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Transverse thermoelectric conductivity and magnetization in high- T_c superconductors

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Abstract. We use the time-dependent Ginzburg-Landau (TDGL) equation with thermal noise to calculate the transverse thermoelectric conductivity α_{xy} describing the Nernst effect and magnetization M_z in type-II superconductor in the vortex-liquid regime. The nonlinear interaction term in dynamics is treated within self-consistent Gaussian approximation. The expressions of the transverse thermoelectric conductivity and magnetization including all the Landau levels are presented in explicit form which are applicable essentially to the whole phase. Our results are compared to recent simulation data on high- T_c superconductor.

1 Introduction

The observation of large Nernst signal (e_N) in cuprates at temperatures much greater than T_c [1] has drawn much attention to the Nernst effect over the past decade. The transverse electric field is induced in a metal under magnetic field by the temperature gradient ∇T perpendicular to the magnetic field **H**, which is a phenomenon known as Nernst effect [2]. In the normal state and in the vortex lattice or glass states it is typically small [3], while in the mixed state the Nernst effect is larger due to vortex motion. Since then, an extensive investigation on the subject has been done, both experimentally [1,4–7] and theoretically [2,8–12], producing different proposals on the origin of the phenomenon. Most of these competing interpretations focus on the dynamics of either vortices [1,2,4,8–12] or quasiparticles [13].

In recent years, much attention has been paid to the anomalously enhanced positive Nernst signal observed well above T_c in La_{2-x}Sr_xCuO₄ in a wide range of doping x [1,4,5]. Wang et al. [1,4] argued that the large Nernst signal supports a scenario [14] where the superconducting order parameter does not disappear at T_c but at a much higher (pseudogap) temperature. Theory of the Nernst effect based on the phenomenological TDGL equations with thermal noise describing strongly fluctuating superconductors was developed long time ago [2,15,16]. Recent theoretical investigations of the Nernst effect in fluctuating superconductors include the analysis of Gaussian fluctuations above the mean-field transition temperature [8] and a Ginsburg-Landau (GL) model with interactions between fluctuations of the order parameter [9]. These models are good in agreement with experiments on thin amorphous samples [7] and with cuprate data in overdoped and

optimally doped samples. More recently, there are some closely related theoretical studies of the strong superconducting fluctuations in the 2-dimensional cuprates based on: Quantum Monte Carlo simulations [17], renormalization group scaling [18], diagrammatic expansion [19]. Podolsky et al. [10] numerically simulated the two dimensional TDGL equation with thermal noise and obtained results of the transverse thermoelectric conductivity α_{xy} and the diamagnetic response M_z in 2D at low T and analytic results at high T, and found the ratio $|M_z|/T\alpha_{xy}$ reaches a fixed value at high temperatures. However, the result of the transverse thermoelectric conductivity α_{xy} [8] was only lowest Landau level contribution and the simulation of this system, even in 2D, is not easy and it was one of our goals to supplement it with a reliable analytical expression including all Landau levels in the region of the vortex liquid.

In this paper we obtain explicit expressions for the transverse thermoelectric conductivity α_{xy} and the magnetization M_z in 2D by using TDGL equation with thermal noise. The interaction term in dynamics is treated within self-consistent Gaussian approximation sufficient for description of the vortex liquis. Our results summing all Landau levels in an explicit form are compared with recent simulation data in the cuprates.

2 Relaxation dynamics and thermal fluctuations in 2D

We can start with the GL free energy in 2D:

$$F_{GL} = s' \int d^2r \left\{ \frac{\hbar^2}{2m^*} |\mathbf{D}\Psi|^2 + a|\Psi|^2 + \frac{b'}{2}|\Psi|^4 \right\}, \quad (1)$$

where s' is the order parameter effective "thickness", the covariant derivatives are defined by $\mathbf{D} \equiv \nabla + i(2\pi/\Phi_0)\mathbf{A}$,

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where the vector potential describes constant and homogeneous magnetic field $\mathbf{A} = (-By, 0)$ and $\Phi_0 = hc/e^*$ is the flux quantum with $e^* = 2 |e|$. For simplicity we assume $a = \alpha T_c^{mf}(t-1), t^{mf} \equiv T/T_c^{mf}$, this critical temperature T_c^{mf} depends on UV cutoff, τ_c , of the "mesoscopic" or "phenomenological" GL description, specified later. The two scales, the coherence length $\xi^2 = \hbar^2/(2m^*\alpha T_c)$, and the penetration depth, $\lambda^2 = c^2 m^* b'/(4\pi e^{*2}\alpha T_c)$ define the GL ratio $\kappa \equiv \lambda/\xi$, which is very large for high- T_c superconductors. In this case of strongly type-II superconductors the magnetization is by a factor κ^2 smaller than the external field for magnetic field larger than the first critical field $H_{c1}(T)$, so that we take $B \approx H$.

In the presence of thermal fluctuations, which on the mesoscopic scale are represented by a complex white noise [20,21], dynamics of the order parameter (called TDGL) reads:

$$\frac{\hbar^2 \gamma'}{2m^*} D_\tau \Psi = -\frac{1}{s'} \frac{\delta F_{GL}}{\delta \Psi^*} + \zeta, \qquad (2)$$

where $D_{\tau} \equiv \partial/\partial \tau - i(e^*/\hbar)\Phi$ is the covariant time derivative, with $\Phi = -Ey$ being the scalar electric potential describing the driving force in a purely dissipative dynamics.

The variance of the thermal noise, determining the temperature T is taken to be the Gaussian white noise:

$$\langle \zeta^*(\mathbf{r},\tau)\zeta(\mathbf{r}',\tau')\rangle = \frac{\hbar^2\gamma'}{m^*s'}k_BT\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau').$$
(3)

The total heat current density in GL model [2,8,15,16] is:

$$\mathbf{J}^{h} = -\frac{\hbar^{2}}{2m^{*}} \left\langle \left(\frac{\partial}{\partial\tau} + i\frac{e^{*}}{\hbar}\phi\right)\Psi^{*}\left(\nabla + i\frac{2\pi}{\Phi_{0}}\mathbf{A}\right)\Psi\right\rangle + c.c.$$
(4)

Throughout most of the paper we use the coherence length ξ as a unit of length, $H_{c2} = \Phi_0/2\pi\xi^2$ as a unit of the magnetic field, $\tau_{GL} = \gamma'\xi^2/2$ as a unit of time, $E_{GL} = H_{c2}\xi/(c\tau_{GL})$ as a unit of electric field. After rescaling by $x \to \xi x, y \to \xi y, s' \to \xi s, \tau \to \tau_{GL}\tau, B \to$ $H_{c2}b, E \to E_{GL}\mathcal{E}, T \to t^{mf}T_c^{mf}, \Psi^2 \to (2\alpha T_c^{mf}/b')\psi^2$, the dimensionless Boltzmann factor (1) in these units is:

$$\frac{F_{GL}}{T} = \frac{s}{\omega t} \int d^2 r \left\{ \frac{1}{2} \left| D\psi \right|^2 - \frac{1 - t^{mf}}{2} \left| \psi \right|^2 + \frac{1}{2} \left| \psi \right|^4 \right\},\tag{5}$$

and equation (2) can be written as:

$$\left(D_{\tau} - \frac{1}{2}D^2\right)\psi - \frac{1 - t^{mf}}{2}\psi + |\psi|^2\psi = \overline{\zeta}.$$
 (6)

Here the covariant time derivative is $D_{\tau} = \frac{\partial}{\partial \tau} + i\mathcal{E}y$, the covariant derivatives are defined by $D_x = \frac{\partial}{\partial x} - iby$, $D_y = \frac{\partial}{\partial y}$. The Langevin white-noise forces $\overline{\zeta}$ are correlated through

$$\left\langle \overline{\zeta}^*(\mathbf{r},\tau)\overline{\zeta}(\mathbf{r}',\tau')\right\rangle = 2\omega t^{mf}\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau')$$

with $\omega = \sqrt{2Gi_{2D}\pi}$, where the Ginzburg number is defined by:

$$Gi_{2D} = \frac{1}{2} (8e^2 \kappa^2 \xi^2 k_B T_c^{mf} / c^2 \hbar^2 s')^2.$$

The dimensionless heat current density along x-direction is $J_x^h = J_{GL}^h j_x^h$ where

$$j_x^h = -\frac{1}{2} \left\langle \left(\frac{\partial}{\partial \tau} - i\mathcal{E}y\right) \psi^* \left(\frac{\partial}{\partial x} - iby\right) \psi \right\rangle + c.c., \quad (7)$$

with $J_{GL}^{h} = \hbar c H_{c2}/(2\pi e^{*}\xi\kappa^{2}\tau_{GL})$ being the unit of the heat current density. Consistently the transverse thermoelectric conductivity will be given in units of $\alpha_{GL} = J_{GL}^{h}/E_{GL} = \hbar c^{2}/(2\pi e^{*}\xi^{2}\kappa^{2})$.

3 The self-consistent Gaussian approximation for vortex-liquid phase

The cubic term in the TDGL equation (6) will be treated in the self-consistent Gaussian approximation [22] by replacing $|\psi|^2 \psi$ with a linear one $2 \langle |\psi|^2 \rangle \psi$

$$\left(D_{\tau} - \frac{1}{2}D^2 - \frac{b}{2}\right)\psi + \varepsilon\psi = \overline{\zeta},\tag{8}$$

leading the "renormalized" value of the coefficient of the linear term:

$$\varepsilon = -a_h + 2\left\langle |\psi|^2 \right\rangle,\tag{9}$$

where the constant is defined as $a_h = (1 - t^{mf} - b)/2$.

The relaxational linearized TDGL equation with a Langevin noise, equation (8), is solved using the retarded $(G = 0 \text{ for } \tau < \tau')$ Green function (GF) $G(\mathbf{r}, \tau; \mathbf{r}', \tau')$:

$$\psi(\mathbf{r},\tau) = \int d\mathbf{r}' \int d\tau' G(\mathbf{r},\tau;\mathbf{r}',\tau') \overline{\zeta}(\mathbf{r}',\tau').$$
(10)

The GF satisfies

$$\left\{D_{\tau} - \frac{1}{2}D^2 - \frac{b}{2} + \varepsilon\right\}G(\mathbf{r}, \mathbf{r}', \tau - \tau') = \delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau').$$
(11)

The GF is a Gaussian

$$G(\mathbf{r}, \mathbf{r}', \tau'') = C(\tau'')\theta(\tau'') \exp\left[\frac{ib}{2}X(y+y')\right]$$
$$\times \exp\left[-\frac{X^2 + Y^2}{2\beta} - \nu X\right], \qquad (12)$$

with

$$X = x - x' - \nu \tau'', \quad Y = y - y', \quad \tau'' = \tau - \tau'.$$

 $\theta\left(\tau^{\prime\prime}\right)$ is the Heaviside step function, C and β are coefficients.

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Substituting the ansatz (12) into equation (11), we obtain following conditions:

$$\varepsilon - \frac{b}{2} + \frac{\nu^2}{2} + \frac{1}{\beta} + \frac{\partial_\tau C}{C} = 0, \qquad (13)$$

$$\frac{\partial_{\tau}\beta}{\beta^2} - \frac{1}{\beta^2} + \frac{b^2}{4} = 0.$$
 (14)

Equation (14) determines β , subject to an initial condition $\beta(0) = 0$,

$$\beta = \frac{2}{b} \tanh\left(\frac{b\tau''}{2}\right),\tag{15}$$

while equation (13) determines C:

$$C = \frac{b}{4\pi} \exp\left\{-\left(\varepsilon - \frac{b}{2} + \frac{\nu^2}{2}\right)\tau''\right\} \sinh^{-1}\left(\frac{b\tau''}{2}\right).$$
(16)

The normalization is dictated by the delta function term in definition of the Green function equation (11).

The thermal average of the superfluid density (density of Cooper pairs) without electric field can be expressed via the Green functions

$$\left\langle \left| \psi(\mathbf{r},\tau) \right|^2 \right\rangle = 2\omega t^{mf} \int d\mathbf{r}' \int d\tau'' \left| G(\mathbf{r},\mathbf{r}',\tau'') \right|$$
$$= \frac{\omega t^{mf}b}{2\pi} \int_{\tau_c}^{\infty} d\tau'' \frac{\exp\left\{ -\left(2\varepsilon - b\right)\tau''\right\}}{\sinh(b\tau'')}.$$
(17)

Substituting it into the "gap equation", equation (9), the later takes a form

$$\varepsilon = -a_h + \frac{\omega t^{mf} b}{\pi} \int_{\tau_c}^{\infty} d\tau'' \frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\sinh(b\tau'')}.$$
 (18)

In order to absorb the divergence into a renormalized value a_h^r of the coefficient a_h , it is convenient to make an integration by parts in the last term for small τ_c

$$b \int_{\tau_c}^{\infty} d\tau'' \frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\sinh(b\tau'')} \\ = -\int_{0}^{\infty} d\tau'' \ln[\sinh(b\tau'')] \frac{d}{d\tau''} \left[\frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\cosh(b\tau'')}\right] \\ -\ln(b\tau_c). \tag{19}$$

Then equation (18) can be written as:

$$\varepsilon = -a_h^r - \frac{\omega t}{\pi} \int_0^\infty d\tau'' \ln[\sinh(b\tau'')] \\ \times \frac{d}{d\tau''} \left[\frac{\exp\left\{ - (2\varepsilon - b)\tau'' \right\}}{\cosh(b\tau'')} \right] - \frac{\omega t}{\pi} \ln(b), \quad (20)$$

where

$$a_h^r = a_h + \frac{\omega t^{mf}}{\pi} \ln(\tau_c) = \frac{1 - b - T/T_c}{2},$$

 $t = T/T_c$ and $\omega = \sqrt{2Gi_{2D}\pi}$, where

$$Gi_{2D} = \frac{1}{2} \left(8e^2 \kappa^2 \xi^2 k_B T_c / c^2 \hbar^2 s' \right)^2,$$

 $(T_c^{mf} \mbox{ is now replaced by } T_c \mbox{ after renormalization}).$ The formula is cutoff independent.

4 Theoretical calculation and comparison

4.1 The transverse thermoelectric conductivity

The heat current density, defined by equation (7), can be expressed via the Green functions as:

$$j_x^h = -\frac{1}{2} \int d\mathbf{r}' \int d\tau' \left(\frac{\partial}{\partial \tau} - i\mathcal{E}y\right) G^* \left(\mathbf{r}, \mathbf{r}', \tau - \tau'\right) \\ \times \left(\frac{\partial}{\partial x} - iby\right) G\left(\mathbf{r}, \mathbf{r}', \tau - \tau'\right) + c.c.,$$
(21)

where $G(\mathbf{r}, \mathbf{r}', \tau - \tau')$ as the Green function of the linearized TDGL equation (6) in the presence of the scalar potential.

Substituting the full Green function (12) into expression (21), and performing the integrals in linear response to electric field, we obtain:

$$j_x^h = \frac{\omega t b}{2\pi s} \mathcal{E} \int_0^\infty d\tau'' \frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\cosh^2\left(\frac{b\tau''}{2}\right)}.$$
 (22)

In physical units the current density reads:

$$J_x^h = \alpha_{GL} E \frac{\omega t b}{2\pi s} \int_0^\infty d\tau'' \frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\cosh^2\left(\frac{b\tau''}{2}\right)}.$$
 (23)

By an Onsager relation, α_{xy} can be obtained from the heat and magnetization currents response to an electric field [2,8,23]

$$\alpha_{xy} = \frac{1}{T} \left(\frac{J_x^h}{E} + cM_z \right). \tag{24}$$

Magnetization M_z will be shown in the following section.

4.2 Magnetization

In order to calculate magnetization, we substitute expressions (10) and (12) into (5), the Boltzmann factor can be written as:

$$f = \frac{F_{GL}}{T} = -\frac{\omega t b^2}{4\pi s} \int_{\tau_c}^{\infty} d\tau'' \frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\sinh^2(b\tau'')} + \frac{\omega t b^2}{8\pi s} \int_{\tau_c}^{\infty} d\tau'' \frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\sinh^2(\frac{b\tau''}{2})} - \frac{1 - t}{2} \frac{\omega t b}{2\pi s} \int_{\tau_c}^{\infty} d\tau'' \frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\sinh(b\tau'')} + \left(\frac{\omega t b}{2\pi s} \int_{\tau_c}^{\infty} d\tau'' \frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\sinh(b\tau'')}\right)^2.$$
(25)

To extract the divergent part, one can make an integration by parts for small τ_c , the Boltzmann factor (25) becomes

$$f = F_1(\varepsilon, b) - F_2(\varepsilon, b) - \frac{1-t}{2} F_0(\varepsilon, b) + \frac{\omega t}{2\pi s} F_0^2(\varepsilon, b) - \frac{\omega t}{8\pi s} \frac{1}{\tau_c} + \frac{1-t}{2} \ln(\tau_c) - \frac{\omega t}{2\pi s} \ln^2(\tau_c), \qquad (26)$$

where

$$F_1(\varepsilon, b) = -\frac{\omega t b}{4\pi s} \int_0^\infty d\tau'' \frac{1}{\sinh(b\tau'')} \\ \times \frac{d}{d\tau''} \left[\frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\cosh(b\tau'')} \right], \tag{27}$$

$$F_2(\varepsilon, b) = -\frac{\omega t \sigma}{4\pi s} \int_0^{\infty} d\tau'' \frac{1}{\sinh(\frac{b\tau''}{2})} \times \frac{d}{d\tau''} \left[\frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\cosh(\frac{b\tau''}{2})} \right], \quad (28)$$

$$F_0(\varepsilon, b) = -\frac{\omega t b}{2\pi s} \int_0^\infty d\tau'' \ln\left[\sinh(b\tau'')\right] \\ \times \frac{d}{d\tau''} \left[\frac{\exp\left\{-\left(2\varepsilon - b\right)\tau''\right\}}{\cosh(b\tau'')}\right] - \ln\left(b\right).$$
(29)

Magnetization can be obtained by taking the first derivative of free energy (26) with respect to magnetic field b

$$M_{z} = -\frac{H_{c2}}{2\pi\kappa^{2}} \frac{\partial f}{\partial b}$$

= $-\frac{H_{c2}}{2\pi\kappa^{2}} \left[\frac{\partial F_{1}(\varepsilon, b)}{\partial b} - \frac{\partial F_{2}(\varepsilon, b)}{\partial b} - \frac{1-t}{2} \frac{\partial F_{0}(\varepsilon, b)}{\partial b} + \frac{\omega t}{\pi s} F_{0}(\varepsilon, b) \frac{\partial F_{0}(\varepsilon, b)}{\partial b} \right].$ (30)

4.3 Discussion and comparison with simulation

The analytical expressions (24) and (30) are the main result of the present paper. We compare the transverse thermoelectric conductivity equation (24) and the ratio $|M_z|/T\alpha_{xy}$ with the simulation results in the same model of Podolsky et al. [10] on underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ with $T_c = 28$ K. The comparison is presented in Figures 1 and 2. The parameters we obtained from the fit are: $H_{c2}(0) = 70$ T (corresponding to $\xi = 21.7$ Å), $\kappa = 62$, s' = 7 Å. The value $H_{c2}(T)$ does match the result of of Podolsky et al. [10]. With these values, our caculation gives good agreement with numerical simulation in the same model [10] as one would expect. The simulation of this system, even in 2D, is difficult and our expressions are supplemental with simulation results only when necessary.

5 Conclusion

We calculated the transverse thermoelectric conductivity α_{xy} and the magnetization M_z in 2D under magnetic field in the presence of strong thermal fluctuations on the mesoscopic scale in linear response. Time dependent Ginzburg-Landau equations with thermal noise describing the thermal fluctuations is used to study the vortexliquid regime. The nonlinear term in dynamics is treated using the renormalized Gaussian approximation. We obtained the analytically explicit expressions for the transverse thermoelectric conductivity α_{xy} and the magnetization M_z including all Landau levels, so that the approach





Fig. 1. Points are the transverse thermoelectric conductivity for different temperatures in reference [10]. The solid lines are the theoretical values of the transverse thermoelectric conductivity calculated from equation (24) with fitting parameters (see text).



Fig. 2. Points are the ratio $|M_z|/T\alpha_{xy}$ for different temperatures in reference [10]. The solid lines are the theoretical values of the ratio $|M_z|/T\alpha_{xy}$ calculated from equations (24) and (30) with same fitting parameters.

is valid for arbitrary values of the magnetic field not too close to $H_{c1}(T)$. Our results were compared to the simulation data on underdoped $\text{La}_{2-x}\text{Sr}_x$ CuO₄. The comparison is in good qualitative and even quantitative agreement with simulation data.

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