Unconventional Superconductivity from the Kohn-Luttinger Perspective

Work done in collaboration with
Sri Raghu and Doug Scalapino
Also
Aharon Kapitulnik, Weejee Cho, Andrey Chubukov

KITP, UCSB 2016

My connections with Walter started before I was born

Born	Julian Seymour Schwinger February 12, 1918 New York City, New York, USA
Died	July 16, 1994 (aged 76) Los Angeles, California, USA
Nationality	United States
Fields	Physics
Institutions	University of California, Berkeley Purdue University Massachusetts Institute of Technology Harvard University University of California, Los Angeles
Alma mater	City College of New York Columbia University
Doctoral advisor	Isidor Isaac Rabi
Doctoral students	Roy Glauber Ben R. Mottelson Sheldon Lee Glashow Walter Kohn Bryce DeWitt Daniel Kleitman Sam Edwards Gordon Baym Lowell S. Brown Stanley Deser Lawrence Paul Horwitz Margaret G. Kivelson
Known for	Quantum electrodynamics

Inhomogeneous Electron Gas*

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AND

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(Received 18 June 1964)

This paper deals with the ground state of an interacting electron gas in an external potential $v(\mathbf{r})$. It is proved that there exists a universal functional of the density, $F[n(\mathbf{r})]$, independent of $v(\mathbf{r})$, such that the expression $E\equiv\int v(\mathbf{r})n(\mathbf{r})d\mathbf{r}+F[n(\mathbf{r})]$ has as its minimum value the correct ground-state energy associated with $v(\mathbf{r})$. The functional $F[n(\mathbf{r})]$ is then discussed for two situations: (1) $n(\mathbf{r})=n_0+\tilde{n}(\mathbf{r})$, $\tilde{n}/n_0<<1$, and (2) $n(\mathbf{r})=\varphi(\mathbf{r}/r_0)$ with φ arbitrary and $r_0\rightarrow\infty$. In both cases F can be expressed entirely in terms of the correlation energy and linear and higher order electronic polarizabilities of a uniform electron gas. This approach also sheds some light on generalized Thomas-Fermi methods and their limitations. Some new extensions of these methods are presented.

INTRODUCTION

DURING the last decade there has been considerable progress in understanding the properties of a homogeneous interacting electron gas.[1] The point of view has been, in general, to regard the electrons as similar to a collection of noninteracting particles with the important additional concept of collective excitations.

On the other hand, there has been in existence since the 1920's a different approach, represented by the Thomas-Fermi method[2] and its refinements, in which the electronic density $n(\mathbf{r})$ plays a central role and in which the system of electrons is pictured more like a classical liquid. This approach has been useful, up to now, for simple though crude descriptions of inhomogeneous systems like atoms and impurities in metals.

Lately there have been also some important advances along this second line of approach, such as the work of Kompaneets and Pavlovskii,[3] Kirzhnits,[4] Lewis,[5] Baraff and Borowitz,[6] Baraff,[7] and DuBois and Kivelson.[8] The present paper represents a contribution in the same area.

In Part I, we develop an exact formal variational principle for the ground-state energy, in which the density $n(\mathbf{r})$ is the variable function. Into this principle enters a universal functional $F[n(\mathbf{r})]$, which applies to all electronic systems in their ground state no matter what the external potential is. The main objective of theoretical considerations is a description of this functional. Once known, it is relatively easy to determine the ground-state energy in a given external potential.

In Part II, we obtain an expression for $F[n]$ when n deviates only slightly from uniformity, i.e., $n(\mathbf{r})=n_0+\tilde{n}(\mathbf{r})$, with $\tilde{n}/n_0\rightarrow 0$. In this case $F[n]$ is entirely expressible in terms of the exact ground-state energy and the exact electronic polarizability $\alpha(q)$ of a *uniform* electron gas. This procedure will describe correctly the long-range Friedel charge oscillations[9] set up by a localized perturbation. All previous refinements of the Thomas-Fermi method have failed to include these.

In Part III we consider the case of a slowly varying, but *not* necessarily almost constant density, $n(\mathbf{r})=\varphi(\mathbf{r}/r_0)$, $r_0\rightarrow\infty$. For this case we derive an expansion of $F[n]$ in successive orders of r_0^{-1} or, equivalently of the gradient operator ∇ acting on $n(\mathbf{r})$. The expansion coefficients are again expressible in terms of the exact ground-state energy and the exact linear, quadratic, etc., electric response functions of a uniform electron gas to an external potential $v(\mathbf{r})$. In this way we recover, quite simply, all previously developed refinements of the Thomas-Fermi method and are able to carry them somewhat further. Comparison of this case with the nearly uniform one, discussed in Part II, also reveals why the gradient expansion is intrinsically incapable of properly describing the Friedel oscillations or the radial oscillations of the electronic density in an atom which reflect the electronic shell structure. A partial summation of the gradient expansion can be carried out (Sec. III.4), but its usefulness has not yet been tested.

I. EXACT GENERAL FORMULATION

1. The Density as Basic Variable

We shall be considering a collection of an arbitrary number of electrons, enclosed in a large box and moving

* Supported in part by the U. S. Office of Naval Research.
† NATO Post Doctoral Fellow.
‡ Guggenheim Fellow.
[1] For a review see, for example, D. Pines, *Elementary Excitations in Solids* (W. A. Benjamin Inc., New York, 1963).
[2] For a review of work up to 1956, see N. H. March, Advan. Phys. **6**, 1 (1957).
[3] A. S. Kompaneets and E. S. Pavlovskii, Zh. Eksperim. i. Teor. Fiz. **31**, 427 (1956) [English transl.: Soviet Phys.—JETP **4**, 328 (1957)].
[4] D. A. Kirzhnits, Zh. Eksperim. i. Teor. Fiz. **32**, 115 (1957) [English transl.: Soviet Phys.—JETP **5**, 64 (1957)].
[5] H. W. Lewis, Phys. Rev. **111**, 1554 (1958).
[6] G. A. Baraff and S. Borowitz, Phys. Rev. **121**, 1704 (1961).
[7] G. A. Baraff, Phys. Rev. **123**, 2087 (1961).
[8] D. F. Du Bois and M. G. Kivelson, Phys. Rev. **127**, 1182 (1962).
[9] J. Friedel, Phil. Mag. **43**, 153 (1952).

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I. EX

1. T

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[9] J. Friedel, Ph

I came to ITP in Feb. 1980 – among the first cadre of post docs.

Walter was the director, and already one of my scientific heros.

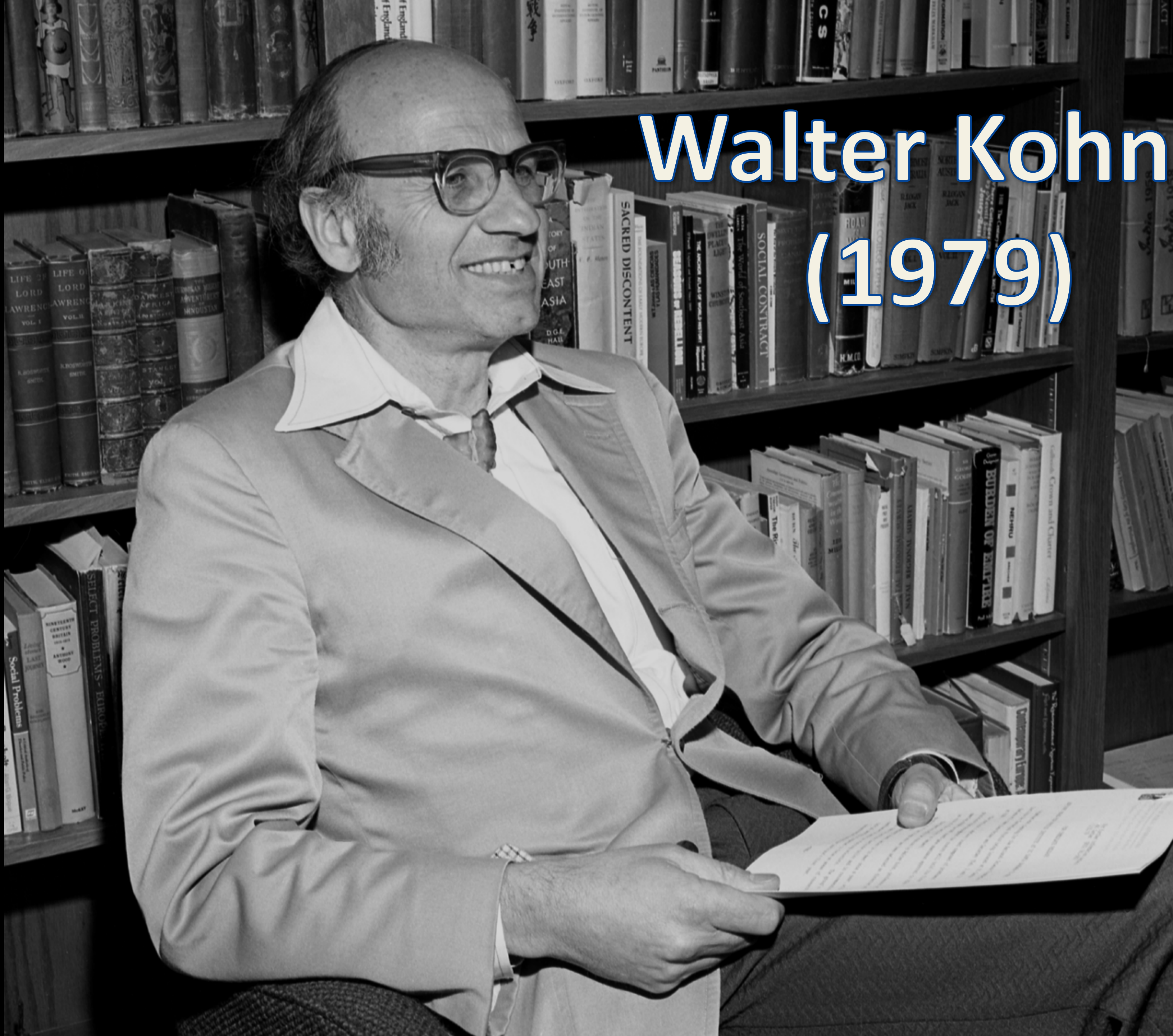
The man I encountered was kind, scholarly, encouraging, demanding,

and while physics is a serious business …
he made it clear that it can be great fun,

and that it is a human activity,
not a monastic abstraction.

His gravitas only emphasized the warmth of his gentle smile
and the good humor he radiated.

Also, he must have been 56 at the time!!!!


Walter Kohn
(1979)

NEW MECHANISM FOR SUPERCONDUCTIVITY*

W. Kohn

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and

J. M. Luttinger

Columbia University, New York, New York

(Received 16 August 1965)

It is the purpose of this note to point out a new mechanism which provides an instability against Cooper-pair formation. We find that a weakly interacting system of fermions cannot remain normal down to the absolute zero of temperature, no matter what the form of the interaction. This mechanism has nothing to do with the conventional electron-phonon attractive interaction in metals, or the long-range attractive van der Waals forces in He^3. It is present even in the case of purely repulsive forces between the particles, and is due to the sharpness of the Fermi surface for the normal system.

To understand what is involved, we first take an over-simplified view of the effect. It has the dielectric constant as a function of the momentum transfer $\vec{q}$, when $q = 2k_F$.[1] This singularity in the Fourier transform of the interaction gives rise to a long-ranged oscillatory force in ordinary space. All that is necessary for this effect is a sharp Fermi surface; a rounding of the Fermi surface due to (say) finite temperature or impurities will give rise to an interaction which drops off exponentially at very large distances.

It is plausible to suppose that, similarly, the effective interaction between the fermions themselves will have a long-range oscillatory part. By taking advantage of the attractive regions, Cooper pairs can form thus giving rise to superconductivity.

It is the purpose of this note to point out a new mechanism which provides an instability against Cooper-pair formation. We find that a weakly interacting system of fermions cannot remain normal down to the absolute zero of temperature, no matter what the form of the interaction. This mechanism has nothing to do with the conventional electron-phonon attractive interaction in metals, or the long-range attractive van der Waals forces in He^3. It is present even in the case of purely repulsive forces between the particles, and is due to the sharpness of the Fermi surface for the normal system.

What is the status of "the theory" of high temperature superconductivity

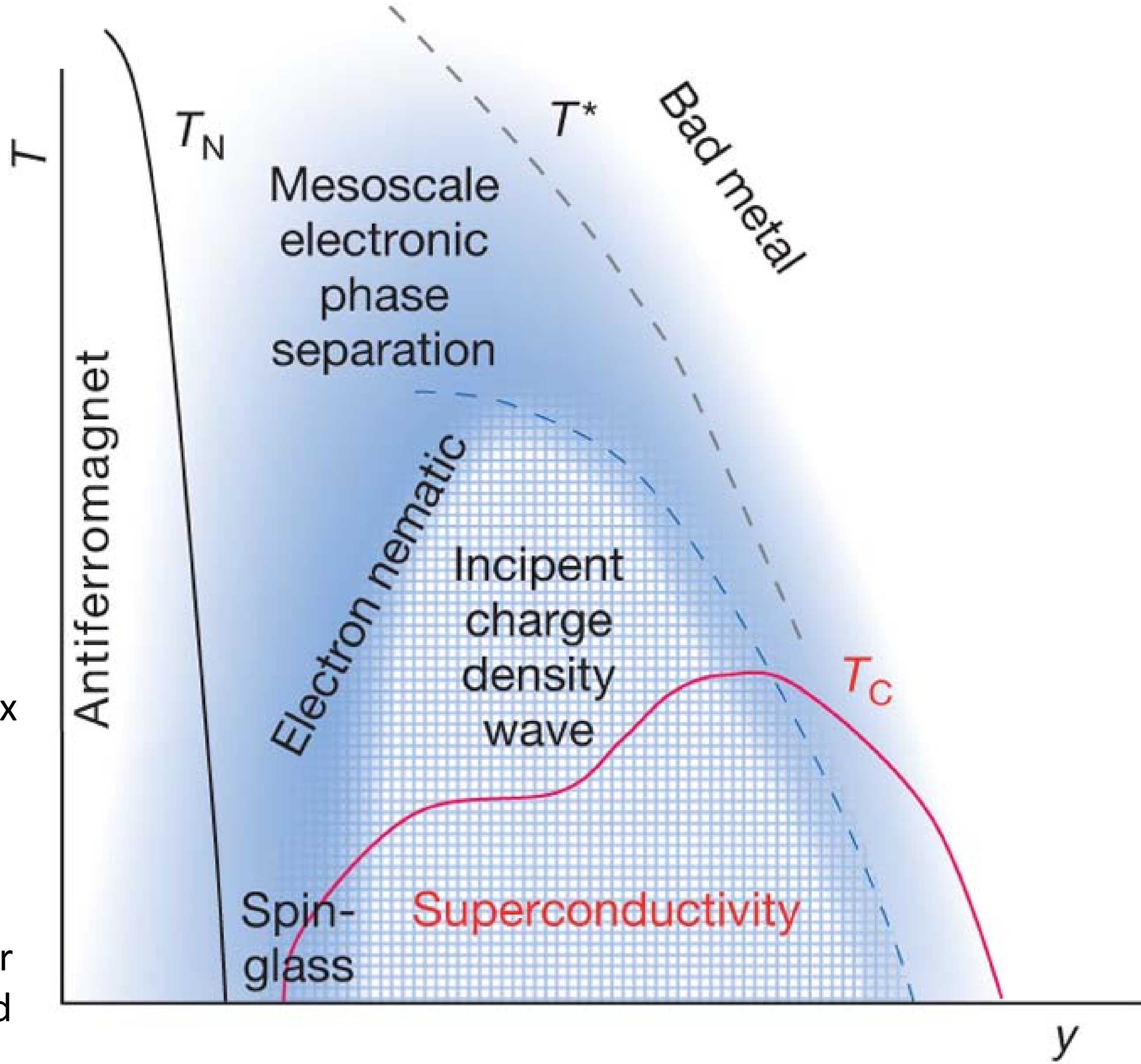
Why is T_c so much higher than in "conventional" superconductors?

What is the relation between HTC and magnetism?

Is there a general mechanism of unconventional SC & pairing directly from repulsive interactions?

What gives rise to the complex phase diagrams … intertwined orders?

How does one understand the "bad metal" behavior in many highly correlated materials at T ~ 300K?



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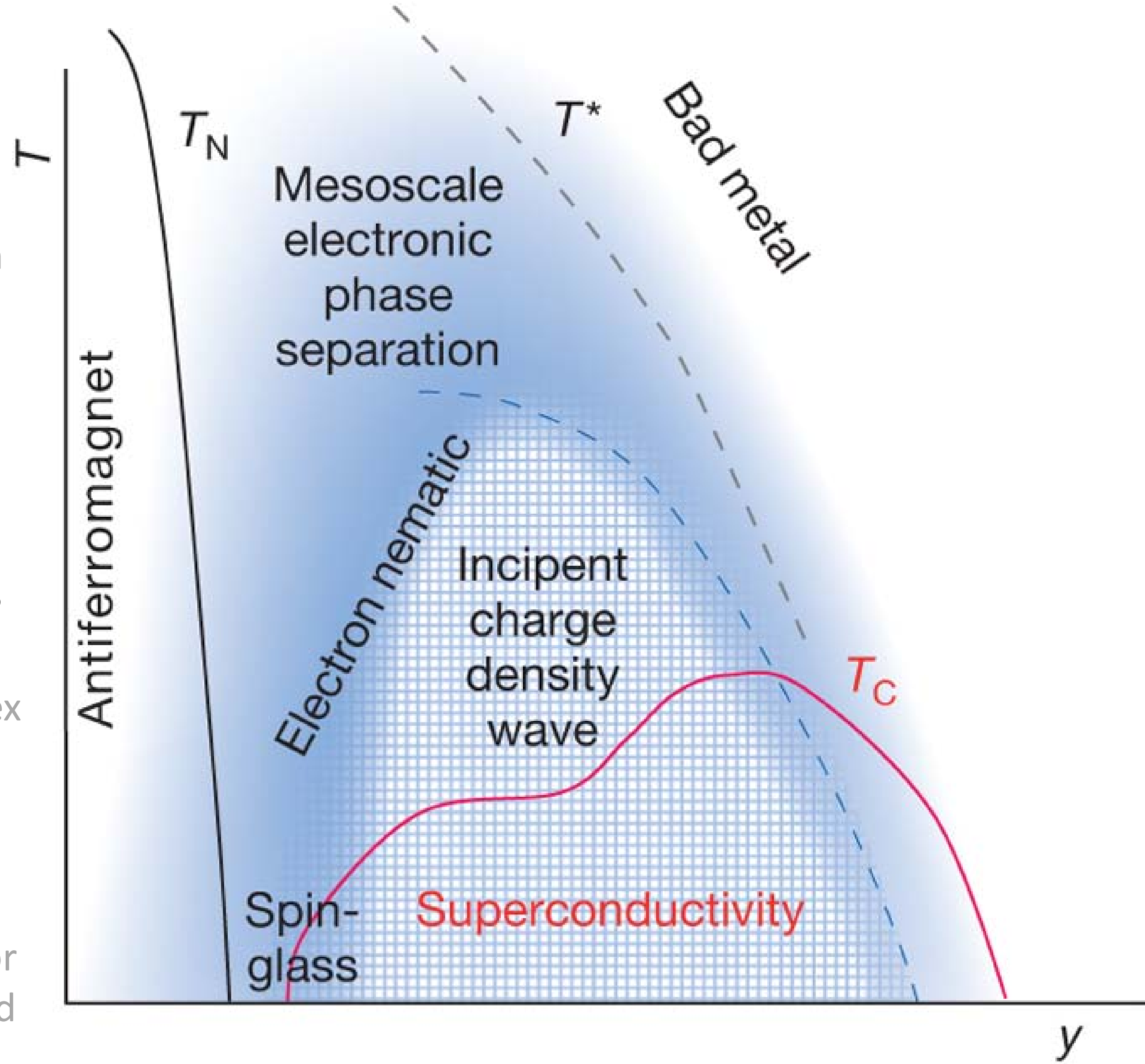

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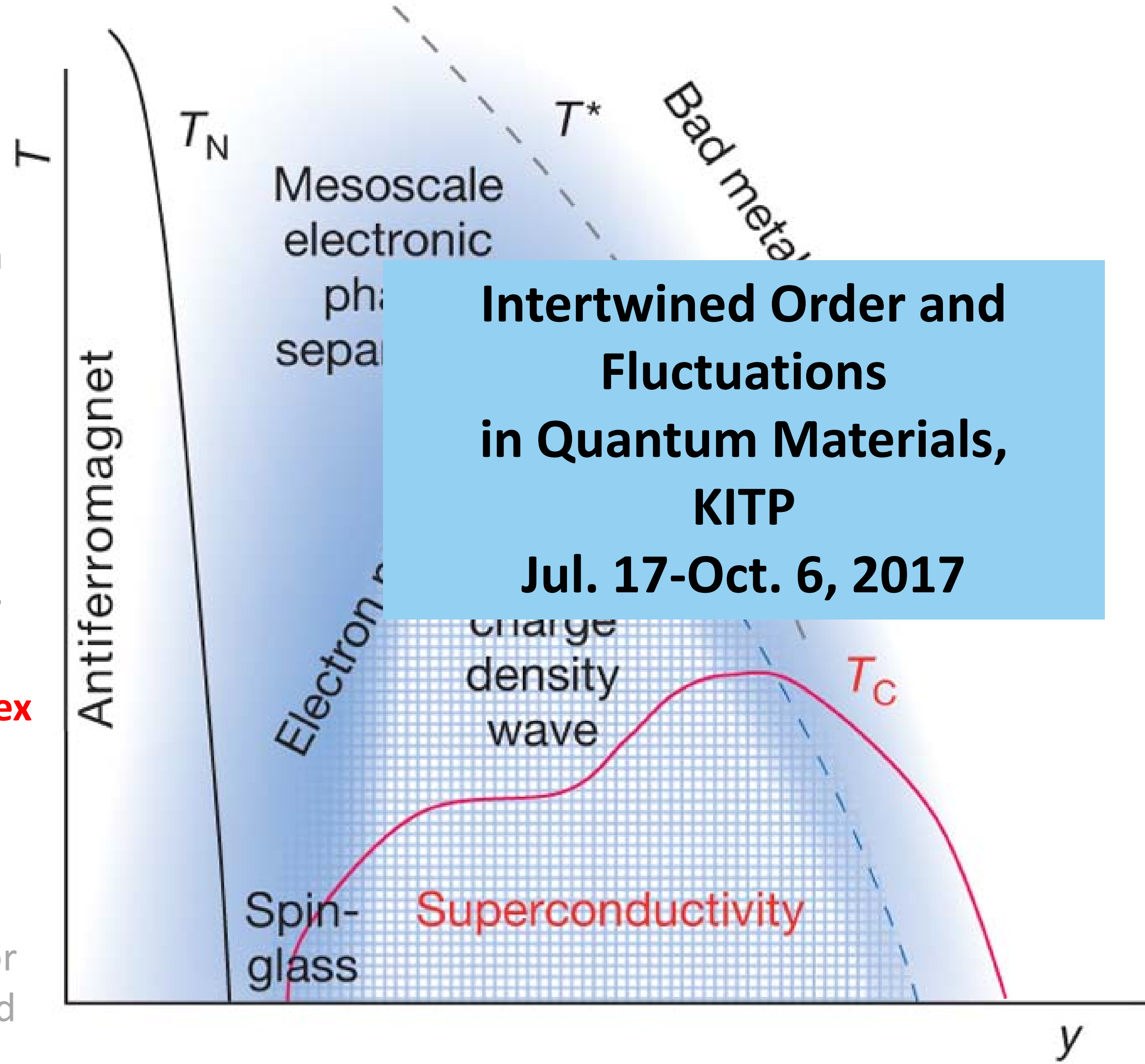

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Intertwined Order and Fluctuations in Quantum Materials, KITP
Jul. 17-Oct. 6, 2017

"Although it has been a really long time and billions of papers have been written on the subject, there is still no *understanding* of high temperature superconductivity, and therefore our paper should be published in a glossy magazine with pornographic pictures on the cover."

***i.e.* theorists are useless parasites and enemies of the working class.**

Approximate beginning line in billions of papers.

In contrast, I will argue:

We have an satisfactory understanding of the mechanism of "unconventional superconductivity."

(Which does not mean we have a satisfactory understanding of any particular "high temperature superconductor.")

Defining feature of unconventional superconductors:

$$\Big|\sum_{\vec{k}} \Delta_{\vec{k}}\Big|^2 \ll \sum_{\vec{k}} \Big|\Delta_{\vec{k}}\Big|^2$$

Including sign-changing s-wave, d-wave, p-wave, f-wave, …

What constitutes "understanding" the mechanism?

(Compare with the case of the BCS theory of conventional superconductors.)

1) **A compelling theoretical solution of a paradigmatic model which is clearly correct in an appropriate limit.**

For the conventional superconductors, this means a Fermi liquid weakly coupled to phonons with $E_F >> \omega_0$ and $\omega_0 >> T_c$.

What constitutes “understanding” the mechanism?

(Compare with the case of the BCS theory of conventional superconductors.)

1) **A compelling theoretical solution of a paradigmatic model which is clearly correct in an appropriate limit.**

2) **Some successful semi-quantitative but precise “predictions” of experimentally verifiable consequences of the mechanism.**

For the conventional superconductors, this means the isotope effect (sometimes) and phonon wiggles in the tunneling spectrum.

What constitutes "understanding" the mechanism?

(Compare with the case of the BCS theory of conventional superconductors.)

1) **A compelling theoretical solution of a paradigmatic model which is clearly correct in an appropriate limit.**

2) **Some successful semi-quantitative but precise "predictions" of experimentally verifiable consequences of the mechanism.**

3) **A theory which can predict T_c and other dimensional quantities quantitatively and can make specific predictions concerning new superconducting materials.**

Even for conventional superconductors, this is difficult at best -
and may not be possible. (Opinions differ.)

What constitutes "understanding" the mechanism?

For the case of unconventional superconductivity without phonons

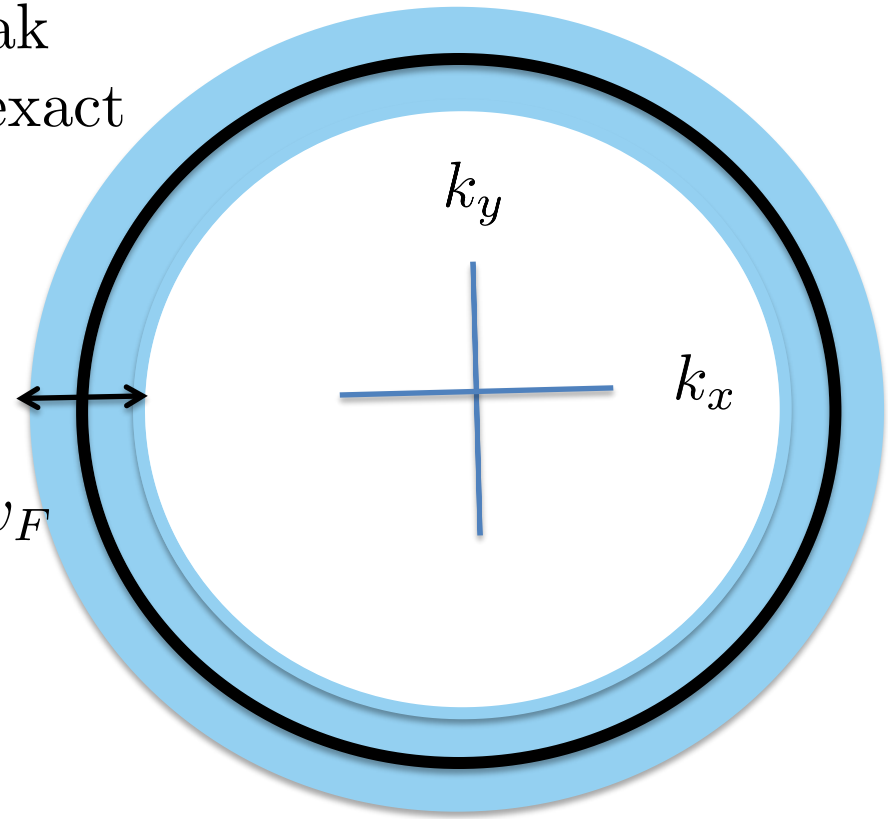
1) **A compelling theoretical solution of a paradigmatic model which is clearly correct in an appropriate limit.**

Superconductivity as a (weak-coupling) instability of a Fermi liquid

Integrate out high energy degrees of freedom with $|\nu| > \Lambda$

If residual interactions are weak
a presumably asymptotically exact
perturbative RG solution
is possible.

$\Delta k = 2\Lambda / v_F$



Superconductivity as a (weak-coupling) instability of a Fermi liquid

$\mathrm{BCS\ (mean-field)\ gap\ equation}$

$$\Delta_{\vec{k}} = -\frac{1}{N} \sum_{|\vec{v}_F \cdot \vec{k}'|<\Lambda} \tilde{V}(\vec{k}, \vec{k}') \ \frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}} \ \tanh\left(\frac{E_{\vec{k}'}}{2T}\right)$$

$$g_{\hat{k},\hat{k}'} \equiv \frac{V(\hat{k}, \hat{k}')}{\sqrt{|\vec{v}_F(\hat{k})||\vec{v}_F(\hat{k}')|}} \qquad E_{\vec{k}} = \sqrt{\tilde{\epsilon}^2_{\vec{k}} + |\Delta_{\vec{k}}|^2}$$

$$\lambda_a \ \phi^{(a)}_{\hat{k}_F} = -\int \frac{d\hat{k}'_F}{\Omega_F} \ g_{\hat{k}_F,\hat{k}'_F} \ \phi^{(a)}_{\hat{k}'_F} \qquad \lambda_0 \geq \lambda_n$$

If $\lambda_0 > 0$ $\qquad T_c \sim \Lambda \exp[-1/\lambda_0]$

Superconductivity as a (weak-coupling) instability of a Fermi liquid

Perturbative R.G.

$$\frac{\partial \underline{g}}{\partial \ell} = -\underline{g} \cdot \underline{g}$$

$$\ell = \log[\Lambda/T]$$

$$\underline{g}(\Lambda)\ \phi^{(a)} = -\lambda_a(\Lambda)\ \phi^{(a)}$$

$$\frac{\partial \lambda_a}{\partial \ell} = -\lambda_a^2$$

$$T_c \sim \Lambda\ \exp[\ -1/\lambda_0(\Lambda)\ ]$$

If $\lambda_0 > 0$

$$g_{\hat{k},\hat{k}'} \equiv \frac{V(\hat{k},\hat{k}')}{\sqrt{|\vec{v}_F(\hat{k})||\vec{v}_F(\hat{k}')|}}$$

J. Polchinski, arXiv:9210046 TASI 1992

R. Shankar, RMP **66**, 129 (1994)

Superconductivity as a (weak-coupling) instability of a Fermi liquid

Two step solution electron phonon problem

$$\Lambda \sim \omega_0$$

$$g_{\hat{k},\hat{k}'}(\Lambda) \approx -\lambda_{el-ph} + \mu^*(\Lambda)$$

$$\phi^{(0)}_{\hat{k}} \approx \text{const.} \qquad\qquad \Delta_{\hat{k}} \approx \Delta$$

$$T_c \sim \omega_0 \; \exp[-1/(\lambda_{el-ph} - \mu^*)]$$

Central role of retardation : $E_F \gg \omega_0 \gg T_c$

Superconductivity as a (weak-coupling) instability of a Fermi liquid

$$\text{Two step solution electron} - \text{electron problem}$$

$$U^2/E_F \gg \Lambda \gg E_F \exp[-1/U\rho(E_F)]$$

$$g_{\hat{k},\hat{k}'}(\Lambda) = U + U^2\chi(\hat{k},\hat{k}') + \dots$$

$$\text{Even for ``purely repulsive'' interactions } g_{\hat{k},\hat{k}'} > 0$$

$$\text{typically } \lambda_0 > 0$$

$$e.g. \;\; \underline{g} = g_0 \, \underline{1} + g_1 \, \underline{\tau}_1 \;\; \rightarrow \;\; \lambda_0 = g_1 - g_0$$

$$\text{However, the resulting SC state is ``unconventional''}$$

$$\phi^{(0)} = \langle 1, -1 \rangle \quad \rightarrow \;\; \Delta_{\vec{k}_1} = -\Delta_{\vec{k}_2}$$

S. Raghu, S.A. Kivelson, D. J. Scalapino, Phys. Rev. B **81**, 224505 (2010)

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$$g_{\hat{k},\hat{k}'}(\Lambda) = U + U^2\chi(\hat{k},\hat{k}') + \dots$$

$$T_c \sim \Lambda \;\exp[-1/\lambda_0(\Lambda)]$$

$$\lambda_0(\Lambda) = U^2\mathbf{A} + U^3\mathbf{B} + U^4\left\{\mathbf{A}^2\log[E_F/\Lambda] + C\right\} + \dots$$

$$\underline{g}(\Lambda)\;\phi^{(a)} = -\lambda_a(\Lambda)\;\phi^{(a)}$$

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$$T_c \sim E_F \; \exp[-1/\lambda]$$

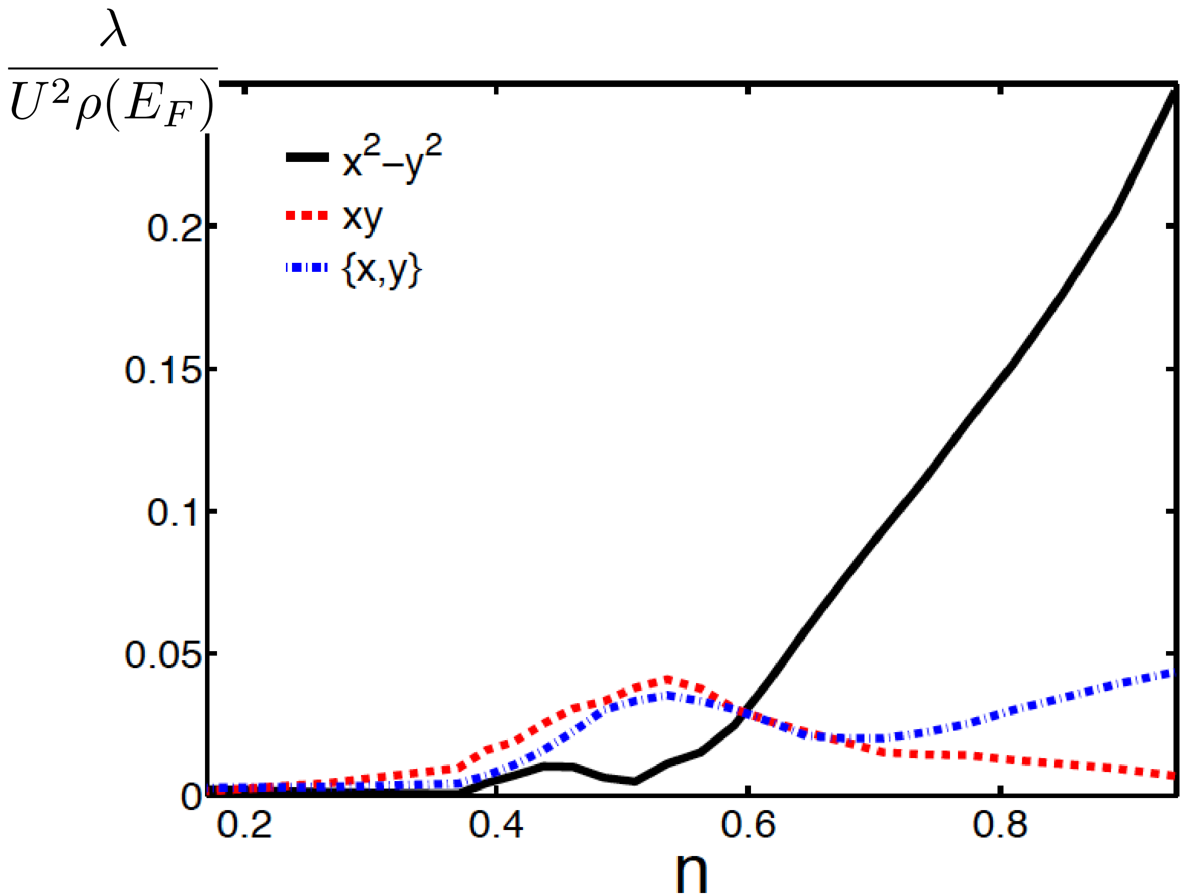
$$\Delta_{\hat{k}} = \sqrt{|\vec{v}_F(\hat{k})|}\; \phi^{(0)}_{\hat{k}}$$

$$\lambda = U^2\mathbf{A} + U^3\mathbf{B} + \ldots$$

S. Raghu, S.A. Kivelson, D. J. Scalapino, Phys. Rev. B **81**, 224505 (2010)

Small U/t limit of the Hubbard-like Models:

$T_c = 4t \exp\{-1/\lambda\}$ $\lambda = (U/t)^2 [A + B(U/t) + C(U/t)^2 + \ldots]$



Can calculate **A** and **B** exactly from band-Structure properties of non-interacting model

Depends on band-structure at all energies - not just on "Friedel oscillations"

A =0 (but B≠0) for circular Fermi surface.

What constitutes "understanding" the mechanism?

For the case of unconventional superconductivity without phonons

1) A compelling theoretical solution of a paradigmatic model which is clearly correct in an appropriate limit.

What's missing?

Theory of low $T_c \sim \exp[- \alpha(E_F/U)^2]$

Normal state is an excellent Fermi liquid

No fluctuating order, competing orders, intertwined orders, exotic orders …

Requires considerable faith in adiabatic continuity.

What constitutes "understanding" the mechanism?

For the case of unconventional superconductivity without phonons

1) A compelling theoretical solution of a paradigmatic model which is clearly correct in some limit.

2) Some successful semi-quantitative but precise "predictions" of experimentally verifiable consequences of the mechanism.

In some senses, the d-wave character of the SC in the cuprates was “predicted” from K-L considerations

Scalapino *et al* 1986-88, Emery 1987,
Monien and Pines 1990, …

(Also from strong-coupling perspective
Kotliar 1988, Gros 1988, Trivedi 1989, …)

There has been a growing effort to use a weak-coupling approach to predict new features of known unconventional SC's or even predict new SC's

Topological $p + ip$ superconductivity in doped graphene-like single-sheet materials BC_3

Renormalization group analysis of a neck-narrowing Lifshitz transition in the presence of weak short-range interactions in two dimensions

Topological odd-parity superconductivity at type-II two-dimensional van Hove singularities

Superconductivity from weak repulsion in hexagonal lattice systems

Spin-orbit coupling and odd-parity superconductivity in the quasi-one-dimensional compound $Li_{0.9}Mo_6O_{17}$

Spin-orbit coupling induced enhancement of superconductivity in a two-dimensional repulsive gas of fermions

Superconductivity from repulsive interactions in the two-dimensional electron gas

Evidence for spin-triplet odd-parity superconductivity close to type-II van Hove singularities

Manipulating superconductivity in ruthenates through Fermi surface engineering

Pairing symmetry and dominant band in Sr_2RuO_4

Thomas Scaffidi, Jesper C. Romers, and Steven H. Simon

Weak coupling two-step RG solution applied to Sr_2RuO_4

PRL **105,** 136401 (2010) PHYSICAL REVIEW LETTERS week ending 24 SEPTEMBER 2010

Hidden Quasi-One-Dimensional Superconductivity in Sr_2RuO_4

S. Raghu, A. Kapitulnik, and S. A. Kivelson

PHYSICAL REVIEW B **89**, 220510(R) (2014)

Pairing symmetry and dominant band in Sr_2RuO_4

Thomas Scaffidi, Jesper C. Romers, and Steven H. Simon

Sr_2RuO_4 is well described by FL theory below T_{FL} ~ 30K
Becomes an unconventional (probably chiral p-wave)
SC below T_c =1.5K. (Quasi-2D electronic structure.)

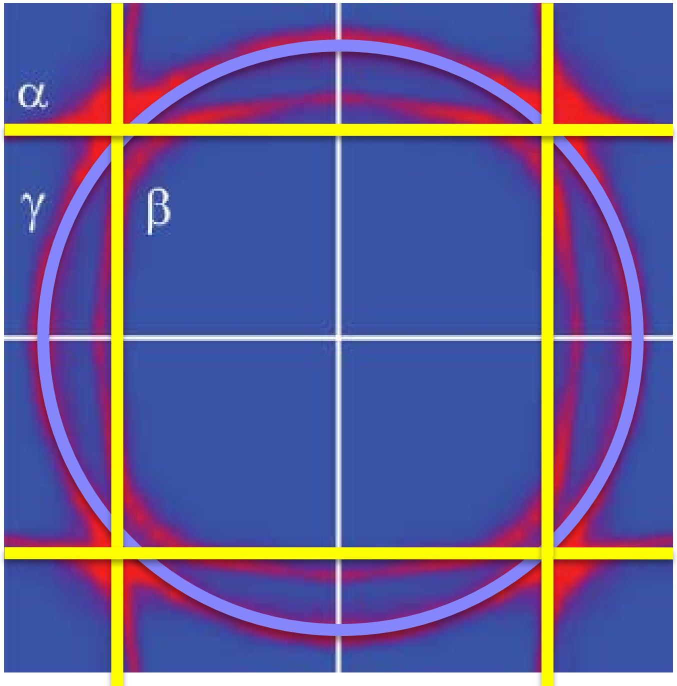
Is Sr_2RuO_4 like ^3He or like the cuprates?

p-wave pairing due to induced, long-ranged attraction mediated by ferromagnetic (q=0) paramagnons

Sigrist and Rice, J. Phys. C **7**, L643 (1996).

p-wave pairing due to strongly q-dependent repulsive interactions associated with antiferromagnetic fluctuations

Raghu, Kapitulnik, and SAK, - Phys. Rev. Lett. **105**, 136401 (2010).



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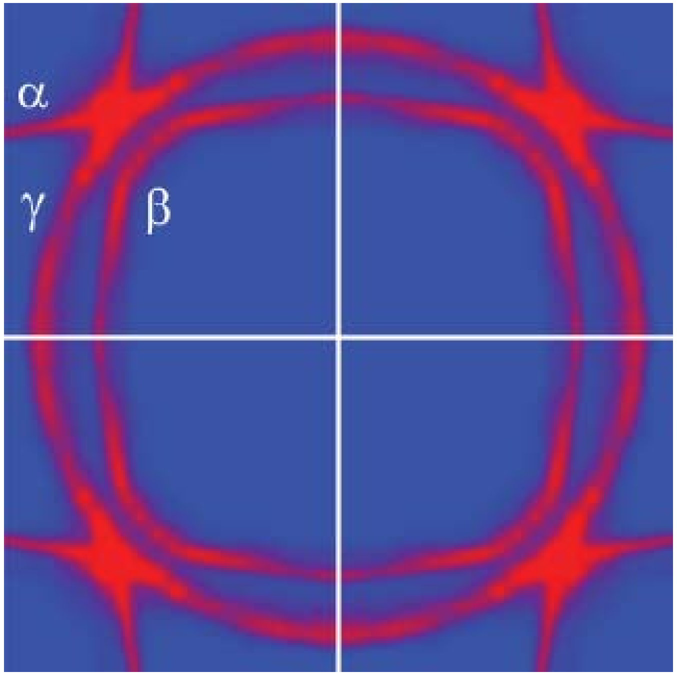

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Despite direct experimental evidence that the SC state breaks time-reversal symmetry, there exist deep (near) gap nodes.

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Preliminary evidence from microscopic measurements of gap structure in STM have corroborated some of the most dramatic features of the predicted gap structure on the quasi 1D bands

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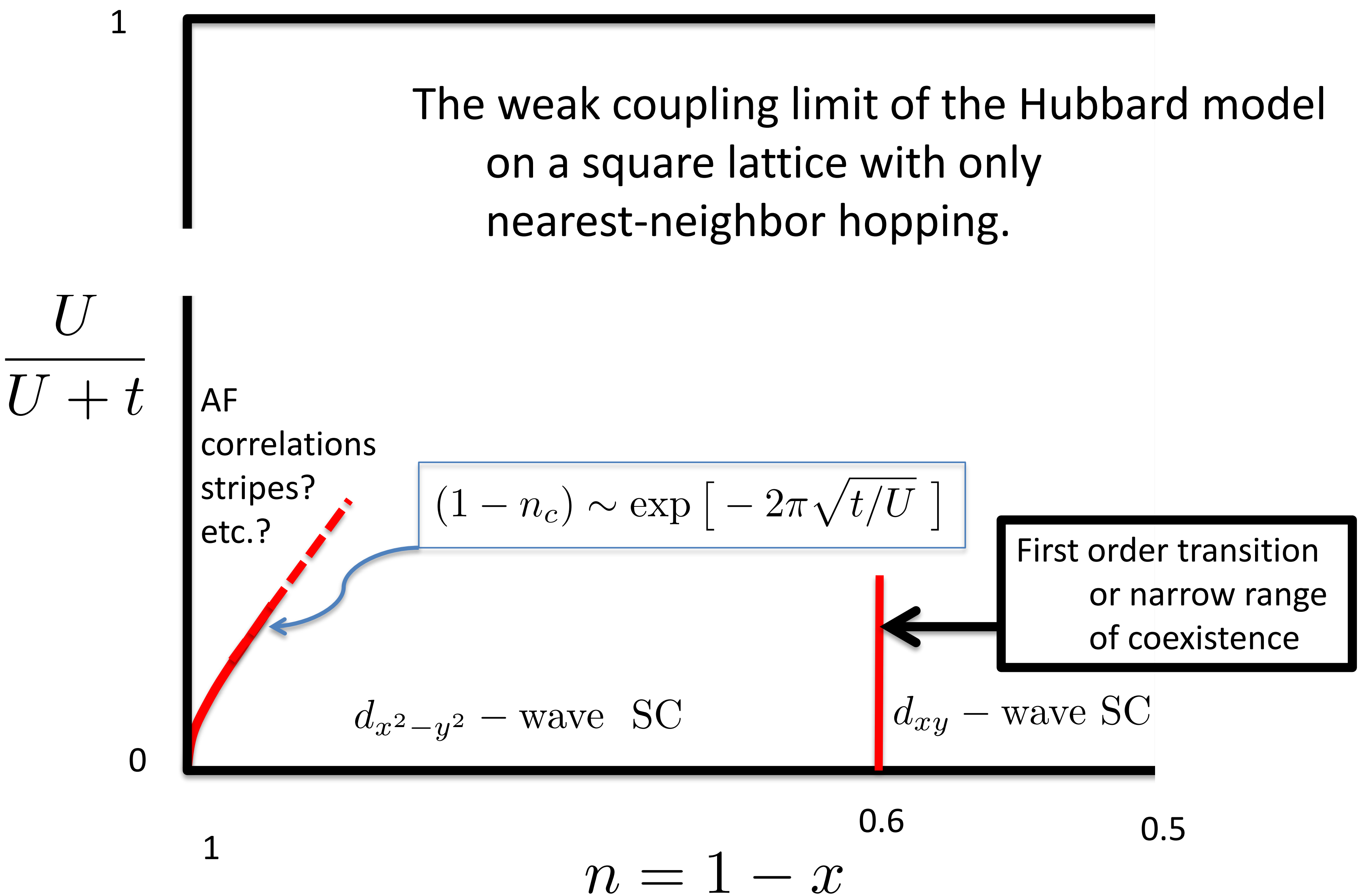
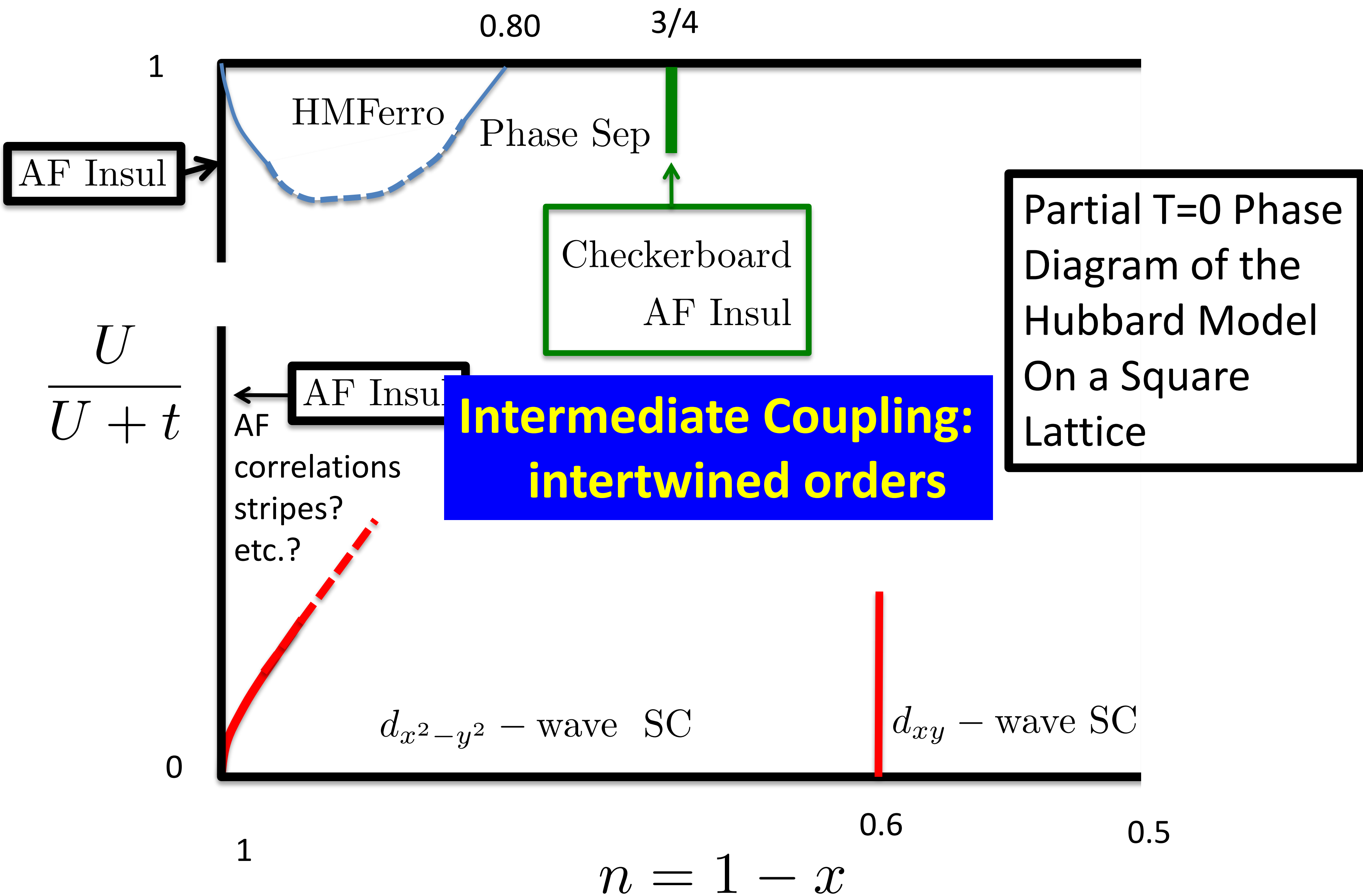
I. Firmo, S. Lederer, C. Lupien, A. P. Mackenzie, J. C. Davis, SAK, Phys. Rev. B (2013)

T=0 Phase diagram of the Hubbard model



T=0 Phase diagram of the Hubbard model



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One may easily see that a flattening of the Fermi surface or an abnormally high density of states can result in a considerable enhancement of phonon anomalies[10] as well as of the mechanism discussed here. A factor of 10 in the exponent does not appear out of the question.

Thanks