Superfluid density of the two-dimensional strong-coupling attractive Hubbard model

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Abstract

The low-temperature result for the superfluid density of the attractive (negative-U) Hubbard model in two dimensions and in the strong-coupling limit is obtained, applying a field-theoretic representation of the model and utilizing a hydrodynamic relation between the order parameter field, the correlation function for soft planar fluctuations, and the superfluid density. This microscopic derivation does not involve self-consistency arguments and allows to include the influence of the out-of-plane pseudo-spin fluctuations which become singular at half band-filling and suppress a Kosterlitz-Thouless transition at finite temperature. The result is in good agreement with quantum Monte Carlo data.

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The negative-U Hubbard model describes strongly correlated electronic systems in which both itinerant behavior and short-ranged attractive interactions are present [1]. Doped away from half band-filling, it exhibits XY-like symmetry and in two dimensions is believed to undergo [2] a Kosterlitz-Thouless (KT) transition [3] at finite temperature, while at half filling the transition temperature should vanish due to the full Heisenberg symmetry which is restored in this case. This picture is very suggestive especially in the limit of strong coupling, where the negative-U Hubbard Hamiltonian can be mapped on the anisotropic pseudo-spin quantum Heisenberg model [4]. A peculiar feature of the Kosterlitz-Thouless transition is the discontinuous jump [5] of the superfluid density (or spin-stiffness) from zero to finite values below T_{KT}. Both numerical [2, 6, 7] and analytical [8] approaches have been reported to study the KT transition of the attractive Hubbard model and to calculate the spin-stiffness [9] for various band-fillings and temperatures. While quantum Monte Carlo results [6] indicate a depression of the superfluid density as one approaches half filling, a BCS-like mean-field theory [8] fails to capture this symmetry-related behavior. For purely planar classical magnets, renormalization group techniques [10] have been applied to obtain the spin-stiffness in the vicinity of T_{KT} [5], and also for low temperatures [11]. The effect of an easy-plane anisotropy of the Heisenberg model [12] on the spin-stiffness in two dimensions has been studied [13] in the framework of an extended [14] self-consistent harmonic approximation [15] neglecting vortices. To estimate T_{KT} in such classical easy-plane systems including the role of vortices, the deformation of a single vortex into an instanton and crossover scaling arguments have been considered [16].

In the present paper we apply a field-theoretic representation [17] of the strong-coupling negative-U Hubbard model in order to derive the low-temperature result for the superfluid density for arbitrary band-filling and in two dimensions. We start with a Grassmann functional integral representation of the model and obtain an effective field theory which incorporates the effect of both the in-plane and out-of-plane pseudo-spin fluctuations. Within this field theory, the superfluid density is expressed by a hydrodynamic relation which involves the effective 1-point and 2-point vertices of the order parameter fluctuations. Such a microscopic derivation conserves the full symmetry of the model and does not have to invoke further self-consistency arguments which were necessary in previous studies of anisotropic two-dimensional magnets [14]. However, since this approach does not capture the influence of vortex excitations of the Hubbard model [18], we have to restrict our consideration to low temperatures, and evaluate momentum integrals in the approximation of the leading singularities.

We start with the Hubbard Hamiltonian

$$\mathcal{H} = -t \sum_{\langle rr'\rangle\sigma} c^{+}_{r\sigma} c_{r'\sigma} + U \sum_{r} n_{r\uparrow} n_{r\downarrow} - \mu \sum_{r\sigma} n_{r\sigma}, \tag{1}$$

where we consider attractive on-site interaction $U < 0$, the chemical potential μ, and hopping $t > 0$ between adjacent sites on a simple cubic lattice. $c^{+}_{r\sigma}$ creates an electron with spin σ at site r. The sum $\langle rr'\rangle$ extends over nearest neighbors of the lattice. In the limit of strong coupling, $|U| \gg t$, an expansion of the Hubbard model [4] in t/U, truncated after the leading order, results in the anisotropic quantum Heisenberg model,

$$\mathcal{H} = -\frac{J}{2} \sum_{\langle rr'\rangle} \left(A^{+}_{r} A^{-}_{r'} - N_r N_{r'} \right) - 2\mu \sum_{r} N_r, \tag{2}$$

with the coupling constant $J = 4t^2/|U|$ and the spin-like pair operators $A^{-}_{r} = c_{r\downarrow} c_{r\uparrow}$,

$A_r^+ = c_{r\uparrow}^+ c_{r\downarrow}^+$, and $N_r = n_{r\uparrow} n_{r\downarrow} = \frac{1}{2}\sum_\sigma n_{r\sigma}$. These operators are defined on the restricted local fermionic Hilbert space which contains only pair states, excluding single occupancy of sites. This constraint can be modelled exactly by a spin-dependent Popov-Fedotov potential [19] which leads to a shifted Matsubara frequency spectrum, $z_{n\sigma} = \frac{\pi}{\beta\hbar}(2n+1+\frac{\sigma}{2})$, with $\sigma = \pm 1$. The partition function of the model (2) is now written as a functional integral over Grassmann fields,

$$Z = \int \prod_{r\sigma\tau} \mathcal{D}\overline{\psi}_{r\sigma}(\tau)\mathcal{D}\psi_{r\sigma}(\tau)\ \exp\mathcal{S}\{\overline{\psi}_{r\sigma}(\tau), \psi_{r\sigma}(\tau)\}, \tag{3}$$

with the action

$$\mathcal{S} = \int_0^\beta \mathrm{d}\tau \left(\sum_{r\sigma} \overline{\psi}_{r\sigma}(\tau)\left(\partial_\tau + \mu\right)\psi_{r\sigma}(\tau) - \mathcal{H}(\overline{\psi}, \psi) \right). \tag{4}$$

The quartic Grassmann products in the interaction terms of the action (4) are decoupled by introducing the local Hubbard-Stratonovitch fields Δ_r and X_r, which correspond to the order parameters for superconductivity and charge-ordering, $\langle \Delta_r \rangle = \frac{J}{2}\sum_{r'}\langle c_{r'\downarrow} c_{r'\uparrow}\rangle$ and $\langle X_r \rangle = \frac{J}{4}\sum_{r'\sigma}(-1)^{r'}\langle c_{r'\sigma}^+ c_{r'\sigma}\rangle$, where the r'-sum is over the nearest neighbors of r. The action then reduces to bilinear products of Grassmann variables which can be integrated out to yield the effective action for the pair fields,

$$\mathcal{S} = -\sum_{q,m} \frac{\beta}{J_q}\left(\overline{\Delta}_{q,m}\Delta_{q,m} + X_{q,m}X_{-q,-m} \right) + \sum_r \ln\det \beta\mathbf{M}_r, \tag{5}$$

where $J_q = Jd\gamma_q$, and $\gamma_q = \frac{1}{d}\sum_{l=1}^{d}\cos(q_l a)$ is the coupling in momentum space. The fermion determinant contains the bilinear kernel

$$(\mathbf{M}_r)_{n+m,n} = (i\hbar z_{n\sigma}\,\rho_z + \mu\,\rho_0)\delta_{m,0} + (-1)^r X_{r,m}\,\rho_0 - \Delta_{r,m}\,\rho_+ + \overline{\Delta}_{r,-m}\,\rho_-, \tag{6}$$

where ρ denotes a Pauli matrix. Dividing the effective action $\mathcal{S}$ into a static and homogeneous part $\mathcal{S}_0$ and the fluctuation contribution $\mathcal{S}_{\mathrm{fl}}$, we now identify the saddle-point solutions. Since charge-ordering is suppressed for nonzero chemical potential, we may set $\langle X_{0,0}\rangle \equiv 0$, which corresponds to purely planar ordering of the pseudo-spins in the low-temperature phase. In this way one finds

$$\mathcal{S}_0 = -\frac{\beta\Delta^2}{J_0} + \ln\cosh\beta\sqrt{\mu^2+\Delta^2}, \tag{7}$$

which immediately leads to a self-consistency equation for the superconducting order parameter $\Delta = \langle \Delta_{0,0}\rangle$. The chemical potential in the low-temperature phase is given by $\mu = J_0(\nu - \frac{1}{2})$, where $\nu = \langle n_\uparrow n_\downarrow\rangle$ is the band-filling. For $T = 0$, this implies $\Delta = J_0|\alpha_0| = J_0\sqrt{\nu(1-\nu)}$. Introducing now the fluctuation fields

$$(\Phi_r)_{n+m,n} = (-1)^r X_{r,m}\,\rho_0 + \phi_{r,m}\,\rho_+ - \overline{\phi}_{r,-m}\,\rho_-, \tag{8}$$

allows the separation $\mathbf{M}_r = \mathbf{M}_0 + \Phi_r$, where $\mathbf{M}_0$ is the saddle-point value of the kernel (6). The fermionic propagator matrix $\mathbf{G} = (\mathbf{M}_0)^{-1}$ is spin-dependent, local, and diagonal in the frequencies, $(\mathbf{G}_{rr'})_{n+m,n} = \delta_{r,r'}\delta_{m,0}\mathbf{G}_n$, and describes lattice fermions with infinite mass,

$$\mathbf{G}_n = \frac{-i\hbar z_{n\sigma}\,\rho_z + \mu\,\rho_0 + i\Delta\,\rho_y}{(\hbar z_{n\sigma})^2 + \mu^2 + \Delta^2}. \tag{9}$$

Inserted in (5), this results in the effective action that describes the fluctuations, $\mathcal{S}_{\text{fl}} = \mathcal{S}_2 + \mathcal{S}_{\text{int}}$. Its free part is given by

$$\mathcal{S}_2 = -\frac{\beta}{J_0}\sum_m \int \mathrm{d}^d q \frac{1}{C_m \gamma_q} \chi^T_{q,m} \mathbf{A}_{q,m} \chi_{-q,-m}, \tag{10}$$

where $C_m = \mu^2 + \Delta^2 + \frac{1}{4}(\hbar\omega_m)^2$, and the new basis $\chi^T_{q,m} = (i\phi^-_{q,m}, \phi^+_{q,m}, X_{\pi+q,m})$ with the components $\phi^\pm_{q,m} = \frac{1}{2}(\overline{\phi}_{-q,-m} \pm \phi_{q,m})$ has been introduced. For $q \approx 0$, the fields ϕ^- correspond to the soft transversal phase fluctuations of the complex order parameter Δ, while the massive longitudinal ones are related to ϕ^+. $\mathcal{S}_2$ encapsulates two massless modes, whose leading components at half band-filling are $\phi^-_{q,m}$ for $q \approx 0$, and $X_{\pi+q,m}$ for $q \approx \pi$. These excitations correspond to the Bogoliubov-Anderson phase fluctuation mode, and alternating charge-density fluctuations which become soft at half band-filling and suppress the KT transition, respectively. In the massless ($\mu = 0$) case, both exhibit the linear dispersion $\omega = ck$, with the velocity $c = 2\Delta a/\hbar\sqrt{d}$, which for $\nu = \frac{1}{2}$ agrees with the result of spin-wave calculations [20]. In the static case, $\omega_m = 0$, the structure of the inverse propagator for the fluctuation fields is given by the matrix

$$\mathbf{A}_{q,0} = \begin{pmatrix} C_0(1-\gamma_q) & 0 & 0 \\ 0 & C_0 - \mu^2\gamma_q & -\mu\Delta\gamma_q \\ 0 & -\mu\Delta\gamma_q & -C_0 - \Delta^2\gamma_q \end{pmatrix}. \tag{11}$$

The saddle-point value for the static effective 2-point vertex related to the ϕ^- fluctuations in $\mathcal{O}(q^2)$ is therefore given by

$$\Gamma_2^{(0)}(q) = \frac{\beta}{J_0}(1-\gamma_q). \tag{12}$$

The higher order terms of the fluctuation expansion contribute to the interacting part of the effective action,

$$\mathcal{S}_{\text{int}} = \sum_r \sum_{k=3}^{\infty} \frac{(-1)^{k+1}}{k} \mathrm{Tr}(\mathbf{G}\Phi_r)^k. \tag{13}$$

To derive the low-temperature result of the superfluid density, it is sufficient to evaluate the one-loop corrections for the superconducting order parameter field and for the correlation function of the phase fluctuations. This is because for low temperatures the loop-expansion is equivalent to an expansion in powers of T. Therefore, it is necessary to obtain $\mathcal{S}_{\text{int}}$ up to fourth order in the fluctuation fields. We also restrict the calculation to the contributions which are leading in the dimensional singularities near $d = 2$. This implies to consider only diagrams related to singular internal propagators, therefore we may set $\omega_m = 0$ in the free bosonic Matsubara sums and neglect contributions from massive fluctuations. Introducing the new fields λ, with $J_0\lambda_{q,m} = \mu X_{\pi+q,m} - \Delta\phi^+_{q,m}$, we find for the interacting part of the effective action, $\mathcal{S}_{\text{int}} \simeq \mathcal{S}_3 + \mathcal{S}_4$, the low-temperature results which enter into the calculations,

$$\begin{aligned} \mathcal{S}_3 &= \frac{\beta}{J_0^2}\sum_r \left[16\,\lambda^3_{r,0} - 4\,\lambda_{r,0}(\chi^T_{r,0}\chi_{r,0})\right], \\ \mathcal{S}_4 &\simeq -\frac{\beta}{J_0^3}\sum_r (\chi^T_{r,0}\chi_{r,0})^2. \end{aligned} \tag{14}$$

In accordance with our discussion, in these expressions we have considered only the static contributions, and in the prefactors terms which are exponentially small in the temperature have been neglected.

We now proceed to obtain the one-loop results for the order parameter field and for the correlation function of the soft in-plane fluctuations. To the fluctuation correction of Δ at one-loop order only the diagram depicted in Fig. 1 (a) contributes. Introducing the reduced temperature $\theta = kT/\pi J_0\,\nu(1-\nu)$, the result [17] is given by

$$\Delta - \langle\phi^+_{0,0}\rangle = \Delta\left(1 - \frac{\theta}{2}\left[I_d(0) + I_d(m)\right]\right), \tag{15}$$

with the momentum integral

$$I_d(m) = \frac{1}{2}\int_0^{\Lambda^2} \frac{\mathrm{d}x\; x^{d/2-1}}{x + m^2}, \tag{16}$$

and the filling dependent mass $m^2 = 8\mu^2/\Delta^2$ which becomes zero at the band center. Since the one-loop correction of the chemical potential vanishes [17], in (15) no further terms arise.

The one-loop contribution to the effective 2-point vertex $\Gamma_2(q)$ related to the ϕ^- fluctuations involves the evaluation of the diagrams (b)-(d). They are readily derived

$$\begin{aligned}
\Gamma^{(1)}_{2,\mathrm{b}}(q) &= -\frac{4}{\pi J_0^2} I_d(0)\left(1 - \frac{1}{4|\alpha_0|^2}(1-\gamma_q)\right), \\
\Gamma^{(1)}_{2,\mathrm{c}}(q) &= -\frac{2}{\pi J_0^2}\left[I_d(0) + I_d(m)\right], \\
\Gamma^{(1)}_{2,\mathrm{d}}(q) &= +\frac{2}{\pi J_0^2}\left[3\,I_d(0) + I_d(m)\right].
\end{aligned} \tag{17}$$

Adding up these contributions, one finds that the ϕ^- fluctuations remain massless, $\Gamma^{(1)}_2(0) = 0$, which is required by Goldstone's theorem (or a generalized Ward identity). The 2-point vertex at one-loop order is then given by

$$\Gamma_2(q) = \Gamma^{(0)}_2(q)\left[1 + \theta I_d(0)\right]. \tag{18}$$

Having derived the one-loop order parameter and effective 2-point vertex, we are now ready to obtain the low-temperature result for the superfluid density. We first decompose the pair operators in cartesian components, $A^{\pm}_r = A^x_r \pm i A^y_r$, which are related to the fluctuation fields,

$$i\langle A^y_r\rangle = \langle\phi^-_r\rangle \qquad \text{and} \qquad \langle A^x_r\rangle = \Delta - \langle\phi^+_r\rangle, \tag{19}$$

where we have chosen Δ to be real. In the low-temperature phase, and above two dimensions, the $U(1)$ gauge symmetry is broken, $\langle A^x\rangle \neq 0$. The symmetry-restoring operator $A^y_r = i[A^x_r, N]$ is related to the soft phase fluctuations of the order parameter A^x. In the low-temperature phase, the pseudo-spin stiffness (corresponding to the superfluid density ρ_s) can then be expressed by the homogeneous expectation value of A^x and the static correlation function of A^y in the limit of low momenta [21],

$$\rho_s = \frac{\langle A^x_{0,0}\rangle^2}{\beta\langle A^y_{q,0}, A^y_{-q,0}\rangle\,(qa)^2} \qquad \text{for} \quad q \to 0. \tag{20}$$

Since we consider low temperatures, and therefore may neglect the effect of vortex excitations [3], this relation gives the correct result for the superfluid density for $T \ll T_{\rm KT} \sim J$. At higher temperature, $T \approx T_{\rm KT}$, vortices cannot be neglected, and the definition of ρ_s has to be modified [22]. Inserting now the results (12), (15) and (18) into the expression (20), the low-temperature value of the superfluid density near two dimensions is finally obtained,

$$\rho_s = J|\alpha_0|^2[1 - \theta I_d(m)]. \tag{21}$$

Although both the order parameter and the correlation function exhibit one-loop corrections which become singular in two dimensions [*cf.* Eqs. (15) and (18)], indicating the breakdown of long-range order, these singularities do not appear in the superfluid density, which only contains a term with a logarithmic singularity in the band-filling, reflecting the vanishing mass of the out-of-plane fluctuations. Taking now $d = 2$, one finds

$$\rho_s = J|\alpha_0|^2 + \frac{kT}{2\pi} \ln|1 - 2\nu|. \tag{22}$$

For half filling and $T = 0$, the corresponding result for the $S = 1/2$ Heisenberg antiferromagnet [23] is retrieved, $\rho_s = J/4$. The expression (22) is also in accordance with the low-temperature result of the self-consistent harmonic approximation [13] for a classical Heisenberg magnet in an external field corresponding to the chemical potential. However, invoking the scaling behavior for the superconducting order parameter as expected from the XY and Heisenberg limit of the nonlinear σ-model [24] suggests

$$\rho_s = J\,\nu(1 - \nu)\,|1 - 2\nu|^\theta. \tag{23}$$

The filling dependence of this result is shown in Fig. 2 for $J = t$ and $\beta t = 10$. It is in quite good agreement with quantum Monte Carlo simulations of finite lattices [6] and captures the depression of ρ_s near half band-filling. If one considered only the saddle-point value of the quantities which enter into the relation (20), the result $\rho_s = J|\alpha_0|^2$ would follow, which misses the effect of the full Heisenberg symmetry for the $\mu = 0$ case. The out-of-plane fluctuations restore this symmetry and suppress a Kosterlitz-Thouless transition at finite temperature.

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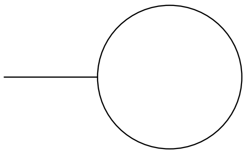
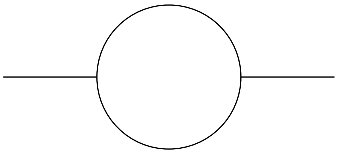
Figure captions

Figure 1. One-loop diagrams for the 1-point (a) and 2-point vertex (b)-(d).

Figure 2. The superfluid density ρ_s/t versus the band-filling ν, as given by Eq. (23) for $\beta t = 10$ and $U = -4t$ (solid line), and the corresponding quantum Monte Carlo data of Scalapino *et al.* (Ref. 6) obtained from an 8×8 lattice.



(a)



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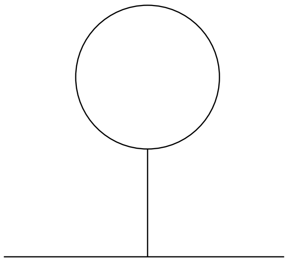

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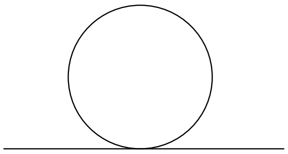
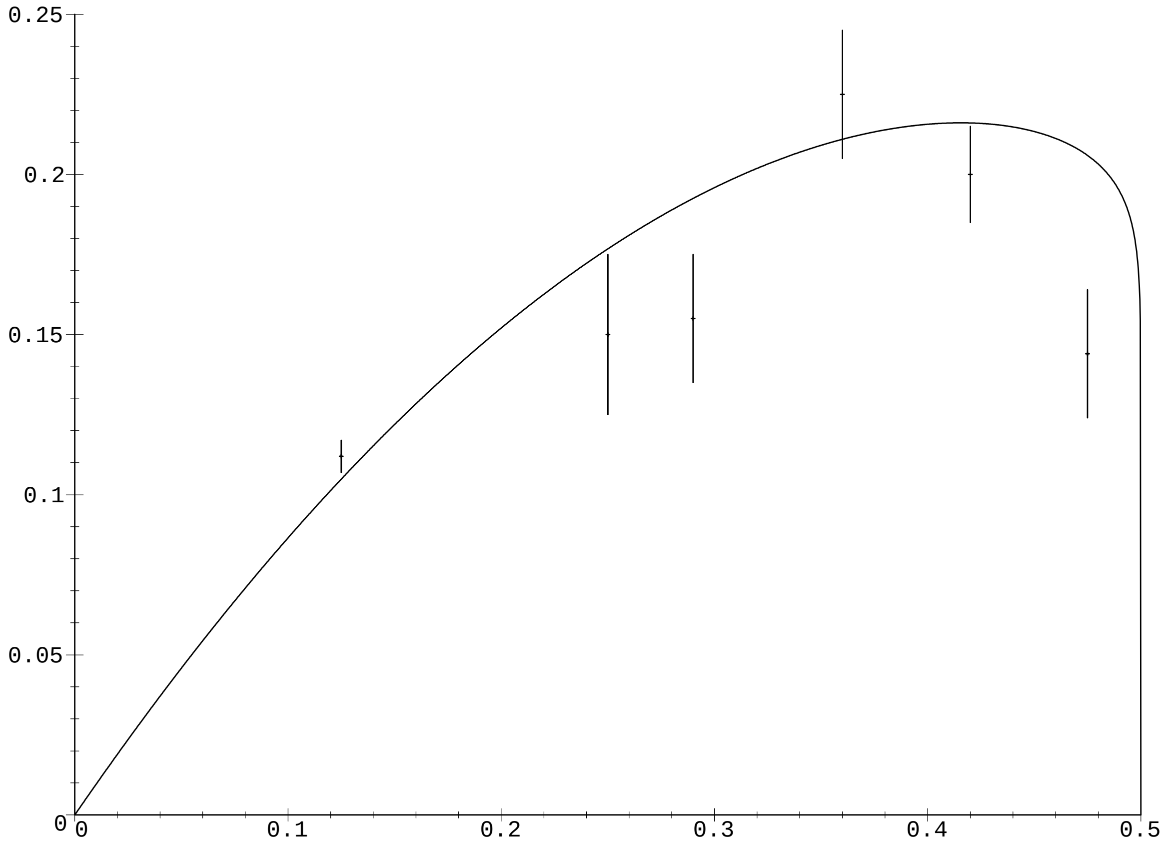


(d)

Figure 1.



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0.2
0.15
0.1
0.05
0
0
0.1
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0.4
0.5