Emergent BCS regime of the two-dimensional fermionic Hubbard model: ground-state phase diagram

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(Dated: December 3, 2014)

A significant part of the phase diagram of the two-dimensional fermionic Hubbard model for moderate interactions and filling factors ($U < 4, n < 0.7$) is governed by effective Fermi liquid physics with weak BCS-type instabilities. We access this regime in a controlled way by a combination of the bold-line diagrammatic Monte Carlo method with an additional ladder-diagram summation trick and semi-analytic treatment of the weak instability in the Cooper channel. We obtain the corresponding ground-state phase diagram in the $(n, U)$ plane describing the competition between the $p$– and $d$–wave superfluid states. We also claim the values of the dimensionless BCS coupling constants controlling the superfluid $T_c$ at the phase boundaries, which prove to be very small up to $U = 4, n = 0.6$.

PACS numbers: 71.10.Fd, 02.70.Ss, 74.20.Fg

The fermionic Hubbard model [1, 2],

$$H = - \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i \sigma} \hat{c}_{j \sigma} + U \sum_i (\hat{n}_{i \uparrow} \hat{n}_{i \downarrow}) - \mu \sum_i \hat{n}_{i \sigma}$$ (1)

($\hat{c}_{i \sigma}$ creates a fermion with spin projection $\sigma = \uparrow, \downarrow$ on site $i; \hat{n}_{i \sigma} = \hat{c}_{i \sigma} \hat{c}^\dagger_{i \sigma}; \langle \ldots \rangle$ restricts summation to neighboring lattice sites; $U$ and $\mu$ are, respectively, the on-site repulsion and the chemical potential in units of the hopping amplitude) is one of “standard models” of condensed matter physics. The metal-insulator transition at half filling $\langle \hat{n}_{i \uparrow} + \hat{n}_{i \downarrow} \rangle = 1$, along with the antiferromagnetism promoted by it, was the main context of the original formulation of the model and subsequent two decades of its intensive theoretical studies. The advent of high-temperature superconductivity dramatically enhanced (and changed the focus of) the interest to Eq. (1). The model became paradigmatic for high-temperature superconductors [2], at least as a minimalistic Hamiltonian featuring (not far from half filling) the relevant $d_{x^2-y^2}$ Cooper instability, solely due to repulsive interaction between fermions. The third wave of interest to the model has been generated recently by its direct realization with ultracold atoms in optical lattices [3–5].

Decades of theoretical studies of Cooper instability in the model (1) have seen a number of remarkable successes. Controlled results were obtained in certain limiting cases: perturbatively small interaction or/and low filling [6–13], half-filling [14–16], system with restricted transverse size [17]. An impressive numeric progress has been achieved with methods based on the dynamical mean-field approximation and its extensions [18–25].

For the 2D case we are interested in here, it has been found that, at a fixed filling factor and $U \rightarrow 0$ (whithin the second-order perturbation theory in $U$) the ground state of the system is either $d_{x^2-y^2}$-wave (smaller fillings) or $d_{x^2+y^2}$-wave (higher fillings) BCS superfluid, with a pocket of a $p$-wave phase near quarter filling [13]. It has been also shown that, in the low-density limit at any fixed $U$, the ground state of the system is the $p$-wave BCS superfluid [9]. The dynamic-cluster-approximation (DCA) simulations convincingly revealed (see [25] and references therein) a region of high-temperature $d_{x^2-y^2}$-wave pairing developing at $U \gtrsim 6$. Nevertheless, the rich ground-state phase diagram guaranteed by the above-mentioned findings remains elusive: So far, none of the phase boundaries is known.

In this Letter, we report accurate controllable results (Fig. 1) for a significant part of the ground-state phase diagram of Hamiltonian (1) on the square lattice. We study the region of moderate bare coupling $U \leq 4$ and filling $n < 0.7$ where the system demonstrates Landau Fermi-liquid behavior at temperatures $T_c < T < E_F$; i.e., between the Fermi energy $E_F$ and the temperature of the superfluid phase transition $T_c \ll E_F$. Our method is a combination of bold diagrammatic Monte Carlo (BDMC)—a numeric technique for stochastic summation of skeleton diagrammatic series—and semi-analytic BCS treatment of weak instability in the Cooper channel. The overall theoretical framework is based on the asymptotically exact (in the $T_c/E_F \rightarrow 0$ limit) diagrammatic theory of Cooper instability in the Fermi liquid [26, 27]. We employ the skeleton expansion in terms of the fully dressed interaction vertex in the particle-particle channel, as used in Ref. [28] for the resonant Fermi gas, with an additional trick leading to near cancellation of large-
amplitude contributions in the interaction vertex, which crucially improves numerical efficiency of BDMC. In the considered regime of moderate interactions and fillings the skeleton series is known to produce exact results [29], which we also explicitly check by benchmarking the obtained Green’s function against corresponding bare-series calculations.

The emergent low-energy property. By definition, $T$ is the sum of all four- pole diagrams that can not be split into disconnected pieces by cutting two particle lines. From the Bethe-Salpiter relation, Fig. 2, for the full four-pole vertex $\Gamma^{(4)}$, we see that the smallness of the attractive part of $T$ is a natural condition preventing $\Gamma^{(4)}$ from dramatic growth at $T \ll E_F$. Indeed, in the FL state, the leading contribution to the integral over $k_3$ in the second term in the r.h.s. of Fig. 2 comes from \( \int d^d k_3 \sum \xi_3 G(p_3) G(-p_3) \) in close vicinity to the Fermi surface, where only the finite temperature (i.e., discreteness of Matsubara frequency $\xi_3$) prevents it from logarithmic divergence. With the logarithmic accuracy at $T \ll E_F$, we have

$$\Gamma^{(4)}_{k_{1,2}} \approx T_{k_{1,2}} + \ln \frac{E_F}{T} \int T_{k_{1,3}} Q_{k_3} \Gamma^{(4)}_{k_3,2} d^{-1} k_3, \quad (3)$$

where $\Gamma^{(4)}_{k_{1,2}}$ and $T_{k_{1,2}}$ are $\Gamma^{(4)}$ and $T$ at vanishing frequencies projected to the Fermi surface:

$$\Gamma^{(4)}_{k_{1,2}} \equiv \Gamma^{(4)}(k_1 \to k_1, \xi_1, \xi_1 \to 0; k_2 \to k_2, \xi_2 \to 0),$$

and $Q_k$ is the product of $z^2(\hat{k})$ and the single-component density of states at the $k$-point on the Fermi surface. The systematic error in (3) comes from the ultra-violet cutoff scale, $E_F \to c E_F$, where $c$ is some order-unity factor [30].

Switching to the matrix notations, $\Gamma^{(4)}_{k_{1,2}} \to \hat{\Gamma}^{(4)}$, $T_{k_{1,2}} \to \hat{T}$, $T_{k_{1,2}} Q_{k_2} \to \hat{M}$, we find

$$\hat{\Gamma}^{(4)} \approx \left[ 1 - \ln(E_F/T)^\hat{M} \right]^{-1} T, \quad (4)$$

implying that $\Gamma^{(4)}$—and thus the static response function in the Cooper channel—diverges at the critical temperature

$$T_c = c E_F e^{-1/\lambda}, \quad (5)$$

where $\lambda$ is the largest positive eigenvalue of $\hat{M}$. The consistency of the emergent BCS picture based on weak Cooper instability requires $\lambda \ll 1$. Solving the problem with logarithmic accuracy amounts then to finding the eigenvalues/eigenvectors of a real symmetric matrix

$$T_{k_{1,2}} \psi_{k'} = \lambda \psi_{k'}, \quad T_{k_{1,2}} = Q_k^2 T_{k_{1,2}} Q_k^2, \quad (6)$$
where the eigenvector $\psi_k$ is the wave function of the Cooper pair in the momentum representation.

In two dimensions, it is convenient to parameterize $\hat{k}$ with the polar angle $\theta$, and to write the eigenvalue/eigenvector problem explicitly as

$$
\int_0^{2\pi} T_{0,\theta'} \psi_{\theta'} \frac{d\theta'}{2\pi} = \lambda \psi_{\theta}, \quad T_{0,\theta'} = Q_{\theta}^{1/2} T_{\theta,\theta'} Q_{\theta}^{1/2}, \quad Q_{\theta} = k_F (\theta) z^2(\theta)/[2\pi \hat{v} \cdot \nu_F(\theta)].
$$

By the $D_{4h}$ symmetry of the square lattice, $T_{0,\theta'}$ splits into five independent blocks corresponding to $s, p, d_{x^2-y^2}, d_{xy}$, and $g$ eigenvector sectors. The $p$-sector is doubly degenerate and can be further split into two independent sectors, $p_x$ and $p_y$, related to each other by $\pm \pi/2$ rotations. For each of the six (sub)sectors, the symmetry propagator matrix $\Sigma$ is symmetric/anti-symmetric with respect to reflections $\pi/2, \pi$. These propagators change their sign when rotated by $\pi/2, \pi$, respectively; they are related to $D_{x^2-y^2}$, $d_{xy}$, and $g$ eigenvector sectors.

To parameterize $\tau$, we choose the time parameter $\tau$ to parameterize the spin and momentum indexes are suppressed for clarity): $\Pi_{13} \equiv \Pi_{(\tau_1 - \tau_2)}, \Pi_{13} \equiv \Pi_{(\tau_1 - \tau_2)}$, etc. Integration over internal times is assumed. Pair self-energy $\Pi_{13}$ is the sum of all vertex-irreducible diagrams starting, at time $\tau_3$, and ending, at time $\tau_1$, with spin-up and spin-down outgoing (incoming) single particle propagators. A diagram is vertex-irreducible if it remains connected after cutting across any single interaction vertex. The lowest-order diagram contributing to $\Pi_{13}$ is a sum of all ladder diagrams, $\bar{\Pi}$, is a continuous function of $\tau$ and will be referred to as $\bar{\Gamma}$. Hence, $\bar{\Gamma}(\tau, \mathbf{k}) = -U \delta(\tau) + \bar{\Gamma}(\tau, \mathbf{k})$.

The solution is to transform the functional form of the bare vertex to make it (i) compatible with that of $\bar{\Gamma}(\tau)$ at the level of integrands, and (ii) such that the diagram value remains intact under integration. To this end we introduce a function $\Gamma_U$ with the following properties

$$
\int_0^\beta \bar{\Gamma}_U(\tau) d\tau = -U.
$$

The particular design of $\bar{\Gamma}_U(\tau)$ still has a freedom. We choose $\bar{\Gamma}_U(\tau) = -\bar{\Gamma}(\tau) + c_0$, where $c_0$ is a constant of order unity or much smaller. This guarantees that, for $|U| > 1$, the condition of compensation, $\bar{\Gamma}_U(\tau) \approx -\bar{\Gamma}(\tau)$, is satisfied.

We then formally—and identically—represent each coupling constant $U$ in the diagrammatic series as an integral over the auxiliary variable $\tau$, thereby replacing the bare vertex with the $I_{13}$ function as pictured graphically in Fig. 4. Since $\bar{\Gamma}_U$ has the same functional structure as $\bar{\Gamma}$, we sum up the two elementary diagrammatic contributions into one, $A_{1234}$, as shown in Fig. 4. Thereby, we arrive at the diagrammatic formulation identical to that for resonant fermions [28], but with a modified rule for reading the diagram value: The single diagram element $A_{1234}$, now contributes a factor (momenta are suppressed

![FIG. 3](image-url)
for clarity)

\[ A_{1234} = \tilde{\Gamma}_U(\tau_1 - \tau_2) G_1(\tau_1 - \tau_3) G_4(\tau_1 - \tau_4) + \tilde{\Gamma}(\tau_1 - \tau_2) G_1(\tau_2 - \tau_3) G_4(\tau_2 - \tau_4), \]  

(11)

to the integrand of the diagram it enters. It contains two terms that become close in absolute values and opposite in sign when \(|\tau_1 - \tau_2| \lesssim 1/|U|\). This is how the large-

\(|U|\) compensation is achieved at the level of integrands. Apart from this specific way of evaluating the diagram value, the rest of the BDMC protocol is essentially identical to that for resonant fermions \([28]\).

![Diagram](image)

FIG. 4. The compensation trick. The diagram element \(A_{1234}\) is understood as the sum of two terms with different assignment of the end point for incoming fermionic propagators.

**Numeric procedure and results.** We employ the following protocol of data collection and analysis based on FL physics. Start with the BDMC simulation of the single-particle Green’s function at some temperature \(T \ll E_F\), low enough for observing sharp Fermi-step in the momentum distribution, and extract all quasiparticle FL parameters. Use this Green’s function to perform the BDMC simulation of the irreducible vertex \(\hat{T}_{k_1,k_2}\). Extract eigenvalues/eigenfunctions for all Cooper channels by solving the eigenvalue problem (7), and locate phase boundaries shown in Fig. 1 from points where \(\lambda\) for the two competing ground-state phases coincide. We have verified that spin and density correlations (particle-hole channels) do not exhibit any flow towards instability at low temperature for \((n = 0.6, \ U = 4)\).

With simulations done at different temperatures we ensure that final results are temperature independent and employ special procedure for eliminating the slowly vanishing (and quite substantial in the \(n \rightarrow 0\) limit) finite-temperature correction to \(T_{k_1,k_2}\). Having observed that the leading term in this correction is coming from the second-order diagram, we calculate the corresponding contribution (semi-analytically) directly at \(T = 0\). All simulations are performed with explicit truncation of diagrammatic series at some maximum order \(N\). Extrapolation with respect to \(N\) brings the corresponding systematic error under control, see Fig. 5.

The small-\(|U|\) limit of the \(p-d_{xy}\) phase boundary is consistent with the linear law, \(n_c = 0.139U\), implied (qualitatively [31]) by analytic results derived in Ref. [7, 8] (the term \(\propto U^2\) in the \(n \rightarrow 0\) limit) and Ref. [9] (terms \(\propto U^3\) in the \(n \rightarrow 0\) limit).

![Graph](image)

FIG. 5. Critical density and dimensionless coupling constant as functions of maximum diagram order, \(N\), at various points on the phase boundaries (parameterized by \(U\)) with extrapolation to the \(N \rightarrow \infty\) limit.

For densities \(n\) between 0.5 and 0.6 the \(p\)-wave state is rather peculiar (we denote it \(p'\) to emphasize the difference with the conventional \(p\)-wave); this point was not addressed in [13]. In a typical case of \(p\)-wave instability, the real eigenvector \(\psi_0\) has two nodes, in direct analogy with the case of continuous rotation group (justifying the usage of the same symbol \(p\)). The eigenvector \(\psi_0\) of the \(p'\) phase features six nodes. In terms of the expansion (9), the nodal structure of the \(p\)-wave state \(\psi_0\) is dominated by the first term, while the nodal structure of the \(p'\)-eigenvector comes from the second term. The dominant role of the second term in (9) renders the \(p'\) phase akin to the \(f\) phase in a continuous space.

We are grateful to A. Chubukov, M. Baranov, E. Gull, J. Gukelberger, and M. Troyer for valuable discussions. We also thank X.-W. Liu for his participation in the study of convergence of skeleton diagrammatic series. This work was supported by the Simons Collaboration on the Many Electron Problem, National Science Foundation under the grant PHY-1314735, the MURI Program “New Quantum Phases of Matter” from AFOSR, and the Swiss National Science Foundation, NSFC Grant No. 11275185, CAS, and NKBRSFC Grant No. 2011CB921300. We acknowledge the hospitality of
Kavli Institute for Theoretical Physics China at Beijing.

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[30] Methods for systematic (in parameter $g \ll 1$) evaluation of $\epsilon$ are well-known [27] and will be discussed elsewhere.
[31] Actually, the analytic results in Refs. [8, 9] would imply $n_{\epsilon} = 0.060U^2$, instead of $n_{\epsilon} = 0.138U^2$. Our eigenvalues in all Cooper channels are a quarter of those for the $U^2$ term in Ref. [8] and half of those for the $U^3$ term in Ref. [9]. When directly comparing our results for the irreducible vertex $T$ to the analytical formula in Ref. [7] (for the $U^2$ term), we find good agreement apart from a factor 1/2 that is missing in Ref. [7].