Dispelling a myth: Fermi liquids do not necessarily exhibit quasiparticle peaks in their spectra nor metallic behaviour

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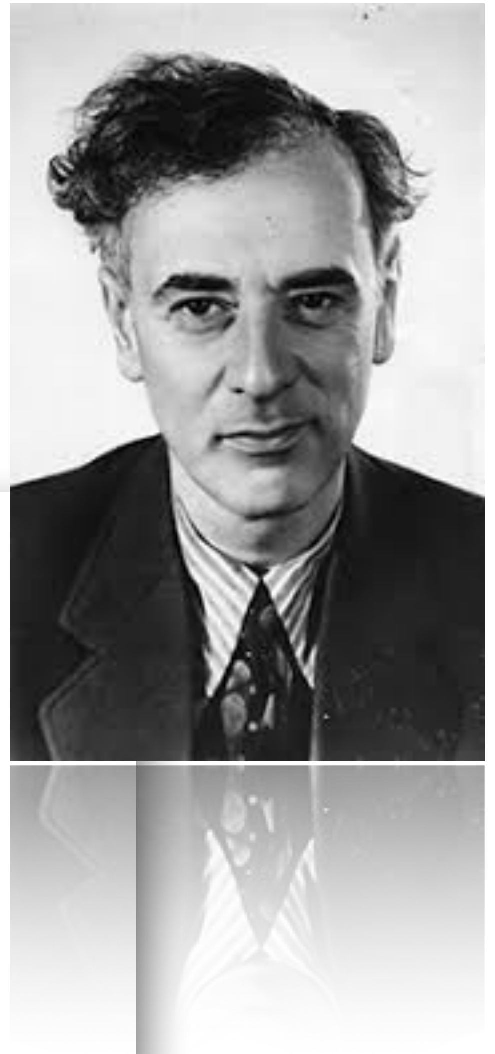
Outline

- Brief overview of Landau's Fermi liquid theory
- A closer look at the microscopic derivation of Nozières and Luttinger and its extension
- A case study: hypothetical non-symmetry breaking Mott insulator exhibiting metallic thermal and magnetic properties
- Conclusions

Landau's Fermi liquid theory

(Landau, 1957)



SOVIET PHYSICS JETP VOLUME 3, NUMBER 6 JANUARY, 1957

The Theory of a Fermi Liquid

L. D. LANDAU

Institute for Physical Problems, Academy of Sciences, USSR

(Submitted to JETP editor March 7, 1956)

J. Exptl. Theoret. Phys. (U.S.S.R.) **30**, 1058-1064 (June, 1956)

A theory of the Fermi liquid is constructed, based on the representation of the perturbation theory as a functional of the distribution function. The effective mass of the excitation is found, along with the compressibility and the magnetic susceptibility of the Fermi liquid. Expressions are obtained for the momentum and energy flow.

Chief paradigm of interacting electrons at low temperature

Landau derived his theory starting from a conjecture

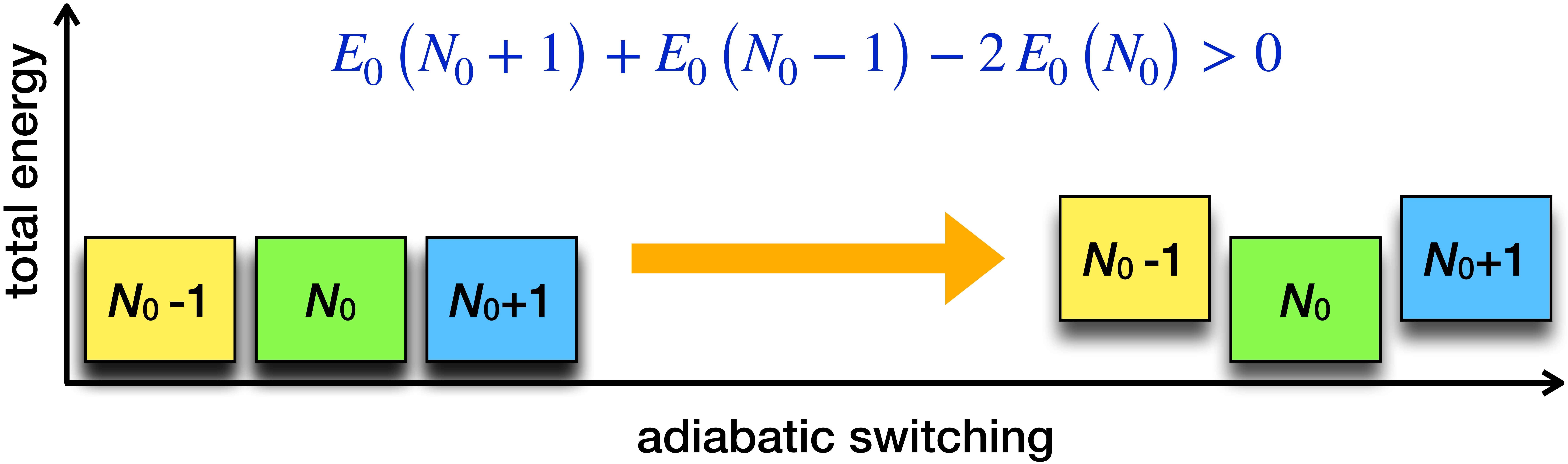
As a basis for the construction of the type of spectrum under consideration is the assumption that, as we gradually "turn on" the interaction between the atoms, i.e., in the transition from the gas to the liquid, classification of the levels remains invariant.

This simple assumption fully characterises the low energy, long wavelength physical properties of interacting electron systems.

A few points are worth noting

- The adiabatic conjecture holds separately in each symmetry subspace. States with different quantum numbers can well cross.
- Therefore, if the ground state resides in the subspace with N_0 electrons, Landau's adiabatic conjecture is not in contradiction with a charge-gap opening between the ground state and the lowest energy states with $N_0 + 1$ and $N_0 - 1$ electrons.

$$E_0\left(N_0+1\right)+E_0\left(N_0-1\right)-2\,E_0\left(N_0\right)>0$$



What then constitutes a sensible definition of a Landau-Fermi liquid?

A system of interacting electrons whose low-frequency, low-temperature and long-wavelength response functions can be obtained by an auxiliary interacting Hamiltonian, the *quasiparticle* Hamiltonian, treated within the Hartree-Fock plus random-phase approximation.

Microscopic justification of Landau's Fermi liquid theory

Nozières and Luttinger, 1962

PHYSICAL REVIEW VOLUME 127, NUMBER 5 SEPTEMBER 1, 1962

Derivation of the Landau Theory of Fermi Liquids. I. Formal Preliminaries*

P. Nozières
Ecole Normale Supérieure, Paris, France

AND

J. M. Luttinger
Columbia University, New York, New York

(Received Nobember 2, 1962)

The formal relationships necessary to derive the Landau theory of Fermi liquids are given. These include relationships between scattering functions for small energy and momentum transfers, vertex functions, and correlation functions. In addition certain identities (of the Ward type in quantum electrodynamics) are established which enable us to evaluate these quantities. Finally, the form of all these relationships when a long-ranged Coulomb force is present is given.

Key assumption of the microscopic derivation

- Dyson's equation relating retarded Green's function and self-energy

$$G(\epsilon, \mathbf{k}) = \frac{1}{\epsilon - \epsilon(\mathbf{k}) - \Sigma(\epsilon, \mathbf{k})}$$

- order by order in perturbation theory

$$\mathrm{Im}\,\Sigma(\epsilon, \mathbf{k}) \xrightarrow[\epsilon \to 0]{} -\gamma(\mathbf{k})\,\epsilon^2 \qquad\qquad \gamma(\mathbf{k}) > 0$$

- one assumes that such perturbative result holds true for the whole perturbative series, i.e., that the **perturbation series converges uniformly in $\epsilon = 0$**

A byproduct of that assumption

- single-particle spectrum for $\epsilon \simeq 0$ and $\mathbf{k} \simeq \mathbf{k}_F$

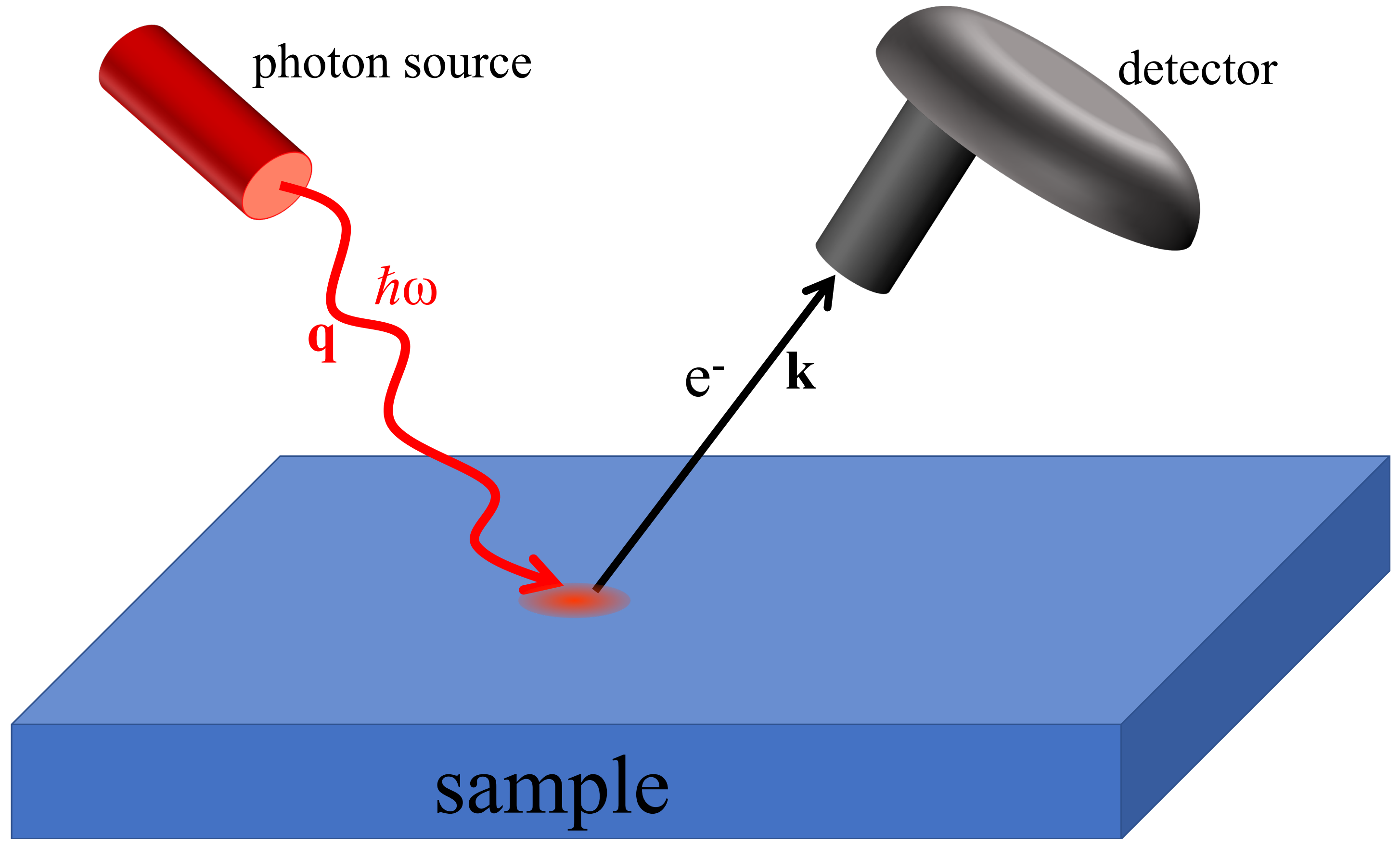
$$A(\epsilon,\mathbf{k}) = -\frac{1}{\pi}\,\mathrm{Im}\,G(\epsilon,\mathbf{k}) \xrightarrow[\epsilon\simeq 0\ \mathbf{k}\simeq\mathbf{k}_F]{} Z(\mathbf{k}_F)\,\delta\big(\epsilon - \boldsymbol{v}_{\mathbf{k}_F}\cdot(\mathbf{k}-\mathbf{k}_F)\big)$$

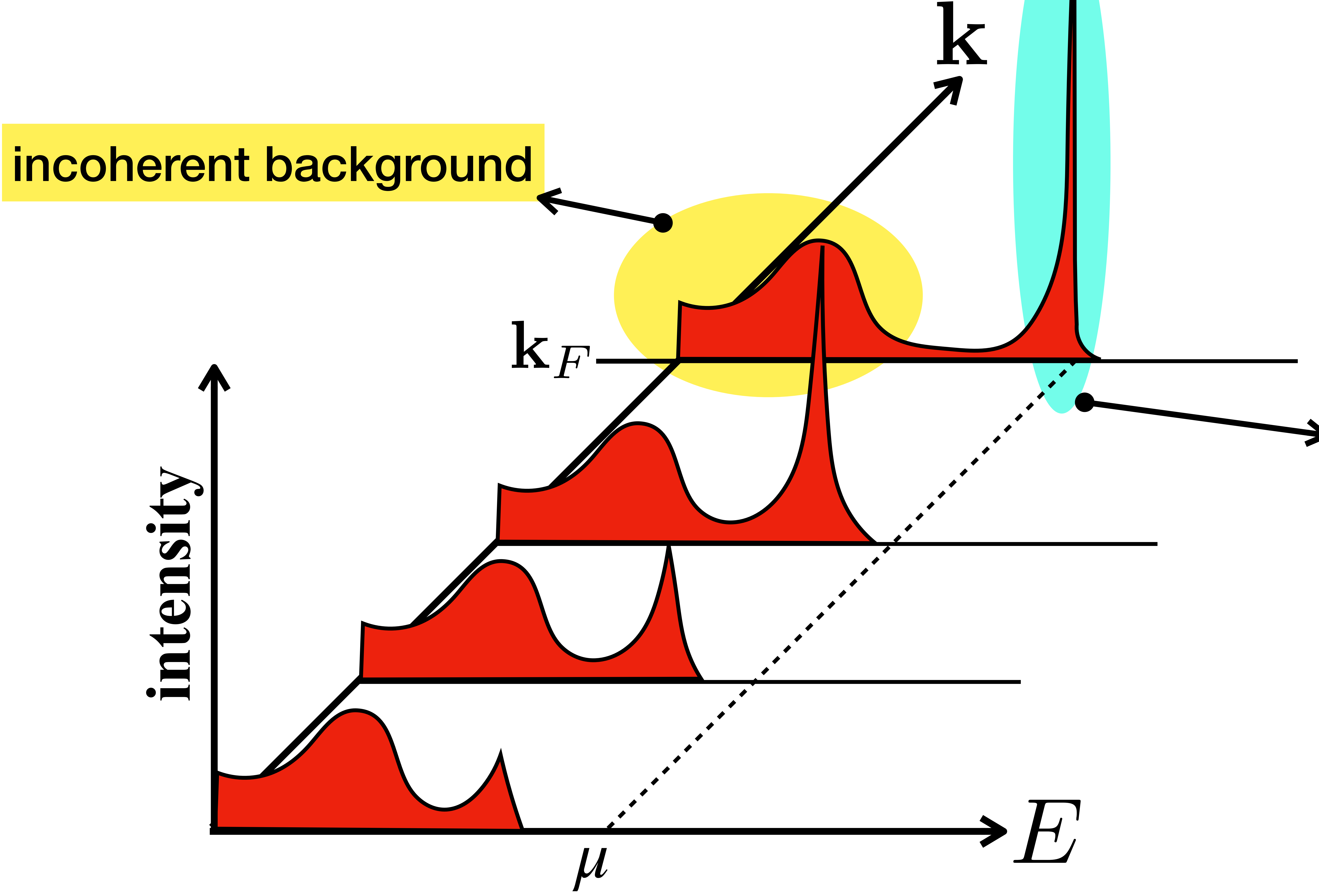
quasiparticle residue

where $\mathbf{k}_F$ defines the physical Fermi surface, i.e., the location in the Brillouin zone of the poles of $G(0,\mathbf{k})$ or, equivalently, the solution of the equation

$$\epsilon(\mathbf{k}_F) + \Sigma(0,\mathbf{k}_F) = 0$$

what that means, e.g., in ARPES





The absence of a quasiparticle peak in the single-particle spectrum, for example measured by ARPES, is therefore typically interpreted as a breakdown of Landau's Fermi liquid theory.

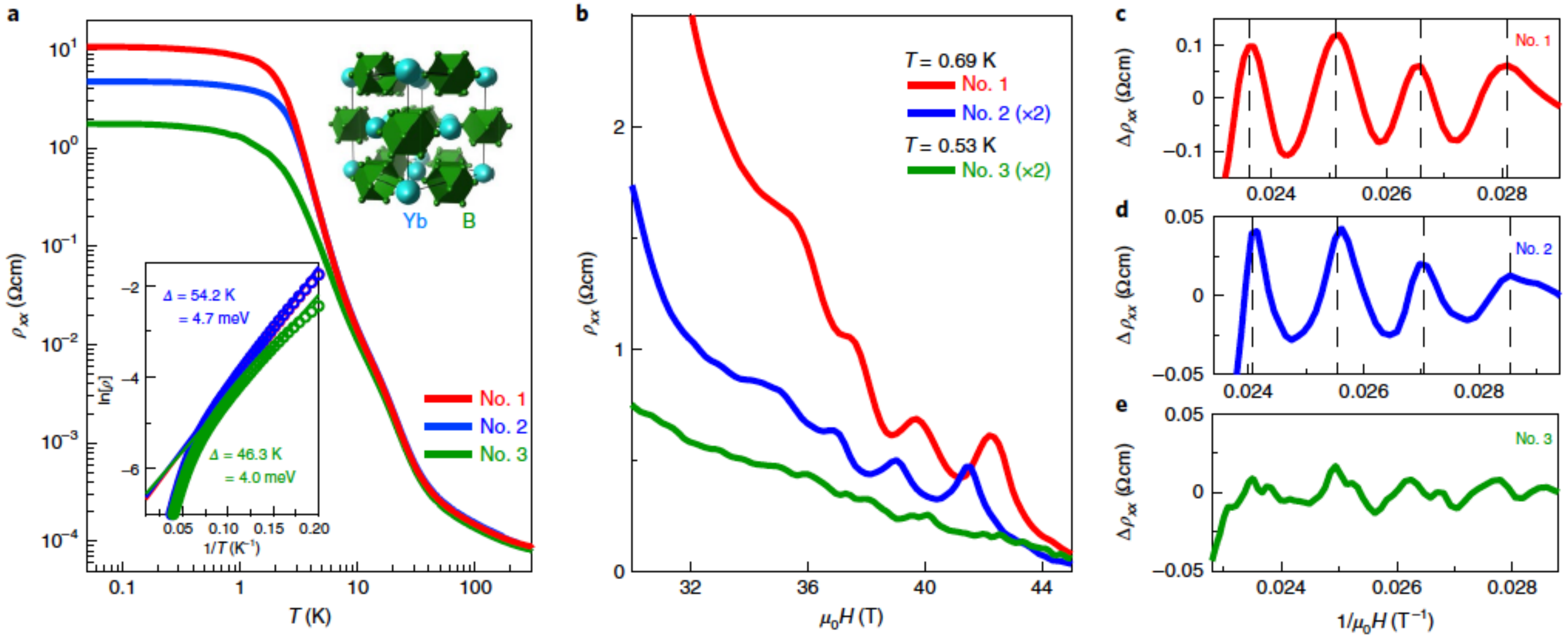
However, there exist strongly correlated materials that, despite lacking quasiparticle peaks in the spectrum, exhibit properties typical of conventional Fermi liquids, up to extreme cases of some correlated insulators.

NATURE PHYSICS | VOL 15 | SEPTEMBER 2019 | 954-959 |

nature physics

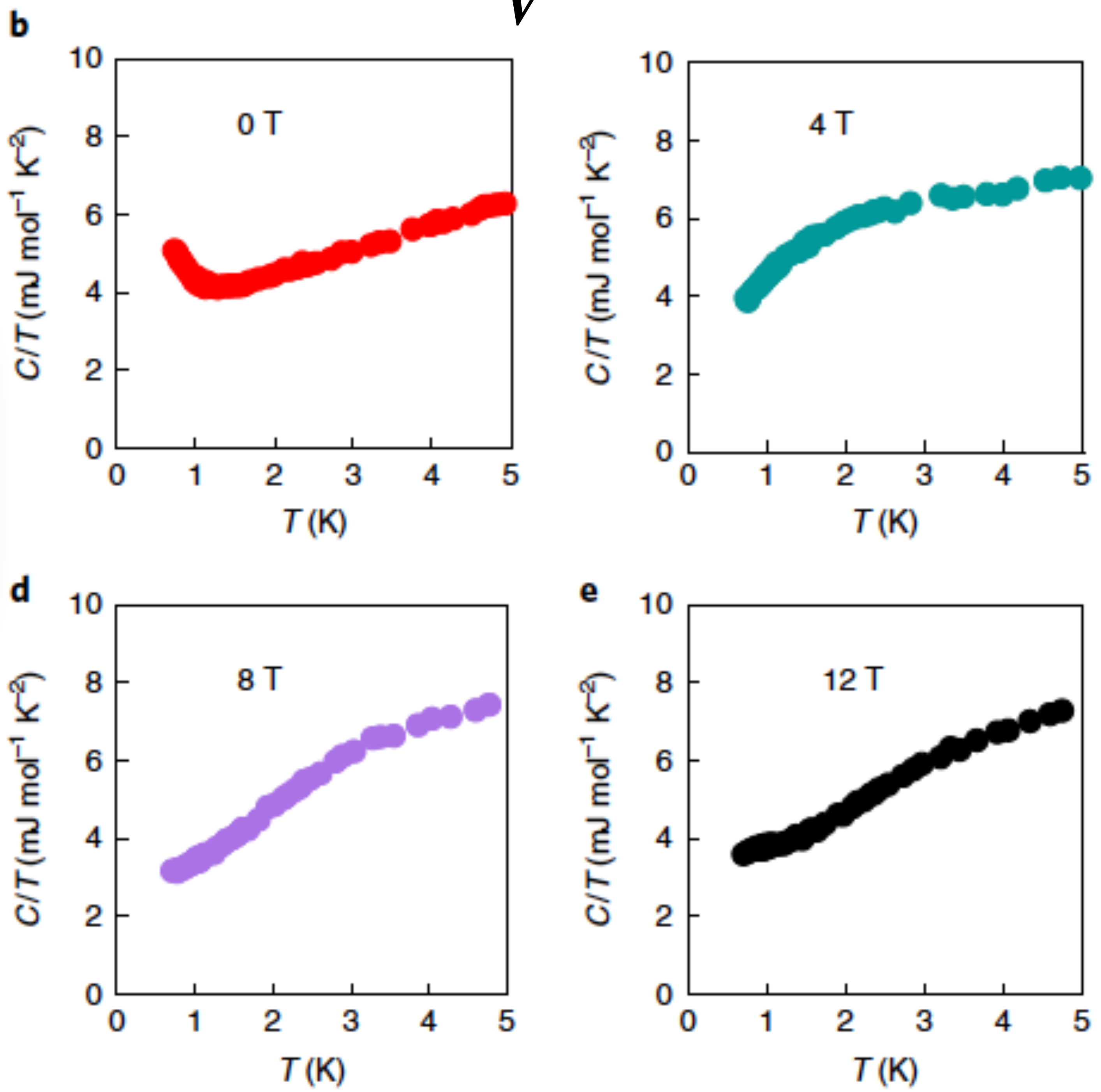
Unconventional thermal metallic state of charge-neutral fermions in an insulator

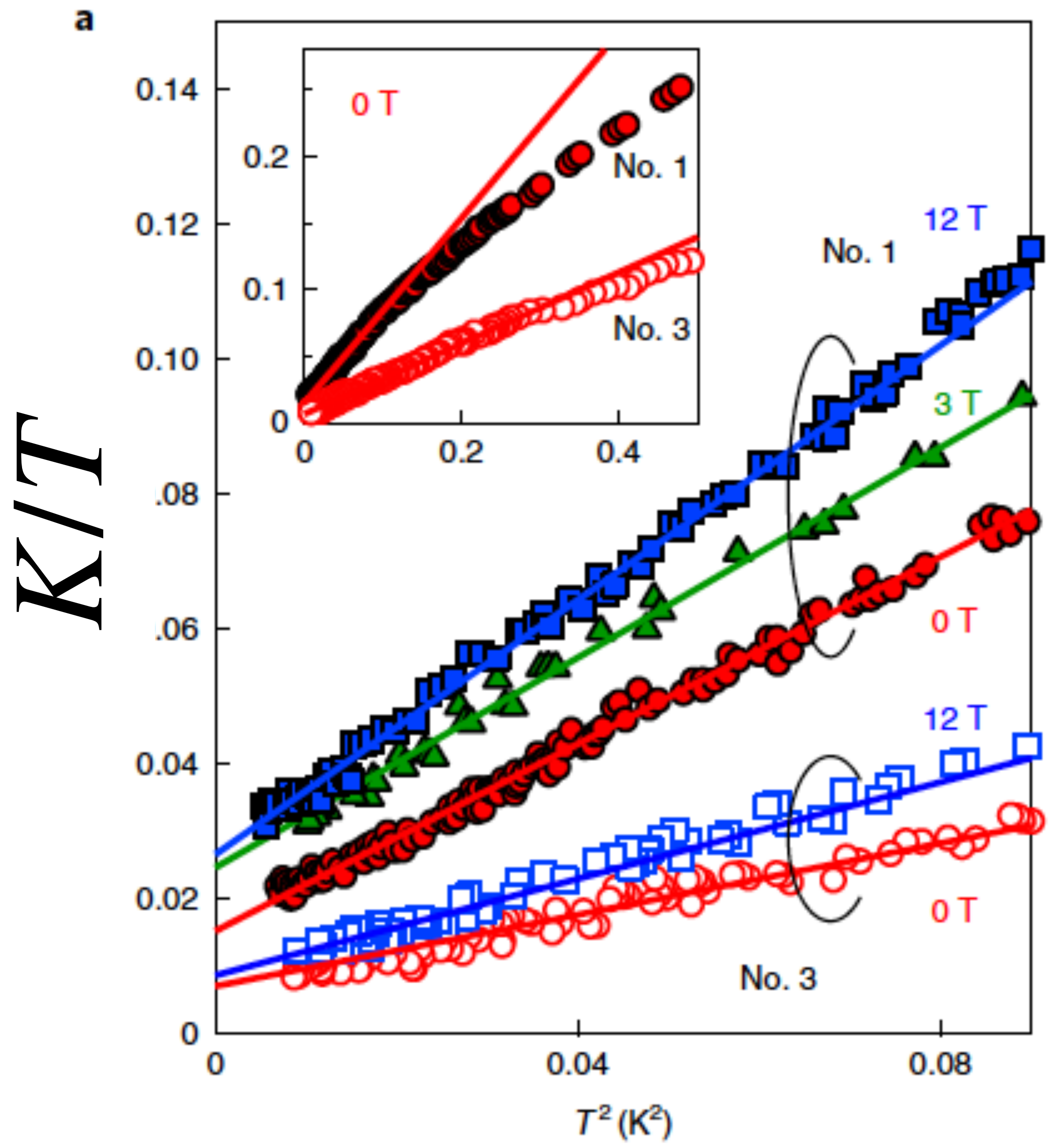
Y. Sato[1], Z. Xiang[2], Y. Kasahara[1], T. Taniguchi[1], S. Kasahara[1], L. Chen[2], T. Asaba[2,3], C. Tinsman[2], H. Murayama[1], O. Tanaka[4], Y. Mizukami[4], T. Shibauchi[4], F. Iga[5], J. Singleton[6], Lu Li[2*] and Y. Matsuda[1*]



YbB_{12}

c_V/T





quantum oscillations, linear in T specific heat and thermal conductivity

PHYSICAL REVIEW B **96**, 195131 (2017)

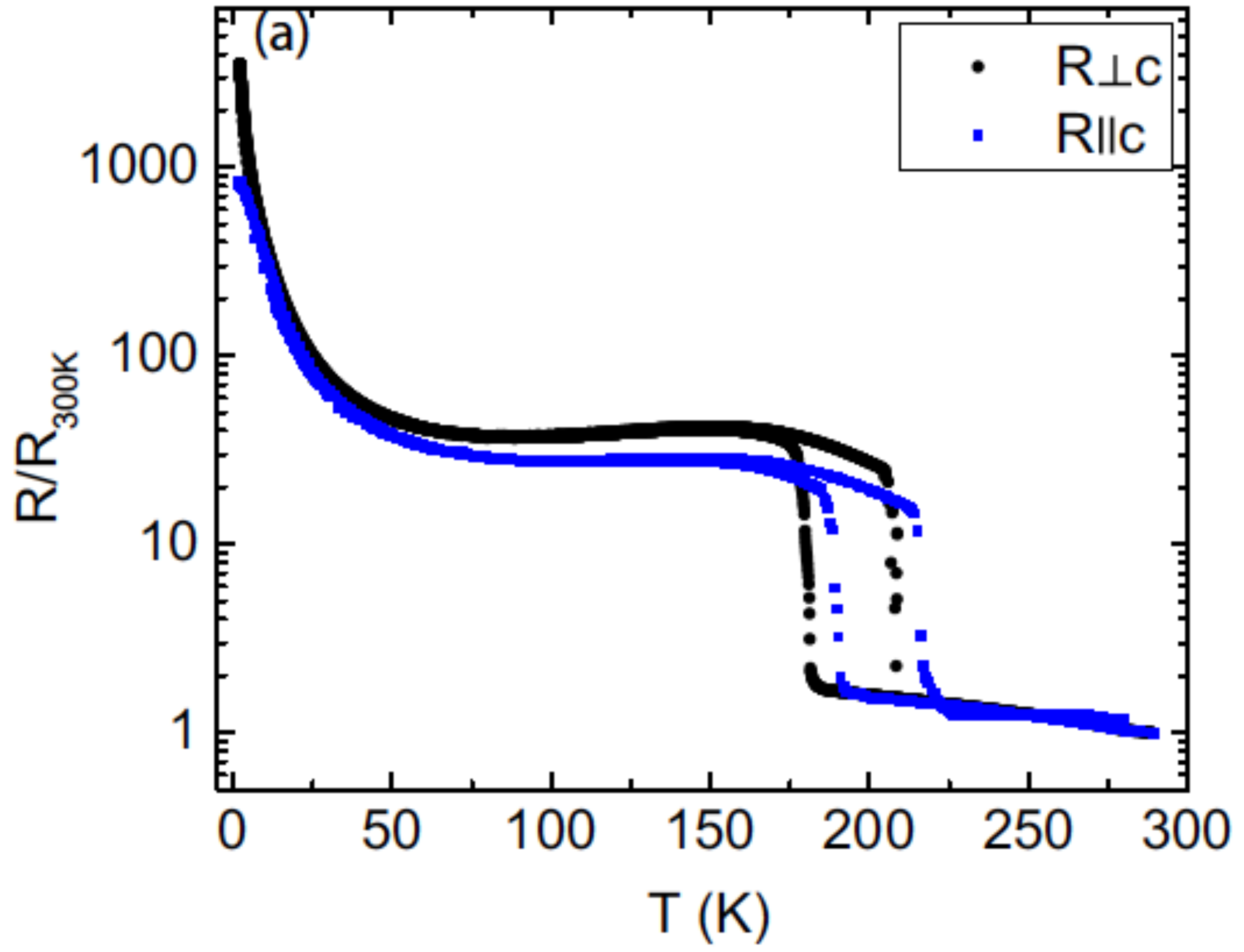
Gapless excitations in the ground state of 1*T*-TaS_2

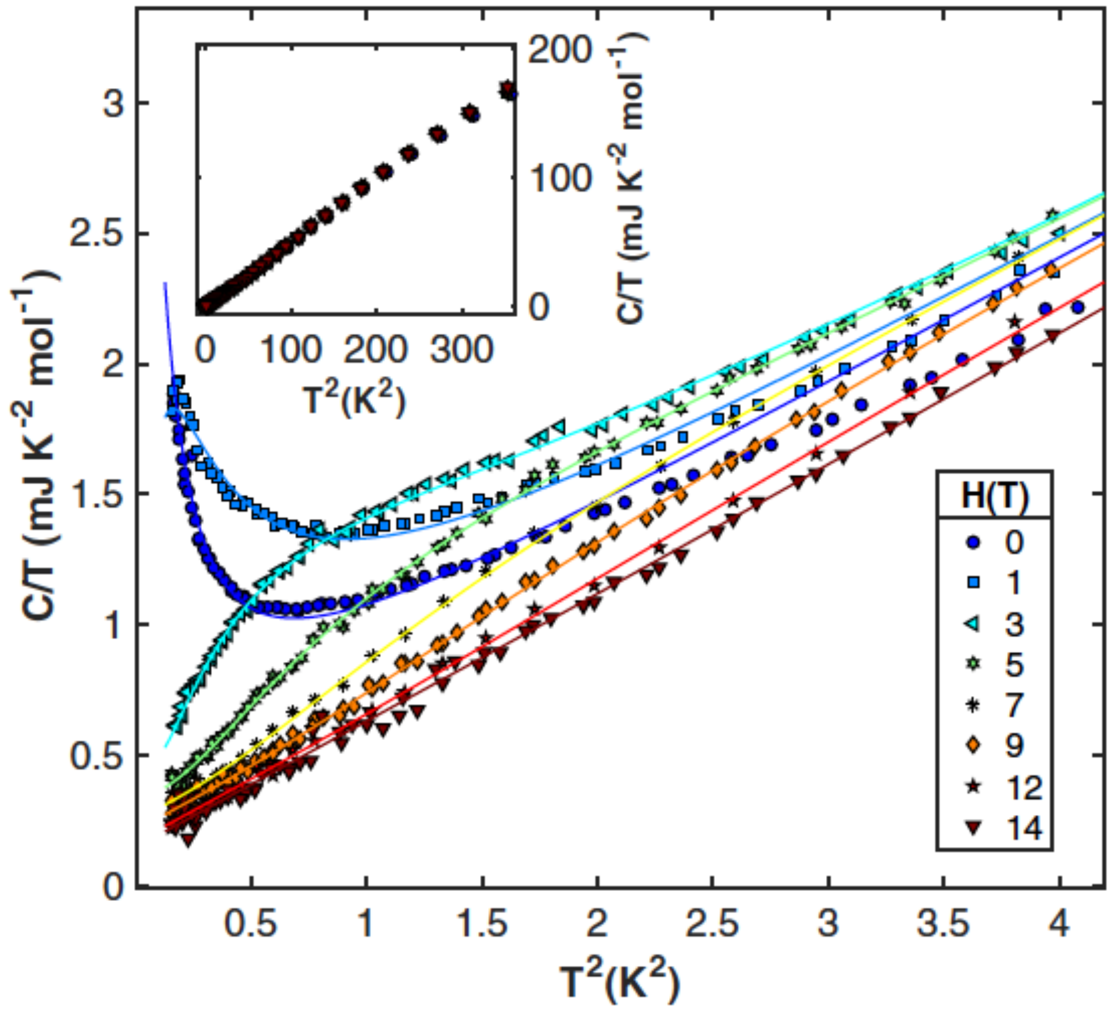
A. Ribak,[1] I. Silber,[2] C. Baines,[3] K. Chashka,[1] Z. Salman,[3] Y. Dagan,[2] and A. Kanigel[1]

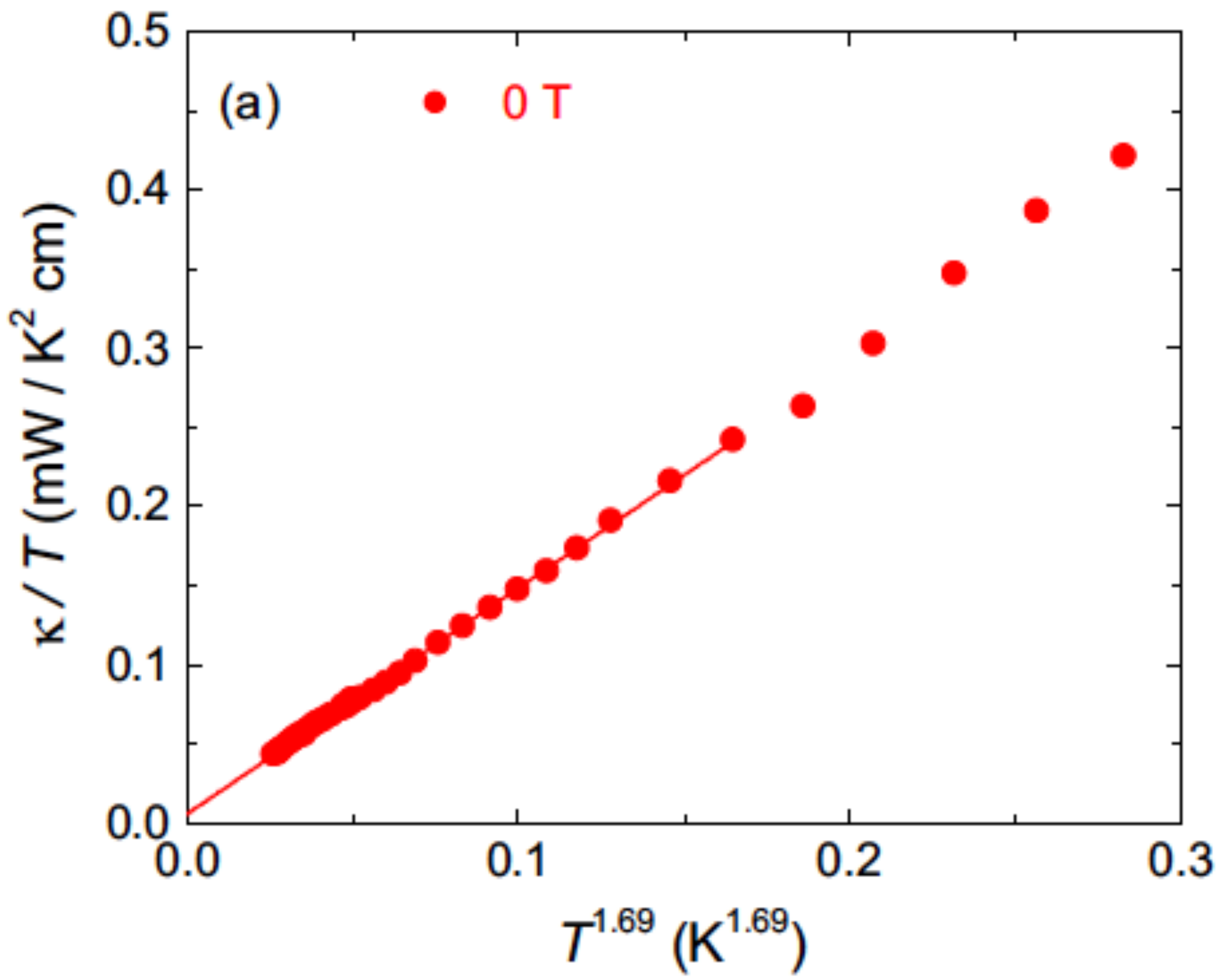
PHYSICAL REVIEW B **96**, 081111(R) (2017)

Heat transport study of the spin liquid candidate 1*T*-TaS_2

Y. J. Yu,[1] Y. Xu,[1] L. P. He,[1] M. Kratochvilova,[2,3] Y. Y. Huang,[1] J. M. Ni,[1] Lihai Wang,[4] Sang-Wook Cheong,[4] Je-Geun Park,[2,3] and S. Y. Li[1,5,*]







1T-TaS_2 is supposed to be a spin-liquid insulator, and yet has $c_V \sim T$ and $K \sim T$, with finite, though small, slope

Do these materials realise a state of matter distinct from Fermi liquids, or is the class of Landau's Fermi liquids broader than commonly believed?

A hint in that direction

- quasiparticles are well defined if, for $\epsilon \to 0$ and $\mathbf{k} \simeq \mathbf{k}_F$, their decay rate

$$\Gamma_*(\epsilon, \mathbf{k}) = -Z(\epsilon, \mathbf{k})\, \mathrm{Im}\Sigma(\epsilon, \mathbf{k}) = -\frac{\mathrm{Im}\Sigma(\epsilon, \mathbf{k})}{1 - \dfrac{\partial \mathrm{Re}\Sigma(\epsilon, \mathbf{k})}{\partial \epsilon}} \sim \epsilon^2$$

which holds true if

1. either $Z(0,\mathbf{k})$ is finite and $\mathrm{Im}\Sigma(\epsilon, \mathbf{k}) \sim -\epsilon^2$, as assumed by Nozières and Luttinger

2. or, $Z(\epsilon, \mathbf{k}) \sim \epsilon^2$ and $\mathrm{Im}\Sigma(0,\mathbf{k}) < 0$, in which case **quasiparticles are still well defined but they are invisible in the physical electron spectrum**

Let us therefore reexamine the microscopic derivation of Nozières and Luttinger

More convenient to switch to thermal Green's functions

$$G(i\epsilon, \mathbf{k}) = G(-i\epsilon, \mathbf{k})^* = \frac{1}{i\epsilon - \epsilon(\mathbf{k}) - \Sigma(i\epsilon, \mathbf{k})}$$

- $\epsilon = (2n+1)\,\pi\,T$ are Matsubara frequencies
- since $\Sigma(i\epsilon, \mathbf{k}) = \Sigma(-i\epsilon, \mathbf{k})^*$

$$\mathrm{Re}\,\Sigma(i\epsilon, \mathbf{k}) = \mathrm{Re}\,\Sigma(-i\epsilon, \mathbf{k}) \qquad \mathrm{Im}\,\Sigma(i\epsilon, \mathbf{k}) = -\mathrm{Im}\,\Sigma(-i\epsilon, \mathbf{k}) \begin{cases} < 0 & \epsilon > 0 \\ > 0 & \epsilon < 0 \end{cases}$$

which allows defining the *quasiparticle* residue

$$Z(\epsilon, \mathbf{k}) = Z(-\epsilon, \mathbf{k}) := \left(1 - \frac{\mathrm{Im}\,\Sigma(i\epsilon, \mathbf{k})}{\epsilon}\right)^{-1} \in [0, 1]$$

A novel exact representation of the thermal Green's function

- it readily follows that

$$G(i\epsilon, \mathbf{k}) \equiv \frac{Z(\epsilon, \mathbf{k})}{i\epsilon - \epsilon_*(\epsilon, \mathbf{k})} := Z(\epsilon, \mathbf{k})\; G_*(i\epsilon, \mathbf{k})$$

where $G_*(i\epsilon, \mathbf{k})$ looks like the Green's function of fictitious non-interacting *quasiparticles* with momentum-space dispersion

$$\epsilon_*(\epsilon, \mathbf{k}) = \epsilon_*(-\epsilon, \mathbf{k}) := Z(\epsilon, \mathbf{k}) \Big(\epsilon(\mathbf{k}) + \mathrm{Re}\,\Sigma(i\epsilon, \mathbf{k})\Big)$$

which is real and depends parametrically on ϵ such that, for $\epsilon \to \pm\infty$, it becomes the Hartree-Fock energy

Quasiparticle Fermi surface

$$G_*(i\epsilon, \mathbf{k}) = \frac{1}{i\epsilon - \epsilon_*(\epsilon, \mathbf{k})}$$

- the *quasiparticle* Fermi surface corresponds to the location in momentum space of the poles of $G_*(0,\mathbf{k}_{*F})$, i.e., of the roots of $\epsilon_*(0,\mathbf{k}_{*F})$

$$0 = \epsilon_*(0, \mathbf{k}_{*F}) = Z(0, \mathbf{k}_{*F}) \left(\epsilon(\mathbf{k}_{*F}) + \mathrm{Re}\,\Sigma(0, \mathbf{k}_{*F})\right)$$

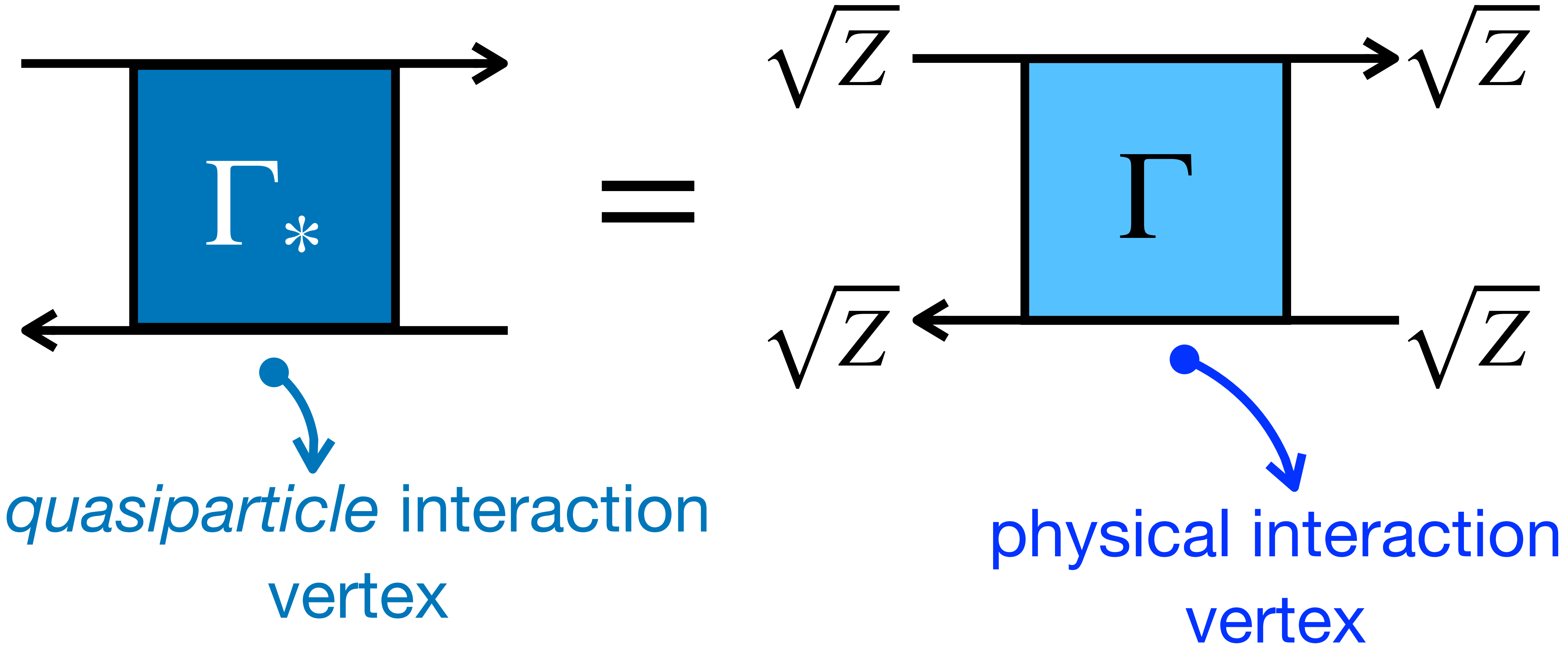
=0 equivalent to the physical Luttinger surface, i.e., the zeros of $G(0,\mathbf{k})$

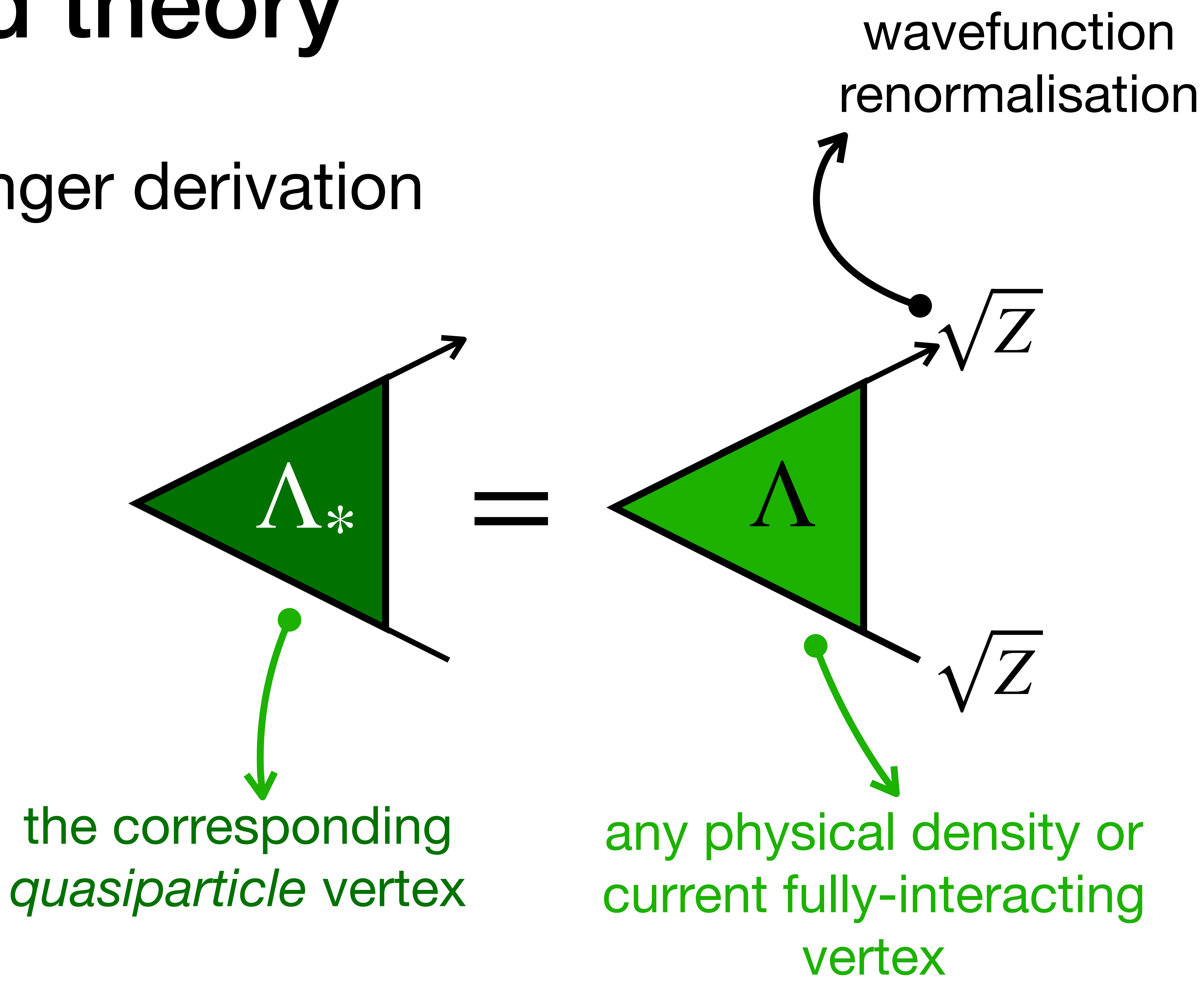
=0 equivalent to the physical Fermi surface, i.e., the poles of $G(0,\mathbf{k})$

in this representation the *quasiparticle* Fermi surface includes the physical Fermi surface as well as the Luttinger surface

Fermi-liquid theory

- straight generalisation of Nozières and Luttinger derivation





- having absorbed the *quasiparticle* residue into the interaction and density/current vertices, the Bethe-Salpeter equations can be rewritten solely in terms of the *quasiparticle* Green's function $G_*(i\epsilon, \mathbf{k})$ and of the *quasiparticle* vertices

Nozières and Luttinger performed an exact, non-perturbative manipulation of the Bethe-Salpeter equations for the dynamic (ω-limit) or static (q-limit) response functions that allows rewriting them in terms of the corresponding *quasiparticle* four-leg vertices, Γ_*^ω and Γ_*^q, and of the density/current vertices directly obtainable from the Ward-Takahashi identities.

The kernel of the resulting equations is simply

$$\Delta(i\epsilon, \mathbf{k}) := \lim_{\omega \to 0} \Big(G_*(i\epsilon + i\omega, \mathbf{k})\, G_*(i\epsilon, \mathbf{k}) - G_*(i\epsilon, \mathbf{k})\, G_*(i\epsilon, \mathbf{k}) \Big)$$

naïvely, it should vanish for $\omega \to 0$

$$\Delta(i\epsilon, \mathbf{k}) := \lim_{\omega \to 0} \overbrace{\Big(G_*(i\epsilon + i\omega, \mathbf{k})\, G_*(i\epsilon, \mathbf{k}) - G_*(i\epsilon, \mathbf{k})\, G_*(i\epsilon, \mathbf{k}) \Big)}$$

in reality, it does not since in the interval $-\omega \leq \epsilon \leq 0$ the function is singular

$$\Delta(i\epsilon, \mathbf{k}) := \lim_{\omega \to 0} \Big(\overbrace{G_*(i\epsilon + i\omega, \mathbf{k})\, G_*(i\epsilon, \mathbf{k}) - G_*(i\epsilon, \mathbf{k})\, G_*(i\epsilon, \mathbf{k})} \Big)$$

- specifically, if $\epsilon_*(\epsilon, \mathbf{k}) = \epsilon_*(-\epsilon, \mathbf{k})$ is analytic at $\epsilon = 0$, so that, for small ϵ,

$$\epsilon_*(\epsilon, \mathbf{k}) = \epsilon_*(0, \mathbf{k}) + O(\epsilon^2) \simeq \epsilon_*(0, \mathbf{k}) := \epsilon_*(\mathbf{k})$$

the actual energies of *quasiparticles*

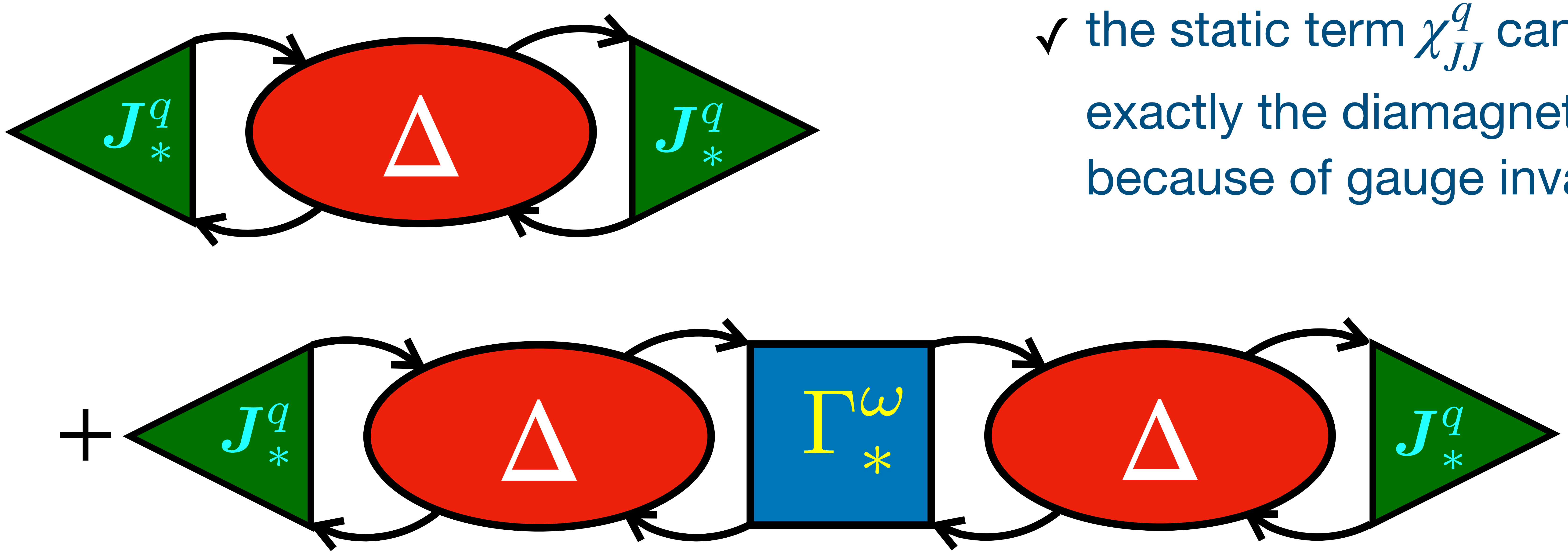
one readily finds that

$$\Delta(i\epsilon, \mathbf{k}) \equiv \frac{\delta_{\epsilon 0}}{T} \left(-\frac{\partial f\big(\epsilon_*(\mathbf{k})\big)}{\partial \epsilon_*(\mathbf{k})} \right) \simeq \delta\big(\epsilon_*(\mathbf{k})\big)$$

Fermi distribution function

- for instance, after Nozières and Luttinger manipulations, the dynamic limit of the current-current response function simply reads

$$\chi^{\omega}_{JJ} = \chi^{q}_{JJ} +$$



✓ the static term χ^{q}_{JJ} cancels exactly the diamagnetic one because of gauge invariance

where the static current vertex $\boldsymbol{J}^{q}_{*}(i\epsilon, \mathbf{k})$ is determined by the Ward-Takahashi identity

$$\boldsymbol{J}^{q}_{*}(i\epsilon, \mathbf{k}) = \boldsymbol{\nabla}_{\mathbf{k}}\epsilon_{*}(\epsilon, \mathbf{k}) + \big(i\epsilon - \epsilon_{*}(\epsilon, \mathbf{k})\big)\, \boldsymbol{\nabla}_{\mathbf{k}} \ln Z(\epsilon, \mathbf{k})$$

- the derivation thus relies on the assumption that $\epsilon_*(\epsilon, \mathbf{k})$ is an analytic function at $\epsilon = 0$, which holds under the condition that

$\Sigma(i\epsilon, \mathbf{k})$ is analytic in a finite interval around the origin, not including $\epsilon = 0$

and it is **less stringent** than Nozières and Luttinger assumption about the validity of perturbation theory, which instead requires that

$\Sigma(i\epsilon, \mathbf{k})$ is analytic in a finite interval around the origin, including $\epsilon = 0$

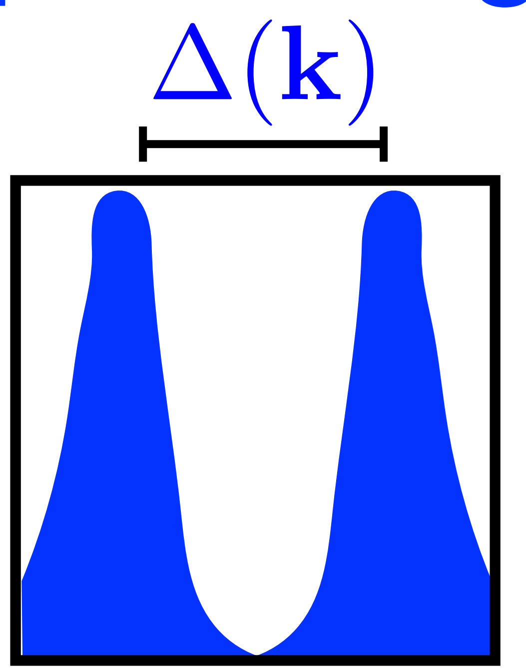
The crucial difference is that $\Sigma(i\epsilon, \mathbf{k})$ is allowed to have a pole at $\epsilon = 0$ without invalidating Landau's Fermi-liquid theory

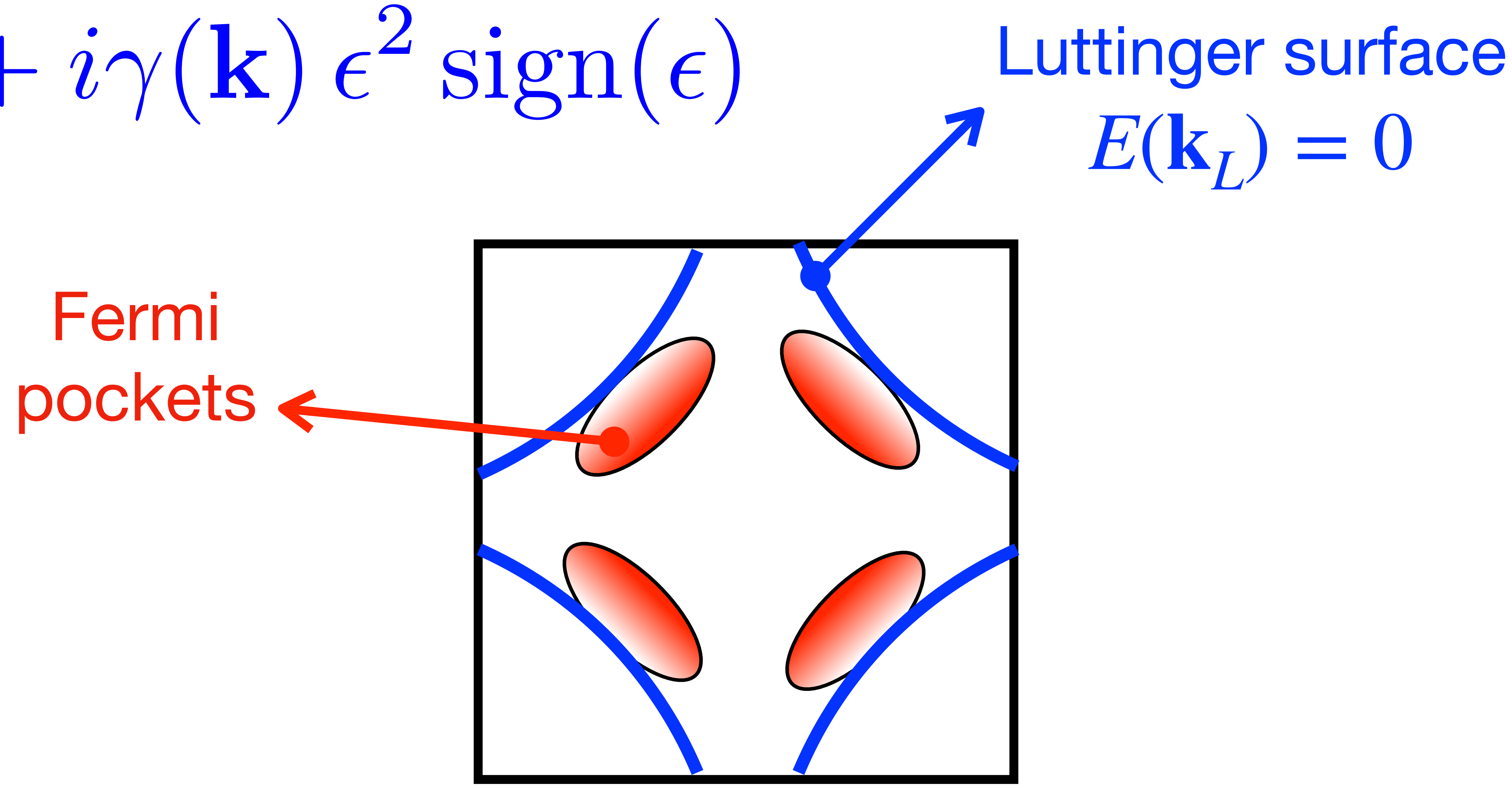
Even more, the derivation of Landau's Fermi liquid theory based on the more general analyticity assumption does not require the system to be metallic

- assuming that a Luttinger surface exists, the derivation works equally well if, for $\epsilon \to 0$,

$$\Sigma(i\epsilon, \mathbf{k}) \simeq \frac{\Delta(\mathbf{k})^2}{i\epsilon - E(\mathbf{k}) + i\gamma(\mathbf{k})\, \epsilon^2 \,\mathrm{sign}(\epsilon)}$$

describing a pseudo gapped metal

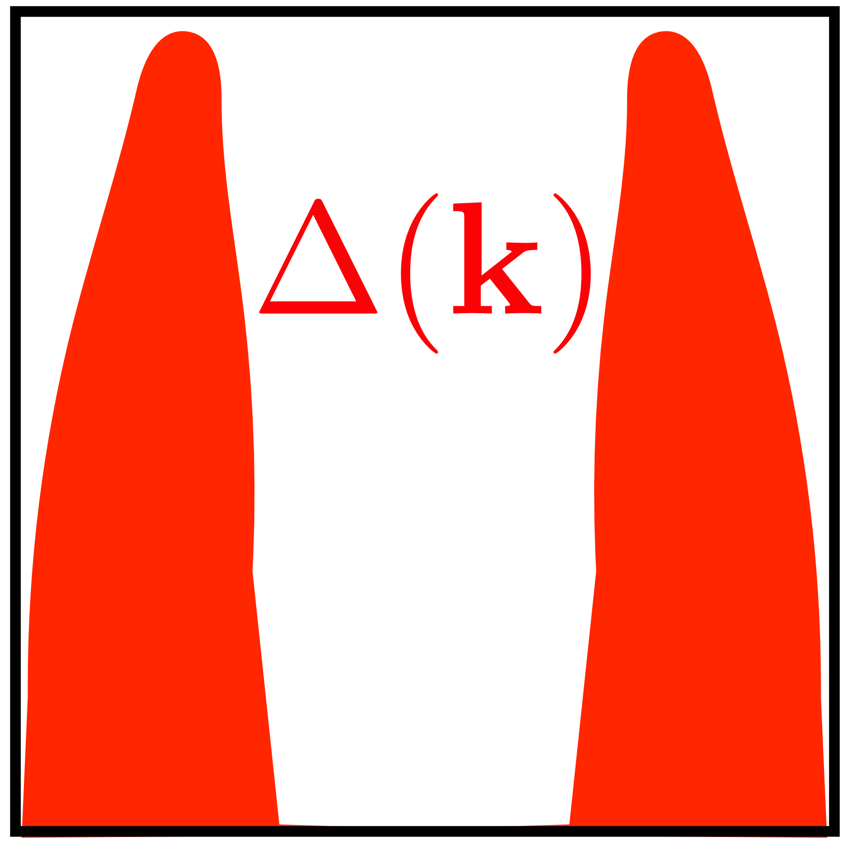




or, instead,

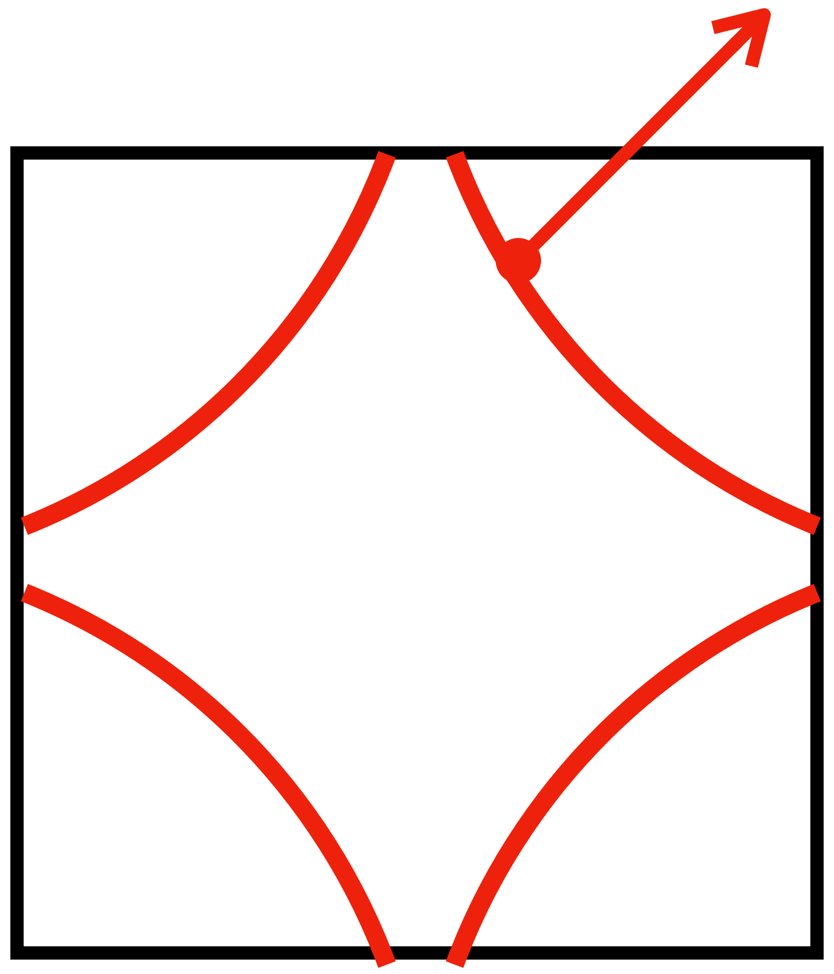
$$\Sigma(i\epsilon, \mathbf{k}) \simeq \frac{\Delta(\mathbf{k})^2}{i\epsilon - E(\mathbf{k})}$$

describing a hard-gap insulator



Luttinger surface

$E(\mathbf{k}_L) = 0$



Let us therefore assume a hypothetical single-band Mott insulator that does not break any symmetry and possesses a Luttinger surface.

Are the *quasiparticles* hosted by this surface compatible with the insulating character?

Fermi-liquid expressions of thermodynamic susceptibilities and transport coefficients

- charge compressibility $\kappa = \rho_* \left(1 - A_{\uparrow\uparrow} - A_{\uparrow\downarrow}\right)$
- charge Drude weight $D = e^2 D_* \left(1 + F^1_{\uparrow\uparrow} + F^1_{\uparrow\downarrow}\right)$
- spin susceptibility $\chi = \mu_B \rho_* \left(1 - A_{\uparrow\uparrow} + A_{\uparrow\downarrow}\right)$
- spin Drude weight $D_s = \mu_B D_* \left(1 + F^1_{\uparrow\uparrow} - F^1_{\uparrow\downarrow}\right)$
- specific heat $c_V = \pi^2 \rho_* T/3$
- heat Drude weight $D_E = \pi^2 D_* T/3$

$$A \propto \Gamma^q_*$$

$$F \propto \Gamma^\omega_*$$

quasiparticle DOS

$$\rho_* = \frac{2}{V} \sum_{\mathbf{k}} \delta\big(\epsilon_*(\mathbf{k})\big)$$

quasiparticle Drude weight

$$D_* = \frac{2\pi}{Vd} \sum_{\mathbf{k}} \delta\big(\epsilon_*(\mathbf{k})\big)\, \boldsymbol{\nabla}_{\mathbf{k}}\epsilon_*(\mathbf{k}) \cdot \boldsymbol{\nabla}_{\mathbf{k}}\epsilon_*(\mathbf{k})$$

Fermi-liquid expressions of thermodynamic susceptibilities and transport coefficients

- charge compressibility $\kappa = \rho_* \left(1 - A_{\uparrow\uparrow} - A_{\uparrow\downarrow}\right)$
- charge Drude weight $D = e^2 D_* \left(1 + F^1_{\uparrow\uparrow} + F^1_{\uparrow\downarrow}\right)$

✓ Mott's localisation implies that $A_{\uparrow\uparrow} \simeq 0$ and $F^1_{\uparrow\uparrow} \simeq 0$ by Pauli principle

✓ If there are well-defined *quasiparticles* then $\rho_* \neq 0$ and $D_* \neq 0$

✓ Since the system is nonetheless an insulator, thus κ and D must vanish, the only possibility is that $A_{\uparrow\downarrow} = 1$ and $F^1_{\uparrow\downarrow} = -1$

Fermi-liquid expressions of thermodynamic susceptibilities and transport coefficients

- charge compressibility $\kappa = \rho_* \left(1 - A_{\uparrow\uparrow} - A_{\uparrow\downarrow}\right) = 0$
- charge Drude weight $D = e^2 D_* \left(1 + F^1_{\uparrow\uparrow} + F^1_{\uparrow\downarrow}\right) = 0$
- spin susceptibility $\chi = \mu_B \rho_* \left(1 - A_{\uparrow\uparrow} + A_{\uparrow\downarrow}\right) = 2\,\mu_B \rho_*$
- spin Drude weight $D_s = \mu_B D_* \left(1 + F^1_{\uparrow\uparrow} - F^1_{\uparrow\downarrow}\right) = 2\,\mu_B D_*$
- specific heat $c_V = \pi^2 \rho_* T/3$
- heat Drude weight $D_E = \pi^2 D_* T/3$

$$A_{\uparrow\uparrow} = F^1_{\uparrow\uparrow} = 0$$
$$A_{\uparrow\downarrow} = -F^1_{\uparrow\downarrow} = 1$$

Wilson ratio

$$\mathrm{R_W} = \frac{\pi^2 T}{3\mu_B} \frac{\chi}{c_V} \simeq 2$$

Perfectly consistent with the insulating character

Do we know a concrete realisation of this physical scenario?

- The half-filled single-band Hubbard model in one dimension is a non-symmetry-breaking Mott insulator. It does possess a Luttinger surface at $k_{*F} = \pm\,\pi/2$ that in fact hosts *quasiparticles,* **the spinons**, giving rise to $c_V \sim T$, Pauli-like magnetic susceptibility and Wilson ratio $R_W \simeq 2$.

- In higher dimensions, it is very likely that the *quasiparticles* at the Luttinger surface become unstable at some temperature T_*. However, they could still be observed if T_* were much smaller than the *quasiparticle* degeneracy temperature T_{*F}.

Can *quasiparticles* at the Luttinger surface exhibit quantum oscillations?

… once again, Luttinger comes to our aid

THE PHYSICAL REVIEW

A journal of experimental and theoretical physics established by E. L. Nichols in 1893

SECOND SERIES, VOL. 121, NO. 5 — MARCH 1, 1961

Theory of the de Haas-van Alphen Effect for a System of Interacting Fermions*

J. M. LUTTINGER
Department of Physics, Columbia University, New York, New York

(Received October 17, 1960)

- Luttinger showed that the leading contribution in B/ϵ_F and T/ϵ_F to the oscillatory part of the free energy arises from

$$\Delta F_{\text{osc}} = T \sum_n \text{Tr}\Big(\ln G\big(i\epsilon_n, \mathbf{K}(\mathbf{r})\big)\Big)$$

- where the operator $G\big(i\epsilon, \mathbf{K}(\mathbf{r})\big)$ is obtained from the Green's function at $B = 0$, $G(i\epsilon, \mathbf{k})$, under the semiclassical substitution

$$\mathbf{k} \to \mathbf{K}(\mathbf{r}) = -i\hbar \frac{\partial}{\partial \mathbf{r}} + \frac{e}{2c} \mathbf{B} \wedge \mathbf{r}$$

$$\Delta F_{\mathrm{osc}} = T \sum_n \mathrm{Tr}\Big(\ln G\big(i\epsilon_n, \mathbf{K}(\mathbf{r})\big)\Big) = - T \sum_n \mathrm{Tr}\Big(\ln G\big(i\epsilon_n, \mathbf{K}(\mathbf{r})\big)^{-1}\Big)$$

poles and zeros of the operator $G(i\epsilon, \mathbf{K}(\mathbf{r}))$ equally contribute to the quantum oscillations, apart from an overall π-shift

Conclusions

- The class of Landau's Fermi liquids is broader than commonly believed.
- It may include states with hidden *quasiparticles* that are invisible in the physical single-particle spectrum, do not contribute to charge transport, and yet exhibit Fermi-liquid-like thermal and magnetic properties, including quantum oscillations in a magnetic field.

Thanks