Superconductivity: Past, Present and Future

Andrew Millis Department of Physics, Columbia University Center for Computational Quantum Physics, Flatiron Institute

Collaborators:

Antoine Georges, Emanuel Gull, Oliver Parcollet, David Reichman, Boris Svistunov, Nikolai Prokof'ev, Malte Roesner, Misch Katsnelsen

John Sous, Chao Zhang, Zhihao Cui, Daniel Munoz-Segovia, Stefan Divic

'Super-C' collaboration (P. Torma)

PRO-QM EFRC (BES DE-SC0019443): Columbia MRSEC (DMR-2011738) The Simons foundation; **KEELE FOUNDATION**





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Serendipitous discovery

Heike Kamerlingh-Onnes 1911-12





Superconductivity:

Many instances

- 'Conventional': Hg, Pb, Nb3Sn, MgB2...
- Unconventional -conventional: A₃C₆₀; LaH₁₀
- Heavy fermion
- Organic: BEDT...
- Copper-Oxide
- Iron-pnictide
- ³He
- Condensed atomic gasses
- Neutron Stars
- High density nuclear matter





Bandwidth











Superconductivity in practice

High field magnets





a b $\frac{1}{2}$ $\frac{1}{2}$

Superconducting Qubits



Dreams: loss-free power transmission

Powering cities with minimal thermal load









Three needs

High Transition temperature



High Critical Current



'Protected' Excitations



?What materials support these behaviors?







Theory

Superconductivity is based on pairing





Pairing => order parameter

$$\Delta(\mathbf{R}) = \int d\mathbf{r} \ \mathbf{D}_{\alpha\beta}(\mathbf{r}) \ \left\langle \mathbf{c}_{\alpha} \left(\mathbf{R} + \frac{\mathbf{r}}{2}\right) \mathbf{c}_{\beta} \left(\mathbf{R} - \frac{\mathbf{r}}{2}\right) \right\rangle$$

- "Pair wave function" D encodes symmetry of pairing state
- $\Delta(\mathbf{R}) = e^{i\theta(\mathbf{R})} |\Delta(\mathbf{R})|$ has magnitude, phase and may depend on internal spin/orbital indices
- Order parameter non-classical: sc state is coherent superposition of states of different particle number. $[\theta, N] \neq 0$
- Long ranged superconducting order implies non-zero 'phase stiffness' $\rho_{\rm S}$: term in free energy ${\rm F} = {1\over 2} \rho_{\rm S} (\nabla \theta)^2$





Theory: Status

- Qualitative properties understood
 - Symmetries classified
 - Elementary excitations determined
- Open questions
 - Mechanism: "what causes that"
 - Transition temperature: "how big can it be"
 - Phase stiffness: "how tough is the superconductor?"





Conventional' superconductors: BCS/Migdal-Eliashberg Theory



Pairing of electrons via exchange of lattice vibrations ("phonons")



Key fact: in conventional metals, phonons are much slower than electrons:

Typical phonon frequency $\omega_{\text{Debve}} \ll \text{typical electron energy } \mathbf{E}_{\mathbf{F}}$

Controlled 'Migdal-Eliashberg' theory

=>





BCS/Migdal-Eliashberg Theory

Scalapino, Schreiffer, Wilkins PR148 263 (1966)



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How do we know this is right? McMillan and Rowell, PRL 14 108 1965

gap function $\Delta(\omega)$ has real and imaginary parts with structure related to phonon frequencies

Scalapino, Schreiffer, Wilkins PR148 263 (1966) McMillan and Rowell PRL 14 108 1965

Rowell, McMillan and Feldman PR 178 897 1969







Implications



Implications

- Electron mass <=> density of states
- Big mass => large coupling (good)
- But: big mass =>low ρ_s (bad)



Normal state conductivity:
$$\sigma(\omega) = \frac{ne^2}{m} \frac{\Gamma}{\omega^2 + \Gamma^2}$$

Stiffness:
$$\rho_{\rm S} = \frac{\rm ne^2}{\rm m} f\left(\frac{\Gamma}{\Delta}\right)$$







Assumptions

- Electrons well described by (effectively non-interacting) density functional (DFT) theory: $-\nabla^2 \psi + V_{KS} [\{n(r), R_n\}] \psi = E\psi$
- Static approximation for electronelectron interaction. Exact (up to corrections $\mathcal{O}\left(\frac{\omega_{\text{Debye}}}{E_{\text{F}}}\right)$) and neglect of anharmonicity for phonon







Extension: Materials Searches High-T_c hydrides at ambient pressure (M. Marques, Super-C)

- Assumption: standard DFT+Migdal-Eliashberg works
- Database:
 - ~10⁶ band structures of compounds
 - ~10⁴ detailed electron-phonon calculations
- =>train neural network to "predict" (identify) high Tc candidates
- Detailed study of candidate materials: verification of transition temperature, material stability





High hydrogen DOS at fermi level

- Good for high Tc
- Bad for thermodynamic stability

Adv Mat. 36, e2307085 2024 Adv. Funct. Mat. 342404043 (2024) No room temperature-stable high Tc compounds found





Relaxing the assumptions

Extending the conventional theory:

=>beyond the static Coulomb approximation; non-adiabatic phonons

Electrons not well described by (effectively non-interacting) density functional (DFT) theory:

=>Hubbard model; quantum critical pairing; doped spin liquids





Dynamical Coulomb interaction in 2d materials Yann in 't Veldt; M. Roesner, M. Katsnelson, AJM. 2D Materials 10, 045031 (2023) and to appear





- Low carrier density superconductivity (NbSe2, MoTe2..). Can be fabricated in monolayer form with controllable surroundings
- Soft tunable plasmon (variable ϵ and layer number) mixes with longitudinal phonons





Model system square lattice tight binding k_F=0.2, E_F=2



One loop theory k-dependent self energy





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Pairing strength as function of r_S for different interaction models

Here: show leading eigenvalue of gap operator at because in 2023, getting to T=Tc is too expensive



Dynamical Coulomb interactions enhance Tc





Essential technical step: compact low rank representations

Ex: Discrete Lehmann representation J. Kaye, O. Parcollet et. Al; CCQ/Flatiron

Interpolative decomposition=> controllable accuracy low rank representation of in terms of small number of frequencies and basis functions.

Generalized to 3 point vertices

Phys. Rev. B105, 235115 (2022) Phys. Rev. B111, 035135 (2025)

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Beyond one loop approximation: Diagrammatic Monte Carlo for extended systems

Van Houcke; Prokof'ev and Svistunov; Kozik; Rossi; Ferrero; Haule, Chen...

Evaluate Feynman Diagram series stochastically



Work in progress (Kun Chen): Coulomb repulsion term in gap equation: standard formula is a significant underestimate



Convergence w.r.t. order (for uniform electron gas)



Haule/Chen arXiv:20103146



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Beyond weak coupling: Bipolarons revisited



Sous, Zhang, Berciu, Prokof'ev, Reichman, Svistunov

Polaron: self-trapped state of electron bound to lattice distortion

3 models:

Holstein: coupling to density

Peierls: coupling to hopping via bond-length modulation

Bond-Peierls: coupling to hopping via oscillator on-bond

 $g \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} X_{i}$ $g \sum_{i,j\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} (X_{i} - X_{j})$ $g \sum_{i,j\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} X_{ij}$ $\bullet t \rightarrow \bullet$ $X_{ij} \bullet$

 $\begin{array}{l} \text{Linearization} \\ \text{of te}^{-a-(X_i-X_j)} \end{array}$

From interference of hopping pathways





Sous, Chakraborty, Krems, Berciu: `Peierls' Bipolarons can be light

One dimensional Peierls model

$$\mathcal{H}_{e} = -t \sum_{i,\sigma} \left(c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + h.c. \right) + \sum_{i\delta} U(\delta) \hat{n}_{i,\uparrow} \hat{n}_{i+\delta,\downarrow}$$
$$g \sum_{i,\sigma} \left(c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + h.c. \right) \left(b_{i}^{\dagger} + b_{i} - b_{i+1}^{\dagger} - b_{i+1} \right)$$









Phys. Rev. Lett. 121, 247001 (2018)

Diagrammatic Monte Carlo for Bipolaarons

Diag MC: evaluate terms in Feynman diagram series stochastically



sample series stochastically (diagram order, topology, internal integrals)

Zhang, Prokof'ev, Svistunov, Phys Rev B105 L020501(2022): for the special case of bipolarons (2 electrons +phonons) on a lattice this can be simplified, extended, and done in a signproblem-free way. Can also do (with somewhat more computational effort) Holstein bipolarons





For Bond-Peierls Polarons in 2D

Phys. Rev. X 13, 011010



In 2D, up to ln[ln[corrections:





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Maximum Transition temperature





long ranged Coulomb interaction

$$\mathcal{V}_{ij} = rac{Va}{|r_i - r_j|}$$

arXiv:2210.14236



Long ranged interaction increases the coupling threshold





Effect of long ranged interaction on superconductivity





Bipolaron phase diagram

At fixed density



- Controlled calculations can be done!
- Bipolarons dont have to be heavy (at reasonable couplings)
- Long ranged part of Coulomb interaction is important but not disastrous

Open questions:

—identifying systems with strongly phonon-mediated hopping

—results beyond the dilute limit





Beyond DFT: Superconductivity in strongly correlated ("quantum") materials







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Families of superconductor

- 'Conventional': Hg, Pb, Nb3Sn, MgB2...
- Unconventional -conventional: A₃C₆₀; LaH₁₀
- Heavy fermion
- Organic: BEDT...
- Copper-Oxide
- Iron-pnictide
- ³He
- Condensed atomic gasses
- Neutron Stars
- Quark matter



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Where are we?



Matthias' rules for finding superconductivity



- 1 Symmetric (pref. cubic) lattices
- 2 Avoid oxygen or similar elements
- 3 Avoid magnetism,
- 4 Avoid insulators,
- **5** Avoid theorists
- 'Conventional': Hg, Pb, Nb3Sn, MgB2...
- Unconventional -conventional: A₃C₆₀; LaH₁₀
- Heavy fermion
- Organic: BEDT...
- Copper-Oxide
- Iron-pnictide
- ³He

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- Condensed atomic gasses
- Neutron Stars
- Quark matter

All except first one on the list violate one or more of Matthias' rules



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'Novel' superconductivity





- Apparently has unconventional (non swave) order parameter symmetry.
- Can have quite high transition temperature









Copper -oxide superconductors Adapted from H. Hwang slide



J. G. Bednorz & K. A. Müller, Z. Phys. B - Condensed Matter **64**, 189 (1986)



B. Keimer, S. A. Kivelson, M. R. Norman, S. Uchida & J. Zaanen, *Nature* **518**, 179 (2015)

Superconductivity emerges in a material with a complicated but basically layered crystal structure, in proximity to a 'pseudogap' phase (or regime) with unusual properties





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Is this specific to Cu-based materials

Adapted from H. Hwang slide

Question:

Can you make Re³⁺Ni¹⁺O₂ look like Ca²⁺Cu²⁺O₂?





PHYSICAL REVIEW B 70, 165109 (2004)

Infinite-layer LaNiO₂: Ni¹⁺ is not Cu²⁺

K.-W. Lee and W. E. Pickett Department of Physics, University of California, Davis, California 95616, USA



Large Ni *d*_{x2-y2} hole band, 2 *Re* 5*d*-derived electron pockets – "self-doped" system





Answer: Yes

Kyuho Lee et al., Nature 619, 288 (2023)

Adapted from H. Hwang slide







Copper and Ni -oxide superconductors Adapted from H. Hwang slide

Theoretical model: the Hubbard model



$$H = -t \sum_{\langle i,j \rangle} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

After ~50 years, solution now in sight—key has

been algorithm development and comparison of

multiple methods. Cf A Georges talk Thursday

Fermi

liquid

ρ_{max}



 T_{c}

d-SC

 $f_{\rho_{c^2}}^{0.2}$

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Phase Diagram



0.06

0.10

 h_d

0.15

0 20



 $T^*/t \approx 0.25$

p = 1/16



0.1

0.0

0.3

0.2

T/t

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0.06

0.04_) ∛

ł

0 06

0.04

0.08

0.02-

0.00

0.00

0.05



What causes superconductivity in the Hubbard Model

 $\hat{\mathbf{H}} = -\sum_{ij} \mathbf{t}_{ij} \left(\mathbf{c}_{i\sigma}^{\dagger} \mathbf{c}_{j\sigma} + \mathbf{H} \cdot \mathbf{c} \cdot \right) + \mathbf{U} \sum_{i\uparrow} \hat{\mathbf{n}}_{i\uparrow} \mathbf{n}_{i\downarrow}$

Xinyang Dong Nat. Phys. 18 1293 (2022) Emanuel Gull



Weak coupling: SC (low TC) Deng et al EPL 2015



Intermediate coupling, x=1/8 SC preempted by stripes Chan et al Science 2017





Dynamical Mean Field Theory

Yields an approximation to electron self energy by solving auxiliary problem of cluster of impurity sites coupled to a bath.

Broken symmetries treated as in usual mean field theory (ask—do you want to break this sym?)=>can see if stable sc phase exists

Not enough resolution to see stripes=>cant tell if stripes preempt sc



`DCA: piecewise constant self energy

$$\Sigma(\mathbf{k},\omega) = \sum_{\mathbf{a}} \Theta(\mathbf{k} \in \mathbf{a}) \Sigma_{\mathbf{a}}(\omega)$$

Example: 8 patches=>8 site cluster





DMFT superconducting phase diagram



Deng et al EPL 2015

Parcollet, Gull, AJM PRL 2013

d_{x2-y2} sc near insulator but cut off by pseudogap Tc Max: t/20~250K



Superconducting /Pseudogap properties

Raman spectra in normal and SC state



DMFT finds a well defined SC state. Is it from (low frequency) spin fluctuations?

Our approach:

- Independently compute spin fluctuation spectrum and normal and anomalous self energies
- Partition normal self energy into spin fluctuation and Mott parts. $\Sigma = \Sigma_{SF} + \Sigma_{rest}$
- Fix the electron-spin fluctuation coupling constant from SF part of normal component of self energy
- Solve Eliashberg equation for SC. Compare to directly calculated result





Normal State Analysis









Now the superconducting part



Spin fluctuations account for at most half of the superconductivity



Implications

- Spin fluctuation as `pairing glue' is not the whole story higher energy processes are important
- the coulomb interaction is not just a pseudopotential (or source of spin fluctuations)



'Moire' Materials

- Moire=>large unit cell
 Win dia/Indexedition
 - Kinetic/Interaction energy ratio controllable by twist angle, gates
 - By adjusting top gate (TG) and bottom gate (BG) voltages independently, can control mean chemical potential and displacement field (<=> inversion symmetry, band structure, occupation of different layers)
 - New feature: quantum geometry

Effect of displacement field



chemical potential above this line: `layer polarized' Van Hove point appears





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Homobilayer + Twist

WSe₂

WSe₂ Pt

BN

BG



а

TMD Moire Bands:



Topological bands; twist angle-tunable dispersion



Three band tight binding model reproduces dispersion and topology of upper two bands

Relative roles of the orbitals depend on displacement field

V. Crepel and AJM arXiv:2403.15546

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Interaction scales (project screened Coulomb onto Wannier orbitals): ~50 meV—LARGE







Superconductivity in Moire WSe2

Columbia and Cornell Experimental Groups

5º twist (Columbia group)





Consequences of nonzero quantum geometry: II Superfluid weight and quantum metric

Slide text from P. Torma

Isolated flat band: $W \ll U \ll E_{\text{band gap}}$

Uniform pairing: $\Delta_{orbital} \ \# = \Delta$



Quantum geometry enhances superfluid stiffness



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Theory: I

Kohn-Luttinger mechanism: arXiv:2408.16075

• Interaction: screened Coulomb + form factors from projection onto top band. Similar spatial structure from spin fluct

$$V_{gg'}(q, i\omega) = [1 - V_0(q)\Pi(q, i\omega)]_{gg'}^{-1} V_0(q + g')$$

$$\Pi_{gg'}(i\omega,q) = \frac{1}{A} \sum_{k\sigma} \frac{f(\xi_{k\sigma}) - f(\xi_{k+q\sigma})}{i\omega + \epsilon_{k\sigma} - \epsilon_{k+q\sigma}} \Lambda^{k,k+q}_{-g\sigma} \Lambda^{k+q,k}_{g'\sigma}$$



• $\Lambda_{g\sigma}^{k,p}$ expresses quantum geometry, inversion symmetry breaking

leading instability: 2D "E" irrep. Strong SOC + no inversion means SC state is of mixed singlet/triplet character. Chiral (d+id/p+ip, C=2 Altland-Zirnbauer A) over most of parameter range; small region of non-topological nematic SC. Chiral state is gapped, with Dirac edge modes







Theory

FRG: arXiv:2412.14296 based on arXiv:2403.15546

3 orbital t.b. model (V. Crepel): reproduces bands and topology. Wannierizable=>purely local interactions. Functional Renormalization Group calculations





Subtle relation of phase diagram to van Hove points



Complicated structure of phase of SC





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Theory: evolution of AF phase with twist angle

D.Munoz Segovia arXiv:2503.11763



At high twist angle, competing phase is associated with the van Hove singularity; at lower twist angle, detaches from van Hove and locks to n=1 and exists only at nonzero displacement field. ??Implications for superconductivity





Twisted WSe2

5° twist angle: Superconductivity in proximity to fermi surface reconstructed phase at particular combination of displacement field and carrier concentration

3.65° twist angle: superconductivity at n=1 in proximity to insulating phase

Proposal: the superconductivity is topological and is understandable from spin fluctuations in proximity to magnetic phase

Role of quantum geometry to be determined









Inducing superconductivity with optical drive (A. Cavalleri and collaborators)

Images from A. Cavalleri





Fundamentally new questions in non equilibrium physics—see Demler talk



Superconductivity: The gift that keeps on giving

- Understanding where the superconductivity comes from and using the knowledge to raise Tc: a continuing challenge in quantum many-body physics.
- Progress in theory of conventional, nearly conventional and unconventional superconductors comes from from new methods (machine learning, DMRG, DMFT, Diag-MC, AF-QMC..) working in tandem to cross compare results and allow 'handshake' between methods
- New experimental platforms allow new classes of systematic theory-experiment comparisons and raise new conceptual challenges



Consequences of nonzero quantum geometry

*If $C \neq 0$, 'Edge states' at interface between topological and vacuum or non-topological material

*Wannierization:
$$W_{n,R}(r) = \sum_{k} e^{i \vec{k} \cdot \vec{R}} M_k \psi_{mk}(r)$$

Marzari/Vanderbilt: if C=0 can choose M so w's are exponentially localized around sites R If C \neq 0, only power-law localization possible

*Broken Galilean invariance, even in dilute limit=> Enhancement of stiffness (Torma), polarizability (Queiroz)



*(FCI) Quantized-Hall like states at 0 field



Bockrath





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Consequences of nonzero quantum geometry: II Superfluid weight and quantum metric

Slide text from P. Torma

Isolated flat band: $W \ll U \ll E_{\text{band gap}}$

Uniform pairing: $\Delta_{orbital} \ \# = \Delta$



Quantum geometry enhances superfluid stiffness



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Theory II: Mott transition in an orbital field S. Divic, V. Crepel, M. Zalatel, AJM arXiv:2406.15348 Tscheppe, Schaefer, AJM in preparation

See also Kuhlenkamp, Kadow, Imamoglu, and Knap, Phys. Rev. X 14, 021013 (2024)

Triangular lattice Hubbard model Flux Φ_{\bigwedge} per unit cell

Focus on
$$\Phi_{\triangle} = \frac{\pi}{2}$$



Small U: integer quantized Hall effect Very large U: conventional 120° antiferromagnet **?Is there an intermediate topological Mott insulator phase?**





Theory: DMRG on small radius cylinders



Kuhlenkamp et al Phys. Rev. X 14, 021013 (2024): measure charge-charge correlator (averaged over cylinder circumference) $\langle n(x)n(0) \rangle$



Weak maximum at U~10t suggests transition to CSL







Theory: DMRG on small radius cylinders



Stefan's idea:

(1) Gauge choice: commuting translations T_x^2 ; $T_y =$ >magnetic unit cell (2 segments)

(2) Gauss' law: $\Phi_{x+1} = \Phi_x - 2L_y \Phi_{i}$ =>for even radius cylinders: flux invariant under T_x odd radius: T_x not a symmetry; PT_x is a symm. (3) Spontaneously breaking of PT_x at CSL transition



Divergent correlation length

correlations; exponentially decaying spin correlations







=>If proximal spin liquid phase, then interesting SC





Transition IQH->CSL: close and reopen a charge gap. Transition CSL->120° AFM: close a spin gap

arXiv:2410.18175: Single particle gap remains non-zero=>gapless mode is a collective charge mode; in simple model, Yang ``eta-pairing" triplet. =>Doping leads to novel superfluid

(see also arXiv:2308.10935 (Sahay, ... Divic...Zalatel)





Summary

Interactions and topology: new physics

Topological Mott Insulators



And (possibly) superconductors





Topological Kondo Insulators



Superconductors: Possibly Topological





