at moderate r_s

DMC: B.J.Alder, PRB
50, 14838 (1994)



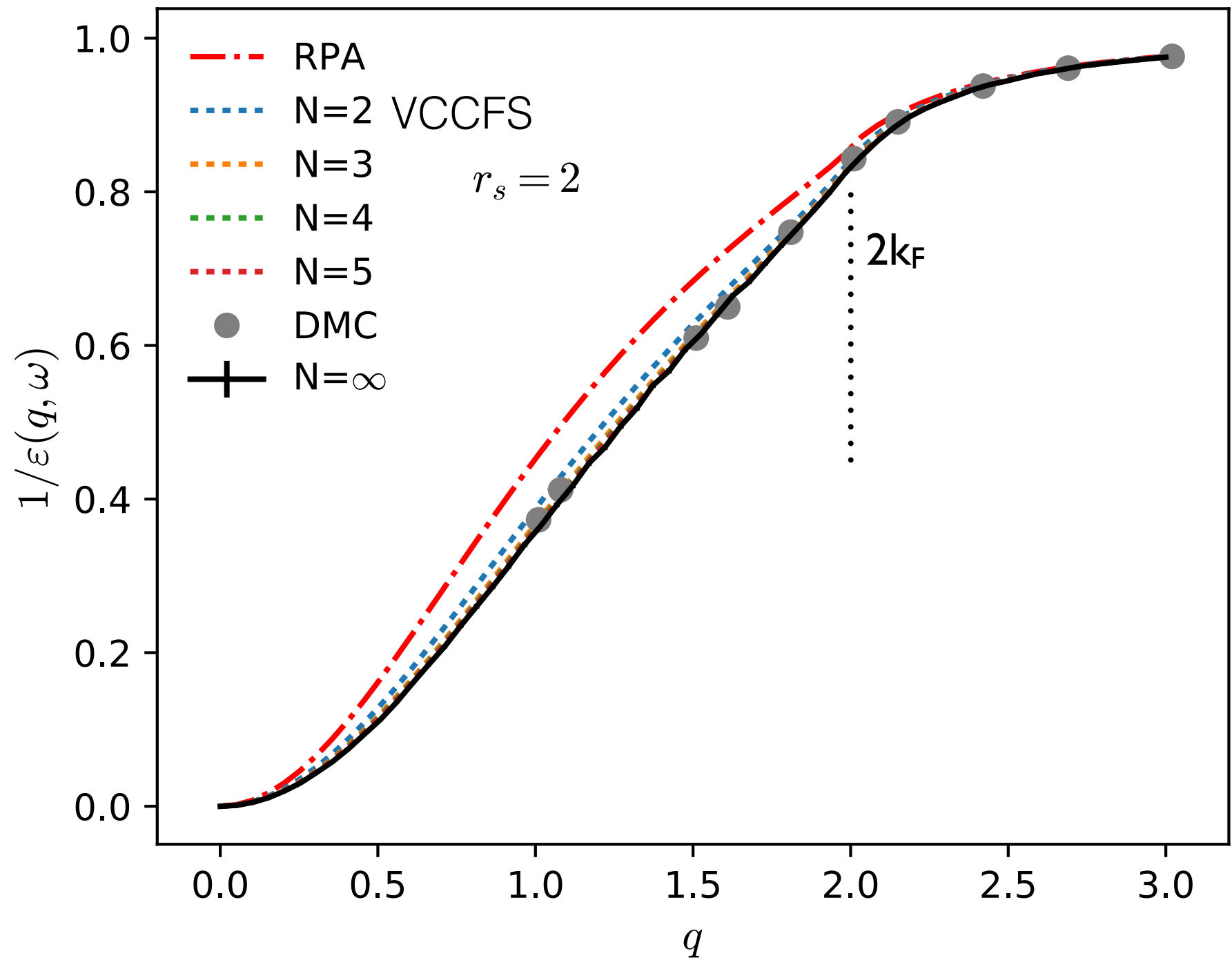
Charge response $r_s=2$

New result superior
to DMC.

VDMC can give full
momentum and
frequency response.

DMC only $\omega=0$ or $t=0$.

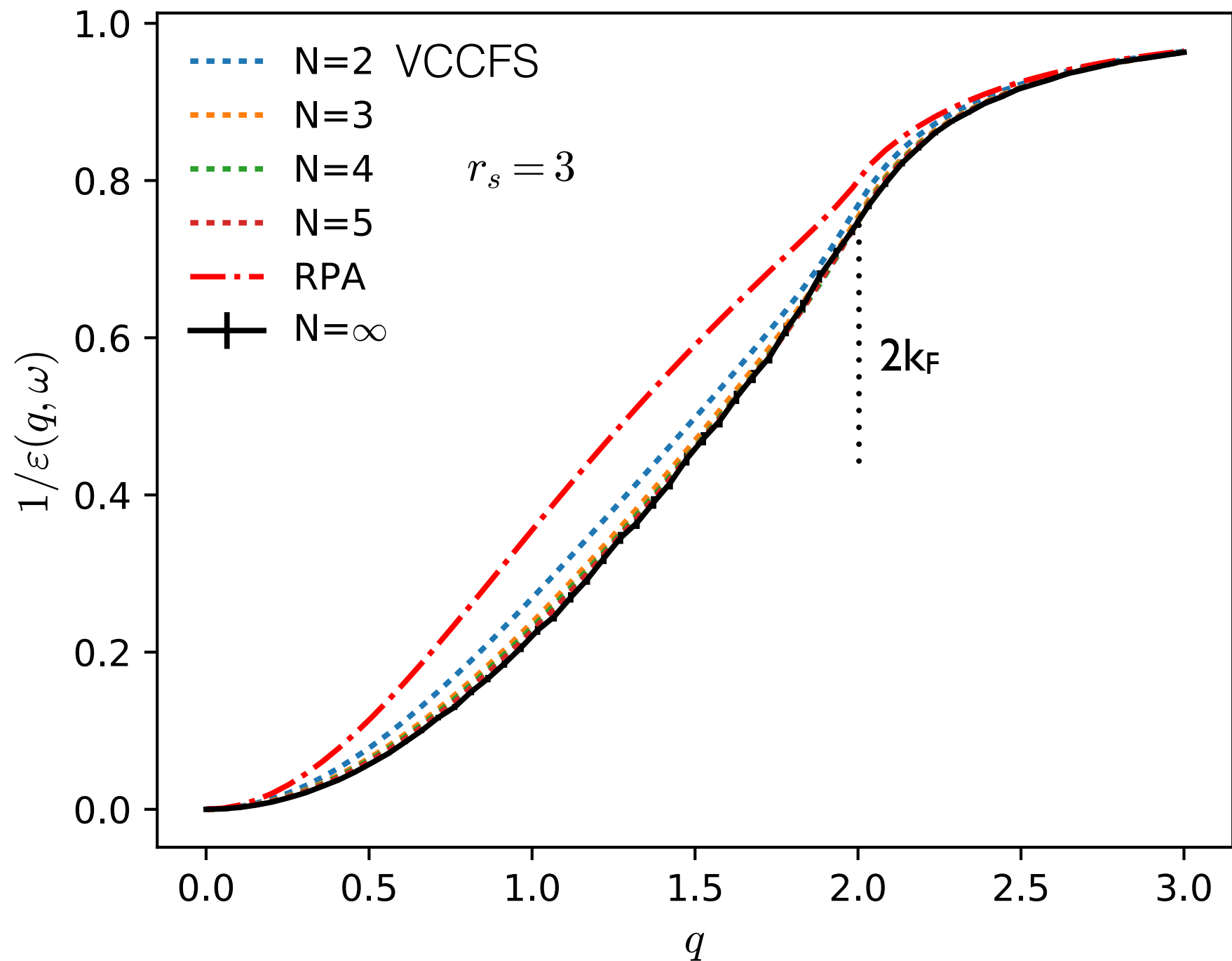
DMC treats finite
system, hence no
small q -points



DMC: B.J.Alder, PRB
50, 14838 (1994)

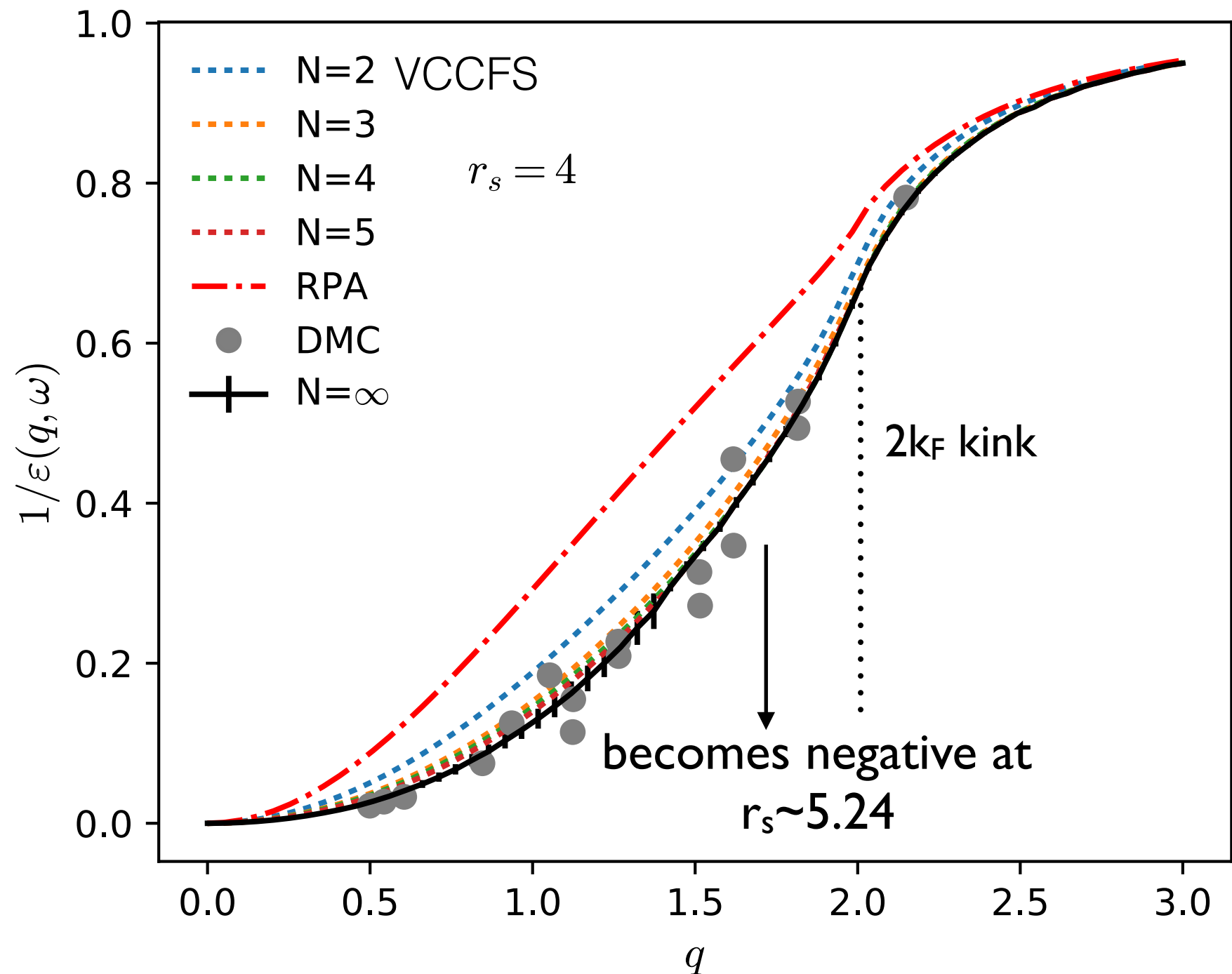
Kun Chen & K. Haule, [arXiv:1809.04651](https://arxiv.org/abs/1809.04651)

Charge response $r_s=3$



Charge response $r_s=4$

Extrapolation needed, convergence becomes hard



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Some charge instability, remains unresolved after 90 years.

Ongoing work : extending convergence to larger r_s

Calculate self-consistently vertex function from Dyson-Schwinger equation

$$\Gamma_4 = \text{tree} + \frac{1}{2} \times \text{loop1} \times 3 + \frac{1}{2} \times \text{loop2} \times 3 - \frac{1}{6} \times \text{loop3}$$

But do not want to store entire information of

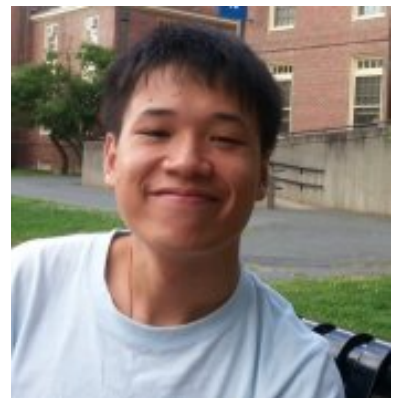
but only the “relevant” part $\mathbf{R} = \left. \Gamma_4 \right|_{\substack{\nu_0 = \nu_1 = \Omega = 0 \\ |\mathbf{k}_0| = |\mathbf{k}_1| = k_F}}$

$$\mathbf{R} = R(q, \theta_1, \theta_2, \phi)$$

$$\cos(\theta_1) = \mathbf{e}_{\mathbf{k}_0} \cdot \mathbf{e}_{\mathbf{k}_1}$$

$$\cos(\theta_2) = \mathbf{e}_{\mathbf{k}_0} \cdot \frac{\mathbf{q}}{q}$$

$$\tan(\phi) = \frac{\mathbf{q} \cdot \mathbf{e}_{\mathbf{k}_1} - (\mathbf{q} \cdot \mathbf{e}_{\mathbf{k}_0})(\mathbf{e}_{\mathbf{k}_0} \cdot \mathbf{e}_{\mathbf{k}_1})}{(\mathbf{q}, \mathbf{e}_{\mathbf{k}_0}, \mathbf{e}_{\mathbf{k}_1})}$$



One loop expansion of Schwinger Dyson

(one loop): $\textcircled{R} = \text{direct} + \text{exchange}$

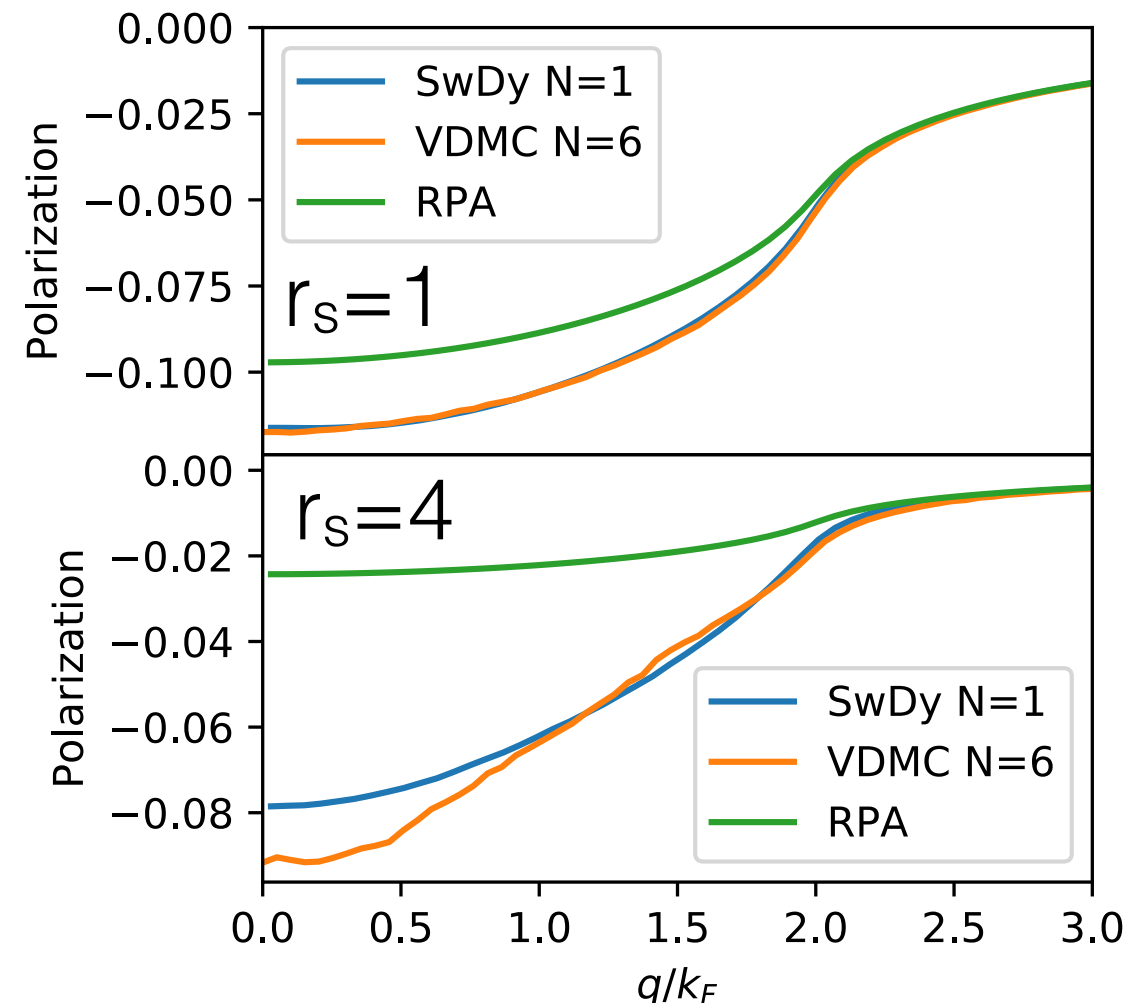
reduc. direct: $\text{wavy} = \frac{1}{\frac{q^2}{8\pi} - \text{loop}} \left[1 + \text{self-energy} + \text{vertex} \right] + \text{irreducible}$

irreduc. direct: $\text{wavy} = \text{self-energy} + \text{vertex} + \text{irreducible}$

$P_q = \text{bubble} + \text{polarization}$

$\Sigma_k = \text{self-energy}$

The first order SwDy comparable to 4th order in VDMC



Conclusion

- Variational Diag. MC very promising direction to extend DFT (or DFT+DMFT) towards controlled solution of solid state problem.
- Long range Coulomb repulsion makes even Hartree-Fock in solids very expensive (similar to GW). By leveraging the emergent locality of correlations, we can avoid the expensive description in terms of bare long-range interaction.
- Sign-problem can be turned into sign-blessing by grouping Feynman diagrams, using crossing symmetry and BK generating functional. Need to choose integration variables (momentum and times) optimally.
- Renormalization of four-point vertex function is a promising direction to explore.