DISORDER AND TRANSPORT IN STRANGE METALS -LESSONS FROM THEORY AND COMPUTATION

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C. Li, D. Valentinis, A. A. P., H. Guo, J. Schmalian, S. Sachdev, I. Esterlis arXiv:2406.07608





Principles and phenomenology

Metals



Fermi surface (*k*-space: translationally invariant metals)

- States of fermionic matter at finite density.
- Compressible: $\partial Q/\partial \mu \neq 0$ as $T \to 0$.
- Large number of gapless excitations (the most gapless systems!).

Fermi liquid theory





$$G_{\psi}(\mathbf{k}, i\omega) = \frac{Z}{i\omega - \varepsilon(\mathbf{k}) + i\Gamma} \qquad \Gamma \sim \max(\omega^2, T^2)$$

Fermions interact with gapped boson and become renormalized quasiparticles.

Fermi liquid theory

Screened interaction is similar to a weak contact interaction





$$\Gamma \sim \max(\omega^2, T^2)$$
 $\Gamma \ll \max(\omega, T)$

The small damping rate means that fermion quasiparticles are well defined additive excitations in a Fermi liquid (d > 1)

The momentum bottleneck



- Current carries momentum
- Resistance requires current relaxation -> momentum relaxation



• Generic sources of momentum relaxation in solids: Umklapp, phonons, disorder. Translational invariance has to be broken.

Transport in conventional metals

- Low $T: \rho(T) \sim T^2$ from Fermi liquid Umklapp processes.
- High $T: \rho(T) \sim T$ from phonons
- Residual resistivity $\rho(0) > 0$ from impurities

• Both Umklapp and phonons are "gapped" $2k_F$ processes that can't produce anything more than $\rho(T) \sim T^2$ at low T





Strange metals



- 2D or quasi-2D (layered) materials.
- T-linear electrical resistivity
- Sometimes proximate to putative quantum critical points.

Transport in strange metals

<u>*T*-linear resistivity down to $T \rightarrow 0$ </u>



Transport in strange metals

Inelastic scattering from optical measurements



$$\sigma(\omega) = \frac{K}{\frac{1}{\tau(\omega)} - i\omega \frac{m^*(\omega)}{m}}$$
$$\frac{1}{\tau(\omega)} \propto |\omega| \Phi\left(\frac{\hbar\omega}{k_B T}\right)$$

Large, frequency dependent (therefore inelastic) scattering rate in optical conductivity.

Also seen in photoemission

(Reber et al, Nat. Comm. 10, 5737 (2019))

Michon et al, Nat. Comm. 14, 3033 (2023)

Transport constraints in strange metals

- Need T-linear DC resistivity at low T
- Finite DC resistivity requires momentum relaxation
- -> 3 generic options: Umklapp, phonons, disorder
- Finite activation gap for phonons and Umklapp \rightarrow weak scattering at low T, doesn't give T-linear as $T \rightarrow 0$

Transport constraints in strange metals

- Furthermore, ω -linear AC scattering rate
- -> Inelastic scattering
- Electron-phonon scattering is elastic in *T*-linear regime
- Electron-potential disorder scattering is also elastic

Transport constraints in strange metals

- None of phonons, Umklapp, potential disorder seem to work
- Disordered <u>interactions</u> can overcome inadequacies of these mechanisms, by providing momentum-relaxing inelastic scattering that can be strong at low T

Origin of Disordered Interactions

A simple example



• Randomness in hopping strengths leads to randomness in exchange interactions.

Microscopic disorder in correlated electron materials



34nm

Randomness in dopant and charge density in cuprates

Campi et al, Nature **525**, 359–362 (2015)

Twist angle disorder in moiré materials

Andrei and MacDonald, Nat. Mater. 19, 1265–1275 (2020)

• These can lead to randomness in hopping strengths (and also randomness in U itself) in effective Hubbard-type models

Zhou and Ceperley, Phys. Rev. A 81, 013402 (2010)

Theoretical models

non-Fermi Liquid Metal

Strong electron-electron interactions



non-Fermi Liquid Metal

$$\mathcal{L} = \psi_{\mathbf{k}}^{\dagger} \left(\frac{\partial}{\partial \tau} + \varepsilon(\mathbf{k}) \right) \psi_{\mathbf{k}} + \frac{1}{2} \left[(\partial_{\tau} \phi)^2 + (\nabla \phi)^2 + (\lambda - \lambda_c) \phi^2 \right]$$

"Yukawa" coupling: $g \int d^2 r d\tau \, \psi^{\dagger}(r, \tau) \psi(r, \tau) \phi(r, \tau)$

Eliashberg solution for electron (G) and boson (D) Green's functions at small ω :

$$\Sigma(\hat{k}, i\omega) \sim -i \operatorname{sgn}(\omega) |\omega|^{2/3}, \quad G(k, i\omega) = \frac{1}{i\omega - \varepsilon(k) - \Sigma(\hat{k}, i\omega)}, \quad D(q, i\Omega) = \frac{1}{\Omega^2 + q^2 + \gamma |\Omega|/q} \quad \text{P.A. Lee, Phys. Rev. Lett 63, 680 (1989)}$$
(in two spatial dimensions)
Strong inelastic forward scattering, no well-defined quasiparticles, but no momentum relaxation.
(Boson is massless but damped at QCP)

Translationally invariant, $\rho_{DC}(T) = 0$.

I. Esterlis, H. Guo, A. A. P and S. Sachdev, <u>Phys. Rev. B 103, 235129 (2021)</u>
H. Guo, A. A. P., I. Esterlis and S. Sachdev, <u>Phys. Rev. B 106, 115151 (2022)</u>

Strong and disordered electron-electron interactions

$$\mathcal{L} = \psi_{\mathbf{k}}^{\dagger} \left(\frac{\partial}{\partial \tau} + \varepsilon(\mathbf{k}) \right) \psi_{\mathbf{k}} + \frac{1}{2} \left[(\partial_{\tau} \phi)^2 + (\nabla \phi)^2 + (\lambda - \lambda_c) \phi^2 \right]$$

Random potential $\int d^2 r d\tau \, v(r) \, \psi^{\dagger}(r, \tau) \psi(r, \tau)$
"Yukawa" coupling: $\int d^2 r d\tau \, \left[g + g'(r) \right] \psi^{\dagger}(r, \tau) \psi(r, \tau) \phi(r, \tau)$

Spatially random Yukawa coupling g'(r) with $\overline{g'(r)} = 0$, $\overline{g'(r)g'(r')} = g'^2\delta(r-r')$

• Hubbard-Stratonovich decomposition of random 4-Fermi term (such as exchange) produces random Yukawa coupling.

> A. A. P., H. Guo, I. Esterlis and S. Sachdev, Science 381 (6659) 790-793 (2023)

Strong and disordered electron-electron interactions



• Self-consistent 1-loop calculation (Eliashberg), equivalent to a large-N saddle point

A. A. P., H. Guo, I. Esterlis and S. Sachdev, Science 381 (6659) 790-793 (2023)





Conductivity:
$$\sigma(\omega) \sim [1/\tau_{\text{trans}}(\omega) - i\omega m^*(\omega)/m]^{-1}$$

 $\frac{1}{\tau_{\text{trans}}(\omega)} \sim v^2 + g'^2 |\omega| \quad ; \quad \frac{m^*(\omega)}{m} \sim \frac{2g'^2}{\pi} \ln(\Lambda/\omega)$
Residual resistivity is determined by v^2 ; Linear-in-*T* resistivity determined by g'^2 .

C. Li, D. Valentinis, A. A. P., H. Guo, J. Schmalian, S. Sachdev, I. Esterlis arXiv:2406.07608

Numerics beyond mean-field/Eliashberg

Model for sign-free Quantum Monte Carlo

$$\begin{split} \mathcal{S}[\boldsymbol{\phi}, \boldsymbol{\psi}, \boldsymbol{\psi}^{\dagger}] &= \int d\tau \sum_{\boldsymbol{r}, \boldsymbol{r}'} \sum_{\alpha = a, b} \sum_{\sigma = \uparrow, \downarrow} \sum_{j=1}^{2} \psi_{\alpha, \sigma, j, \boldsymbol{r}}^{\dagger} \left[(\partial_{\tau} - \mu_{\alpha}) \delta_{\boldsymbol{r}, \boldsymbol{r}'} - t_{\alpha, \boldsymbol{r}, \boldsymbol{r}'} \right] \psi_{\alpha, \sigma, j, \boldsymbol{r}'} \\ &+ \int d\tau \sum_{\boldsymbol{r}} \left[\frac{1}{2c^{2}} (\partial_{\tau} \boldsymbol{\phi}_{\boldsymbol{r}})^{2} + \frac{1}{2} (\nabla \boldsymbol{\phi}_{\boldsymbol{r}})^{2} + \frac{\lambda}{2} (\boldsymbol{\phi}_{\boldsymbol{r}})^{2} + \frac{u}{4} (\boldsymbol{\phi}_{\boldsymbol{r}} \cdot \boldsymbol{\phi}_{\boldsymbol{r}})^{2} \right] \\ &+ \frac{1}{\sqrt{2}} \sum_{\sigma, \sigma' = \uparrow, \downarrow} \sum_{j=1}^{2} \int d\tau \sum_{\boldsymbol{r}} g_{\boldsymbol{r}}' \; e^{i\boldsymbol{Q}_{\mathrm{AF}} \cdot \boldsymbol{r}} \; \boldsymbol{\phi}_{\boldsymbol{r}} \cdot \left[\psi_{\alpha, \sigma, j, \boldsymbol{r}}^{\dagger} \; \boldsymbol{\tau}_{\sigma, \sigma'} \; \psi_{b, \sigma', j, \boldsymbol{r}} + \mathrm{h.c.} \right]. \end{split}$$



Two-band structure: Berg, Metlitski, Sachdev, Science **338** 1606-1609 (2012).

A. A. P., P. Lunts, M. Albergo, arXiv:2408.xxxxx

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• Integrate out fermions
$$\psi$$
: $\mathcal{Z} = \int \mathcal{D}[\phi] e^{-S_B[\phi]} \det[A(\phi)]$

 $\bullet~A$ is Hermitian positive definite, legitimate probability distribution.

Facing the determinant

- Need large system size to see enough disorder
- Lattice: L^2 sites, N_t imaginary time points.
- Compute det[A] directly: $O(L^6N_t^3)$ cost, very bad.
- Usual determinant QMC method with low-rank updates: $O(L^6N_t)$.
- Requires storing and applying an extensively-sized dense matrix A^{-1} , prohibitive memory and bandwidth costs for large L, N_t .

Hybrid Monte Carlo

$$\mathcal{Z} = \int \mathcal{D}[\vec{\phi}] e^{-S_B[\vec{\phi}]} \det[A(\vec{\phi})]$$
$$\mathcal{Z} = \int \mathcal{D}[\vec{\phi}] \mathcal{D}[\varphi, \varphi^*] e^{-S_B[\vec{\phi}]} e^{-\varphi^* A^{-1}(\vec{\phi})\varphi}$$

- Avoid evaluating det by sampling over $\varphi.$
- Solve linear system with A at each step to determine $A^{-1}(\vec{\phi})\varphi$.
- Cost of the (iterative) linear solve depends upon the condition number of A which can become large at low T, preconditioning is generally required.
- Uses far less memory and bandwidth, GPU friendly, $O(L^2 N_t^{a \gtrsim 1})$, scales to large sizes
- We go up to L = 40, $N_t = 800$ ($\beta = 80$).

Hybrid Monte Carlo

$$\mathcal{Z} = \int \mathcal{D}[\vec{\phi}] \mathcal{D}[\varphi, \varphi^*] e^{-S_B[\vec{\phi}]} e^{-\varphi^* A^{-1}(\vec{\phi})\varphi}$$

- Sample φ from distribution, use fictitious Hamiltonian dynamics to update $\phi,$ repeat iteratively.

$$\frac{d\phi}{dt} = M^{-1}\pi$$
 and $\frac{d\pi}{dt} = -\frac{\partial S(\phi, \varphi)}{\partial \phi}$ (randomly sampled fictitious momentum π)

- Integrator time step size and number of steps are chosen in a warmup phase to maximize change in ϕ . (P. Lunts et al, Nat. Comm. 14, 2547 (2023)).
- M^{-1} is set equal to a running estimate of the $\vec{\phi}$ propagator for optimal updates (P. Lunts et al, Nat. Comm. 14, 2547 (2023)).

S. Duane et al, Phys. Lett. B **195**, 216-222 (1987) P. Lunts et al, Nat. Comm. **14**, 2547 (2023)

Mean-field (Eliashberg) phase diagram



A. A. P., H. Guo, I. Esterlis and S. Sachdev, Science 381 (6659) 790-793 (2023)

C. Li, D. Valentinis, A. A. P., H. Guo, J. Schmalian, S. Sachdev, I. Esterlis, arXiv:2406.07608

Non-perturbative phase diagram



Non-perturbative phase diagram



- Extended region of *T*-linear resistivity (λ_s < λ < λ_G)
- Gapless SRO boson phase, eventual crossover to LRO for $\lambda < \lambda_*$, no sharp QPT to LRO.

Dirty bosons

• Key to new physics: strongly disordered bosons at low energies



$$D(i\omega_n = 0, \mathbf{q}_1, \mathbf{q}_2 \neq \mathbf{q}_1) \neq 0$$

A. A. P., P. Lunts, M. Albergo, arXiv:2408.xxxx

Boson density of states



A. A. P., P. Lunts, M. Albergo, arXiv:2408.xxxxx

Boson density of states



- Gapless constant low-energy DOS for $\lambda_s < \lambda < \lambda_G$ similar to $\lambda = \lambda_c$ in mean field (quadratic dispersion in 2D)
- But, boson eigenmodes are not planewave states
- Spatial correlation length is <u>not</u> large
- Not a QCP

Boson eigenmodes



A. A. P., P. Lunts, M. Albergo, arXiv:2408.xxxxx

Boson eigenmodes



• Gradual crossover to LRO for $\lambda < \lambda_*$ associated with localized low-energy modes slowly delocalizing again

A. A. P., P. Lunts, M. Albergo, arXiv:2408.xxxxx

Dirty bosons, clean fermions







Fermi surface in momentumspace occupation

$$\lambda = \lambda_s$$

• Measure $\sigma(i\omega_n)$ from Kubo formula

• Reparametrize
$$\sigma(i\omega_n) = \frac{\tilde{D}}{|\omega_n| + \Gamma(\omega_n, T)}$$

 $\tilde{D} = \text{non-interacting Drude weight}$

- Analyze functional form of $\Gamma(\omega_n, T)$
- Extrapolation $\Gamma(\omega_n \rightarrow 0, T)$ gives DC scattering rate



- Universal form $\Gamma(i\omega_n \ge 2\pi T) = -a\omega_n \ln \omega_n + b\omega_n + d\omega_n \ln^2 \omega_n + c$ for $\lambda \le \lambda_G$
- "Marginal Fermi liquid" with extra $\omega \ln^2 \omega$ correction that becomes significant for $\lambda < \lambda_s$





- Polynomial spline extrapolation of $\Gamma(\omega_n \to 0, T)$
- Largest slope of T-linear at $\lambda = \lambda_s$
- Planckian $\Gamma \approx 0.4 k_B T/\hbar$, large RRR (clean fermions)





- Residual resistivity onsets for $\lambda < \lambda_s$, associated with SRO
- T-dependence changes to $T \ln(b/T)$ (recall extra log term in ω -dependence). RRR becomes small(er)



Transport universality



- At $\lambda = \lambda_s$, slope of *T*-linear is independent of interaction disorder g'
- Boson DOS $\rho(e) \sim f(e/g'^2)/g'^2$, $\rho(e \to 0) \sim 1/{g'}^2$
- Compatible with $\Gamma \sim \text{fermion DOS} \times \text{boson DOS} \times {g'}^2 \times T$

Transport universality

Material		n (10 ²⁷ m ⁻³)	m^* (m ₀)	$\frac{A_1 / d}{\left(\Omega / \mathrm{K}\right)}$	$h / (2e^2 T_{\rm F}) \ ({f \Omega} / { m K})$	α
Bi2212	<i>p</i> = 0.23	6.8	8.4 ± 1.6	8.0 ± 0.9	7.4 ± 1.4	1.1 ± 0.3
Bi2201	$p \sim 0.4$	3.5	7 ± 1.5	8 ± 2	8 ± 2	1.0 ± 0.4
LSCO	<i>p</i> = 0.26	7.8	9.8 ± 1.7	8.2 ± 1.0	8.9 ± 1.8	0.9 ± 0.3
Nd-LSCO	<i>p</i> = 0.24	7.9	12 ± 4	7.4 ± 0.8	10.6 ± 3.7	0.7 ± 0.4
PCCO	x = 0.17	8.8	2.4 ± 0.1	1.7 ± 0.3	2.1 ± 0.1	0.8 ± 0.2
LCCO	<i>x</i> = 0.15	9.0	3.0 ± 0.3	3.0 ± 0.45	2.6 ± 0.3	1.2 ± 0.3
TMTSF	P = 11 kbar	1.4	1.15 ± 0.2	2.8 ± 0.3	2.8 ± 0.4	1.0 ± 0.3

 $\Gamma = \alpha k_B T / \hbar$

Legros et al al, Nat. Phys. 15, 142 (2019)

Table 1 | Slope of *T*-linear resistivity vs Planckian limit in seven materials.

• Universality of α is a non-perturbative phenomenon

Strange metals near Mott transitions



Ghiotto et al, Nature **597**, 345–349 (2021)

- Twisted WSe₂ has a metal-insulator (Mott) transition, near which a strange metal is observed
- Need to include Coulomb repulsion (Hubbard U) in model of strange metals...

Effects of Hubbard U

- Use EDMFT to study SU(2) fermions with spatially-random Yukawa coupling to a 2D constant DOS bosonic bath and Hubbard U
- Disorder average over random Yukawa coupling g' yields impurity problem with dynamical spin interactions. Solve coupled fermion and boson problems.

$$H_{c} = -\sum_{ij,\sigma} \left(t_{ij} + \mu \delta_{ij} \right) c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow},$$
$$H_{Y} = \sum_{ir} \frac{g'_{ir}}{\sqrt{V}} (-1)^{i} \vec{S}_{i} \cdot \vec{\phi}_{r}, \quad \ll g'_{ir} g'_{jr'} \gg = {g'}^{2} \delta_{ij} \delta_{rr'}.$$



A. Hardy, O. Parcollet, A. Georges and A. A. P, arXiv:2407.21102

Effects of Hubbard U

- Hubbard U enhances marginal Fermi liquid and T-linear scattering rate Γ
- The effects of a weak random Yukawa coupling can therefore be amplified by Coulomb repulsion



A. Hardy, O. Parcollet, A. Georges and A. A. P, arXiv:2407.21102

Conclusions

- 2D metallic quantum criticality with disordered Yukawa interactions leads to strange metal behavior in both DC and AC transport in a disorder-averaged mean-field (Eliashberg) description
- Without mean-field and disorder-averaging, exact QMC shows strong disorder in the bosonic sector, which still leads to robust strange metal behavior not associated with a QCP
- Even though the bosonic sector is disordered, the fermions in the strange metal are clean, with large mean free path and a clear FS
- Strongly disordered bosonic sector produces localized overdamped bosonic modes that serve as microscopic inelastic scatterers of electrons
- T-linear transport scattering rate in the non-perturbative strange metal is universal (Planckian) and independent of the interaction disorder strength
- Hubbard Ustrongly amplifies the effects of disordered Yukawa interactions, important near Mott transitions