Correlated density and superconductivity

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MAX-PLANCK-GESELLSCHAFT

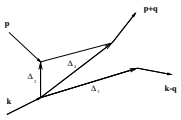
Nonlocal kinetic equation

Unifies achievements of dense quantum gases (Enskog) with Landau theory of quasiparticle transport

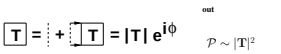
$$\frac{\partial f_1}{\partial t}+\frac{\partial \varepsilon_1}{\partial k}\frac{\partial f_1}{\partial r}-\frac{\partial \varepsilon_1}{\partial r}\frac{\partial f_1}{\partial k}=\int\frac{dpdq}{(2\pi)^3}\mathcal{P}\,\delta\left(\varepsilon_1+\varepsilon_2^-\!-\varepsilon_3^-\!-\varepsilon_4^-\!-2\Delta_E\right)\times\left[\left(1\!-\!f_1\right)\left(1\!-\!f_2^-\right)f_3^-f_4^--f_1f_2^-\left(1\!-\!f_3^-\right)\left(1\!-\!f_4^-\right)\right]$$

where

$$f_1\equiv f(k,r,t)$$
$$f_2^-\equiv f(p,r-\Delta_2,t)$$
$$f_3^-\equiv f(k-q-\Delta_K,r-\Delta_3,t-\Delta_t)$$
$$f_4^-\equiv f(p+q-\Delta_K,r-\Delta_4,t-\Delta_t)$$



with T-matrix



$\mathcal{P}\sim|\mathbf{T}|^2$

$$\Delta_t=\frac{\partial\phi}{\partial\Omega}\Big|_{\varepsilon_1+\varepsilon_2}\qquad\Delta_E=-\frac{1}{2}\frac{\partial\phi}{\partial t}\Big|_{\varepsilon_1+\varepsilon_2}\qquad\Delta_K=\frac{1}{2}\frac{\partial\phi}{\partial r}\Big|_{\varepsilon_1+\varepsilon_2}$$

$$\Delta_2=\left(\frac{\partial\phi}{\partial p}-\frac{\partial\phi}{\partial q}-\frac{\partial\phi}{\partial k}\right)_{\varepsilon_1+\varepsilon_2}\qquad\Delta_3=-\frac{\partial\phi}{\partial k}\Big|_{\varepsilon_1+\varepsilon_2}\qquad\Delta_4=-\left(\frac{\partial\phi}{\partial k}+\frac{\partial\phi}{\partial q}\right)_{\varepsilon_1+\varepsilon_2}$$

P. Lipavský, K. M., and V. Špička: *Kinetic equation for strongly interacting dense Fermi systems*, Annales de physique, 26,1 (2001) ISBN 2-86883-541-4

Summary of Correlated Observables

Quasiparticle parts (Landau theory – like)

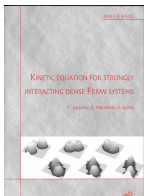
$$n^{\rm qp}=\sum_k f\qquad \mathcal{Q}^{\rm qp}=\sum_k k f\qquad j^{\rm qp}=\sum_k\frac{\partial\varepsilon}{\partial k}f$$
$$\mathcal{E}^{\rm qp}=\sum_k(\tfrac{k^2}{2m}+\tfrac{1}{2}\Sigma_{mf})f_k\qquad \mathcal{J}_{ij}^{\rm qp}=\sum_k\left(k_i\tfrac{\partial\varepsilon}{\partial k_i}+\delta_{ij}\varepsilon\right)f-\delta_{ij}\mathcal{E}^{\rm qp}$$

Two-particle correlated parts with probability to form a molecule per time $d\mathcal{P}=\delta_{1234}|t_{\rm sc}|^2f_1f_2(1-f_3-f_4)$

$$n^{\rm mol}=\int d\mathcal{P}\,\Delta_t\qquad j^{\rm mol}=\int d\mathcal{P}\,\Delta_3$$
$$\mathcal{Q}^{\rm mol}=\int d\mathcal{P}\,\tfrac{k_3+q}{2}\Delta_t\qquad \mathcal{E}^{\rm mol}=\int d\mathcal{P}\,\tfrac{(k_3+q}{2}\Delta_t$$
$$\mathcal{J}_{ij}^{\rm mol}=\frac{1}{2}\int d\mathcal{P}\left\{k_j\Delta_{3i}+p_j(\Delta_{4i}-\Delta_{2i})+q_j(\Delta_{4i}-\Delta_{3i})\right\}$$

Conservation laws

$$\frac{\partial(n^{\rm qp}+n^{\rm mol})}{\partial t}+\frac{\partial(j^{\rm qp}+j^{\rm mol})}{\partial r}=0$$
$$\frac{\partial(\mathcal{Q}_j^{\rm qp}+\mathcal{Q}_j^{\rm mol})}{\partial t}+\sum_i\frac{\partial(\mathcal{J}_{ij}^{\rm qp}+\mathcal{J}_{ij}^{\rm mol})}{\partial r_i}=0$$
$$\frac{\partial\mathcal{E}}{\partial t}=\frac{\partial(\mathcal{E}^{\rm qp}+\mathcal{E}^{\rm mol})}{\partial t}=0$$



Internal energy- $\mathcal{I}_{\rm gain}=\int d\mathcal{P}\Delta_E$ and momentum–gain $\mathcal{F}^{\rm gain}=\int d\mathcal{P}\Delta_K$

Correlated density in superconducting state

Luttinger theorem: Fermi liquids in ground state no correlated density, but:

- Many systems turns not to ideal Fermi liquid at low temperatures
- Electrons in metals and nucleons develop coherent state
- There is a small fraction of correlated density in superconducting state
- Correlated density shifts Fermi momentum and chemical potential μ
- Electrochemical potential $\mu+e\varphi$=const, → electrostatic potential

Total density $n=n_0-\left(e\varphi+\frac{1}{2}mv^2\right)\frac{h(\mu)}{2\pi}+n_{\rm corr}(\Delta)$, density of states h, from the two-pole structure of spectral function, $\epsilon_{\mathbf{k}}=\sqrt{\xi_{\mathbf{k}}^2+\Delta^2}$,

$$A=\frac{1}{2}\left(1+\frac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\right)2\pi\delta\left(\omega-\epsilon_{\mathbf{k}}\right)+\frac{1}{2}\left(1-\frac{\xi_{\mathbf{k}}}{\epsilon_{\mathbf{k}}}\right)2\pi\delta\left(\omega+\epsilon_{\mathbf{k}}\right),$$

one finds the correlated density $n_{\rm corr}\approx\frac{\partial h}{\partial\mu}\frac{\Delta^2}{4\pi}\ln\left(\frac{2\omega_D}{\sqrt{e}\Delta}\right)$

System stays neutral, therefore the two contributions cancel
→ follows electrostatic potential of Bernoulli type

$$e\varphi=-\frac{1}{2}mv^2+\frac{\Delta^2}{4\mu}\ln\left(\frac{2\omega_D}{\sqrt{e}\Delta}\right)$$

- Shift of chemical potential causes internal electric fields
- Bernoulli potential argument for our nonlocal kinetic theory

History of Bernoulli potential in sc - Theory

Equation of motion for condensate, London condition $m\mathbf{v}=-e\mathbf{A}$

$$m\dot{\mathbf{v}}=-e\frac{\partial\mathbf{A}}{\partial t}-e(\mathbf{v}\nabla)\mathbf{A}=e(\mathbf{E}+\mathbf{v}\times\mathbf{B})+\nabla\left(e\varphi+\frac{1}{2}mv^2\right)$$

Compare with Newton $m\dot{\mathbf{v}}=e(\mathbf{E}+\mathbf{v}\times\mathbf{B})+\mathbf{F}_s$

$$\boxed{\nabla e\varphi=\mathbf{F}_s-\nabla\frac{1}{2}mv^2}$$

Hydrodynamics of charged ideal gas
F. Bopp, Z. f. Phys. **107** (1937) 623, F. London, *Superfluids* (1950)
diamagnetic currents in SC are maintained by electrostatic potential
V. S. Sorokin, JETP **19** (1949) 553 free energy responsible for sc contributes

$$e\varphi=-\frac{1}{2}mv^2$$

Quasiparticle Screening:
Force resulting from interaction between electrons and condensate acting on electrons to keep them at rest $\mathbf{F}_n+e\mathbf{E}=0$
A.G. van Vijfeijken and F. S. Staas, Phys. Lett. 12 (1964) 175
Interaction between superfluid and normal electrons (fountain effect) reduces Bernoulli potential

$$\mathbf{F}_n=e\nabla\varphi$$
$$n_n\mathbf{F}_n+n_s\mathbf{F}_s=0$$
$$\mathbf{F}_s=-\frac{n_n}{n_s}e\nabla\varphi$$
$$e\varphi=-\frac{n_s}{n}\frac{1}{2}mv^2$$

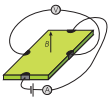
Thermodynamic correction:
Condensate kinetic energy $f_{kin}=n_s\frac{1}{2}mv^2$ determines chemical potential
G. Ryckaizen, J. Phys. C **2** (1969) 1334

$$e\varphi=-\mu=-\frac{\partial}{\partial n}f_{kin}$$
$$=\left(-\frac{n_s}{n}+4\frac{n_s}{n}\frac{\partial\ln T_c}{\partial\ln n}\right)\frac{1}{2}mv^2$$

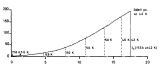
Thermodynamic corrections: Idea to measure material parameters

History of Bernoulli potential in sc - Experiment

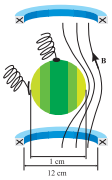
Ohmic contacts: *Null results* due to constant electrochemical potential
H. W. Levis, Phys. Rev 92 (1953) 1149, T. K. Hunt, Phys. Lett. 22 (1966) 42



Capacitive coupling: *No thermodynamic corrections observed !*
J. Bok, J. Klein, PRL 20 (1968) 660; T. D. Morris, J. B. Brown, Physica 55 (1971) 760



$$e\varphi=-\frac{n_s}{n}\frac{1}{2}mv^2=-\frac{1}{n}\frac{B^2}{2\mu_0}$$



It should be $\delta f=\frac{1}{2}n_smv^2$ and (Pb at $T=7$K)
$e\varphi=-\frac{\partial}{\partial n}\delta f=-\left(\frac{n_s}{n}-4\frac{n_s}{n}\frac{\partial\ln T_c}{\partial\ln n}\right)\frac{m}{2}v^2=-(0.1+3.2)\frac{m}{2}v^2$
Why no signal of thermodynamic corrections?

Budd-Vannimenus theorem for superconductors

Answer (after 30 years) due to surface dipoles:
Modification of Budd-Vannimenus theorem

$$e\varphi_{\rm surf}-e\varphi=n\frac{\partial}{\partial n}\left(\frac{f_{\rm el}}{n}\right)$$

- Potential step at surface due to surface dipole in terms of free energy with no regards of potential inside
- With $e\varphi=-\frac{\partial}{\partial n}f_{\rm el}$ and $f_{\rm el}=n_s\frac{1}{2}mv^2$

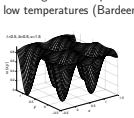
$$e\varphi_{\rm surf}=e\varphi+n\frac{\partial}{\partial n}\left(\frac{f_{\rm el}}{n}\right)=e\varphi+\frac{\partial}{\partial n}f_{\rm el}-\frac{f_{\rm el}}{n}=-\frac{n_s}{n}\frac{1}{2}mv^2$$

Surface dipole compensates thermodynamic corrections for homogeneous superconductors
P. Lipavský and J. Koláček and J.J. Mareš, K. Morawetz, PRB 65 (2002) 2507
Hope: inhomogeneous superconductors, vortices

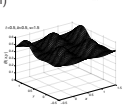
Abrikosov vortex lattices at temperatures below T_c

Ginzburg-Landau equation extended to low temperatures (Bardeen)

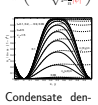
$$\frac{(i\hbar\nabla+e^*\mathbf{A})^2}{2m^*}\psi-\frac{\gamma T^2}{2n}\left(1-|^1\frac{I^2}{\sqrt{I^2+\frac{1}{2}n}}|^2\right)\psi=0$$



Condensate density



Magnetic field



Condensate density at various T

$T/T_c=0.5$, mean magnetic field $B/B_{c2}=0.5$, GL parameter $\kappa_0=1.5$

- n_s smaller at boarders than nonmagnetic value → nonlocal effects
- B higher than applied field in core → B compressed in vortices

P. Lipavský, J. Koláček, K. Morawetz, E. H. Brandt, PRB 65 (2001) 144511

Surface potential within the Ginzburg-Landau theory

Bardeen's low temperature extension of GL (free energy by Gorter Casimir two-fluid, subtraction of free energy of normal state)

$$f_{\rm el}=\frac{1}{2}\gamma T^2+\frac{1}{2m^*}\bar{\psi}\left(-i\hbar\nabla-e^*\mathbf{A}\right)^2\psi-\varepsilon_{\rm con}\frac{2|\psi|^2}{n}-\frac{1}{2}\gamma T^2\sqrt{1-\frac{2|\psi|^2}{n}}$$

From GL equation $\frac{(-i\hbar\nabla-e^*\mathbf{A})^2}{2m^*}\psi=-\alpha\psi-\beta|\psi|^2\psi$ follows $f_{\rm el}=-\frac{1}{2}\beta|\psi|^4$ and surface potential reads (Budd-Vannimenus) $e\phi_0=\frac{1}{2n}\beta|\psi|^4$, without surface dipole, surface potential equals to internal potential

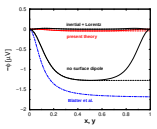
$$e\phi=-\frac{1}{2m^*n}\bar{\psi}\left(-i\hbar\nabla-e^*\mathbf{A}\right)^2\psi+\frac{\partial\varepsilon_{\rm con}2|\psi|^2}{\partial n}\frac{}{n}-\frac{T^2}{2}\frac{\partial\gamma}{\partial n}\left(\frac{|\psi|^2}{n}+\frac{|\psi|^4}{2n^2}\right)$$

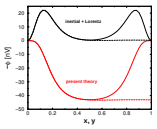
-Inertial and Lorentz forces: neglecting pairing forces
-Khomskii/Kusmartsev/Blatter approximation : $e\phi_{\rm BK}=\frac{\gamma T_c}{n}\frac{\partial T_c}{\partial n}|\psi|^2$
Possible cases for which presented theory can be tested:

- at vortex core $|\psi|^2\propto r^2$ so that $\phi_0\propto r^4$ while $\phi_{\rm BK}\propto r^2$
- B close to B_{c2} for thin layer mean value becomes

$$\langle\omega\rangle=\frac{(1-b)}{\beta_\Lambda},\ \langle\omega^2\rangle=\frac{(1-b)^2}{\beta_\Lambda}\qquad\langle e\phi_0\rangle=\frac{\varepsilon_{\rm con}}{n\beta_\Lambda}\left(1-t^2\right)^2(1-b)^2$$
$$\text{with }\omega=\frac{|\psi|^2}{|\psi_\infty|^2},\ b=\frac{B}{B_{c2}}\qquad\langle e\phi_{\rm BK}\rangle=\frac{\varepsilon_{\rm con}}{n\beta_\Lambda}\frac{\partial\ln T_c}{\partial\ln n}2\left(1-t^4\right)(1-b)$$

Effect of surface dipole





Niobium

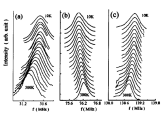
$\frac{T}{T_c}=0.95$
$\kappa=1.5$
$\frac{B}{B_{c2}}=0.7818$

- internal potential and Blatter's result similar (Clem model, neglect of $\frac{\partial\gamma}{\partial n}$)
- full theory and inertial/Lorentz forces are much smaller
- surface dipole cancels major part of pairing forces
- full theory and inertial/Lorentz forces result in different profiles and sign

Charged vortices in HTSC probed by NMR

K. I. Kumagai, K. Nozaki and Y. Matsuda, PRB **63** (2001) 144502

- NMR frequency depends on B, $\gamma_{\rm Cu}$ and number N of holes per Cu/plane
- Polarization of Cu, coupling of spin with electrical field gradient leads to splitting of quadrupole resonance $\nu_Q^{NQR}=E_{\pm3/2}-E_{\pm1/2}=AN+C$.



NQR NMR lower NMR upper satellite

$\nu_0(B)=E_2-E_1=\gamma_{\rm Cu}B+\nu_Q^{NQR}$

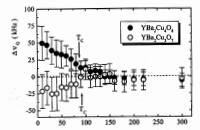


FIG. 7. T dependence of $\Delta\nu_Q=\nu_Q(0)-\nu_Q(H)$ for $YBa_2Cu_3O_6$ and $YBa_2Cu_3O_7$. In both materials nonzero $\Delta\nu_Q$ is clearly observed below T_c, showing that the electron density outside the core differs from that in zero field.

Problems:

- Charge in vortex core(BCS) $Q\sim\frac{d\ln T_c}{d\ln\mu}\sim10^{-5}e-10^{-6}e$ exp : $10^{-2}e$
- Underdoped regime: $Q>0$, overdoped: $Q<0$, contrast to experiment

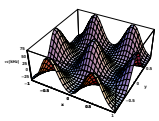
Space variation of NMR lines

averaging of the NMR line over Abrikosov lattice

$$F_{2/3}(\bar{\nu})=\frac{1}{\pi\Omega}\int d\mathbf{r}\frac{\Gamma}{(\bar{\nu}-\bar{\nu}_{2/3}(\mathbf{r}))^2+\Gamma^2}\qquad\nu_{2/3}(\mathbf{r})=\gamma B(\mathbf{r})\mp C\mp AN(\mathbf{r})$$

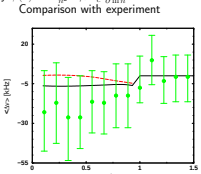
$N(\mathbf{r})=\frac{\Omega_{\rm Cu}}{}(\rho(\mathbf{r})-\rho_\infty)$ by potential via layered structure screening (Lawrence/Doniach):
$\rho(\mathbf{k})=\frac{2k(1+e^{-kD})}{(1-e^{-2kD})(1+e^{-kD\rho-\beta})}\phi(\mathbf{k})$ compare 3D: $\rho(k)=-\epsilon k^2\phi(\mathbf{k})$
$B(\mathbf{r})$ and $\Psi(\mathbf{r})$ from extended GL-theory $\phi(\mathbf{r})=\frac{|\Psi(\mathbf{r})|^2}{n^2}\gamma_c T_c^2\frac{\partial\ln T_c}{\partial\ln n}$

Comparison with experiment



- Space variation of shifts comparable to line width
→ no approximation by mean value

P. Lipavský, J. Koláček, K. Morawetz, E. H. Brandt, PRB 66 (2002) 134525



$\Delta\nu$ ($\Gamma=140$kHz) of single crystal and grain-orientation averaged

Advertisement: *Bernoulli potential in superconductors - how the electrostatic field helps to understand superconductivity*, P. Lipavský, J. Kolácek, K. Morawetz, E. H. Brandt, T. J. Yang
Lecture Notes in Physics 733, Springer, 2007