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Low-temperature specific heat of one-dimensional multicomponent systems at the commensurate-incommensurate phase transition point

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Low-temperature dependence of specific heat of one-dimensional multicomponent systems at the commensurate-incommensurate phase transition point is studied. It is found that for canonical systems, with a fixed total number of particles, low-temperature specific heat linearly depends on temperature with a diverging prefactor.

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Second-order phase transitions in one-dimensional (1D) quantum or two-dimensional statistical systems are often classified by fixed-point Hamiltonians enjoying conformal invariance.[1] In such situations, low-temperature thermodynamic behavior is fixed solely by the central charge,[2] c, the quantity that roughly measures numbers of degrees of freedom, and velocity of the linear excitation, v—"speed of light." Low-temperature specific heat combines these two quantities and has the universal form[3] $C(T)=\pi cT/3v$, depending linearly on temperature. The notable exception from the above picture is provided by the second-order phase transition driven by chemical potential coupled to the conserved quantity,[4] so-called commensurate-incommensurate (C-IC) phase transition.[5,6] At the C-IC phase transition point system, in contrast to conformal invariance, obeys zero scale-factor universality[7] with dynamical critical exponent $z=2$. In particular for the specific heat it implies square-root temperature dependence for $T\rightarrow 0$.

Describing the C-IC phase transitions in multicomponent systems (systems of fermions, bosons or spin S chains) one cannot rely on mode-decoupling approximation.[8] In particular, as a result of spin-charge nonseparation, magnetic susceptibility of spin gapped systems, at the edge point of magnetization plateau, stays finite instead of diverging unless special microscopic symmetries are present (e.g., particle-hole symmetry at half filling for attracting Fermi Hubbard model). This kind of behavior has also been observed for a number of integrable models such as the two component Fermi Hubbard model both on lattice[9,10] as well as in continuum,[11] or spin S generalization of the integrable $t-J$ chain doped with $S-1/2$ carriers.[12] Similar behavior holds for generic systems of multicomponent Fermi or Bose gases, with gapped spin and gapless charge excitation.[8,13] Notable example of bosonic systems, in this respect, is provided by antiferromagnetically interacting spin 1 Bose gas.[13,14]

Zero-temperature magnetization increases linearly with the field at the edge of the magnetization plateau, due to the finite value of magnetic susceptibility. This kind of a behavior is characteristic to conformally invariant systems. The natural question arises whether some kind of conformally invariant theory can be applied to describe the edge points of magnetization plateaus. For this reason we study temperature dependence of specific heat in multicomponent systems at C-IC phase transition point where modes do not decouple. We find that if total number of particles is fixed then square-root temperature dependence, which holds if one works with fixed chemical potential and also is characteristic to mode-decoupled systems undergoing C-IC transition (for both cases with fixed chemical potential or fixed total number of particles, e.g., attractive Hubbard model at half filling at the onset of magnetization), is modified by linear law, however the prefactor diverges as $\ln^2 T$ for $T\rightarrow 0$. To our knowledge no previous studies on finite temperature thermodynamic behavior at C-IC phase transition point have been reported for multicomponent systems where modes do not decouple.

For concrete calculations we will consider a system of two component attractive fermions and place it in an external magnetic field equal to the value of the spin gap. However our main claim on the disappearance of the square-root temperature dependence of the specific heat (at C-IC phase transition point) will hold true for generic situation, where gapped mode (spin), undergoing nonrelativistic softening at the critical point, couples to linearly dispersing excitations (charge). This statement will apply to all situations where magnetic susceptibility stays finite at the edge points of magnetization plateaus in zero-temperature limit.[8]

To simplify things drastically we will consider the dilute limit of the system of attractively interacting two component fermions. Since the dilute limit falls under strong coupling, the ground state (for $T=0$) is made of bound pairs and the low-temperature thermodynamic properties can be modeled by the mixture of noninteracting pairs and thermally created uncompensated spin-up particles (we choose finite temperature magnetization to be positive for nonzero magnetic field). Spin-down particles will also be created thermally, but since they have spectral gap (which is large in strong coupling) their density will be exponentially suppressed at low temperatures and thus they will be ignored in the following. For integrable Fermi Hubbard model (both on lattice[15] and in continuum) the thermodynamic Bethe ansatz method can be applied,[16] and in particular recently it was shown that in dilute limit this method simplifies considerably.[17] However, for finding specific heat at the critical point when magnetization sets in we need not use integrability so that our reasoning will stay both simple and general.

Phenomenological Hamiltonian describing the low energy properties of the two component attractive fermions in strong coupling at the C-IC critical point reads as

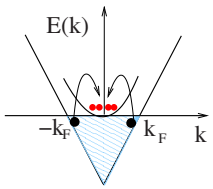

FIG. 1. (Color online) simplified dispersions with purely quadratic and linear behavior adopted in this paper. If total number of particles is conserved creation of each pair of up-spin fermions (smaller bullets) leaves a hole in the Fermi sea of bound pairs (larger bullets).

$$H = \sum (E_p(k) - E_F) a_k^\dagger a_k + \sum E_\uparrow(k) c_k^\dagger c_k, \tag{1}$$

where $a^\dagger(c^\dagger)$ and $a(c)$ are pair (up-spin fermion) creation and annihilation operators. For calculating thermodynamic properties it does not matter whether pairs are modeled by hard-core bosons (which they are) or fermions.[16]

At the edge of the zero magnetization plateau dispersion of up-spin particles is approximated by a purely quadratic expression,

$$E_\uparrow(k) = \sqrt{v_\uparrow^2 k^2 + \Delta^2} - \Delta \simeq v_\uparrow^2 k^2 / 2\Delta. \tag{2}$$

Here Δ is spin gap opened due to strong attraction between spin-up and spin-down fermions, and $v_\uparrow$ is the velocity of gapped excitations. We will see later that in the leading temperature dependence of specific heat Δ and $v_\uparrow$ will not appear. Since low-temperature thermodynamics is determined by low lying modes (states near Fermi wave vector) for the dispersion relation of pairs we can use a simplified strictly linear expression

$$E_p(k) - E_F = v_p(|k| - k_F). \tag{3}$$

Fermi wave vector k_F is related to the linear density of pairs n_p by the usual 1D relation $k_F = n_p \pi$. In the following n_p will stand for the density of pairs strictly at zero temperature: $n_p = n_p(T=0)$. Dispersions $E_\uparrow(k)$ and $E_p(k) - E_F$ considered in our simplified model are plotted on Fig. 1. At zero temperature the ground state is occupied solely by pairs, and density of uncompensated up-spin electrons is zero. Although one might argue that Hamiltonian (1) lacks microscopic derivation, it is expected to exactly reproduce leading low-temperature dependence of the specific heat at C-IC phase transition point in dilute limit, the same way as it yields exact expression for magnetic susceptibility.[8]

The thermodynamic potential of the grand canonical system can be obtained straightforwardly:

$$\frac{\tilde{\Omega}}{L} = -\frac{T}{2\pi} \int dk [\ln(1 + e^{-v_p(|k|-k_F)/T}) + \ln(1 + e^{-v_\uparrow^2 k^2/2\Delta/T})].$$

For specific heat one obtains easily that the leading temperature dependence is linear from pairs (usual conformal contribution[3] with central charge $c=1$ and velocity of pair motion v_p) and square root (which dominates over the linear one in the low-temperature limit), from the up-spin electrons, due to the quadratic low energy dispersion they enjoy. This kind of behavior is also realized for canonical systems at special fillings, e.g., the attractive Fermi Hubbard model at half filling, where spin and charge modes decouple. At half filling charge sector of Hubbard model is described by conformally invariant $SU_1(2)$ Wess-Zumino model,[15] while the spin sector, when magnetic field equals to singlet-triplet spin gap, is characterized by quadratic low energy behavior responsible for the leading, square-root, temperature dependence of specific heat. In the grand canonical systems at finite temperatures, the thermal fluctuations create a finite density of up-spin electrons given by the following expression:

$$\tilde{n}_\uparrow(T) = -\zeta(1/2)\sqrt{2\pi\Delta}(\sqrt{2} - 1)\sqrt{T}/2\pi v_\uparrow, \tag{4}$$

where $\zeta(1/2)$ is the value of the Riemann ζ function at 0.5. The number of pairs also gets modified by temperature fluctuations accordingly

$$\tilde{n}_p(T) = n_p + \frac{T}{\pi v_p}[e^{-v_p k_F/T} + O(e^{-2v_p k_F/T})]. \tag{5}$$

Thus, due to finite ground-state population of pairs, thermal fluctuation of density of pairs is exponentially suppressed, whereas for up-spin electrons, due to Van Hove singularity in their density of states, square-root dependence holds. Already from the above picture it is clear that working at a fixed total number of particles can modify the leading square-root behavior of specific heat at C-IC point, since *thermal occupation of up-spin band will be constrained by the reluctance of depletion of the band of bound pairs*. Since each broken pair produces two up-spin electrons, as depicted on Fig. 1, the constraint that fixes the total number of particles reads as

$$n_\uparrow(T) + 2n_p(T) = 2n_p. \tag{6}$$

To implement the constraint we introduce the temperature dependent chemical potential, which we determine from the equation

$$\int \frac{dk/2\pi}{e^{v_\uparrow^2 k^2/2\Delta - \mu(T)/T} + 1} + \int \frac{dk/\pi}{e^{v_p(|k|-k_F) - 2\mu(T)/T} + 1} = 2n_p. \tag{7}$$

The consistent solution of the above equation requires that $\mu(T)/T \to -\infty$, when $T \to 0$ so that we obtain

$$\mu(T) \simeq -\alpha\sqrt{T} e^{\mu(T)/T}, \tag{8}$$

with positive coefficient $\alpha = \frac{v_p\sqrt{2\Delta\pi}}{8v_\uparrow}$. In the zero-temperature limit we obtain the following solution for the chemical potential:

$$\mu(T) \simeq -T\left(\ln\frac{\alpha}{\sqrt{T}} - \ln\ln\frac{\alpha}{\sqrt{T}} + \frac{\ln\ln\frac{\alpha}{\sqrt{T}}}{\ln\frac{\alpha}{\sqrt{T}}}\right). \tag{9}$$

Now we will use the obtained chemical-potential [Eq. (9)] to calculate the grand canonical potential,

$$\frac{\Omega}{L} = -\frac{T}{2\pi}\int dk\, \ln(1+e^{-v_p(|k|-k_F)-2\mu(T)/T}) - \frac{T}{2\pi}\int dk\, \ln(1+e^{-v_\uparrow^2 k^2/2\Delta-\mu(T)/T}) = -\frac{T^2}{2\pi v_p}\left(\frac{(v_p k_F+2\mu(T))^2}{T^2}+\frac{\pi^2}{3}+\cdots\right) - \frac{T^{3/2}}{2\pi v_\uparrow}\sqrt{2\pi\Delta}e^{\mu(T)/T}+\cdots. \quad (10)$$

Dots stand for subleading terms at low temperatures. Grand canonical potential is related to energy, E, and entropy S, by the following thermodynamic relation:

$$\Omega = E - TS - \mu(T)N_\uparrow(T) - (v_p k_F + 2\mu(T))N_p(T). \quad (11)$$

For the leading temperature dependence of energy we get the following expression:

$$\frac{E}{L} = \frac{(v_p k_F+2\mu(T))^2}{2\pi v_p} + \frac{\pi T^2}{6v_p} - \frac{2T\mu(T)}{\pi v_p} + \cdots \quad (12)$$

For thermally depleted density of pairs we obtain

$$n_p(T) = \frac{v_p k_F + 2\mu(T)}{\pi v_p}, \quad (13)$$

and the density of thermally created up-spin electrons is given by the following expression:

$$n_\uparrow(T) = 2n_p - 2n_p(T). \quad (14)$$

Note, due to constraint of keeping total number of particles fixed, the square-root dependence Eq. (4) is modified in the following way:

$$n_\uparrow(T) \simeq -\frac{2T\ln(T/\Delta)}{\pi v_p}, \quad T/\Delta \ll 1. \quad (15)$$

Using thermodynamic relation Eq. (11) we obtain for the leading temperature dependence of entropy the following expression:

$$s(T) = S(T)/L = \frac{4\mu^2(T)}{T\pi v_p} - \frac{6\mu(T)}{\pi v_p} + \frac{\pi T}{3v_p} + \cdots. \quad (16)$$

Finally substituting chemical potential from Eq. (9) for the leading temperature dependence of specific heat we get,

$$C(T) = T\frac{\partial s(T)}{\partial T} = \frac{T\ln^2(T/\Delta)}{\pi v_p} + \cdots \quad (17)$$

in the limit $T\to 0$. This is our main result: specific heat depends linearly on temperature, albeit with a diverging prefactor. This is kind of an intermediate between the square-root and linear dependences. Recent studies reported similar linear behavior of the specific heat with diverging prefactor for critical two-subband quantum wire[18] when the second band started to fill. However in our case we cannot interpret this as a signal of restoration of Lorentz or conformal invariance.

At this point we would like to comment on the differences between working at fixed chemical potential and fixed total number of particles for attractive Hubbard model away of half filling at the onset of magnetization (C-IC transition point). For the case of fixed total number of particles magnetic susceptibility stays finite and, as we showed here, specific heat depends linearly on temperature (with diverging prefactor). However, for the case of fixed chemical-potential magnetic susceptibility diverges and specific heat shows square-root temperature dependence characteristic to the mode-decoupled theory. One may suspect that if one works with the fixed chemical potential one can use mode-decoupled theory, result of linear bosonization, to describe the C-IC phase transition point. For calculating static magnetic susceptibility and specific heat this statement is true. However, using mode-decoupled theory across the C-IC transition is misleading, because away of half filling and for nonzero magnetization spin and charge modes couple independent of whether one fixes chemical potential or total number of particles. In particular spin and charge stay coupled (spin-charge mixing angle stays *finite*) even in the limit of vanishing magnetization (C-IC point) for both cases with fixed total number of particles or fixed chemical potential. Within spin-charge decoupled theory one cannot calculate correctly e.g., asymptotics of static single-particle correlation functions[8] in the limit of vanishing magnetization (C-IC point). Fixing total number of particles further enhances mode coupling and leaves its traces on magnetic susceptibility as well as specific heat (topic of this manuscript).

The presented analysis is directly applicable also to the phase transition between partially and fully polarized states, when the down-spin fermions band gets empty (at $h=h_{sat}$, where h_{sat} is magnetic field needed to completely polarize the system). In this case one simply has to replace constraint Eq. (6) by: $N_\uparrow(T)+N_\downarrow(T)=\text{const}$, thus specific heat at $h=h_{sat}$ will have the similar temperature dependence as in Eq. (17).

For completeness we write out the leading low-temperature dependence of specific heat in two component attractively interacting fermions in an external magnetic field for all values of the field away from half filling:

$$C(T) \sim \begin{cases} T/v_c & h<2\Delta \quad or \quad h>h_{sat} \\ T\ln^2(T/\Delta) & h=2\Delta \quad or \quad h=h_{sat} \\ T(v_c+v_s)/v_c v_s & 2\Delta<h<h_{sat} \end{cases} \quad (18)$$

where v_c and v_s denote charge and spin velocities.[19] Note that $v_s(m)\sim m$ when $m\to 0$, and $v_s(m)\sim n-2m$ when $m\to n/2$, where m is the magnetization density and n the total density of particles. In the region $\Delta<h<h_{sat}$ spin and charge modes are coupled, and they do not get separated even in the limits $h\to 2\Delta_+$ and $h\to h_{sat\_}$.[8,10] This nonseparation of spin and charge modes explains disappearance of the square-root temperature dependence of specific heat at critical points $h=2\Delta$ and $h=h_{sat}$.[20] Exactly at half filling, where spin-charge separation holds, $C(T)\sim\sqrt{T}$ for $h=2\Delta$ *or* $h=h_{sat}$.

To summarize on simple example of two component attractive fermions placed in an external magnetic field equal to the spin gap we studied the thermodynamic properties of C-IC phase transition point in multicomponent systems. Our

findings are generic, namely, we expect that for multicomponent systems square-root temperature dependence, which holds for the fixed chemical potential, will be changed by linear dependence (with diverging prefactor) if instead total number of particles is fixed. In particular, this statement equally applies to the edge points of magnetization plateaus of 1D bosonic systems, i.e., spin 1 bosons interacting antiferromagnetically.[21] It also holds for the edge points of mid magnetization plateaus of multicomponent systems, i.e., in doped dimerized Hubbard chains.[22] However, currently we cannot determine if the $\ln^2 T$ prefactor in the expression of specific heat Eq. (17) is universal. To answer this question, it will be useful to study, e.g., the same system of two component attractive fermions in the weak-coupling limit. One can make use of integrability of Fermi Hubbard model there. Especially intriguing will be to look close to half filling to follow how does the square-root dependence of specific heat cross over to linear behavior with diverging prefactor as a function of doping.

Our findings may be relevant for real quasi one-dimensional spin gapped materials, where one can study experimentally specific heat as a function of applied magnetic field and doping. Square-root dependence, which is expected at half filling, should be modified by linear with logarithmic prefactor, away from half filling, at critical magnetic field strength equal to the spin gap. One can as well measure the leading temperature dependence of specific heat at saturation magnetization in a generic 1D electron system away of half filling and compare the results to Eq. (17).

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