Coulomb Pseudopotential in metals: When multiple mistakes cancel

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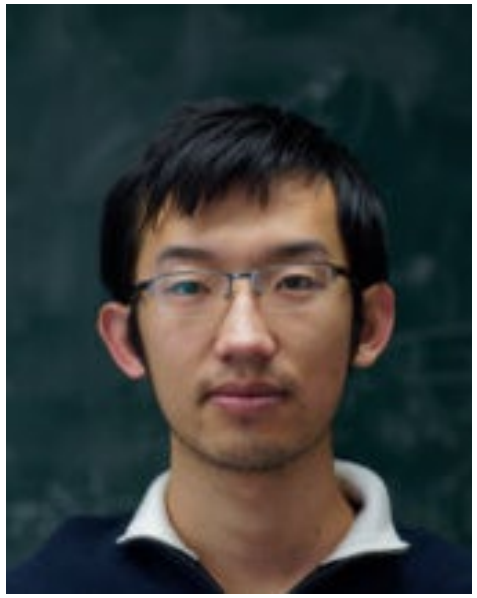
Collaborators



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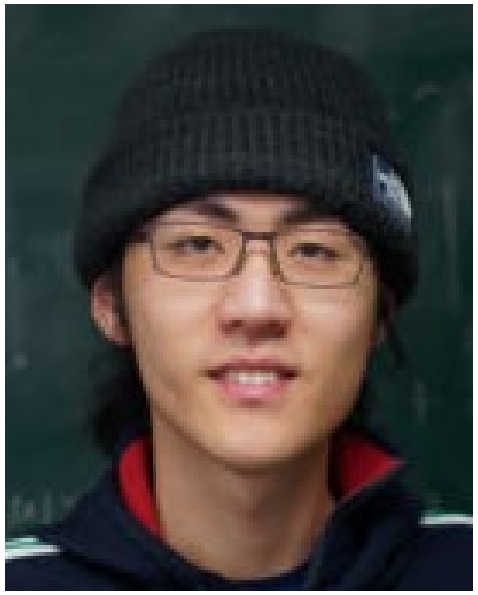

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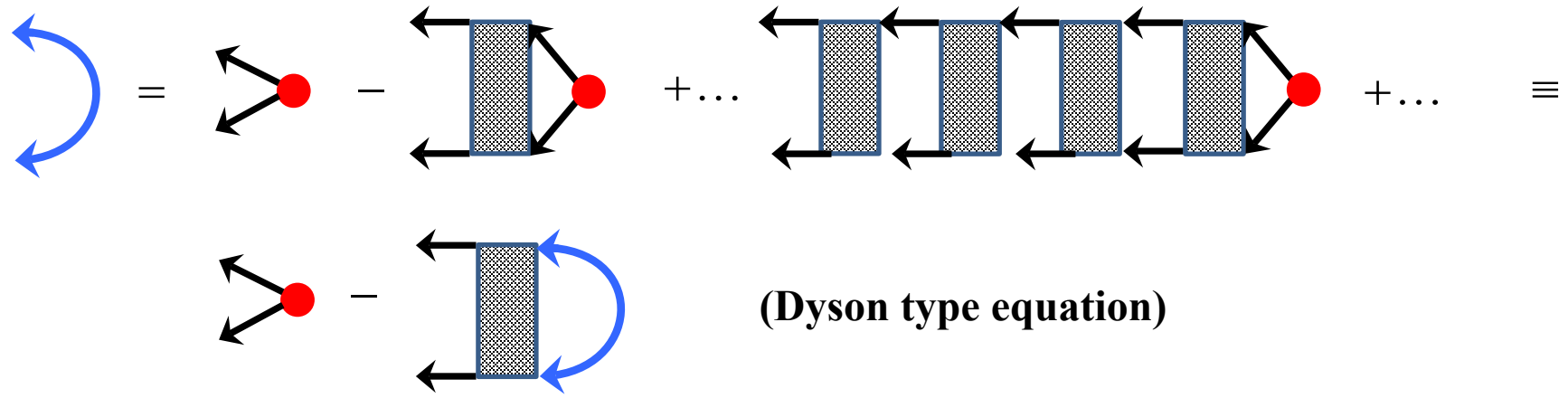
T. Wang, X. Cai, K. Chen, NP, B. Svistunov, PRB 107, L140507 (2023)

T_C: singular response to symmetry breaking field: ● $\delta H = \eta\psi\psi + h.c.$



(Dyson type equation)

$$F_{pn} = \eta G_{pn} G_{-p-n} - G_{pn} G_{-p-n}\, T\sum_{km} \Gamma_{pn,km}\, F_{km}$$

Re-define: $\Delta_{pn} \to T\sum_{km} \Gamma_{pn,km} F_{km}$

$$\Delta_{pn} = \Delta_{pn}(\eta) - T\sum_{km} \Gamma_{pn,km}\, G_{km} G_{-k-m}\, \Delta_{km}$$

singular response when the largest eigenvalue of

$$\hat{A}_{pn,km} = -T\,\Gamma_{pn,km}\,|\,G_{km}\,|^2$$

hits unity

Gap function equation (linear, $T > T_C$)

$$\alpha \Delta_{pn} = -T \sum_{km} \Gamma_{pn,km} \, G_{km} G_{-k-m} \, \Delta_{km}$$

Gap function

Copper channel irreducible vertex function

Green's function

Transition temperature condition: the largest eigenvalue $\alpha(T_C) = 1$

- ideal Green's function $G_{km} = \dfrac{1}{i\omega_m - \xi_k}$ with $\xi_k = \varepsilon_k - \mu$

BCS (weak-coupling):

- attractive coupling $\Gamma_{pn,km} = -g$ at $|\xi_p|, |\xi_k| < \Omega \ll E_F$ and zero otherwise

$$\alpha\Delta_{pn} = -T\sum_{km}\Gamma_{pn,km}\, G_{km}G_{-k-m}\,\Delta_{km} \Rightarrow \alpha\Delta = g\left(T\sum_{km}G_{km}G_{-k-m}\right)\Delta \Rightarrow \boxed{\alpha = g\left(T\sum_{km}G_{km}G_{-k-m}\right)}$$

$$T\sum_{km}G_{km}G_{-k-m} \to \rho_F\int_0^{\Omega/2T} dx\frac{\tanh(x)}{x} = \rho_F \ln\left(1.134\frac{\Omega}{T}\right)$$

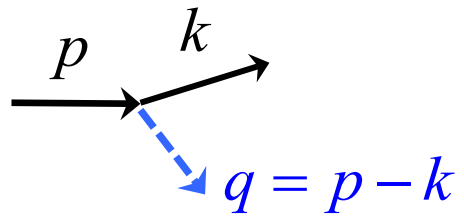
ρ_F: FS density of states (per spin)

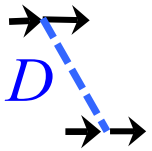
$$\alpha(T_C) = 1 = g\rho_F \ln\left(1.134\frac{\Omega}{T_C}\right) \Rightarrow T_C = 1.134\Omega\exp\left\{-\frac{1}{\lambda}\right\} \quad \text{with} \quad \lambda = g\rho_F \ll 1$$

$$T_C << \Omega << E_F$$

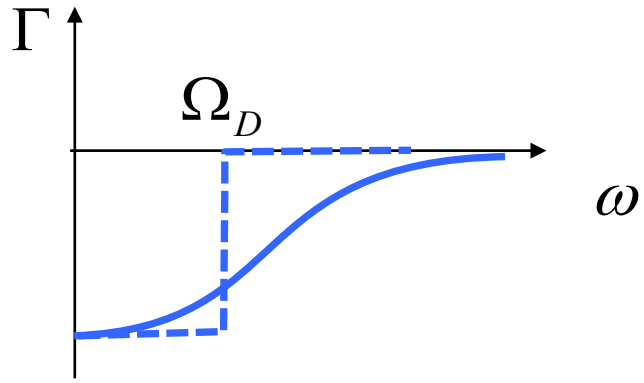
Electron-phonon coupling:
(more realistic modeling)

$$H_{\text{int}} = \sum_{kp\sigma} \left[V(k-p)\, a^{\dagger}_{p,\sigma} a_{k,\sigma} b^{\dagger}_{k-p} + h.c. \right]$$



$\Gamma =$ 

$$D_{pn,km} = -\left|V(q)\right|^2 \frac{2\Omega_q}{\omega_{n-m}^2 + \Omega_q^{\,2}}$$

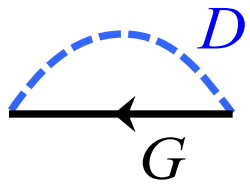


attractive at low frequencies and decays to zero for $\omega_{n-m} \gg \Omega_D$

One step beyond original BCS:

Green's function in an interacting system is always renormalized! $G_{km} = \dfrac{1}{i\omega_m - \xi_k - \Sigma_{km}}$

At least consider the lowest-order diagram based on the same vertex function, say this one for electron-phonon coupling: $\Sigma =$

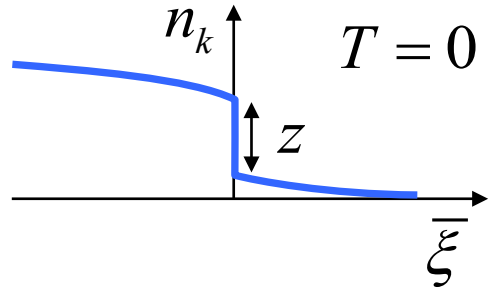


The net result within the Fermi liquid theory at low temperature $T \ll E_F$

smooth across FS even at T=0

$$G = G_{reg} + G_{\text{sing}}$$

$$G_{\text{sing}} = \frac{z}{i\omega_m - \overline{\xi}_k}$$



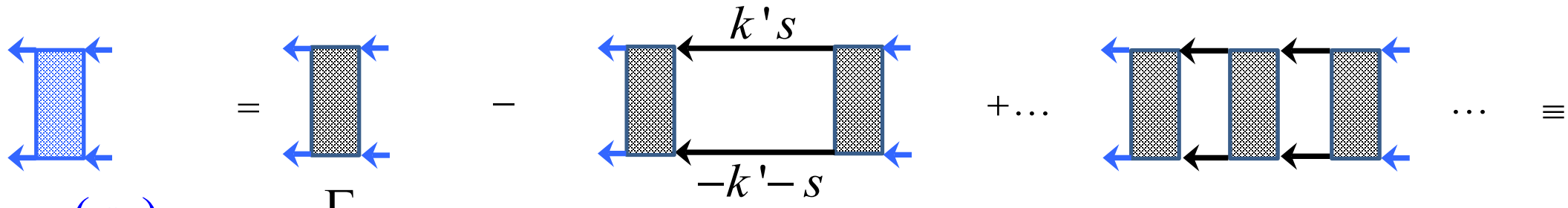
$$T\sum_{km} G_{km}G_{-k-m} = const + z^2\bar{\rho}_F \ln\left(\#\frac{\Omega}{T}\right) \approx z^2 \frac{m_*}{m}\rho_F \ln\left(\#\frac{\Omega}{T}\right) \quad \xrightarrow{f_{FL}} \quad \lambda = z^2\frac{m_*}{m} g\rho_F \ll 1$$

important given exponential dependence of T_C on $1/\lambda$

This setup is the essence of the Migdal-Eliashberg theory

If the sign of g were positive (repulsive) $\lambda = -g\rho_F \ln\left(1.134\frac{\Omega}{T}\right)$ **would never reach unity!**

An alternative point of view: effective low-energy/frequency interactions



$\bar{\Gamma}_{pn,km}(\omega_c)$ = Γ − … + … ≡

external lines are at low energy/frequency below ω_c

internal lines have high energies/frequencies above ω_c

Consider repulsive $\Gamma = g > 0$ **. Then** $\bar{\Gamma}(\omega_c) = g - g\left(T\sum_{km}^{>\omega_c} G_{km}G_{-k-m}\right)g + g^3\rho_F^2 \ln^2\left(E_F/\omega_c\right) - \ldots$

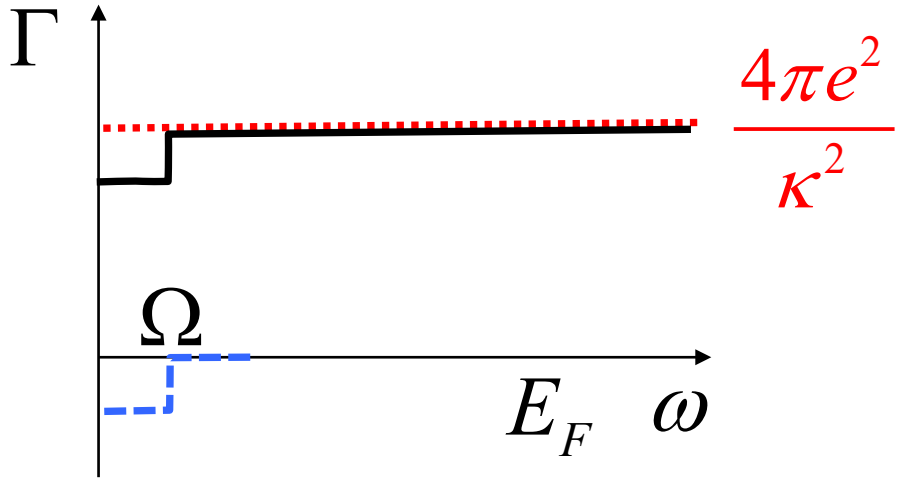
$\approx \rho_F \ln\left(E_F/\omega_c\right)$

$$\bar{\Gamma}(\omega_c) \approx \frac{g}{1+g\rho_F \ln\left(E_F/\omega_c\right)} \underset{\omega_c\to 0}{\to} 0$$

In the particle-particle channel & near the Fermi surface it is renormalized to smaller values

Combining the two:

Bogoliubov & Tolmachev ‘59, ’61
Morel & Anderson ’62
Ratchel & Sham ‘87



$\left(\kappa^2 = 6\pi n e^2 / E_F\right)$

Thomas-Fermi
Screening momentum

$$\bar{\Gamma}(\omega < \Omega) \approx -g_{e-p} + \frac{g_C}{1 + g_C \rho_F \ln\left(E_F / \Omega\right)}$$

$$\lambda_{eff} = \lambda - \mu_*$$

$$\mu_* = \frac{g_C \rho_F}{1 + g_C \rho_F \ln\left(E_F / \Omega\right)}$$

Coulomb pseudopotential

Positive

Rather universal: at RPA level $\frac{4\pi e^2}{\kappa^2}\rho_F = 0.5$

McMillan’s phenomenology for $\ln T_C$
produces $\mu_* \in (0.1 \div 0.15)$

First wrongdoing: $\dfrac{4\pi e^2}{\kappa^2}$ or $\dfrac{4\pi e^2}{q^2+\kappa^2}$ is the **static (zero frequency)** result of screening. and cannot be used for all frequencies!

Screening is dynamic: $W_{qm} = \dfrac{4\pi e^2}{q^2 - 4\pi e^2 \Pi_{qm}}$

RPA approximation (Lindhard function at *T=0*)

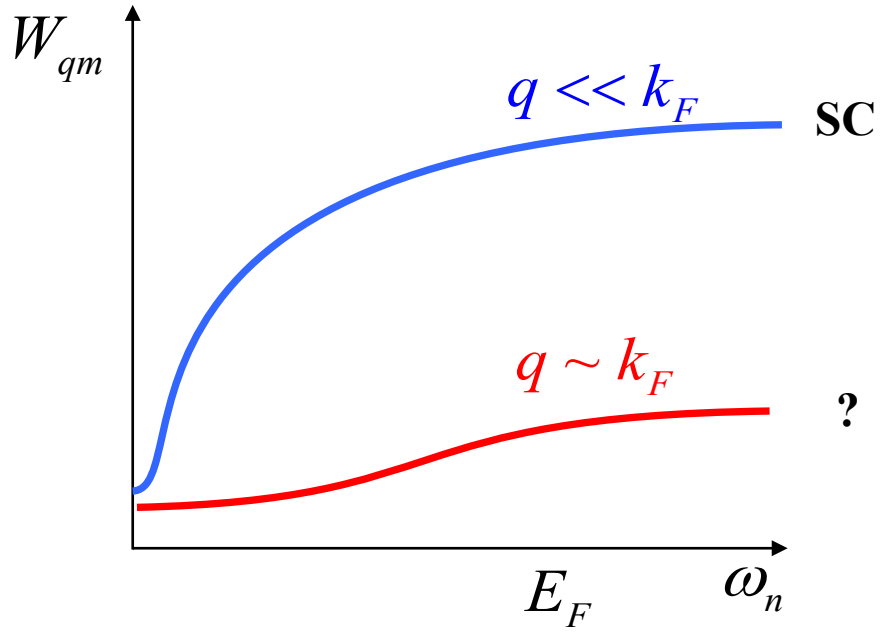
$$\Pi_{qm} = 2\sum_{kn} G_{kn} G_{k+q\, n+m}$$

At $\omega_m >> E_F$ **we have** $W_{qm} \approx V_q$

At $\omega_m = 0$ **we have** W_{q0} :| $W_{q0} = \begin{cases} \dfrac{4\pi e^2}{q^2+\kappa^2} & (q << k_F) \\ V_q & (q >> k_F) \end{cases}$

$\left(\kappa^2 = 6\pi n e^2 / E_F\right)$

Thomas-Fermi
Screening momentum



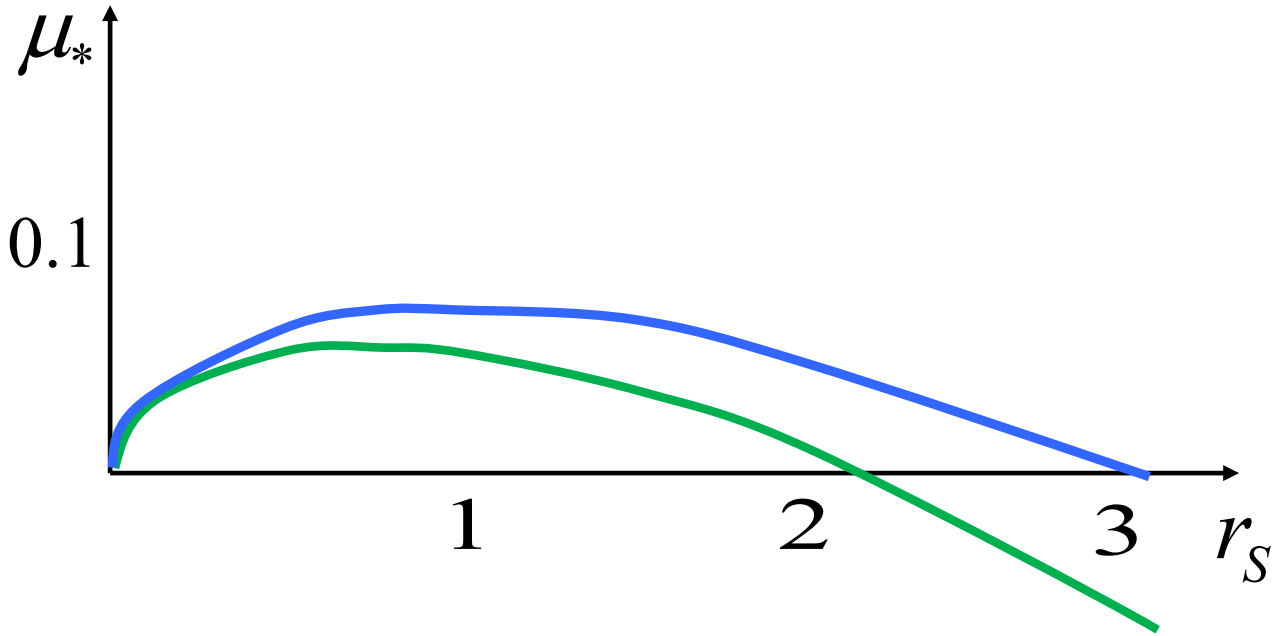
First wrongdoing: $\frac{4\pi e^2}{\kappa^2}$ or $\frac{4\pi e^2}{q^2+\kappa^2}$ is the **static (zero frequency)** result of screening. and cannot be used for all frequencies!

Dynamic screening all by itself leads to effective attraction in the s-wave channel at large enough r_S!

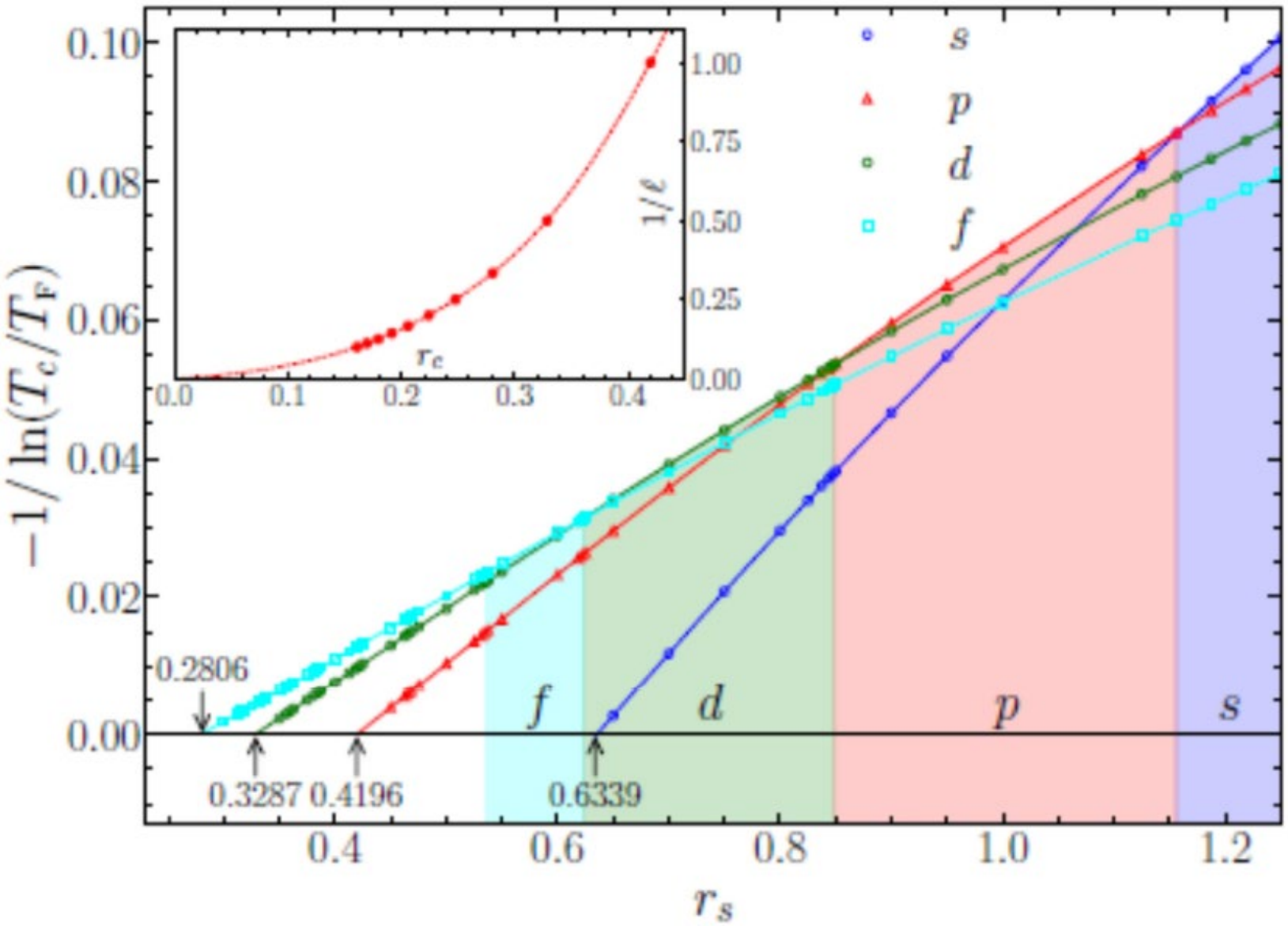
$$\Gamma_C = W_{qm} \quad \rightarrow \quad \overline{\Gamma}_C(\omega \le \Omega) < 0$$

Takada '78, '89
Rietschel, Sham '83
Wang, Cai, Svistunov, NP '22

Critical r_S at the RPA level is close to 2 with leading vertex corrections about 3



RPA phase diagram of superconducting phases in the 2D electron gas at $r_S < 1.3$ (s-channel goes attractive at $r_S > 0.65$)



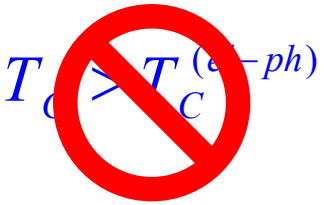
Watch my hands ☺

K. Chen, T. Wang, X. Cai, B. Svistunov, NP

1. Take $\Gamma = \Gamma_{el-ph}$ **and do Migdal-Eliashberg theory → s-wave superconductor with** $T_C^{(el-ph)}$

2. Take $\Gamma = W_{q,n-m}$ **(RPA screened Coulomb interaction) → s-wave superconductor with** $T_C^{(C)}$

3. Combine two attractive mechanisms $\Gamma = \Gamma_{el-ph} + W_{q,n-m}$ **→ s-wave superconductor with** $T_C < T_C^{(el-ph)}$



What is the origin of this counter-intuitive outcome observed in most materials?

Second wrongdoing: Pure math …

If λ_A and λ_B are the largest eigenvalues of $\widehat{A}$ and $\widehat{B}$, respectively, then

$$\boxed{\lambda_{A+B} \leq \lambda_A + \lambda_B}$$

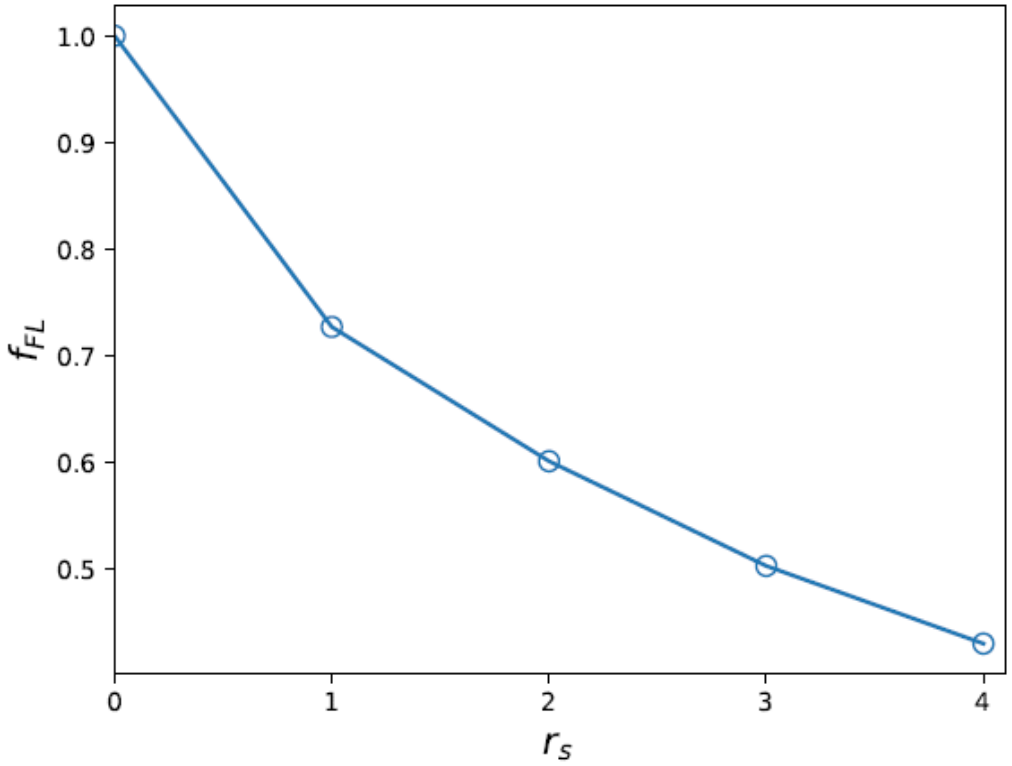
This is generic eigenvector ``mismatch" between the eigenfunctions behind λ_A and λ_B

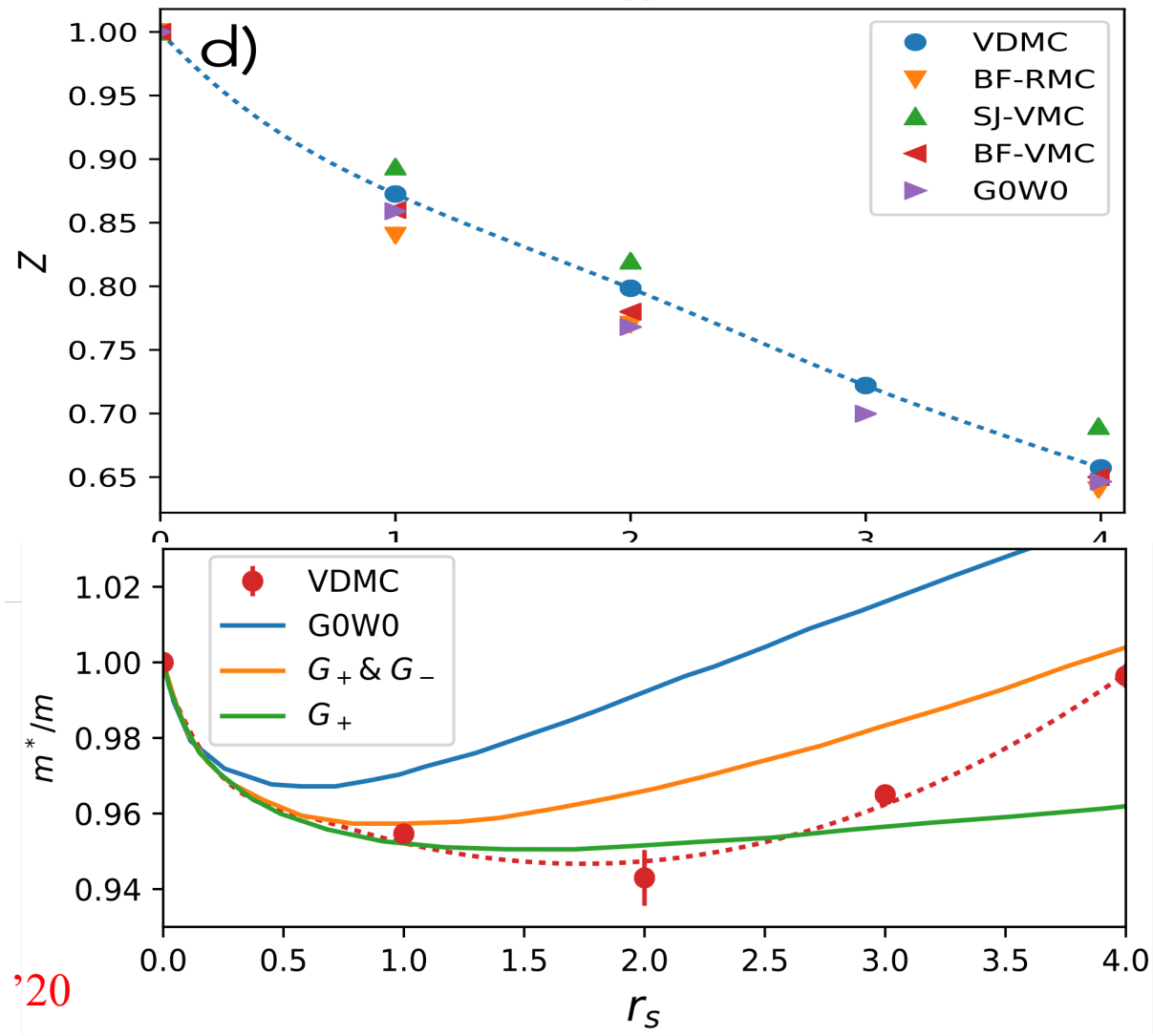
Effective couplings cannot be summed up when combining different pairing mechanisms!

E.g. it is possible to have: Γ_1 with $T_C^{(1)}$ & Γ_2 with $T_C^{(2)}$:| $T_C = 0$ for $\Gamma_1 + \Gamma_2$

Third wrongdoing: Coulomb interactions change $f_{FL} = z^2 \frac{m_*}{m}$ significantly!

Converged high-order (6th) DiagMCcalculation for jellium





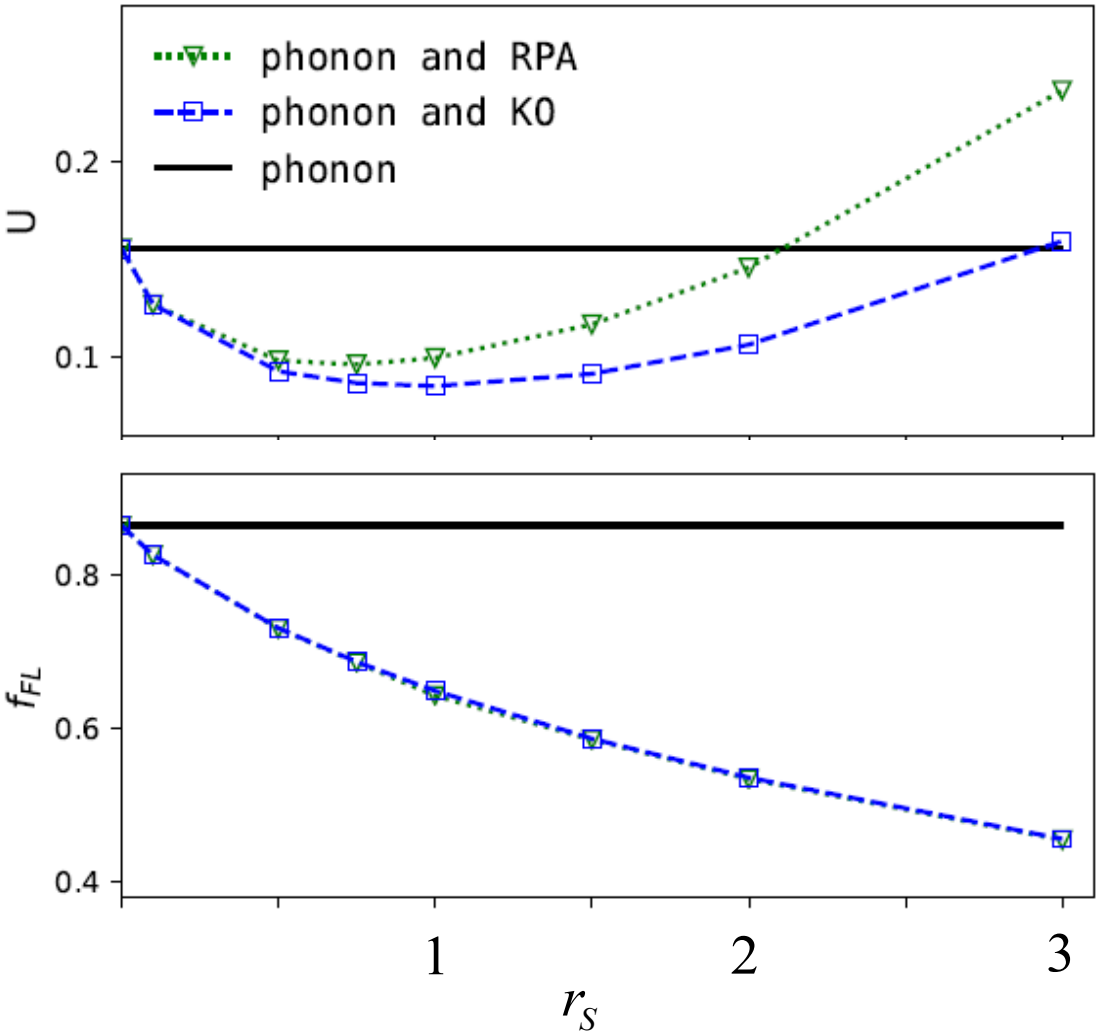
K. Chen, K. Haule '20

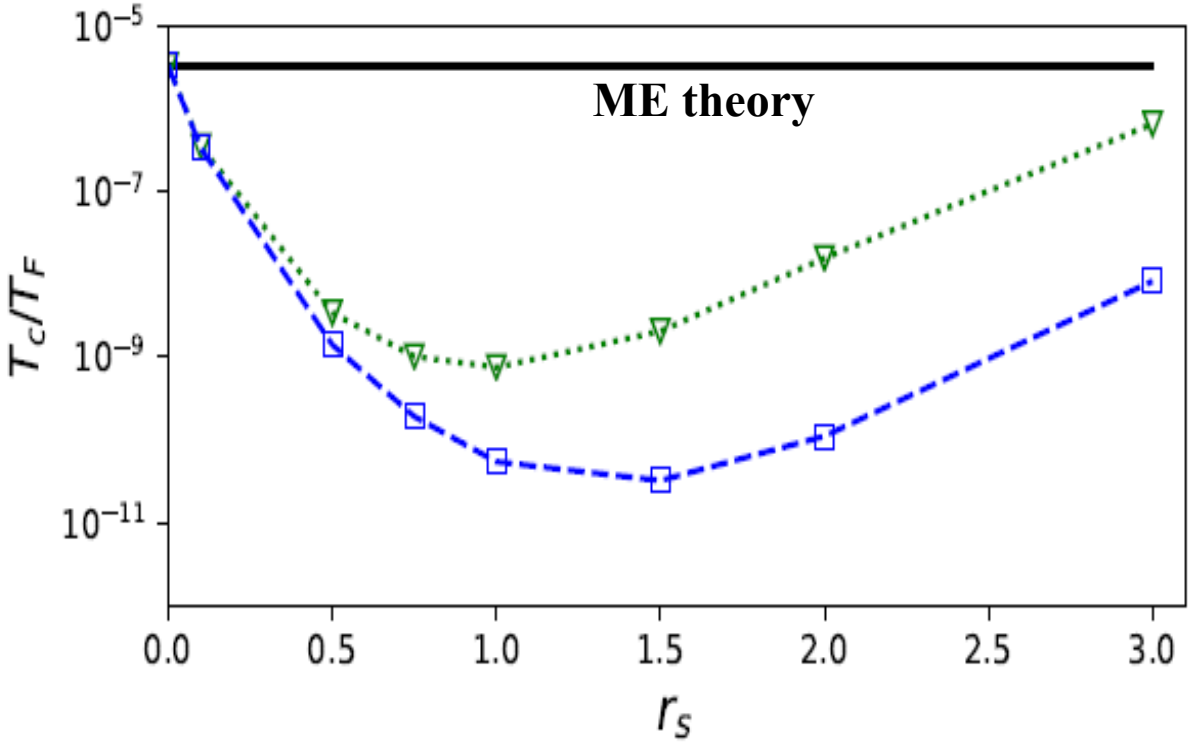
Model calculation: jellium with el-ph interaction

(a la Richardson & Ashcroft '97)

$$\Gamma_{el-ph} = \frac{a\rho_F}{1+(q/2k_F)^2}\frac{\omega^2(q)}{\omega_m^2+\omega^2(q)}$$

$$\omega(q) = \Omega\frac{(q/k_F)^2}{1+(q/k_F)^2}$$

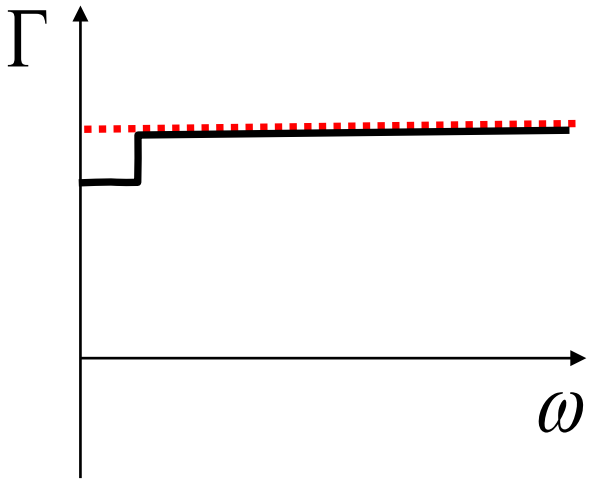




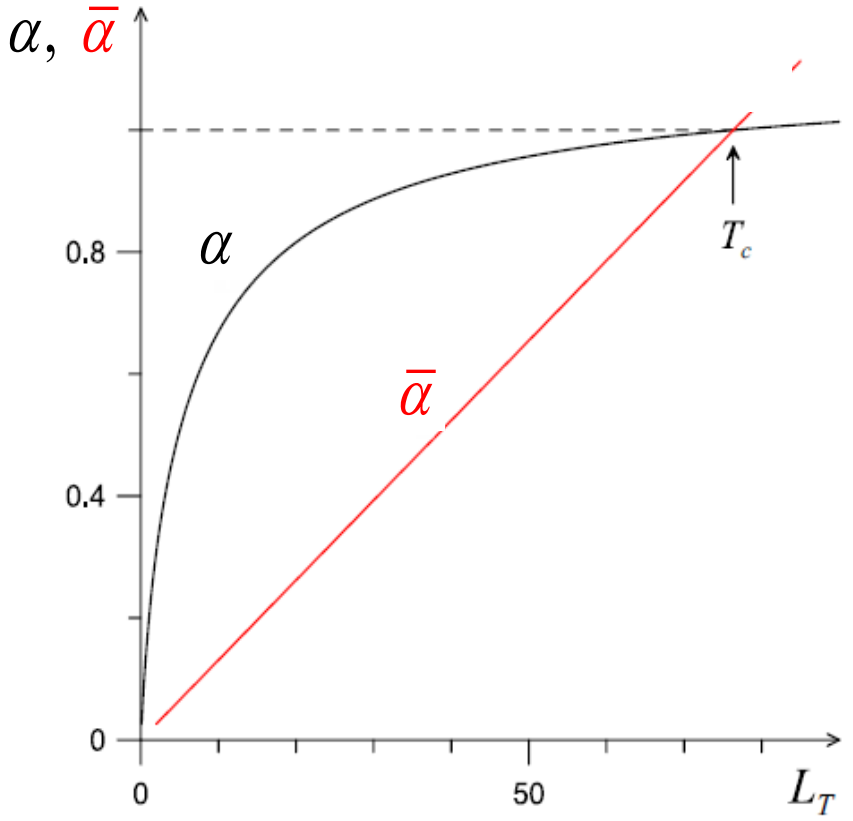
How to determine exponentially small T_C reliably

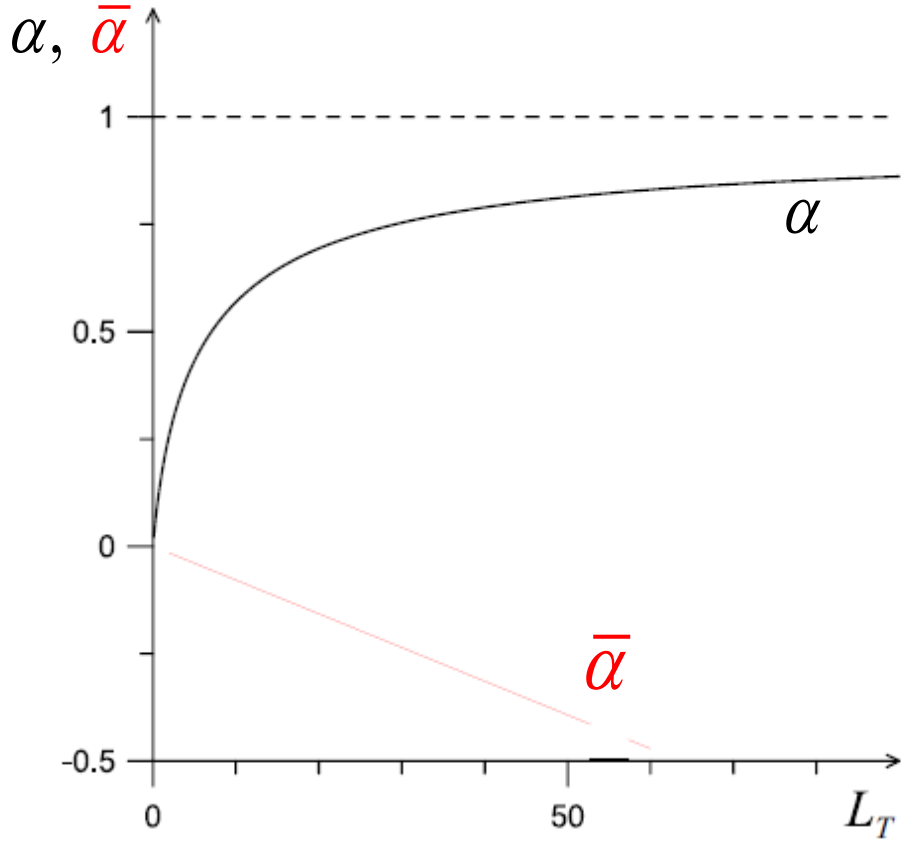
1. Do NOT solve for the largest eigenvalue of $\alpha\Delta_{pn} = -T\sum_{km}\Gamma_{pn,km}\, G_{km}G_{-k-m}\,\Delta_{km}$

Generically, $\alpha(T)$ is a non-linear function of *ln(Ω/T)* and cannot be easily extrapolated to predict T_C, if any!



Exactly solvable case





A. Chubukov, NP, B. Svistunov, Phys. Rev. B '19

How to determine exponentially small T_C reliably

2. No need to invert matrix when solving $\vec{\Delta} = \eta\vec{\Delta}_0 - \left(T\sum_{km} \Gamma \mid G \mid^2 \right)\vec{\Delta} \equiv \eta\vec{\Delta}_0 - \hat{A}\,\vec{\Delta}$

↑

Symmetry breaking "source" term

$(\eta \to 0)$

Damped iterations: $\vec{\Delta}_{i+1} = \eta\vec{\Delta}_0 - \hat{A}\left[\frac{1}{i}\sum_{k=1}^{i}\vec{\Delta}_k\right]$ **Guaranteed fast convergence as long as all eigenvalues < 1**

(i) Much faster than matrix size cubed → large number of frequencies and momenta

(ii) Symmetrized discrete Lehman representation allows one to cover 8-9 orders in frequency domain

J. Kaye, K. Chen, O. Parcollet, PRB '22

J. Kaye, K. Chen, H. U. Strand, Comp. Phys. Comm. '22

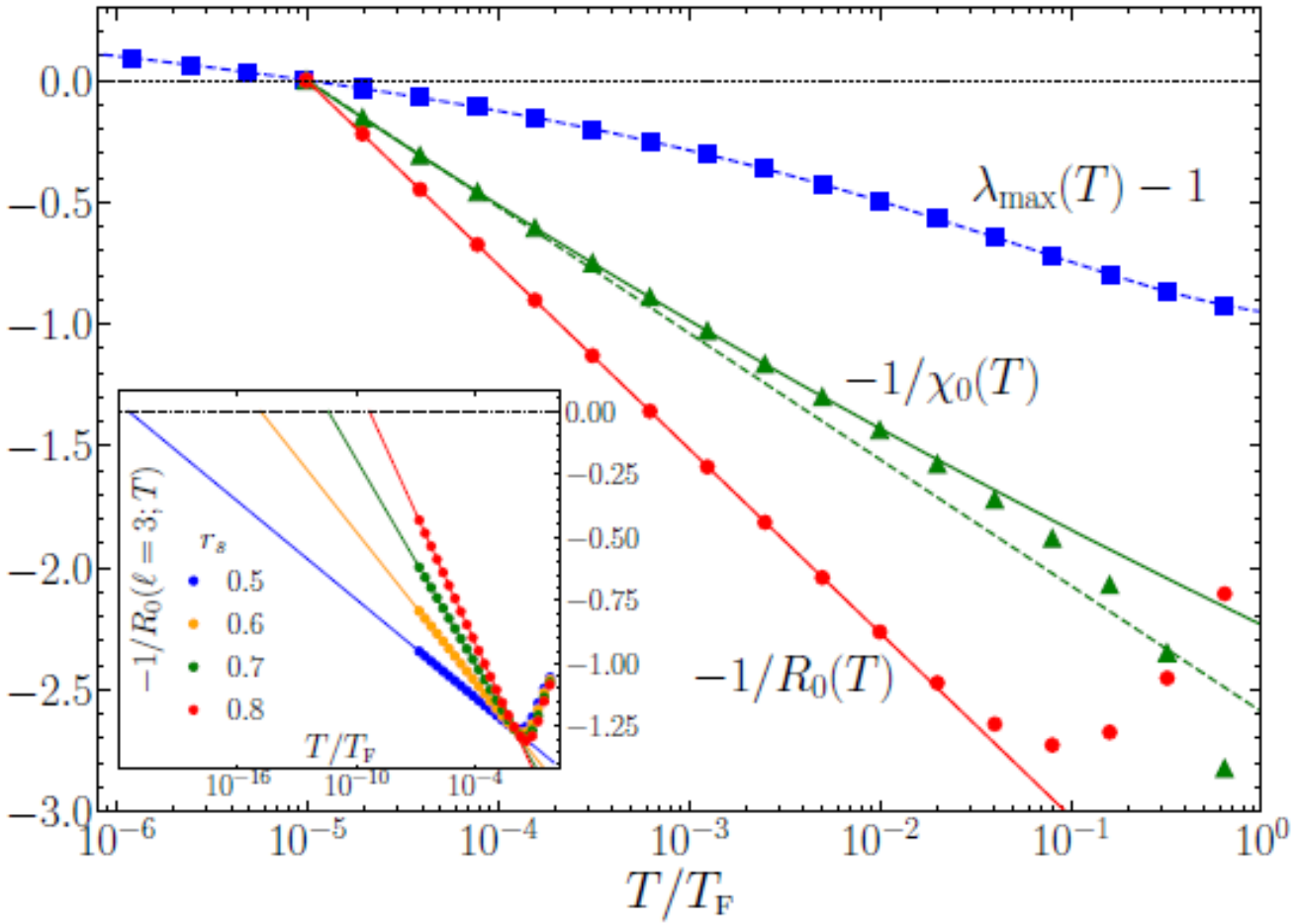
T. Wang, X. Cai, K. Chen, NP, B. Svistunov, PRB '23

(iii) No need to keep matrix A in memory if it is sampled stochastically → perfect Diag.MC setup
High-order calculations are no more complex (memory wise) than G

How to determine exponentially small T_C reliably

3. Instead of eigenvalue compute "linear response" $\vec{\Delta} = I - \hat{A}\,\vec{\Delta}$

and look at the Fermi surface/lowest frequency component: $R_0 = \Delta_{k=k_F,\,\omega=\pi T}$



$1/R_0$ **is a linear function of** $\ln(T)$

at low temperature

$$R_0 = \frac{1}{1 + g \ln \frac{\Lambda}{T}} + \mathcal{O}(T)\,.$$

Material science phenomenological practice (Mc Millan's formula)

Ignore FL renormalization due to Coulomb interactions (unreasonable choice) --- wrong

Reduce Γ by assuming that Coulomb interaction is repulsive at low frequency and described by renormalized static potential (arbitrary choice) --- wrong

When mechanisms are combined their effective couplings are combined --- wrong

The final outcome: three wrongs often make it almost "right" --- Mc Millian's formula

$$T_C = \frac{\omega_{\mathrm{ph}}}{1.45}\exp\left\{-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right\}$$

$0.1 \div 0.15$