Precursory Cooper Flow:
From Physics Phenomenon to Computational Techniques

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The concept of emergent BCS regime

Paradigmatic models:

(i) Uniform electron gas

(ii) Repulsive Hubbard model

The goal: To utilize Feynman diagrammatics (Diagrammatic Monte Carlo) to bridge the emergent long-wave BCS physics with strongly correlated ultraviolet microscopics.

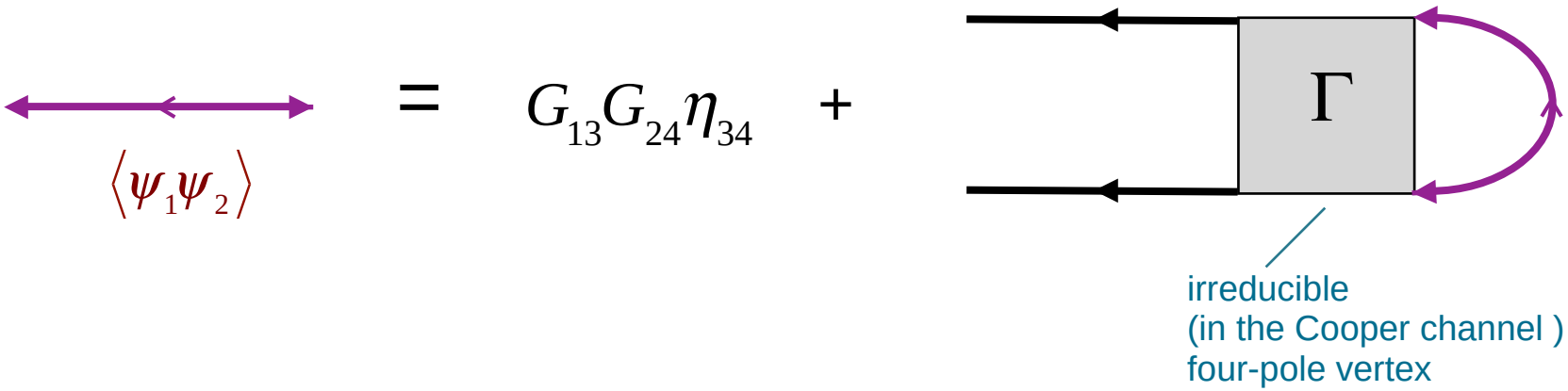
Linear response of the normal state to a pair-creating perturbation

Modify the Hamiltonian: $H \rightarrow H + \left(\eta^{*}_{12}\psi_1\psi_2 + \text{H.c.}\right)$

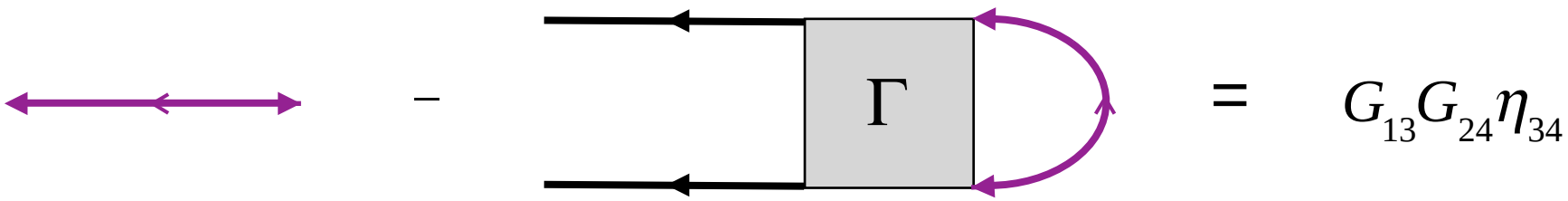
infinitesimally small pair-creating perturbation

(infinitesimal) linear response: $\langle\psi_1\psi_2\rangle$

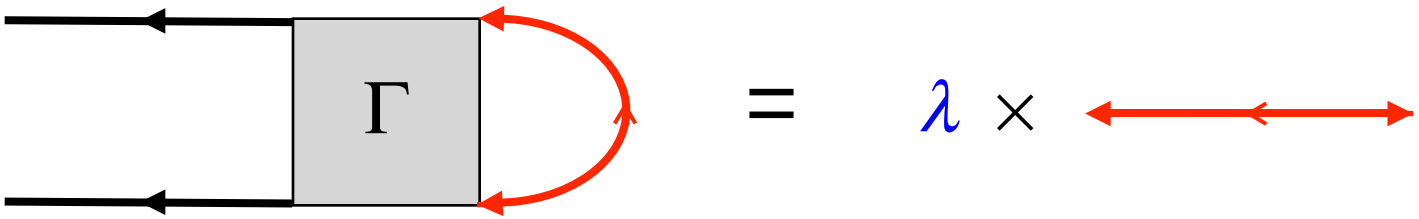
Diagrammatically:



Singular response: eigenvector-eigenvalue problem

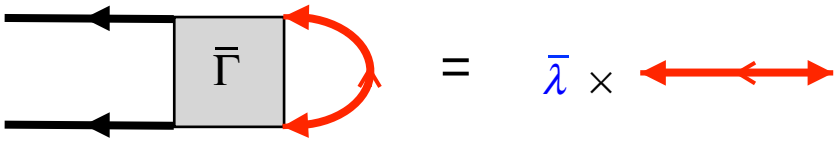


Response diverges (i.e., the critical temperature is reached), when the following eigenvalue becomes equal **1**.



Corresponding eigenvector defines the pairing channel.

Emergent BCS regime: long-wave effective theory



In this regime:

Green's function has a Fermi-liquid form (close to the Fermi surface):

$$G(\mathbf{k},\omega_n) \approx \frac{z(\hat{k})}{i\omega_n - \mathbf{v}_F(\hat{k})\bullet[\mathbf{k}-\mathbf{k}_F(\hat{k})]}$$

The effective four-pole vertex $\bar{\Gamma}$ is small and independent of temperature and frequency.

The eigenvector is temperature and frequency independent.

Temperature dependence of $\bar{\lambda}$ is essentially due to the Green's function factor:

$$\bar{\lambda}(T) = |g|\ln(\Lambda/T) \quad \Rightarrow \quad T_c = \Lambda e^{-1/|g|}, \quad |g| \ll 1$$

Eigenvalue-eigenvector problem for the gap function Δ

$$\lambda(T)\Delta_{\mathbf{k},\omega_n} = -T\sum_m \int \frac{d\mathbf{p}}{(2\pi)^d}\, \Gamma^{\mathbf{k},\omega_n}_{\mathbf{p},\omega_m} G_{\mathbf{p},m} G_{-\mathbf{p},-m}\, \Delta_{\mathbf{p},\omega_m}$$

A crucial obstacle for the (*otherwise straightforward*) DiagMC:
In the majority of interesting cases, the diagrammatic series for Γ is well beyond the convergence radius at $T \sim T_c$.

How about extrapolating $\lambda(T)$ from $T \gg T_c$?

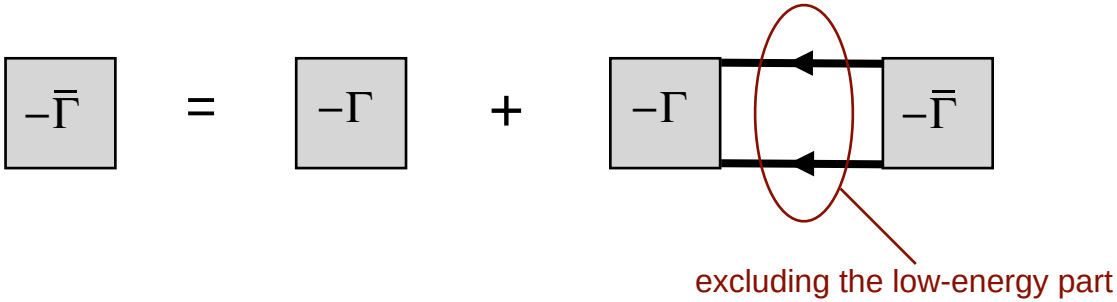
Works with $\bar{\lambda}(T)$ *but not with* $\lambda(T)$ *!*

(As we will see later.)

Implicit renormalization approach

A. Chubukov, N. Prokof'ev, and BS, Phys. Rev. B 100, 064513 (2019)

Renormalization of the interaction in the Cooper channel



Not doable because of the “curse of multivariableness.”

However, $\bar{\lambda}(T)$ can be extracted from a ***modified eigenvalue-eigenvector problem based on bare*** Γ ***.***

A few preliminary steps

matrix-vector notation:

$$\lambda\vec{\Delta} = -\hat{A}\vec{\Delta}, \qquad \vec{\Delta} \equiv \Delta(\mathbf{p},\omega)$$

Introduce low- and high-energy parts with respect to a certain characteristic energy scale Ω_c :

$$\vec{\Delta} = \vec{\Delta}^{(1)} + \vec{\Delta}^{(2)}$$

$$\Delta^{(1)}(\mathbf{p},\omega) \equiv 0 \quad \text{at} \quad \xi_p^2 + \omega^2 > \Omega_c^2 \qquad \text{low-energy part}$$

$$\Delta^{(2)}(\mathbf{p},\omega) \equiv 0 \quad \text{at} \quad \xi_p^2 + \omega^2 \le \Omega_c^2 \qquad \text{high-energy part}$$

$$\hat{A} = \hat{A}^{(11)} + \hat{A}^{(22)} + \hat{A}^{(21)} + \hat{A}^{(12)}$$

$$\begin{cases} \lambda\vec{\Delta}^{(1)} = -\hat{A}^{(11)}\vec{\Delta}^{(1)} - \hat{A}^{(12)}\vec{\Delta}^{(2)} \\ \lambda\ \vec{\Delta}^{(2)} = -\hat{A}^{(22)}\vec{\Delta}^{(2)} - \hat{A}^{(21)}\vec{\Delta}^{(1)} \end{cases}$$

(So far, it is just an identical rewriting.)

Implicit-renormalization formulation

Replace

$$\begin{cases} \lambda\,\vec{\Delta}^{(1)} = -\hat{A}^{(11)}\vec{\Delta}^{(1)} - \hat{A}^{(12)}\vec{\Delta}^{(2)} \\ \lambda\;\vec{\Delta}^{(2)} = -\hat{A}^{(22)}\vec{\Delta}^{(2)} - \hat{A}^{(21)}\vec{\Delta}^{(1)} \end{cases}$$

with:

$$\begin{cases} \bar{\lambda}\,\vec{\Delta}^{(1)} = -\hat{A}^{(11)}\vec{\Delta}^{(1)} - \hat{A}^{(12)}\vec{\Delta}^{(2)} \\ \vec{\Delta}^{(2)} = -\hat{A}^{(22)}\vec{\Delta}^{(2)} - \hat{A}^{(21)}\vec{\Delta}^{(1)} \end{cases}$$

Let us see that $\bar{\lambda}$ and (new) $\vec{\Delta}^{(1)}$ exactly correspond to the renormalized theory.

Substituting $\vec{\Delta}^{(2)} = -[\hat{I} + \hat{A}^{(22)}]^{-1}\hat{A}^{(21)}\vec{\Delta}^{(1)}$ (implied by the second equation) into the first equation, we get:

$$\bar{\lambda}\,\vec{\Delta}^{(1)} = -\hat{B}\vec{\Delta}^{(1)}, \qquad \hat{B} = \hat{A}^{(11)} - \hat{A}^{(12)}[\hat{I} + \hat{A}^{(22)}]^{-1}\hat{A}^{(21)}$$

This is exactly the kernel of the effective theory.

Illustrative simulation of the 3D uniform electron gas

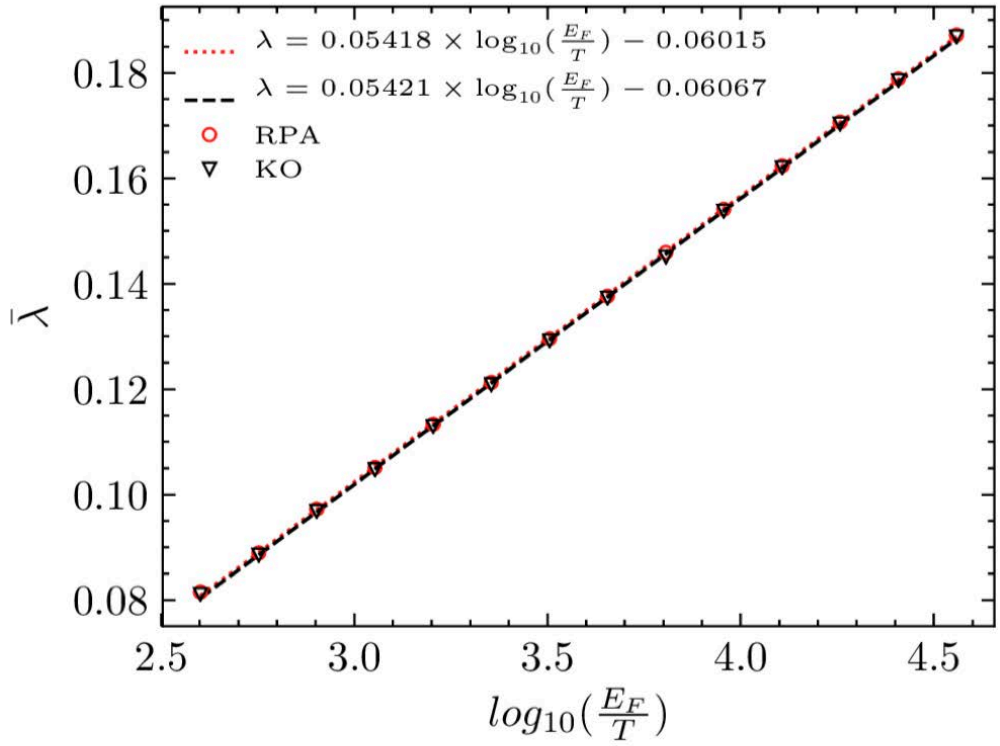


FIG. 3: Temperature dependence of the eigenvalues $\bar{\lambda}(T)$ for RPA (red circles) and KO (black triangles) vertex functions at $r_s = 2.0$ and $\ell = 3$. The linear fits of the RPA (red dotted line) and KO (black dashed line) data are almost identical. The extrapolated value of $T_c = 2.71 \times 10^{-20} E_F$ is extremely small.

(KO stands for Kukkonen-Overhauser approximation.)

Conclusions I

- A protocol for extrapolating numerical data towards T_c from higher temperatures —applicable to first-principle description of real metals, as well as strongly interacting models—has to adequately capture the physics of the emergent weakly-interacting effective theory.

- Implicit renormalization protocol provides a simple, efficient, and unbiased way of solving the extrapolation problem. The scheme has a built-in tool of controlling the systematic error of extrapolation—the only systematics of the otherwise numerically exact method.

- The implicit renormalization approach is perfectly compatible with the DiagMC. One can solve the corresponding eigenvalue problem without invoking the matrix inversion or even explicitly calculating the four-point vertex function Γ.

- The implicit renormalization protocol also allows one to obtain the correct gap function immediately below T_c.

Despite unquestionable success, the Implicit renormalization (IR) approach encounters certain technical limitations and lacks a direct connection with what can be measured experimentally. Technical limitations of IR are most pronounced in the vicinity of the “quantum transition point” at which a given channel undergoes a transition from Cooper-stable to Cooper-unstable regime.

Alternative approach: Trace the flow of the net linear response rather than its singular part (if any)

Well-known result for the linear response in the (emergent) BCS regime:

$$\chi_0(T) \propto 1/\ln\left(T/T_c\right) \qquad (T \to T_c + 0) \qquad (1)$$

Good, but not enough,…

… as is clear from the following accurate formula—*to be derived later* :

$$\chi_0(T) = \frac{c\ln(\Lambda/T)}{1 + g\ln(\Lambda/T)} \qquad (|g| \ll 1, \quad T_c < T \ll \Lambda) \qquad (2)$$

The numerator corresponds to the response of an ideal gas (up the the pre-refactor c taking care of the UV-renormalization of the strength of pair-creating perturbation).

Within a large interval of temperatures where $|g|\ln(\Lambda/T) \ll 1$, expression (2) has little to do with (1).

Derivation and further improvement

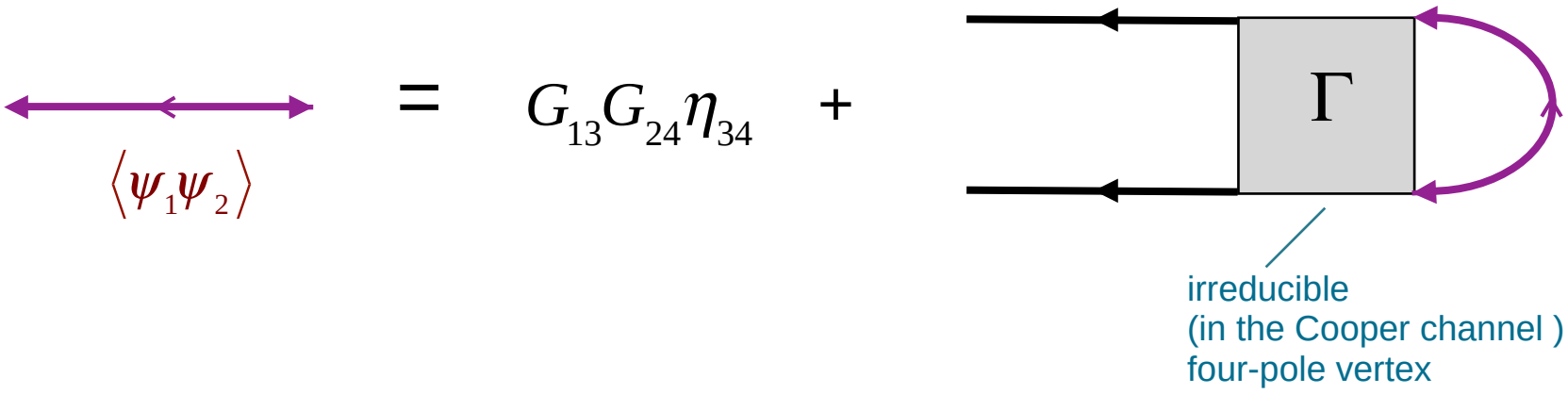
Back to the initial setup, but now solving for the total response

Modify the Hamiltonian: $H \rightarrow H + \left(\eta^{*}_{12}\psi_1\psi_2 + \text{H.c.}\right)$

infinitesimally small
pair-creating perturbation

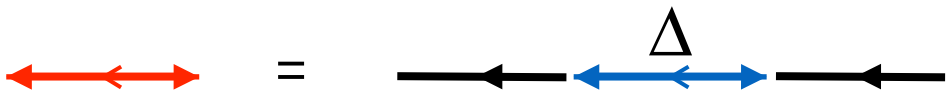
(infinitesimal) linear response: $\langle\psi_1\psi_2\rangle$

Diagrammatically:



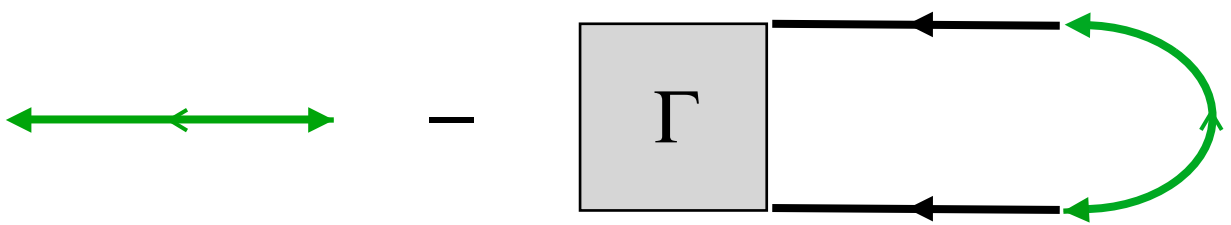
irreducible
(in the Cooper channel)
four-pole vertex

In a direct analogy with the definition of Δ ,



define R:

and get the “gap equation with the right-hand-side”



can be replaced with unity (operator)

$$R_k + \int_p \Gamma_{kp} G_p G_{-p} R_p = 1 \,, \qquad \int_k \equiv T \sum_n \int \frac{\mathbf{dk}}{(2\pi)^d}$$

$$R_k + \int_p \Gamma_{kp} G_p G_{-p} R_p = 1 \quad \Rightarrow \quad R_0(T) = \frac{1}{1 + g' \ln(\Lambda'/T)}, \qquad R_0 \equiv R_{k\to 0}$$

$$\chi_0 = \int_k R_k G_k G_{-k} \propto R_0(T) \ln(\Lambda/T)$$

$$R_0(T) = \frac{1}{1 + g' \ln(\Lambda'/T)}$$

$$\chi_0(T) = \frac{c \ln(\Lambda/T)}{1 + g \ln(\Lambda/T)}, \qquad \ln(\Lambda'/\Lambda) = 1/g - 1/g'$$

Improved response function $R_0(T)$ vs standard $\chi_0(T)$

Definition: $R_0 \equiv R_{k\to 0}$

$$\chi_0(T) = \frac{c\ln(\Lambda/T)}{1+g\ln(\Lambda/T)} \qquad (T_c < T \ll \Lambda)$$

$$R_0(T) = \frac{1}{1+g'\ln(\Lambda'/T)}, \qquad \ln(\Lambda'/\Lambda) = 1/g - 1/g'$$

only two fitting parameters

$$T_c = \Lambda' e^{1/g'} = \Lambda e^{1/g} \qquad (g, g' < 0)$$

Illustrative simulations of the uniform electron gas in 2D

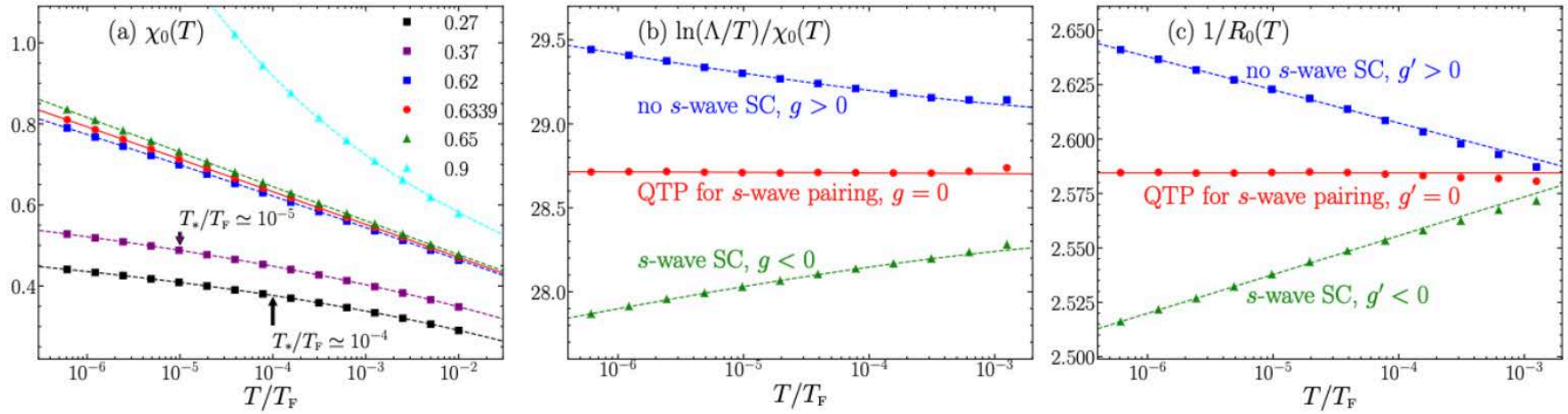


FIG. 2. Temperature evolution of the standard pair susceptibility χ_0 and modified pair susceptibility R_0 of the 2D uniform electron gas in the s-channel for various values of r_s. Red circles correspond to QTP $r_s = 0.6339$, squares stand for stable regimes ($g > 0$), and triangles are used for the unstable regimes ($g < 0$). The lines are the fits with the ansatz (2) for χ_0 and ansatz (3) for R_0. (a) Function $\chi_0(T)$. For stable regimes, $\chi_0(T)$ saturates to a constant at $T \ll T_* \simeq \Lambda e^{-1/|g|}$; for unstable regimes, $\chi_0(T)$ diverges at $T = T_c$; at the QTP, $\chi_0(T)$ diverges as $T \to 0$. (b) Inverse $\chi_0(T)$ rescaled with the ideal-gas logarithmic factor. (c) Inverse R_0.

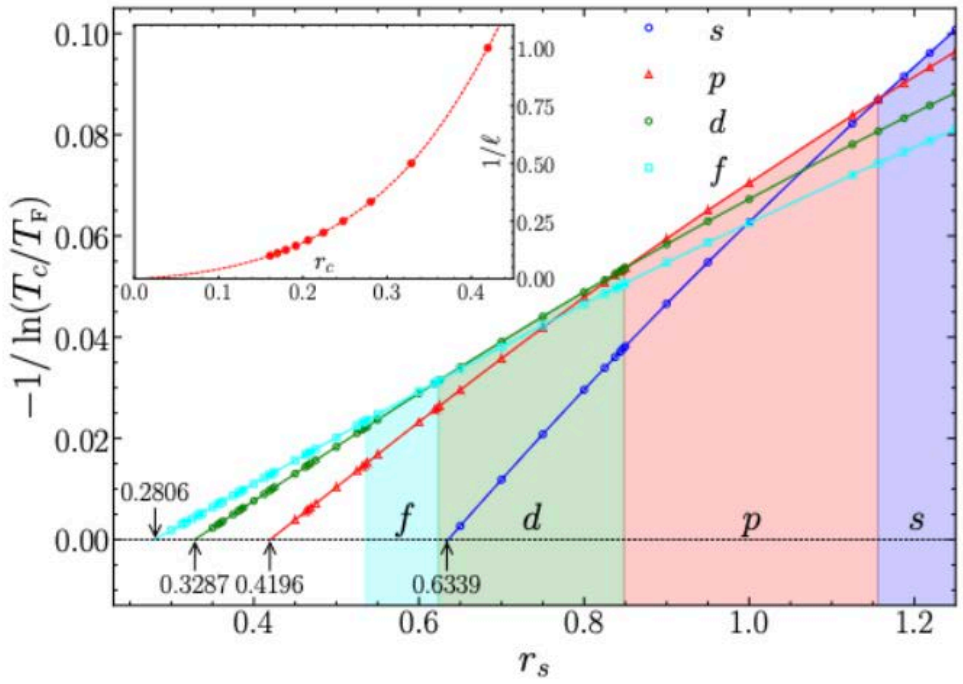


FIG. 3. Superconducting phase diagram of the 2D UEG. For each channel, the line starting at QTP shows the (would-be) critical temperature. Critical values of r_s for ℓ as large at 10 are presented in the inset.

Conclusions II

Pair susceptibility (linear response to a static spatially uniform pair-creating perturbation) of the normal Fermi liquid features universal for all BCS superconductors temperature dependence:

$$\chi_0(T) = \frac{c \ln(\Lambda/T)}{1 + g \ln(\Lambda/T)} \qquad (|g| \ll 1, \quad T_c < T \ll \Lambda)$$

This ansatz applies to both stable and unstable pairing channels. In both cases, the higher-temperature part of the flow is the same, up to small corrections, and represents singular in the $T \to 0$ limit response of an ideal Fermi liquid.

A sharp difference between the stable and unstable cases develops only at exponentially low temperatures: the unstable channel hits finite-temperature singularity at T_c while the stable channel develops non-trivial correlations suppressing the zero-temperature singularity.

The $T = 0$ singularity survives only at the quantum transition points separating the stable and unstable regimes.

Powerful tool for numeric simulations (with Drag MC) and quantum emulations (with ultracold atoms).

Might also be generalized to the proximity tunneling setups.