Nonlocal kinetic theory and field effects

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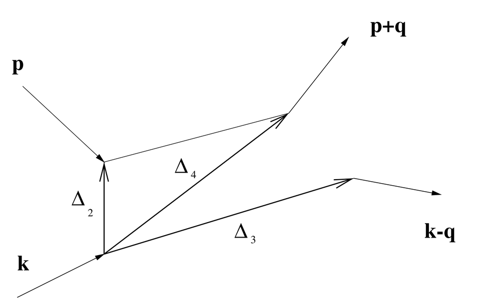
Nonlocal kinetic equation

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

$$\frac{\partial f_1}{\partial t}+\frac{\partial \varepsilon_1}{\partial k}\frac{\partial f_1}{\partial r}-\frac{\partial \varepsilon_1}{\partial r}\frac{\partial f_1}{\partial k}=\int\frac{dpdq}{(2\pi)^5}\mathcal{P}\,\delta\left(\varepsilon_1+\varepsilon_2^--\varepsilon_3^--\varepsilon_4^--2\Delta_E\right)\times\left[(1-f_1)(1-f_2^-)f_3^-f_4^--f_1f_2^-(1-f_3^-)(1-f_4^-)\right]$$

where

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



with T-matrix $\boxed{\mathbf{T}} = \vdots + \vdots\boxed{\mathbf{T}} = |\mathbf{T}|\,e^{i\phi}$ $\qquad \mathcal{P}\sim|\mathbf{T}|^2$

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

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

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)

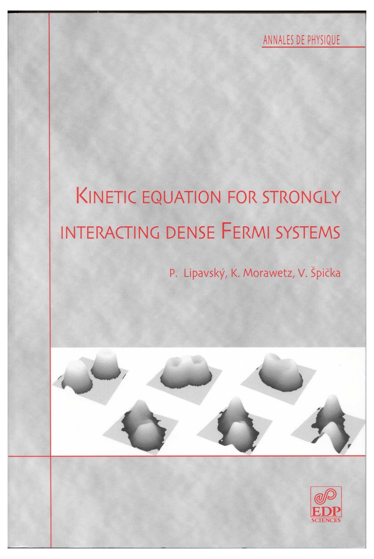
$$n^{\rm qp}=\sum_k f\qquad \mathcal{Q}^{\rm qp}=\sum_k k\,f\qquad j^{\rm qp}=\sum_k\frac{\partial\varepsilon}{\partial k}f$$
$$\mathcal{E}^{\rm qp}=\sum_k\left(\frac{k^2}{2m}+\frac{1}{2}\Sigma_{mf}\right)f_k\qquad \mathcal{J}_{ij}^{\rm qp}=\sum_k\left(k_j\frac{\partial\varepsilon}{\partial k_i}+\delta_{ij}\varepsilon\right)f-\delta_{ij}\mathcal{E}^{\rm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

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

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

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, $\to$ electrostatic potential

Total density $n=n_0-(e\varphi+\frac{1}{2}mv^2)\frac{h(\mu)}{2\pi}+n_{\rm corr}(\Delta)$, 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 $n_{\rm corr}\approx\frac{\partial h}{\partial\mu}\frac{\Delta^2}{4\pi}\ln\left(\frac{2\omega_D}{\sqrt{e}\Delta}\right)$

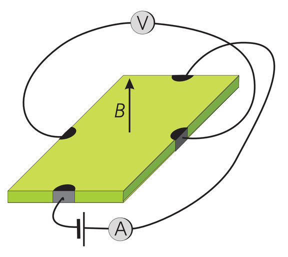
System stays neutral, therefore the two contributions cancel
$\to$ follows electrostatic potential of Bernoulli type

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

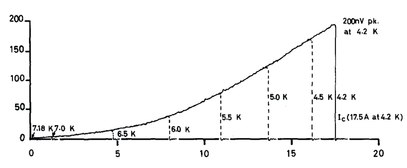
- Shift of chemical potential causes internal electric fields
- Bernoulli potential argument for our nonlocal kinetic theory

History of Bernoulli potential - Experiment

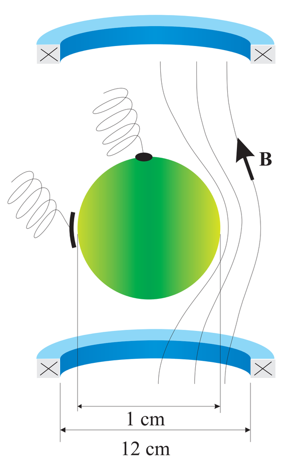
Ohmic contacts: *Null results* due to constant electrochemical potential
H. W. Levis, Phys. Rev 92 (1953) 1149, T. K. Hunt, Phys. Lett. 22 (1966) 42



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)
$e\varphi=-\frac{\partial}{\partial n}\delta f=-\left(\frac{n_s}{n}-4\frac{n_n}{n}\frac{\partial\ln T_c}{\partial\ln n}\right)\frac{m}{2}v^2=-(0.1+3.2)\frac{m}{2}v^2$
Why no signal of thermodynamic corrections?

Budd-Vannimenus theorem for superconductors

Answer (after 30 years) due to surface dipoles: Modification of Budd-Vannimenus theorem $\qquad e\varphi_{\rm surf}-e\varphi=n\frac{\partial}{\partial n}\left(\frac{f_{\rm el}}{n}\right)$

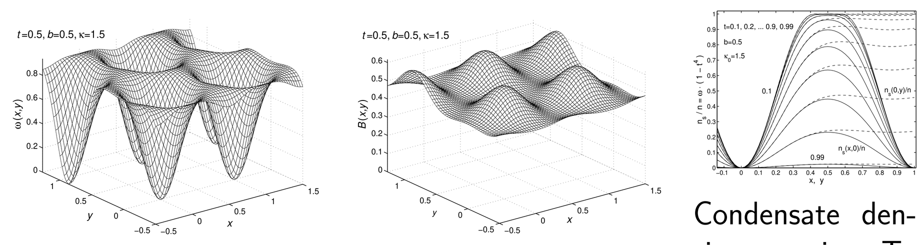
- Potential step at surface due to surface dipole in terms of free energy with no regards of potential inside
- With $e\varphi=-\frac{\partial}{\partial n}f_{\rm el}$ and $f_{\rm el}=n_s\frac{1}{2}mv^2$

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

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



Condensate density $\qquad$ Magnetic field $\qquad$ Condensate density at various T

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

- n_s smaller at boarders than nonmagnetic value $\to$ nonlocal effects
- B higher than applied field in core $\to$ 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)

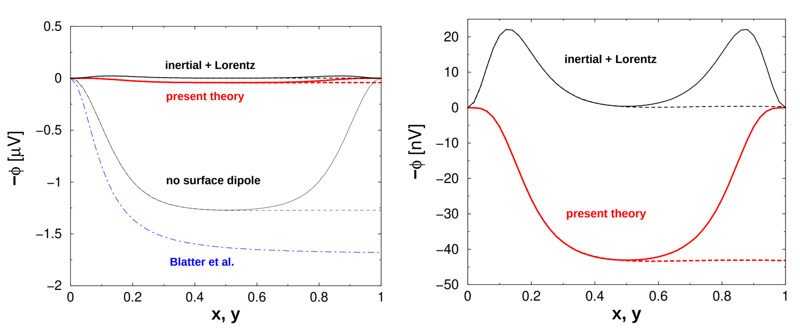
$$f_{\rm el}=\frac{1}{2}\gamma T^2+\frac{1}{2m^*}\bar\psi\left(-i\hbar\nabla-e^*\mathbf{A}\right)^2\psi-\varepsilon_{\rm con}\frac{2|\psi|^2}{n}-\frac{1}{2}\gamma T^2\sqrt{1-\frac{2|\psi|^2}{n}}$$

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

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

-Inertial and Lorentz forces: neglecting pairing forces
-Khomskii/Kusmartsev/Blatter approximation : $e\phi_{\rm Bl}=\frac{2T_c}{n}\frac{\partial T_c}{\partial n}|\psi|^2$

Effect of surface dipole

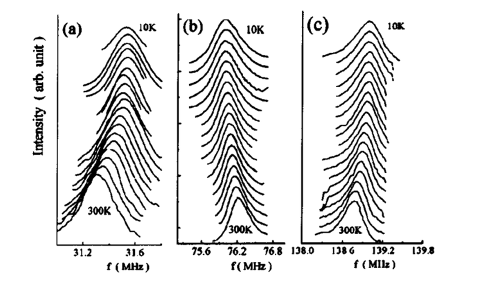


$$\frac{T}{T_c}=0.95\qquad \kappa=1.5\qquad \frac{B}{B_{c2}}=0.7818$$

- 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 $\qquad$ NMR lower $\qquad$ NMR upper satellite

$\nu_3(B)=E_{\frac{3}{2}}-E_{\frac{1}{2}}=\gamma_{\rm Cu}B+\nu_Q^{NQR}$

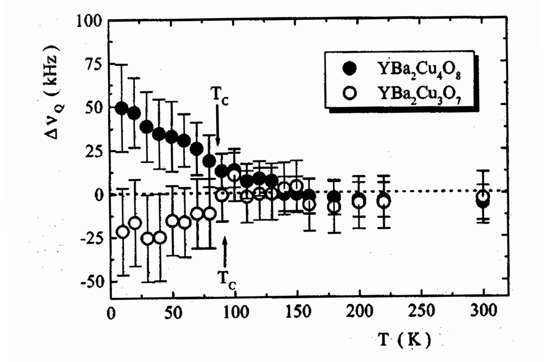


FIG. 7. T dependence of $\Delta\nu_Q=\nu_Q(0)-\nu_Q(H)$ for $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$. In both materials nonzero $\Delta\nu_Q$ is clearly observed below T_c, showing that the electron density outside the core differs from that in zero field.

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

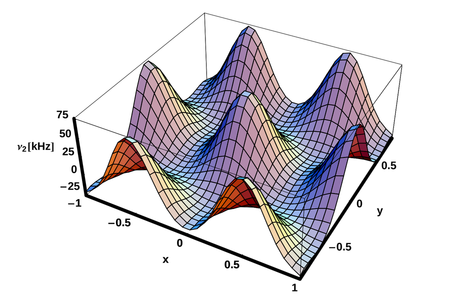
Space variation of NMR lines

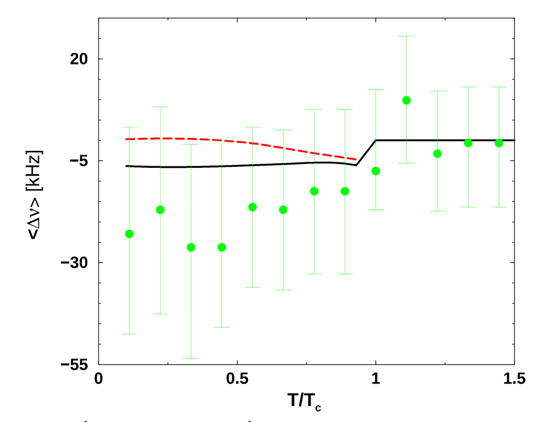
averaging of the NMR line over Abrikosov lattice

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

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

Comparison with experiment





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

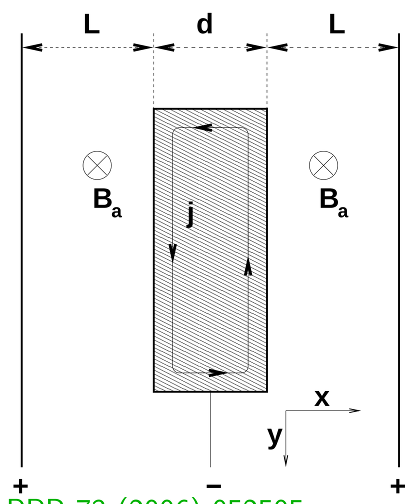
P. Lipavský, J. Kolácek, K. Morawetz, E. H. Brandt, PRB 66 (2002) 134525

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

Effective magnetocapacitance

Aim: effective capacitance and surface critical field in dependence on applied voltage and magnetic field

- Total energy of capacitor with area S, $\frac{1}{2}\epsilon_0E^2LS+\sigma S$
- Capacitance $\frac{S}{C}=\frac{L}{\epsilon_0}+\frac{1}{\epsilon_0^2}\frac{\partial^2\sigma}{\partial E^2}$
- Ginzburg Landau equation with external bias $\frac{1}{2m}(-i\hbar\nabla-e\mathbf{A})^2\Psi+\alpha\Psi+\beta|\Psi|^2\Psi=0$ de-Gennes surface conditions



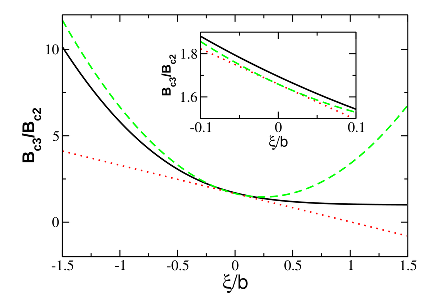
$$\left.\frac{\nabla\Psi}{\Psi}\right|_{x=0}=\frac{1}{b},\qquad \left.\frac{\nabla\Psi}{\Psi}\right|_{x=d}=-\frac{1}{b},$$

where extrapolation length $\frac{1}{b}=\frac{1}{b_0}+\frac{E}{\varphi_{\rm fe}}$,

P. Lipavsky, K. Morawetz, J. Kolacek, T. Yang, PRB 73 (2006) 052505

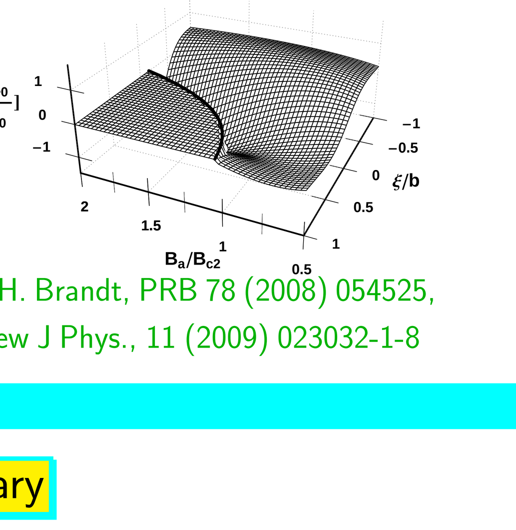
Nucleation of surface superconductivity

Nucleation possible if $-\alpha$ equals eigenvalue of linearized GL equation
- maximal nucleation temperature by maximal $\tilde\alpha=\max[\alpha]$
- corresponds to highest attainable critical magnetic field



Effective capacitance

$$\left.\frac{S}{C_{\rm surf}}\right|_0=\frac{L_0}{\epsilon_0}\left(\frac{l}{\xi}\right)^{3.25}h\left(\frac{\xi}{b}\right)$$



K. Morawetz, P. Lipavsky, J. Kolaček, E. H. Brandt, PRB 78 (2008) 054525,
K. Morawetz, P. Lipavsky, J. J. Mares, New J Phys., 11 (2009) 023032-1-8

Summary

1. Consistent theory unifying Landau - quasiparticle picture for quantum liquids and Enskog - like equations for dense gases
2. No additional computational expenses-modify existing Boltzmann codes by nonlocal and non-instantaneous shifts
3. Consequence is correlated density: shifts Fermi momentum (chemical potential), since electrochemical potential constant, follows electrostatic potential (Bernoulli type)
4. Electrostatic potential above surface of thin superconducting layer with vortex lattice calculated, NMR observation of charge transfer reproduced
5. Influence of external magnetic fields parallel and electric field perpendicular to surface: nonlinear dependence of critical magnetic field, effective capacitance has a jump near B_{c3} to be measured