LPHYS 2013 – Prague, Czech Republic – July 16th, 2013

Seminar 6: *Physics of Cold Trapped Atoms* – talk 6.4.2

Universiteit Antwerpen

Theory of Quantum and Complex systems

Two-bandgap superfluidity in atomic Fermi systems

J.Tempere, S.N.Klimin, J.T. Devreese

From left to right: dr. Kai Ji, Maarten Baeten, dr. Serghei Klimin, Stijn Ceuppens, Dries Sels, prof. Jacques Tempere, Ben Anthonis, prof. Michiel Wouters, dr. Jeroen Devreese, Enya Vermeyen, Giovanni Lombardi, Selma Koghee, dr. Onur Umucalilar, Nick Van den Broeck.
Not shown: prof.em. Jozef Devreese, prof.em. Fons Brosens, dr. Vladimir Gladilin, dr. Wim Casteels

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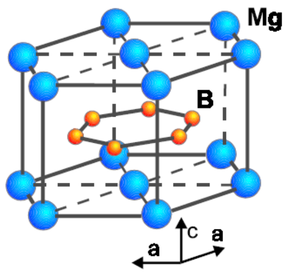
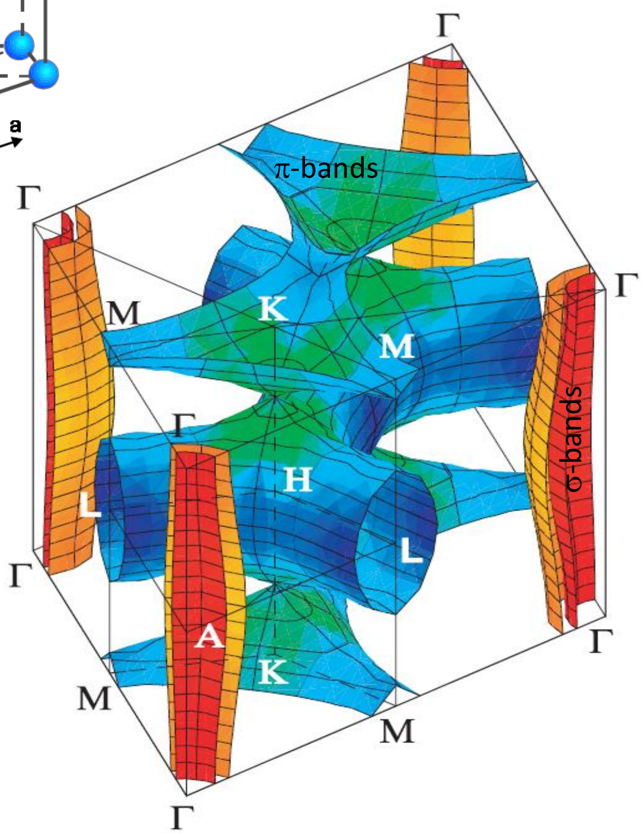
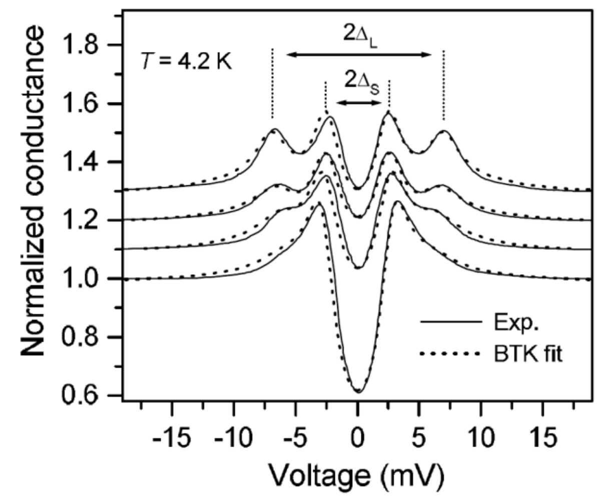
FWO VLAANDEREN Fonds Wetenschappelijk Onderzoek Research Foundation – Flanders

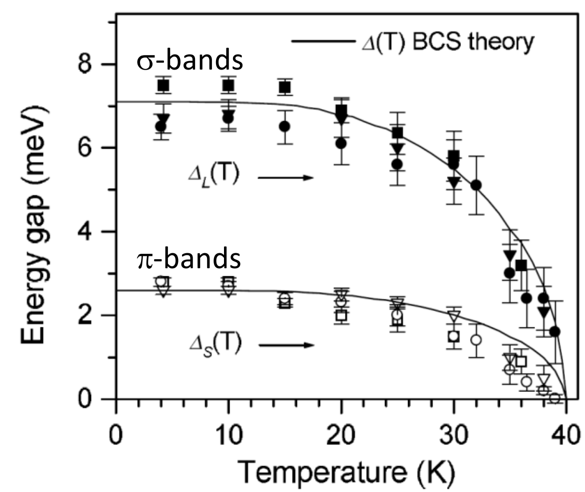
Two-bandgap superconductivity



MgB_2

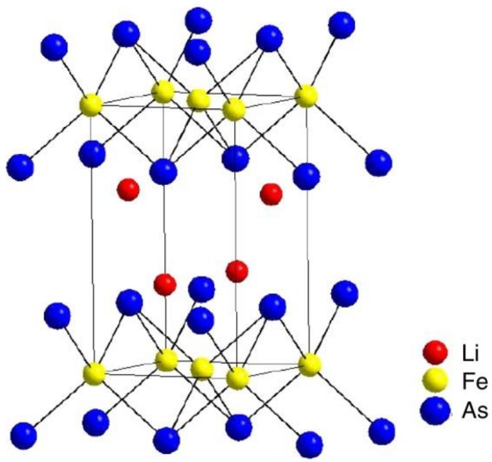




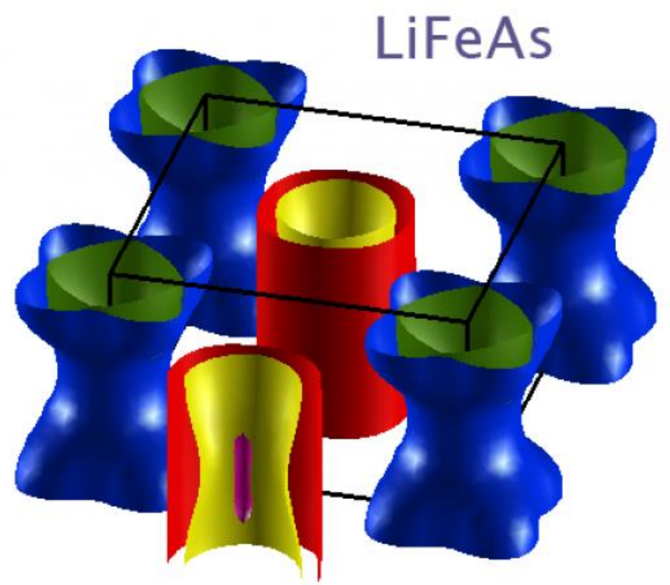


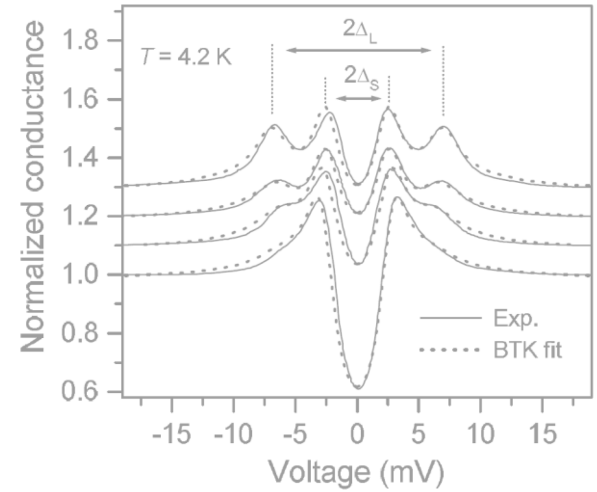
Images from:
P. Szabo et al. , Phys. Rev. Lett. **87**, 137005 (2001).
H.-J. Choi, D. Roundy, H. Sun, M.L. Cohen, S.G. Louie, Nature **418**, 758-760 (2002).

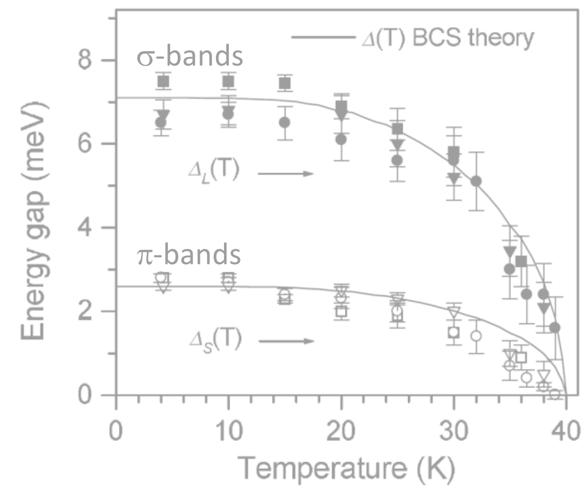
Two-bandgap superconductivity



Also the recently discovered iron pnictide class of superconductors have multiple gaps







Images from:
X.C. Wang et al., Solid State Communications **148**, 538 (2008).
http://www2.physics.ox.ac.uk/research/quantum-matter-in-high-magnetic-fields/fermi-surfaces

The special case of MgB_2 : type 1.5 superconductivity

Gaps[1]:
Δ_π = 2.2 meV
Δ_σ = 7.1 meV

Fermi velocities[2]:
$v_{F,\pi} = 5.4\times10^5$ m/s
$v_{F,\sigma} = 4.4\times10^5$ m/s

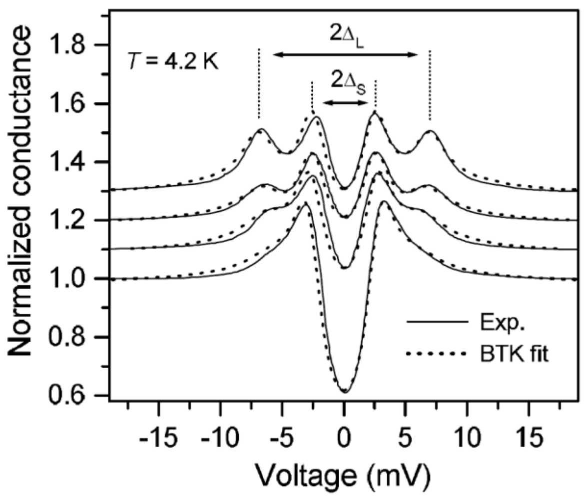
$$\xi(0) = \hbar v_F / \pi\Delta(0)$$

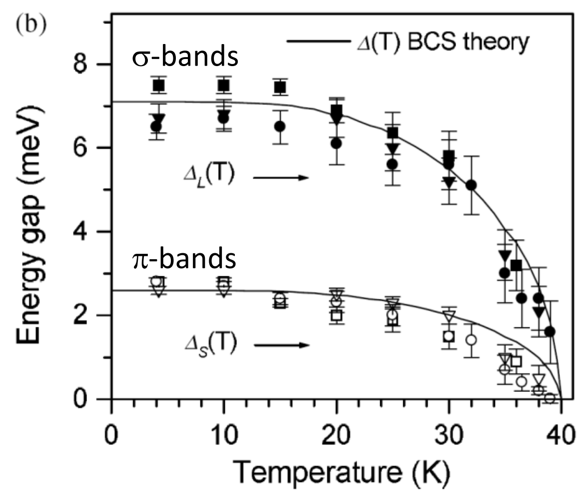
Coherence lengths:
ξ_π = 51 nm
ξ_σ = 13 nm

Penetration depths:
λ_π = 34 nm
λ_σ = 48 nm

SC Plasma frequencies[3]

GL paramater[4]:
κ_π = 0.66 **TYPE I**
κ_σ = 3.68 **TYPE II**





1) H.-J. Choi et al., Nature **418**, 758-760 (2002).
2) A. Brinkman et al., Phys. Rev. B **65**, 180517(R) (2002).
3) I. I. Mazin et al., Phys. Rev. Lett. **89**, 107002 (2002).
4) V. V. Moshchalkov et al., Phys. Rev. Lett. **102**, 117001 (2009).

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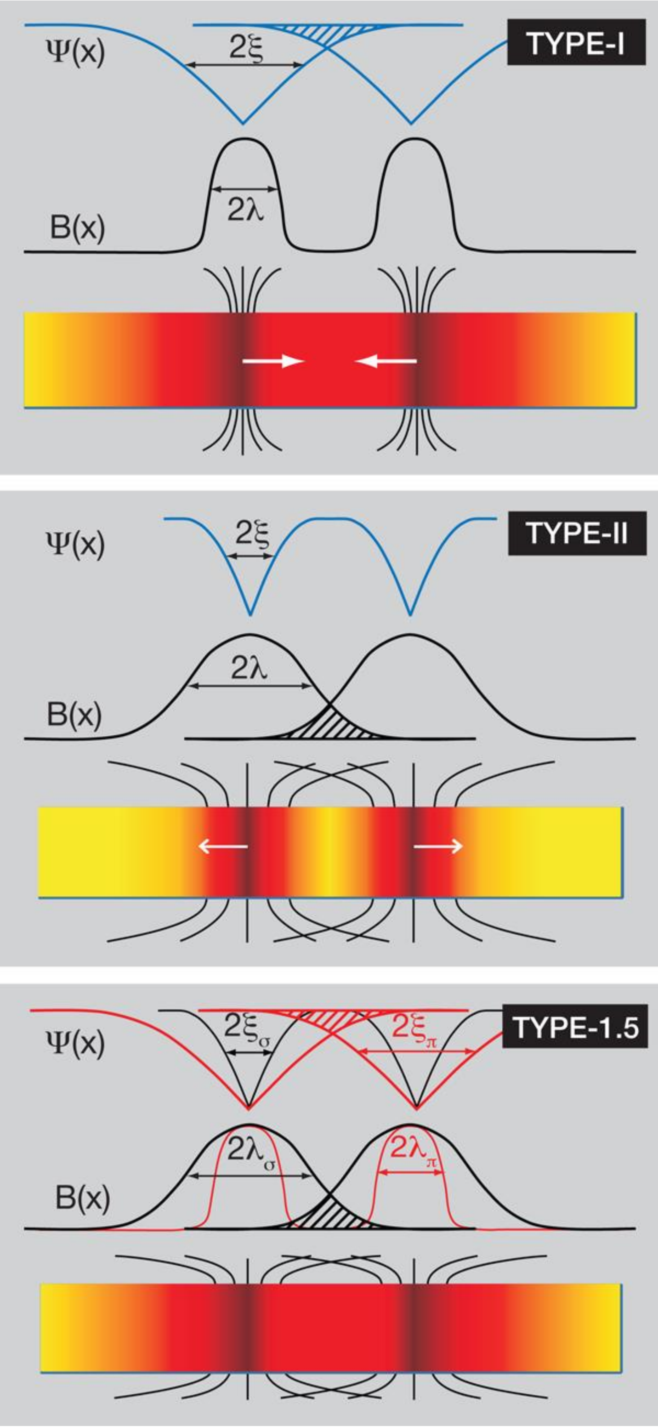

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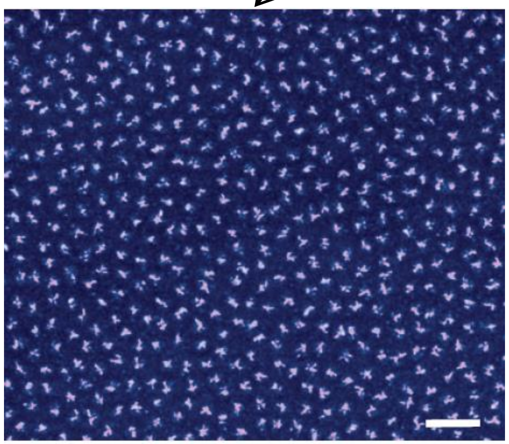
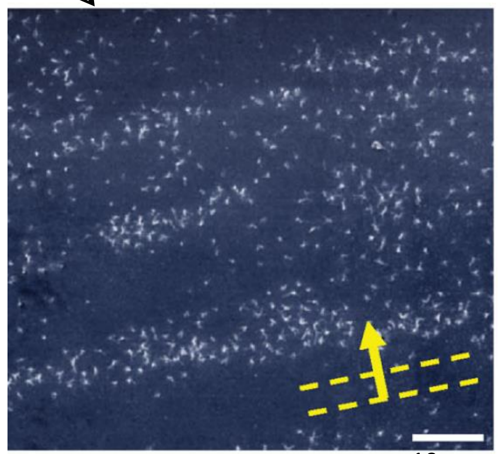
Type 1.5 superconductivity

Vortices made visible with bitter decoration, in a field-cooled experiment

Compare $NbSe_2$ (type II) to MgB_2 :

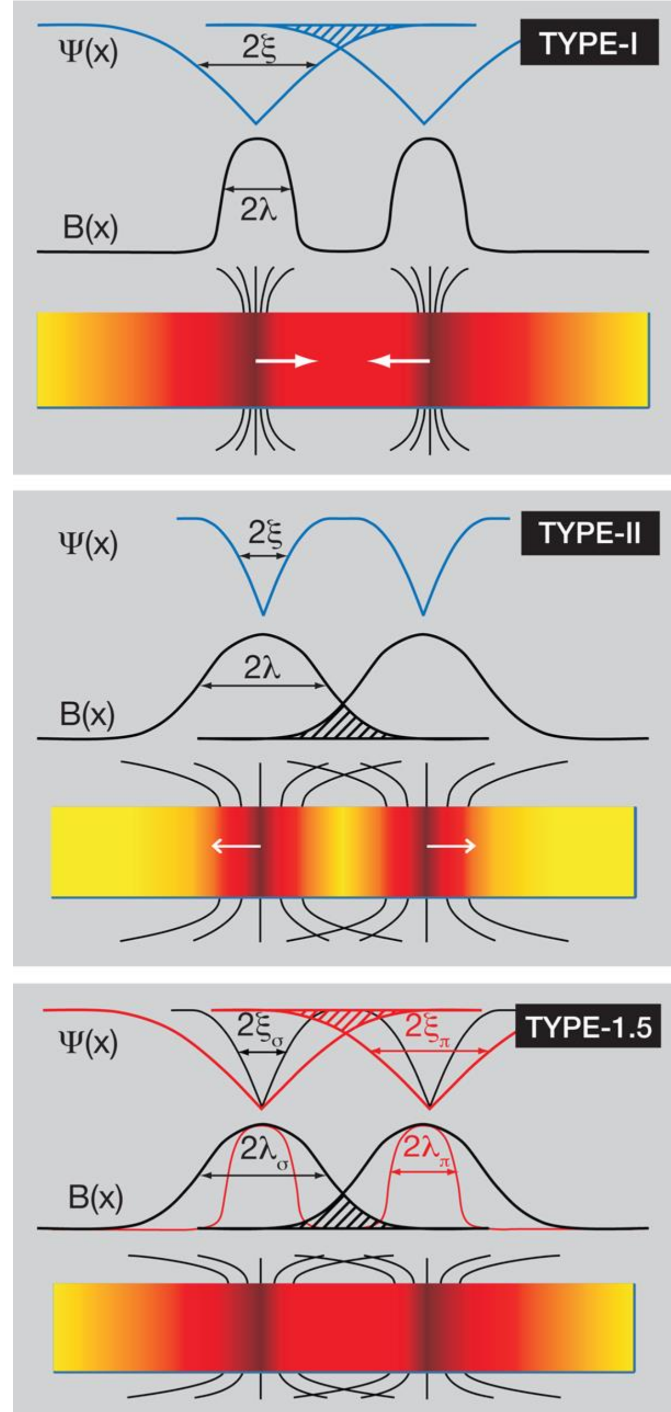


10 μm



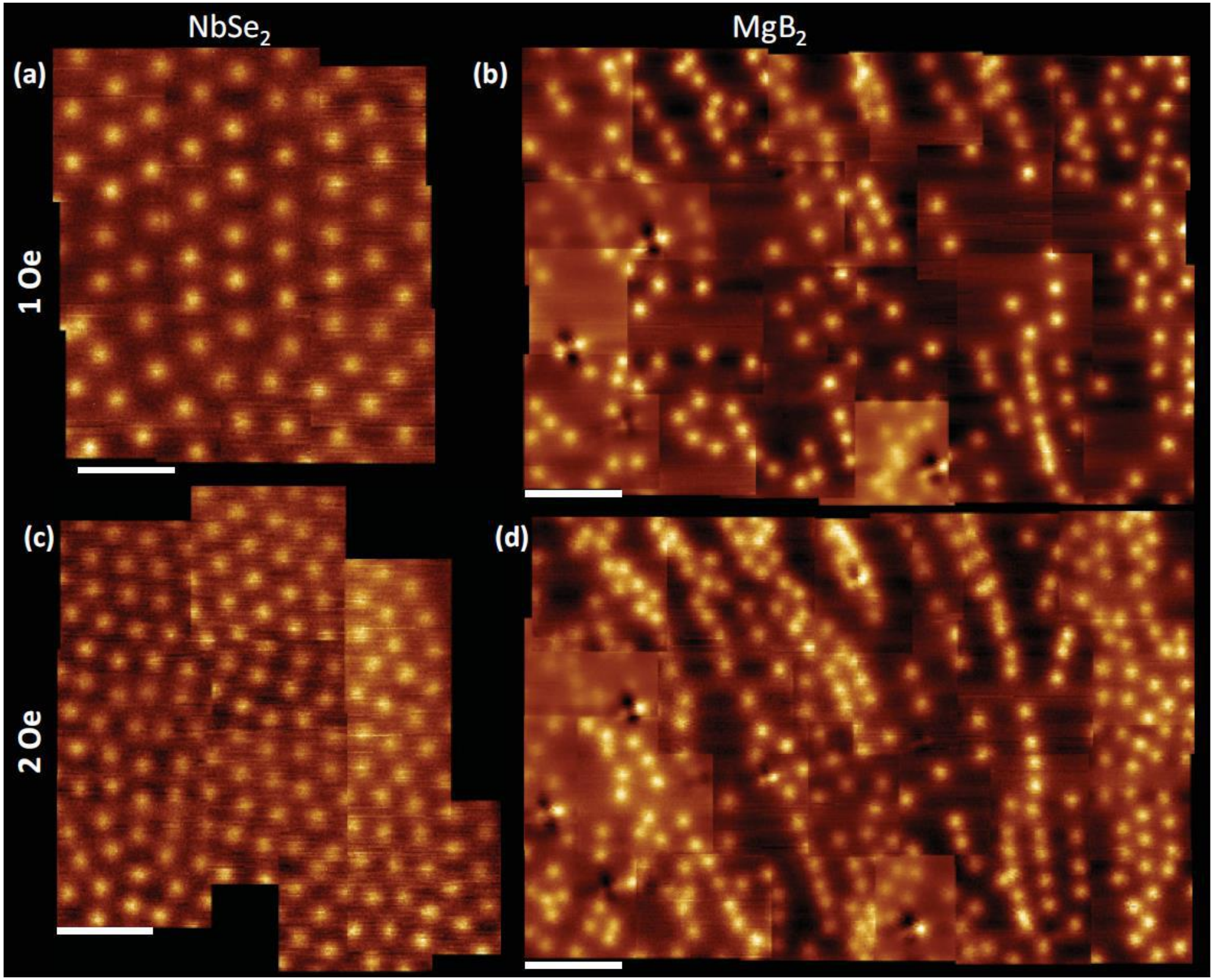
10 μm

Clustering in the case of MgB_2 may point to an in interaction potential with both repulsive and attractive components.



V. V. Moshchalkov, M. Menghini, T. Nishio, Q. H. Chen, A. V. Silhanek, V. H. Dao, L. F. Chibotaru, N. D. Zhigadlo, and J. Karpinski, Phys. Rev. Lett. **102**, 117001 (2009).

Scanning Hall probe microscopy



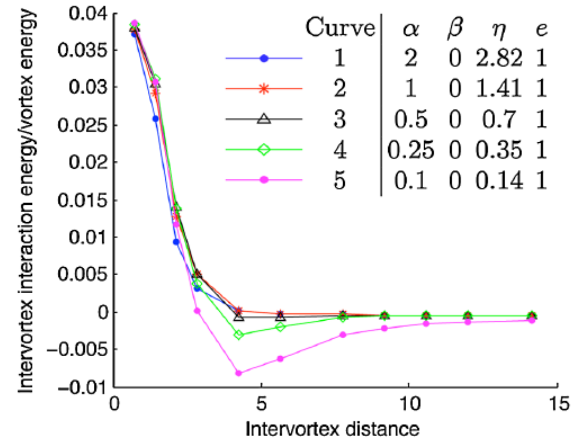
- Stripes rather than clusters
- Direction not related to crystal lattice or edge
- Stripe direction maintained in successive field-cooling runs, but vortex position in stripe is different (no pinning)

J. Gutierrez, B. Raes, A. V. Silhanek, L. J. Li, N. D. Zhigadlo, J. Karpinski, J. Tempere, and V. V. Moshchalkov, Phys. Rev. B **85**, 094511 (2012).

Two-bandgap Ginzburg-Landau theory

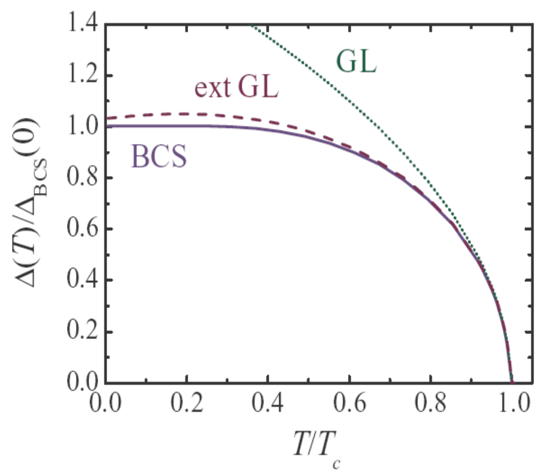
Zhitomirsky and Dao[1] propose a two-bandgap extension to GL theory, with ad-hoc Josephson coupling, and two length scales, and Babaev et al.[2] find that it can lead to the correct vortex behavior.

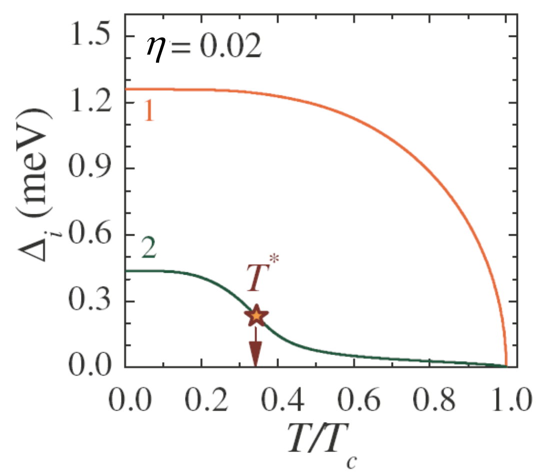
$$\mathcal{F} = \frac{1}{2}\sum_{i=1,2} |(\nabla + ie\mathbf{A})\psi_i|^2 + \frac{1}{2}(\nabla\times\mathbf{A})^2 + \frac{1}{2}(|\psi_1|^2-1)^2$$
$$+\alpha|\psi_2|^2 + \frac{1}{2}\beta|\psi_2|^4 - \eta|\psi_1||\psi_2|\cos(\theta_2-\theta_1).$$



Kogan and Schmalian[3] contest the coupling, in that this term lies outside the temperature validity of GL → only one length scale, since gaps are always proportional to eachother.

Shanenko et al.[4] expand the free energy to higher order in (1–T/T_c) and find that the two length scales are present and revealed through a hidden criticality in $\partial\psi/\partial\eta$ → two length scales.

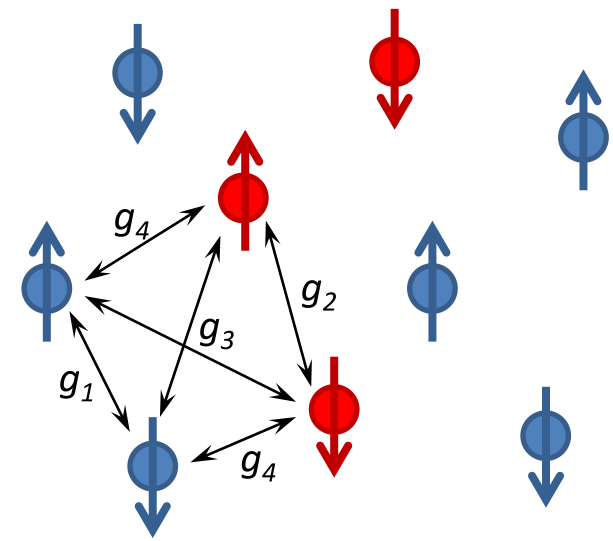




1) M. E. Zhitomirsky and V.-H. Dao, Phys. Rev. B **69**, 054508 (2004).
2) E. Babaev, J. Carlstrom, and M. Speight, Phys. Rev. Lett. **105**, 067003 (2010).
3) V. G. Kogan and J. Schmalian, Phys. Rev. B **83**, 054515 (2011).
4) A. A. Shanenko, M.V. Milosevic, and F. M. Peeters, Phys. Rev. Lett. **106**, 047005 (2011).

Simplify life with a two-bandgap superfluid

We consider a 4-component system with
two "intraband" BCS channels and "interband" scattering:



$$S = \int_0^\beta d\tau \int d\mathbf{r} \sum_{j=1,2} \sum_{\sigma=\uparrow,\downarrow} \bar{\phi}_{j,\sigma} \left(\frac{\partial}{\partial \tau} + H_{j,\sigma} \right) \phi_{j,\sigma}$$

$$+ \int_0^\beta d\tau \int d\mathbf{r} \left\{ \sum_{j=1,2} g_j \bar{\phi}_{j,\uparrow} \bar{\phi}_{j,\downarrow} \phi_{j,\downarrow} \phi_{j,\uparrow} \right.$$

$$+ g_3 \left(\bar{\phi}_{1,\uparrow} \phi_{1,\uparrow} \bar{\phi}_{2,\downarrow} \phi_{2,\downarrow} + \bar{\phi}_{1,\downarrow} \phi_{1,\downarrow} \bar{\phi}_{2,\uparrow} \phi_{2,\uparrow} \right)$$

$$\left. + g_4 \left(\bar{\phi}_{1,\uparrow} \phi_{1,\uparrow} \bar{\phi}_{2,\uparrow} \phi_{2,\uparrow} + \bar{\phi}_{1,\downarrow} \phi_{1,\downarrow} \bar{\phi}_{2,\downarrow} \phi_{2,\downarrow} \right) \right\}$$

The single-particle contributions to the action functional allow for population imbalances and interspecies mass imbalance:

$$H_{j,\sigma} = -\frac{1}{2m_j} \nabla_{\mathbf{r}}^2 - \mu_{\sigma,j} \qquad \mu_{j,\uparrow} = \mu_j + \zeta_j \text{ and } \mu_{j,\downarrow} = \mu_j - \zeta_j$$

From Hubbard-Stratonovic to a Josephson coupling term

The thermodynamic potential is calculated in the functional integral formalism:

$$\mathcal{Z} = e^{-\beta\Omega(T,V,\mu_{j\sigma})} = \int \mathcal{D}\bar{\phi}\mathcal{D}\phi \;\exp\left\{-S[\bar{\phi},\phi]\right\}$$

From Hubbard-Stratonovic to a Josephson coupling term

The four-fermion field interaction terms are decoupled using 2 Hubbard-Stratonovic fields

$$\mathcal{Z} = e^{-\beta\Omega(T,V,\mu_{j\sigma})} = \int \mathcal{D}\bar{\phi}\mathcal{D}\phi \ \exp\left\{-S[\bar{\phi},\phi]\right\} = \int \mathcal{D}\bar{\phi}\mathcal{D}\phi \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi \ \exp\left\{-S_{HS}[\bar{\Psi},\Psi,\bar{\phi},\phi]\right\}$$

with

$$S_{HS} = S_B - \sum_{j=1,2} \int_0^\beta d\tau \int d\mathbf{r} \begin{pmatrix} \bar{\phi}_{j,\uparrow} & \phi_{j,\downarrow} \end{pmatrix} \begin{pmatrix} -\frac{\partial}{\partial\tau} - H_{j,\uparrow} & \Psi_j \\ \bar{\Psi}_j & -\frac{\partial}{\partial\tau} + H_{j,\downarrow} \end{pmatrix} \begin{pmatrix} \phi_{j,\uparrow} \\ \bar{\phi}_{j,\downarrow} \end{pmatrix}$$

$$\Big\downarrow$$

$$S_B = -\int_0^\beta d\tau \int d\mathbf{r} \left[\frac{1}{G_1}\bar{\Psi}_1\Psi_1 + \frac{1}{G_2}\bar{\Psi}_2\Psi_2 - \frac{1}{G_{12}}\left(\bar{\Psi}_1\Psi_2 + \bar{\Psi}_2\Psi_1\right)\right]$$

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The effective coupling constants are

$$\frac{1}{G_1} = \frac{g_2}{g_1 g_2 - (g_4 - g_3)^2} \qquad \frac{1}{G_2} = \frac{g_1}{g_1 g_2 - (g_4 - g_3)^2} \qquad \frac{1}{G_{12}} = \frac{g_4 - g_3}{g_1 g_2 - (g_4 - g_3)^2}$$

and are related to the scattering lengths through following renormalization:

$$\frac{1}{g_j} = m_j \left(\frac{1}{4\pi a_j} - \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{k^2}\right) \qquad \text{for } m_3, m_4 \text{ use } \frac{4m_1 m_2}{m_1 + m_2}$$

Integration over the fermion fields → effective bosonic action

The integration over the fermion fields leads to an effective bosonic field action:

$$\mathcal{Z} = e^{-\beta\Omega(T,V,\mu_{j\sigma})} = \int \mathcal{D}\bar{\phi}\mathcal{D}\phi \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi \; \exp\left\{-S_{HS}[\bar{\Psi},\Psi,\bar{\phi},\phi]\right\} = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi \exp\left\{-S_{eff}[\bar{\Psi},\Psi]\right\}$$

This action functional is given by

$$S_{eff} = S_B - \sum_{j=1,2} \mathrm{Tr}\ln\left(-\mathbb{G}_j^{-1}\right)$$

$$-\mathbb{G}_j^{-1}(\mathbf{r},\tau) = -\mathbb{G}_{j,0}^{-1}(\mathbf{r},\tau) + \mathbb{F}_j(\mathbf{r},\tau)$$

with $\mathbb{G}_{j,0}^{-1}(\mathbf{r},\tau) = \begin{pmatrix} -\partial_\tau - H_{j,\sigma} & 0 \\ 0 & -\partial_\tau + H_{j,\sigma} \end{pmatrix}$ and $\mathbb{F}_j(\mathbf{r},\tau) = \begin{pmatrix} 0 & -\Psi_j(\mathbf{r},\tau) \\ -\bar{\Psi}_j(\mathbf{r},\tau) & 0 \end{pmatrix}$

$$\downarrow$$

$$S_{eff} = S_B \underbrace{- \sum_{j=1,2} \mathrm{Tr}\ln\left[-\mathbb{G}_{j,0}^{-1}\right]}_{S_0} + \sum_{j=1,2}\sum_{p=1}^{\infty} \underbrace{\frac{1}{p}\mathrm{Tr}\left[\left(\mathbb{G}_{j,0}\mathbb{F}_j\right)^p\right]}_{S_{\Psi_j}^{(p)}}$$

In general, the sum over p cannot be taken analytically, except for Ψ constant.
Here, we assume that the pair fields vary slowly in time and space.

Gradient expansion of the bosonic action

The gradient expansion in the effective action

$$S_{eff} = S_B + S_0 + \sum_{j=1,2} \sum_{p=1}^{\infty} S_{\Psi_j}^{(p)} \qquad \text{with} \qquad S_{\Psi}^{(p)} = \frac{1}{p} \operatorname{Tr}\left[(\mathbb{G}_0 \mathbb{F})^p \right]$$

is performed by setting

$$\mathbb{F}(\mathbf{r}+\mathbf{r}', \tau+\tau') = \mathbb{F}(\mathbf{r},\tau) + \tau' \frac{\partial \mathbb{F}(\mathbf{r},\tau)}{\partial \tau} + \mathbf{r}' \cdot \nabla_{\mathbf{r}} \mathbb{F}(\mathbf{r},\tau) + \frac{1}{2} \sum_{i,i' \in \{x,y,z\}} \frac{\partial^2 \mathbb{F}(\mathbf{r},\tau)}{\partial x_i \partial x_{i'}} x'_i x'_{i'} \cancel{+\ldots}$$

In each term of the p summation we have

$$S_{\Psi}^{(p)} = S_{\Psi}^{(p,0)} + S_{\Psi}^{(p,\tau)} + S_{\Psi}^{(p,r)}$$

Zeroth-order term

Term with the time derivatives

Term with the gradients

The subsequent summation over p is performed for each of these three terms separately.

Example: zeroth order term

The action, up to first order time derivatives and up to second order in the gradients:

$$S_{eff} \approx S_B + S_0 + \sum_{j=1,2} \sum_{p=1}^{\infty} \left(S_{\Psi_j}^{(p,0)} + S_{\Psi_j}^{(p,\tau)} + S_{\Psi_j}^{(p,r)} \right)$$

$$S_{\Psi}^{(p,0)} = \frac{1}{p} \frac{1}{\beta V} \sum_{\mathbf{k},n} \int_0^{\beta} d\tau \int d\mathbf{r}\, \mathrm{Tr}\left[(\mathbb{F}(\mathbf{r},\tau)\mathbb{G}_0(\mathbf{k},n))^p \right]$$

$$\mathbb{F}(\mathbf{r},\tau)\mathbb{G}_0(\mathbf{k},n) = \begin{pmatrix} 0 & -\dfrac{\Psi(\mathbf{r},\tau)}{i\omega_n + \xi_{\mathbf{k}}} \\ -\dfrac{\Psi^*(\mathbf{r},\tau)}{i\omega_n - \xi_{\mathbf{k}}} & 0 \end{pmatrix}$$

(p even)

$$\mathrm{Tr}\left[(\mathbb{F}(\mathbf{r},\tau)\mathbb{G}_0(\mathbf{k},n))^p \right] = 2 \left(\frac{|\Psi(\mathbf{r},\tau)|^2}{\omega_n^2 + \xi_{\mathbf{k}}^2} \right)$$

matsubara frequencies

free fermion dispersion

Resumming the zeroth order terms gives:

$$S_B + S_0 + \sum_{j=1,2} \sum_{p=1}^{\infty} S_{\Psi_j}^{(p,0)} = - \sum_{j=1,2} \int_0^{\beta} d\tau \int d\mathbf{r} \left\{ \frac{m_j w_j}{4\pi a_j} + \right.$$

$$\left. + \int \frac{d\mathbf{k}}{(2\pi)^3} \left[\frac{1}{\beta} \ln\left[2\cosh\left(\beta\zeta_j\right) + 2\cosh\left(\beta E_{\mathbf{k},j}\right) \right] - \xi_{\mathbf{k},j} - \frac{m_j w_j}{k^2} \right] \right\}$$

with $w_j = |\Psi_j|^2$ and $E_{\mathbf{k},j} = \sqrt{\xi_{\mathbf{k},j}^2 + |\Psi_j|^2}$

The (gradient-expanded) extended Ginzburg-Landau action

The gradient expansion of the pair fields
+ complete summation of the series in powers of $\Psi_j, \bar{\Psi}_j$
lead to the extended TDGL-like functional

$$\boxed{\begin{aligned} S_{GL} = \int_0^\beta d\tau \int d\mathbf{r} \sum_{j=1,2} \Bigg[\Omega_{s,j} + \frac{D_j}{2} \left(\frac{\partial \bar{\Psi}_j}{\partial \tau} \Psi_j - \bar{\Psi}_j \frac{\partial \Psi_j}{\partial \tau} \right) \\ + \frac{C_j}{2m_j} \left| \nabla_{\mathbf{r}} \Psi_j \right|^2 - \frac{E_j}{2m_j w_j} \left[\left(\bar{\Psi}_j \nabla_{\mathbf{r}} \Psi_j \right)^2 + \left(\Psi_j \nabla_{\mathbf{r}} \bar{\Psi}_j \right)^2 \right] \Bigg] \\ - \frac{m_{12}\gamma}{4\pi} \left(\bar{\Psi}_1 \Psi_2 + \bar{\Psi}_2 \Psi_1 \right) \Big\} . \end{aligned}}$$

The coefficients C_j, D_j, E_j depend on the order parameters $\Psi_j, \bar{\Psi}_j$
and the single-component thermodynamic potentials are

$$\Omega_{s,j} = \int \frac{d\mathbf{k}}{(2\pi)^3} \left[\frac{1}{\beta} \ln \left[2\cosh\left(\beta\zeta_j\right) + 2\cosh\left(\beta E_{\mathbf{k},j}\right) \right] - \xi_{\mathbf{k},j} - \frac{m_j w_j}{k^2} \right] + \frac{m_j w_j}{4\pi a_j}$$

with $w_j = \left|\Psi_j\right|^2$ and $E_{\mathbf{k},j} = \sqrt{\xi_{\mathbf{k},j}^2 + \left|\Psi_j\right|^2}$

The (gradient-expanded) extended Ginzburg-Landau action

The explicit forms of the other coefficients are:

$$
\boxed{
\begin{aligned}
C_j &= \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{k^2}{3m_j}\left[f_2\left(\beta, E_{\mathbf{k},j},\zeta_j\right)\right. \\
&\quad \left. -4\xi_k^2 w_j\ f_4\left(\beta, E_{\mathbf{k},j},\zeta_j\right)\right], \\
D_j &= \int \frac{d\mathbf{k}}{(2\pi)^3}\frac{\xi_{\mathbf{k}}}{w_j}\left[f_1\left(\beta,\xi_{\mathbf{k},j},\zeta_j\right) - f_1\left(\beta, E_{\mathbf{k},j},\zeta_j\right)\right] \\
E_j &= 2w_j\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{k^2}{3m_j}\xi_{\mathbf{k},j}^2\ f_4\left(\beta, E_{\mathbf{k},j},\zeta_j\right).
\end{aligned}
}
$$

The functions $f_p(\beta,\varepsilon,\zeta)$ are based on the Matsubara sums, and can be expressed using the recurrence relations

$$
f_1\left(\beta,\varepsilon,\zeta\right) = \frac{1}{2\varepsilon}\frac{\sinh\beta\varepsilon}{\cosh\beta\varepsilon+\cosh\beta\zeta},
$$

$$
f_{p+1}\left(\beta,\varepsilon,\zeta\right) = -\frac{1}{2p\varepsilon}\frac{\partial f_p\left(\beta,\varepsilon,\zeta\right)}{\partial\varepsilon}.
$$

Comparison with existing TDGL expansions

For single-band Fermi superfluids, time-dependent Ginzburg-Landau (TDGL) type equations have been proposed by

1/ Sa de Melo, Randeria and Engelbrecht[1] *:*

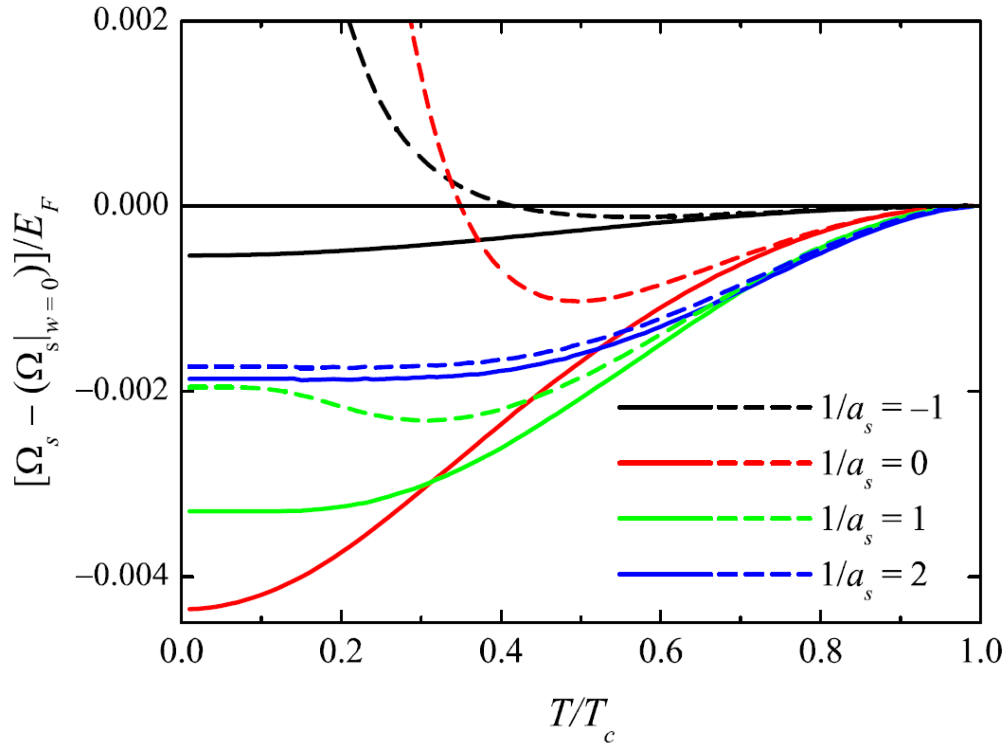
In their seminal BEC-BCS crossover paper, these authors propose a fluctuation expansion around $|\Psi|=0$, which corresponds to setting $E_{\mathbf{k}} \to \xi_{\mathbf{k}}$ in our coefficients. In this limit, our coefficient C corresponds to their "c" and the coefficients of $|\Psi|^2$ and $|\Psi|^4$ in Ω_s correspond to their $-a$ and b respectively.

2/ *Huang, Yu and Yin*[2]

This more recent derivation for a single-bandgap superfluid restricts the summations to $p \leq 2$

present theory

TDGL approach[1]



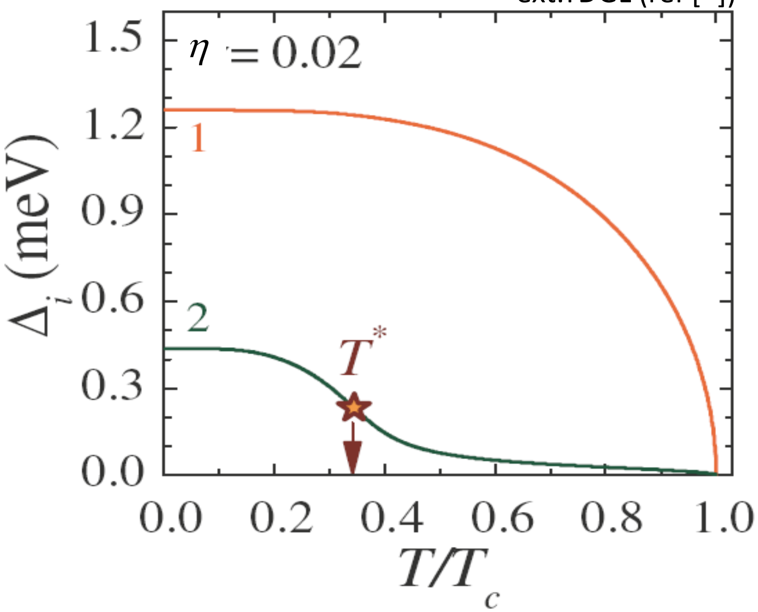
1) C.A.R. Sa de Melo, M. Randeria, and J.R. Engelbrecht, Phys. Rev. Lett. 71, 3202 (1993).
2) K. Huang, Z.-Q. Yu and L. Yin, Phys. Rev. A 79, 053602 (2009).

Comparison with two-band superconductors

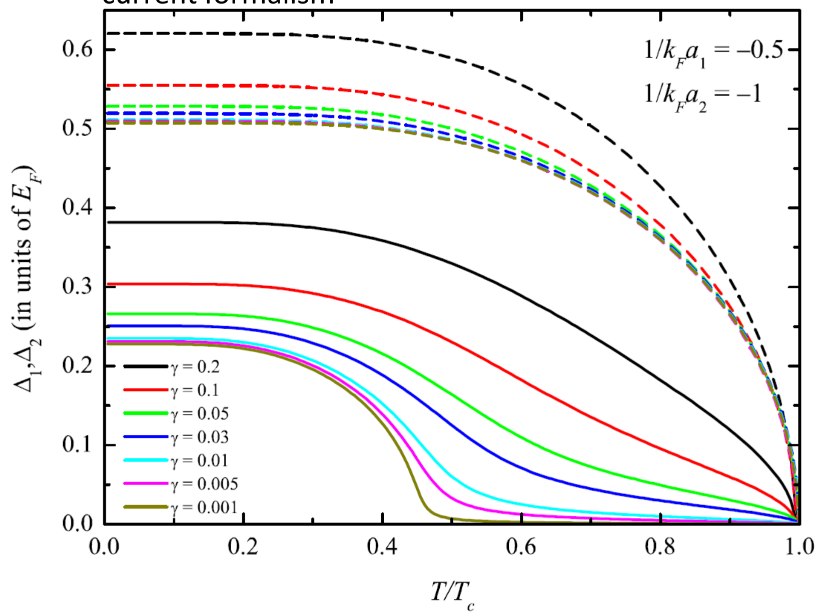
For two-band superconductors, Shanenko et al. developed an extended Ginzburg-Landau formalism[*] by expanding up to $(1-T/T_c)^{5/2}$. This agrees well (<5% error) with Bogoliubov-de Gennes calculations at all T.

This different approach nevertheless gives qualitatively similar results as the present approach, for the band gaps.

ext.TDGL (ref [*])



current formalism



[*] A. A. Shanenko, M.V. Milosevic, and F. M. Peeters, Phys. Rev. Lett. **106**, 047005 (2011); L. Komendova, Y. Chen, A.A. Shanenko, M.V. Milosevic, and F.M. Peeters, Phys. Rev. Lett. 108, 207002 (2012).

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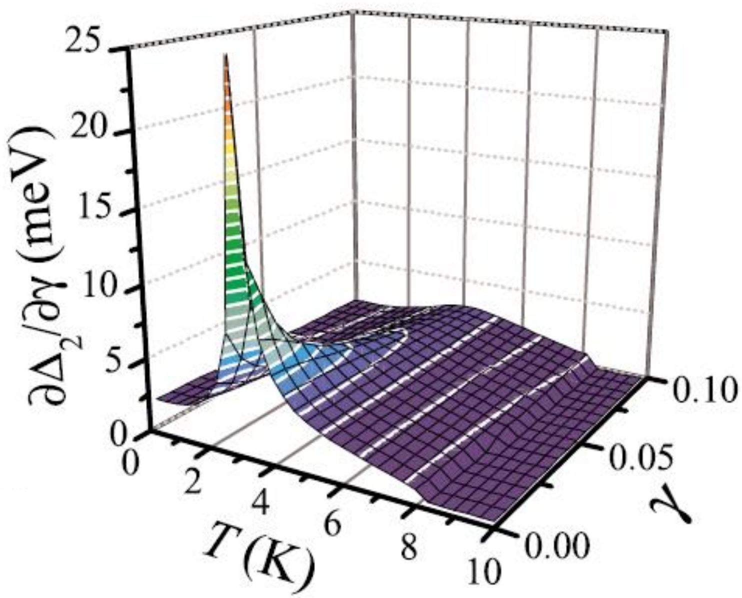

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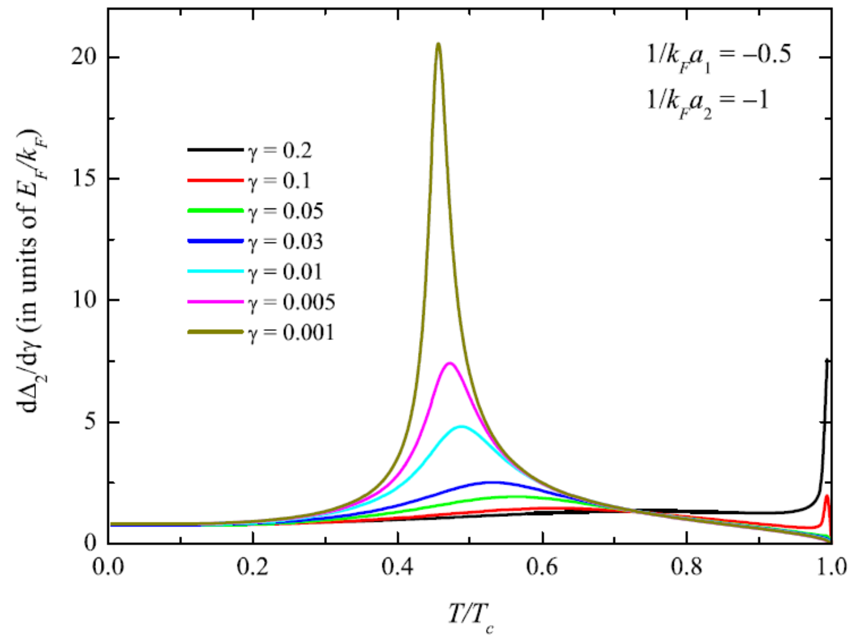

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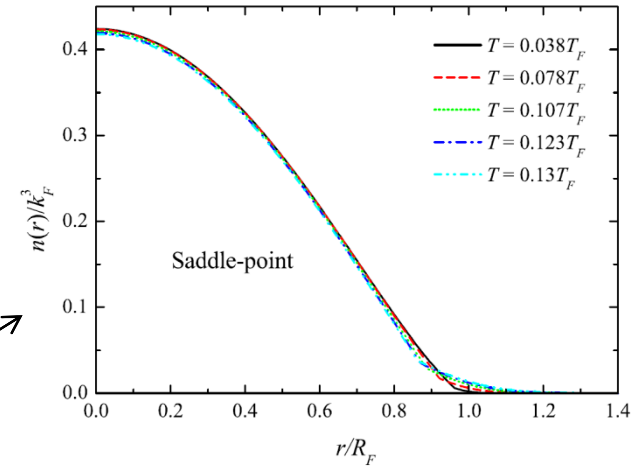
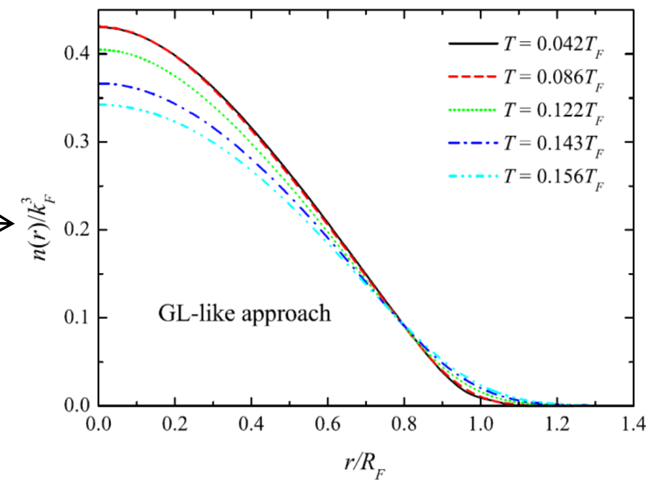
Including external potentials

An external potential is usually taken into account through a local density approximation for the chemical potential. Here we can also take it into account either directly though $H_{j,\sigma}$ or by adding a term $V_j(\mathbf{r})\,|\Psi_j|^2$ to the GL functional. For small order parameters, these methods are equivalent.



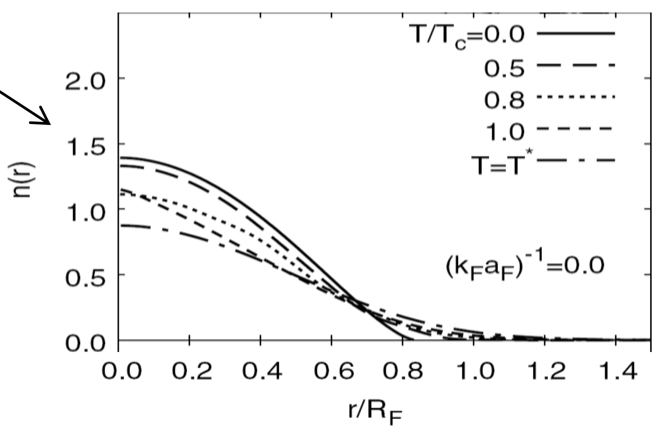
Saddle point result + local chemical potential.

Current approach



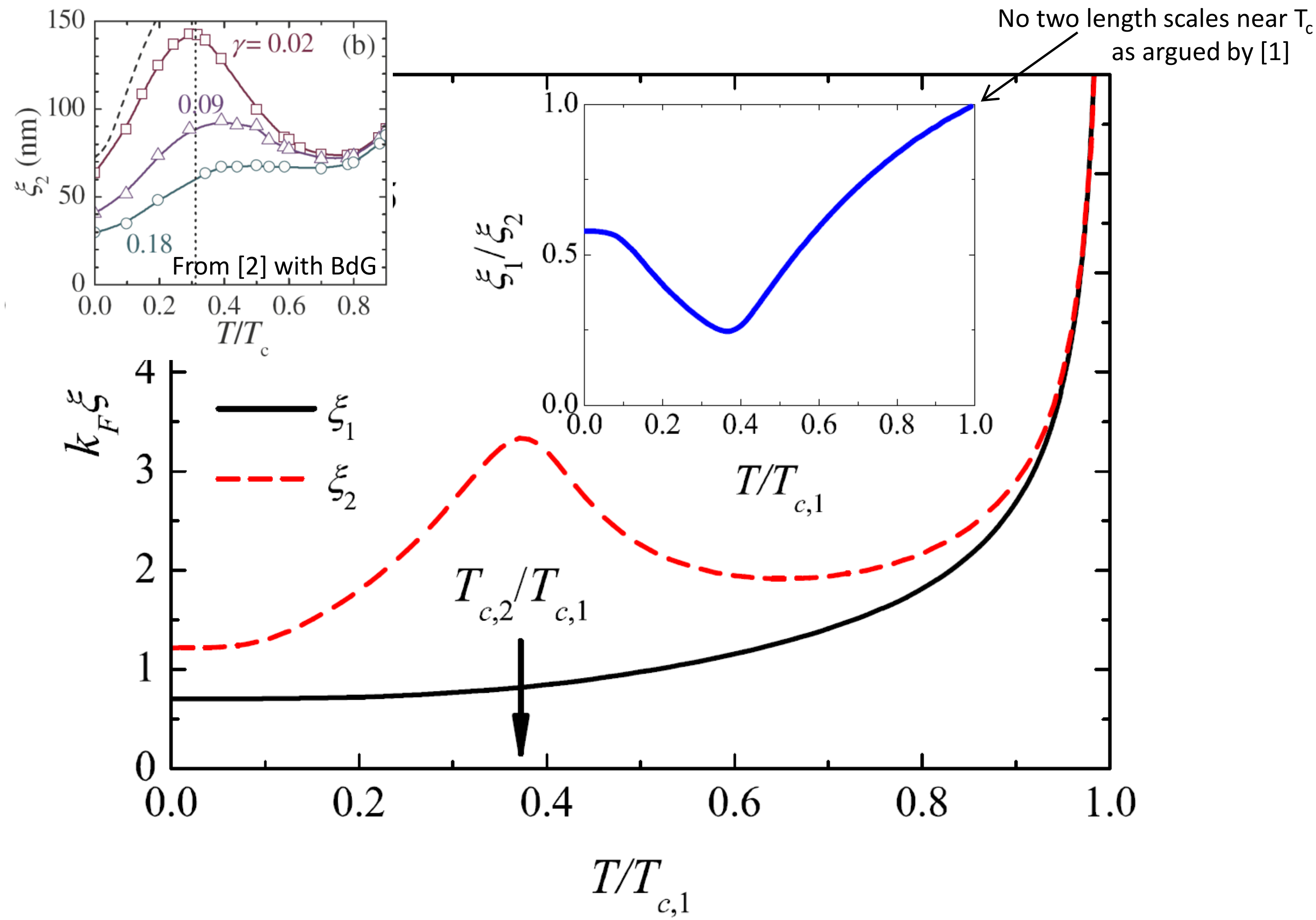
Many-body diagrammatic technique

(from A. Perali, P. Pieri, L. Pisani, and G. C. Strinati, Phys. Rev. Lett. **92**, 220404 (2004)).



Healing lengths & two-band superconductors

Using variational trial functions $\Delta_j \tanh\left[x/\left(\sqrt{2}\xi_j\right)\right]$ with Δ_j the bulk order parameter and ξ_j the variational parameter for the healing lengths, we find:



[1] V. G. Kogan and J. Schmalian, Phys. Rev. B **83**, 054515 (2011).

[2] A. A. Shanenko, M.V. Milosevic, and F. M. Peeters, Phys. Rev. Lett. **106**, 047005 (2011); L. Komendova, Y. Chen, A.A. Shanenko, M.V. Milosevic, and F.M. Peeters, Phys. Rev. Lett. 108, 207002 (2012).

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Conclusions

Theory of Quantum and Complex systems

- The path-integral formalism for interacting fermions has been applied to the two-band system starting from the microscopic Hamiltonian
- The interband Josephson coupling is not introduced ad hoc. Instead, it is derived at the stage of the Hubbard - Stratonovich transformation.
- A TDGL-like variational functional has been derived collecting all terms in powers of the order parameter, being therefore valid also when the order parameter is not small.
- The formalism can find a broad spectrum of applications (two-band superconductors, multi-vortex states, …) .
- The present formalism is applicable in the whole range of the BCS-BEC crossover and allows one to take into account the fluctuations.
- Open question: what is the parameter space for a two-band superfluid with intervortex interactions that have both an attractive and a repulsive component and lead to vortex clustering?

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