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Rapid Note

Kosterlitz-Thouless vs. Ginzburg-Landau description of 2D superconducting fluctuations

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Abstract. We evaluate the charge and spin susceptibilities of the 2D attractive Hubbard model and we compare our results with Monte Carlo simulations on the same model. We discuss the possibility to include topological Kosterlitz-Thouless superconducting fluctuations in a standard perturbative approach substituting in the fluctuation propagator the Ginzburg-Landau correlation length with the Kosterlitz-Thouless correlation length.

PACS. 74.20.De Phenomenological theories (two-fluid, Ginzburg-Landau, etc.) – 74.72.-h High-T_c compounds – 74.25.-q General properties; correlations between physical properties in normal and superconducting states

The discovery of spin and charge pseudogaps in the normal state of underdoped superconducting cuprates [1] has triggered a renewed interest on the physics of preformed Cooper pairs. The actual source of the pseudogaps (pairing, and/or spin-, and/or charge fluctuations) and the leading mechanisms responsible for the reduction of the superfluid density at low temperature (classical phase fluctuations, collective modes, quasiparticle excitations) are still debated. However, many indications support the idea that pairing occurs below some crossover temperature T^*, while the phase coherence is established at a sizably lower temperature. The low density of carriers resulting in a low superfluid density and the short coherence length $\xi_0 \sim 10 \div 30$ Å, support the relevance of the superconducting phase fluctuations in the thermodynamic and dynamic properties of these materials. Moreover, although topological phase fluctuations have been suggested to play a role in the superconductor-to-normal-state phase transition even in three-dimensional extreme type-II superconductors [2], it is clear that these fluctuations are crucial in two dimensions, where they give rise to the Kosterlitz-Thouless (KT) transition *via* the vortex-antivortex unbinding. Although no discontinuity of the superfluid density at T_c is observed, the strong anisotropy due to the layered structure of the cuprates suggests that some features of a KT transition could be present in these systems, in agreement with recent experiments [3]. Therefore it is worth investigating the effects of the topological vortex-antivortex phase fluctuations on the various properties of a 2D superconductor. In particular, an important issue concerns the inclusion of these effects in evaluating thermodynamic quantities like the spin susceptibility or the charge susceptibility. In this context, the aim of the present work is to look for possible connections between the perturbative scheme leading to the standard time-dependent Ginzburg-Landau (TDGL) results and the KT physics.

Halperin and Nelson [4] have shown that, in the KT regime, the contributions of superconducting fluctuations to the conductivity above $T_{\rm KT}$ have the same functional form, in terms of the correlation length ξ, as the Aslamazov-Larkin contributions of the standard TDGL theory, $\sigma_{\rm KT}(\xi) \simeq \sigma_{\rm GL}(\xi) \sim \xi^2$. The same holds for the fluctuation contribution to the diamagnetism $\chi^{\rm d}_{\rm KT}(\xi) \simeq \chi^{\rm d}_{\rm GL}(\xi) \sim \xi^2$. In spite of the same correlation length dependence, conductivity and diamagnetism in KT or TDGL theory have a completely different temperature dependence, induced by the different temperature dependence of the correlation length in the two theories. The KT correlation length diverges exponentially at $T_{\rm KT}$ while the GL correlation length diverges as a power-law with the classical exponent $\nu = \frac{1}{2}$. Therefore the KT conductivity and the diamagnetic susceptibility diverge exponentially at $T_{\rm KT}$ while the same quantities in the TDGL theory diverge as a power-law at T_c with a critical exponent $\gamma = 1$. In the present work we investigate the possibility that, in analogy with conductivity and diamagnetism, the correct behavior of the spin and charge susceptibilities in the KT regime can be simply recovered by inserting the KT

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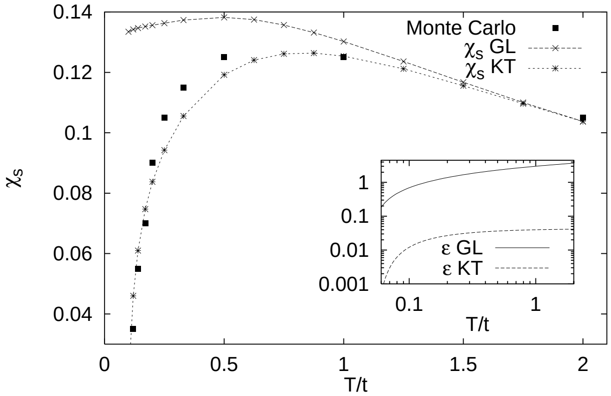

Fig. 1. Comparison between Monte Carlo spin susceptibility (taken from Ref. [6]) and the spin susceptibility calculated using the Ginzburg-Landau (χ_s^{GL}) and the Kosterlitz-Thouless (χ_s^{KT}) correlation length.

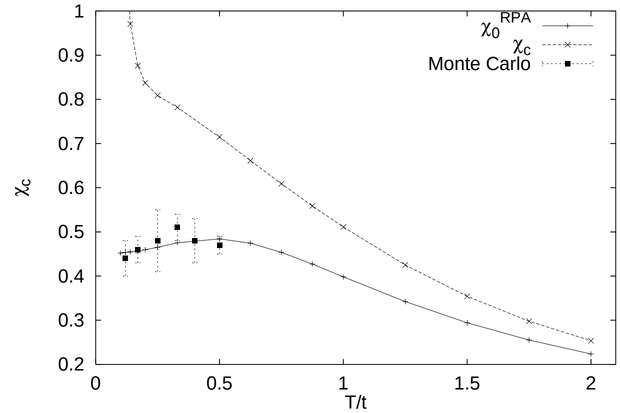

Fig. 2. Comparison between Monte Carlo charge susceptibility (taken from Ref. [8]), the charge susceptibility calculated using the Kosterlitz-Thouless correlation length (χ_c) and the RPA resummation of the bare bubble (χ_0^{RPA}).

correlation length in their TDGL expressions. We shall find that this prescription does work for the spin susceptibility while it does not for the charge susceptibility.

We analyze the two-dimensional negative-U Hubbard model [11] which is the simplest minimal model where the distinct occurrence of pairing and phase coherence can be investigated. Within this model, the spin susceptibility χ_s and the charge compressibility χ_c are calculated on a two-dimensional square lattice by performing a loop expansion with the fermions exchanging the Cooper-fluctuations propagator in the standard form. Before giving the technical details of our treatment, we immediately present our results.

Figure 1 shows the behavior of the spin susceptibility when the correlation length is assumed either of the GL form (dashed line with crosses) or of the KT form (dotted line with stars). Both curves are compared with the Monte Carlo data obtained in reference [7,8] for the negative-U Hubbard model with $U = -4t$ (t is the nearest-neighbor hopping) at filling $n = 0.5$ electrons per cell. The critical temperature T_{KT} of the KT superconducting transition, as extracted from numerical calculations, is $T_{KT} = 0.05t$ and has been used as the input critical temperature for our perturbative calculations. In the Monte Carlo data, for T less then $T^\star \simeq t \gg T_{KT}$, χ_s starts decreasing. This indicates the existence of strong superconducting fluctuations in the temperature range between the mean-field transition temperature ($T_{BCS} \simeq 0.6t$) and the true KT transition. It is apparent from Figure 1 that the rapid decrease of the spin susceptibility in the Monte Carlo results is well fitted by inserting in the correlation length the KT temperature dependence as given by the expression

$$\xi_{KT}(T) = \xi_c \exp\left[b\sqrt{\frac{T(T_{BCS} - T_{KT})}{T_{BCS}(T - T_{KT})}}\right]. \qquad (1)$$

Here ξ_c is an effective size of the core of the vortex that we take of the order of the zero temperature correlation length ξ_0, and b is a positive constant of the order of unity. This specific form of the KT correlation length has been derived along the line of reference [4], although it differs slightly from the one commonly quoted in the literature [5,6]. We shall comment on this later. Notice that the KT mass term (inverse square of the correlation length) of the Cooper propagator remains small and generates strong fluctuations, in a wider range of temperatures than the GL mass with the same critical temperature in agreement with Monte Carlo data. The GL correlation length is instead completely inadequate to reproduce the Monte Carlo data in the all range of temperatures.

The fit in Figure 1 stops at $T \simeq 0.1t$ because there are no numerical data below this value. This also appears to be the lower limit for our approach to work. Indeed for $T \simeq 0.09t$ the TDGL expression for χ_s develops a non physical behavior ($\chi_s < 0$), indicating that the perturbative scheme no longer applies near T_{KT}. Whit this caution in mind, the results of Figure 1 indicate that the simple loop expansion we adopted is able to reproduce the spin susceptibility in a wide range of temperatures. They support the idea that the main effect of the vortex-antivortex phase fluctuations on the spin susceptibility is embedded in (and satisfactorily accounted for by) the temperature dependence of the $\xi_{KT}(T)$ correlation length, in analogy with the conductivity and diamagnetism.

On the other hand, as seen in Figure 2, the same type of calculations for the charge susceptibility fail in describing the nearly constant (but with sizeable error bars) behavior obtained numerically. In particular, we find that the Aslamazov-Larkin (AL) contribution, which does not contribute to the spin susceptibility, strongly enhances $\chi_c(T)$ and eventually leads to a divergent χ_c near T_{KT}. As a consequence $\chi_c(T)$ strongly deviates from the Monte Carlo results for $T < T_{BCS}$. In Figure 2 we also report the RPA resummation of the bare bubble in the charge channel that fits the available Monte Carlo data, to obtain, by extrapolation, the $\chi_c(T)$ at higher temperature.

With this respect χ_c appears to behave as the specific heat C_v, for which the 2D-TDGL expression $C_v^{GL} \sim \xi_{GL}^2$ does not reproduce the correct KT result $C_v^{KT} \sim \xi_{KT}^{-2}$, even when expressed in terms of the correlation length. This failure arises despite the free energies in the two theories have the same leading behavior (but for an overall sign and a subleading logarithmic correction) when written in terms of the respective correlation lengths: $F_{\rm GL} \sim \xi_{\rm GL}^{-2} \ln \xi_{\rm GL}$ and $F_{\rm KT} \sim -\xi_{\rm KT}^{-2}$ [5,6]. The similarity of the free energies indicates that our procedure of replacing $\xi_{\rm KT}$ inside the TDGL expressions nearly holds at least in providing the correct scaling behavior of the free energy at the transition. On the other hand, the temperature dependence of the coherence lengths are quite different within the TDGL and KT theories and therefore, starting from the GL and KT free-energy expressions and differentiating in temperature, one obtains quite different expressions for $C_v^{\rm GL}$ and $C_v^{\rm KT}$ in terms of the ξ's. Notice that, even assuming $F_{\rm GL}(\xi_{\rm KT}) \sim F_{\rm KT}(\xi_{\rm KT})$, $C_v^{\rm KT} \propto \frac{{\rm d}^2 F_{\rm KT}(\xi_{\rm KT})}{{\rm d}T^2}$ has no relation with $C_v^{\rm GL}(\xi_{\rm GL} \to \xi_{\rm KT}) \propto \left.\frac{{\rm d}^2 F_{\rm GL}(\xi_{\rm GL})}{{\rm d}T^2}\right|_{\xi_{\rm KT}}$. According to this example, quantities involving temperature derivatives of the correlation lengths are hardly expected to be reproduced by the replacement $\xi_{\rm GL} \to \xi_{\rm KT}$ in the GL expressions. Our result for $\chi_{\rm c}$ has the same origin: The charge response at $\omega = 0$, $q \to 0$ can be obtained as a chemical potential derivative of the free energy. Now, since the critical temperature depends on the chemical potential $T_{\rm c} = T_{\rm c}(\mu)$, a total derivative with respect to μ also involves derivatives with respect to $T_{\rm c}$, and, in turn, derivatives of ξ. Therefore the temperature dependence in $\chi_{\rm c}$ not only arises from the temperature dependence of $\xi(T)$, but also depends on ${\rm d}\xi/{\rm d}T_{\rm c} \simeq -{\rm d}\xi/{\rm d}T$. In fact one gets the same TDGL singular contribution $\sim \xi^2$ for $\chi_{\rm c}$ and C_v. Our simple perturbative expansion, where the leading temperature dependence only arises from the mass term ξ^{-2} of the Cooper fluctuation propagator in the TDGL expression, fails to reproduce the correct temperature dependence for $\chi_{\rm c}$ in the same way as it fails in evaluating the specific heat.

We now describe the details of our calculations. The model we consider is given by

$$H = -t \sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma} \qquad (2)$$

where t is the hopping between nearest-neighbor sites, $U < 0$ the strength of the attraction and μ the chemical potential. The standard ladder resummation of diagrams leads to the Cooper pair propagator $L(q,\Omega_l) = -U/\left(1 + U\chi_0^{\rm pp}(q,\Omega_l)\right)$ where $\chi_0^{\rm pp}(q,\Omega_l)$ is the bare particle-particle bubble, being q the momenta and Ω_l the Matsubara frequency. In the normal state, within the standard GL approach, at small q and Ω_l one has

$$L^{-1}(q,\Omega_l) = N_0 \left(\epsilon + \eta q^2 + \gamma |\Omega_l|\right) \qquad (3)$$

where N_0 is the density of states at the Fermi energy, $\eta = 7\zeta(3)/(32\pi^2)(v_{\rm F}/T_{\rm c})^2 \simeq \xi_0^2$, and $\gamma = \pi/(8T_{\rm c})$. The mass term $\epsilon = \ln(T/T_{\rm c}) = (\xi/\xi_0)^{-2}$ of the propagator controls the distance from the superconducting transition. In the standard GL approach $\epsilon \sim \xi_{\rm GL}^{-2}$ and near $T_{\rm c}$ it goes to zero as $(T - T_{\rm c})/T_{\rm c}$.

We study the charge and spin susceptibilities by evaluating the one loop corrections $\Delta\chi_{\rm c}$ (charge channel) and $\Delta\chi_{\rm s}$ (spin channel) to the bare particle-hole bubble $\chi_0^{\rm ph}$, $\chi_{\rm c,s}^{\rm ph} = \chi_0^{\rm ph} + \Delta\chi_{\rm c,s}$. The charge (c) and spin (s) bubbles $\chi_{\rm c,s}^{\rm ph}$ are then inserted in the RPA resummation to get the charge and spin susceptibilities (see below). In the one loop expansion, we include diagrams containing only one integration on the bosonic variables (q,Ω_l) (*i.e.* one bosonic loop) of the fluctuation propagator $L(q,\Omega_l)$, obtaining three kinds of diagrams which contribute differently to the spin and charge susceptibilities: the selfenergy diagrams, where $L(q,\Omega_l)$ renormalizes the one particle bare Green function (DOS contribution); the vertex diagrams, where $L(q,\Omega_l)$ renormalizes the vertex, connecting two bare Green function (Maki-Thompson (MT) contribution); the Aslamazov-Larkin (AL) diagrams, containing two fluctuation propagators. Moreover it is necessary to add the counterterms (CT) proportional to the shift of the chemical potential $\delta\mu$, which is required to preserve the number of particles. We notice that the one loop expansion for the charge and the spin susceptibilities satisfies the relation, derived from spin and charge conservation, $\chi_{\rm s,c}(q = 0, \Omega \neq 0) = 0$. One obtains:

$$\Delta\chi_{\rm s} = 4\,DOS - 2\,MT + 4\,CT \qquad (4)$$

$$\Delta\chi_{\rm c} = 4\,DOS + 2\,MT + 4\,AL + 4\,CT. \qquad (5)$$

The absence of the AL contribution and the (opposite) sign of the MT diagrams in the spin susceptibility is the consequence of the vertex spin structure, as shown in reference [12]. Moreover the leading DOS contributions to the charge susceptibility cancel the MT ones. The AL diagrams give therefore the most important contribution to the charge susceptibility (being the CT diagrams subdominant respect to them) [13].

According to the physical assumption outlined above that the TDGL and KT temperature dependencies are essentially ruled by the correlation lengths, we have alternatively taken equation (3) with $\xi = \xi_{\rm GL}$ and $\xi = \xi_{\rm KT}$. In the calculation with $\xi_{\rm GL}$ we used $T_{\rm c} = T_{\rm KT}$ and the mass term $\epsilon = \ln(T/T_{\rm c})$, while in the calculation with $\xi_{\rm KT}$ we used equation (1) with $b = 1.6$ and $\xi_{\rm c} = \xi_0$. In both cases we took the coefficients η and γ given by the corresponding expressions reported below equation (3) calculated with $T_{\rm c} = T_{\rm BCS}$. This choice was motivated by the plausible assumption that η and γ change little once the fluctuations are predominantly in the phase sector. In any case we checked that our results are rather stable with respect to modifications of η and γ.

The charge and the spin susceptibilities are finally obtained by the RPA resummation of the corrected charge and spin bubbles $\chi_{\rm c,s} = \chi_{\rm c,s}^{\rm ph}/\left(1 \pm (\tilde{U}_{\rm c,s}/2)\chi_{\rm c,s}^{\rm ph}\right)$ where the plus (minus) sign is associated to the charge (spin) susceptibility. Notice that, following the analysis of reference [7], the RPA expressions of both susceptibilities contain an effective local interaction $\tilde{U}_{\rm c,s}$ instead of the bare U in order to properly fit the high temperature region of the Monte Carlo data. The validity of the RPA form for the spin susceptibility is also found in the context of the positive-U

Hubbard model [14]. However, while in reference [7] the bare bubbles were resummed and a value $\tilde{U}_\mathrm{s} = -6.5$ was obtained for $U = -4t$ and $\langle n \rangle = 0.5$, in our case we resum the bubbles already containing the $\Delta\chi_\mathrm{s}$ corrections and a different value $\tilde{U}_\mathrm{s} = -4.6$ is needed to match the RPA calculation with the high temperature Monte Carlo data. For the charge susceptibility the comparison with the RPA resummation in terms of the χ_0^ph reported in Figure 2 gives $\tilde{U}_\mathrm{c} = -1.6$.

We now comment on the expression in equation (1) that we used for the KT correlation length. We wrote this expression following Halperin and Nelson [4]. They introduce into the KT correlation length $\xi_\mathrm{KT} \simeq a \exp\left[b(\pi J/k_\mathrm{B}T - 1)\right]$ for the classical XY model (with coupling J and lattice spacing a) a temperature dependent $J(T) = n_\mathrm{s}(T)/8m$ and take $a = \xi_\mathrm{c}$. Here the superfluid density $n_\mathrm{s}(T)$ is taken to vanish linearly at a temperature $T_0(> T_\mathrm{KT})$ to be determined selfconsistently by the request that T_0 should include the effect of the fluctuations at scale lower than ξ_c. Our expression (1) is obtained by taking $T_0 \simeq T_\mathrm{BCS}$ and $\xi_\mathrm{c} \simeq \xi_0$ with the idea that phase fluctuations are the most important effect all over the range of temperatures $T_\mathrm{KT} \leq T \leq T_\mathrm{BCS}$ (at least in evaluating χ_s and χ_c) [15].

The results of the simple procedure outlined above are quite satisfactory for the spin susceptibility. This indicates that the main temperature dependence of this quantity actually arises from the specific KT temperature dependence of the correlation length, which thus brings along the physics of the vortex-antivortex phase fluctuations into a simple perturbative scheme. The same is not true for the compressibility, as for the specific heat, since these quantities also involve temperature derivatives of ξ_KT.

Our method, developed for the 2D attractive Hubbard model, can be useful to understand the role of the superconducting phase fluctuations in quasi-2D cuprate superconductors. In this context the recent finding that KT signatures, which are absent in the static conductivity, are progressively more evident in the dynamical conductivity at shorter timescales [3] encourages to extend our analysis to other frequency-dependent quantities. In particular it is of obvious interest to explore the possibility to include in a simple perturbative scheme along the lines followed in the present work the effects of KT topological phase fluctuations on dynamical quantities like the optical conductivity and single-particle spectra.

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