Well-Defined Quasiparticles in Interacting Metallic Grains

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We analyze spectral functions of mesoscopic systems with large dimensionless conductance, which can be described by a universal Hamiltonian. We show that an important class of spectral functions are dominated by one single state only, which implies the existence of well-defined (i.e., infinite-lifetime) quasiparticles. Furthermore, the dominance of a single state enables us to calculate zero-temperature spectral functions with high accuracy using the density-matrix renormalization group. We illustrate the use of this method by calculating the tunneling density of states of metallic grains, of which we discuss the crossover from the few-electron to the bulk regime.

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The pairing Hamiltonian of Bardeen, Cooper, and Schrieffer (BCS) is established as the paradigmatic framework for describing superconductivity [1,2]. The BCS *solution* is, however, an approximate one, valid (and exceedingly successful) only as long as the mean level spacing d is much smaller than the superconducting band gap Δ_{BCS} [3,4]. One of the main features of the BCS solution is the description of the excitation spectrum by well-defined (i.e., infinite-lifetime) Bogoliubov quasiparticles, responsible for many of the features of the superconducting state.

In this Letter, we address the question whether this quasiparticle picture prevails in the entire regime of parameters—including the case where the samples are so small or so weakly interacting that $d \geq \Delta_{\mathrm{BCS}}$ and the BCS solution is inapplicable—by analyzing spectral functions. For example, the spectral function corresponding to the (noninteracting) particle creation operator $c^\dagger_{k\sigma}$ is given, within the BCS solution, by a sharp line in k-ω space; this reflects the infinite lifetime of the quasiparticles. For an interacting system, this is a very peculiar property, since the interactions usually shift a significant portion of the spectral weight to a background of excitations, responsible for the finite lifetime of the quasiparticles. Here we show that the unusual property of finding well-defined quasiparticles persists to a very good approximation over the entire parameter range of the pairing Hamiltonian and is not merely a property of the mean field approximation in the BCS regime. We also give a condition for more general spectral functions to show analogous behavior.

Of central importance is that this result is relevant not only in the context of mesoscopic superconductivity, but more generally for disordered systems with large dimensionless conductance g (defined as the ratio between the Thouless energy and the mean level spacing d). This is because to lowest order in g^{-1} the electron-electron interactions can be described by a remarkably simple universal Hamiltonian [5,6], which has, besides the kinetic energy term $H^0 = \sum_{i\sigma} \epsilon_i c^\dagger_{i\sigma} c_{i\sigma}$, only three couplings:

$$H^c = E_c \hat{n}^2, \qquad H^s = J_s \hat{\vec{S}}^2, \qquad H^p = -\lambda d \sum_{i,j \in \mathcal{N}} c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow}. \tag{1}$$

Here E_c, J_s, and $-\lambda d$ are coupling constants. The sum includes all energy levels around the Fermi energy ϵ_F up to some cutoff ω_{co} at the Thouless energy, denoted by the set $\mathcal{N}$. It turns out that H^c and H^s do not affect our result because they commute with $H^0 + H^p$ and thus leave the eigenstates invariant. Therefore, it suffices to take H^p—the BCS pairing Hamiltonian—as the only interaction term. Therefore, for our purposes the difference between the BCS model and the universal Hamiltonian is only in the cutoff ω_{co}, being at the Debye energy for the former and at the Thouless energy for the latter. In either case, we define $\Delta_{\mathrm{BCS}} = \omega_{\mathrm{co}} e^{-1/\lambda}$.

The fact that the zero-temperature spectral function $\mathcal{A}_{\hat{O}}(\omega)$ of an operator $\hat{O}$ is sharply peaked translates to a strong condition on the matrix elements of the Lehmann representation, which is given by

$$\mathcal{A}_{\hat{O}}(\omega) = \sum_{|I\rangle} \langle \mathrm{gs}|\hat{O}^\dagger|I\rangle\langle I|\hat{O}|\mathrm{gs}\rangle \delta(\omega - E_I). \tag{2}$$

Here $|\mathrm{gs}\rangle$ denotes the ground state, $|I\rangle$ the excited states with energies E_I. For only one sharp peak to be present in the spectral function, the sum in Eq. (2) must be dominated by one single eigenstate, say, $|I\rangle^0$, whereas all other states $|I\rangle \neq |I\rangle^0$ do not contribute. Obviously, it will depend on the operator $\hat{O}$ whether this is the case, and, if so, which is the state $|I\rangle^0$. We show that it suffices that $\hat{O}$ satisfies a rather unrestrictive condition, given after Eq. (4) below and fulfilled for many physically relevant quantities. Furthermore, we show that under this condition the state $|I\rangle^0$ is from a very limited subset of all possible excitations, which we characterize below as the

"No-Gaudino states." Our finding of well-defined quasiparticles therefore implies that only these No-Gaudino states are relevant for many physical properties of systems that satisfy the conditions of the universal Hamiltonian.

Calculating the spectral function nonperturbatively [e.g., by the route of Eq. (2)] is usually a formidable task, equivalent to diagonalizing the Hamiltonian. Although an exact solution [3,7] exists for the Hamiltonian H^p, its complexity in practice does not allow us to calculate spectral functions from it. Instead, we use the density-matrix renormalization group (DMRG) method [8] for this purpose, a numerical variational approach that has already been proven very useful for analyzing this model [9–11]. For suitable operators $\hat{O}$, we are able to obtain the spectral function from the DMRG without the usual complications [12,13], because the state $|I\rangle^0$—the only one that contributes significantly to the spectral function—can be constructed explicitly. The existence of a sum rule allows us to quantify the contribution of other states $|I\rangle \neq |I\rangle^0$, which we find to be negligibly small. Finally, we illustrate the use of our method of calculating spectral functions by evaluating the tunneling density of states, of which we discuss the crossover from the few-electron to the bulk regime.

Excitation spectrum and No-Gaudino states.—Let us begin by describing the excitations of the Hamiltonian H^p in Eq. (1). H^p has the well-known property that singly occupied energy levels do not participate in pair scattering; hence their labels (and spins) are good quantum numbers. Therefore, the singly occupied levels decouple from the interaction with the other levels, in the sense that all eigenstates with a set of singly occupied levels $\mathcal{B} = \{j_1, \ldots, j_l\}$ are (as far as the remaining levels are concerned) identical to those of a system with $\mathcal{N}$ in Eq. (1) replaced by $\mathcal{N} \setminus \mathcal{B}$ [3].

A given state can thus contain two kinds of excitations: pair-breaking excitations that go hand in hand with a change of the quantum numbers $\mathcal{B}$ and other many-body excitations that do not. The latter were studied in [14] and dubbed "Gaudinos." In this spirit, we define the No-Gaudino state as the lowest-energy state within a certain sector of the Hilbert space characterized by the quantum numbers $\mathcal{B}$, i.e., the state that is mapped onto the ground state in the presence of the levels $\mathcal{N} \setminus \mathcal{B}$. For example, the No-Gaudino state with no singly occupied levels, $\mathcal{B} = \emptyset$, is trivially given by the ground state. In the BCS limit, the No-Gaudino state with singly occupied levels $\mathcal{B} = \{j_1, \ldots, j_l\}$ (with spins $\sigma_1, \ldots, \sigma_l$) is given by

$$|j_1^{\sigma_1} \cdots j_l^{\sigma_l}\rangle^0 \approx \gamma^\dagger_{j_1\sigma_1} \cdots \gamma^\dagger_{j_l\sigma_l} |\mathrm{gs}\rangle_{\mathrm{BCS}}, \tag{3}$$

where $|\mathrm{gs}\rangle_{\mathrm{BCS}}$ is the BCS ground state and γ are the Bogoliubov quasiparticle operators from BCS theory [2]. As is shown below, these states are easily obtained within the DMRG algorithm.

Let us now specify under which condition the spectral function, Eq. (2), is dominated by such a No-Gaudino state. Any operator can be written as a linear superposition of operators:

$$\hat{O} = c_{i_1\sigma_1} \cdots c_{i_k\sigma_k} c^\dagger_{j_1\sigma'_1} \cdots c^\dagger_{j_l\sigma'_l}. \tag{4}$$

Creating linear superpositions poses no difficulties; therefore it is sufficient to consider operators of this form. *The central condition we impose on $\hat{O}$ is that all indices $i_1, \ldots, j_l$ be mutually different.* $\hat{O}$ then takes a state with no singly occupied levels, $\mathcal{B} = \{\}$, to the sector of the Hilbert space characterized by $\mathcal{B} = \{i_1, \ldots, j_l\}$. We show below that under the above condition $\hat{O}$ moreover has the crucial property that, when acting on the ground state, it creates to an excellent approximation just the No-Gaudino state in this sector. Therefore, the state $\hat{O}|\mathrm{gs}\rangle$ contributing to the spectral function, Eq. (2), is seen to be not only a well-defined eigenstate of the system, but moreover a No-Gaudino state. This is our central result. It is ultimately based on the large number of good quantum numbers in the universal Hamiltonian model: they subdivide the Hilbert space into "narrow" sectors, each of which is well represented by the respective No-Gaudino state. Note that the condition stated after Eq. (4) excludes operators such as $\hat{O} = c^\dagger_{i\sigma} c_{i\sigma}$. Such operators do have a substantial amplitude of creating a pair excitation, and therefore a "Gaudino state," as can be easily verified in the BCS limit.

In the BCS limit $d \ll \Delta_{\mathrm{BCS}}$ (i.e., at $\lambda \gg 1/\ln N$, where N is the number of energy levels between the Fermi energy and ω_{co}), our result follows from the identity

$$\hat{O}|\mathrm{gs}\rangle \approx v_{i_1} \cdots v_{i_k} u_{j_1} \cdots u_{j_l} |i_1^{-\sigma_1} \cdots j_l^{\sigma'_l}\rangle^0, \tag{5}$$

where the state $|i_1^{-\sigma_1} \cdots j_l^{\sigma'_l}\rangle^0$ is the BCS limit of a No-Gaudino state of the form of Eq. (3). Here u and v are the coherence factors from BCS theory [2].

In the opposite limit $\Delta_{\mathrm{BCS}} \ll d$ ($\lambda \ll 1/\ln N$), where perturbation theory in λ is valid[4], the same conclusion is obtained: to first order (i.e., up to errors of order λ^2), $\hat{O}|\mathrm{gs}\rangle$ again creates precisely the No-Gaudino state [15].

There is no such simple analytic argument that the Gaudino admixture to $\hat{O}|\mathrm{gs}\rangle$ in Eq. (5) will be negligible also in the intermediate regime. However, this assertion can be checked numerically by a sum rule, which follows from Eq. (2):

$$\int \mathcal{A}(\omega) d\omega = \sum_{|I\rangle} \langle \mathrm{gs}|\hat{O}^\dagger|I\rangle\langle I|\hat{O}|\mathrm{gs}\rangle = \langle \mathrm{gs}|\hat{O}^\dagger \hat{O}|\mathrm{gs}\rangle. \tag{6}$$

The right-hand side (r.h.s.) is a simple ground state expectation value and is therefore easily evaluated using the DMRG. We define the lost spectral weight $w_L \equiv \langle \mathrm{gs}|\hat{O}^\dagger \hat{O}|\mathrm{gs}\rangle - |\langle \mathrm{gs}|\hat{O}^\dagger|I\rangle^0|^2$ as the part of Eq. (6) that is not carried by the No-Gaudino state $|I\rangle^0$ but instead lost

to other background states. As is shown in Fig. 1, this lost weight turns out to be negligibly small.

DMRG algorithm.—We now give a brief description of the DMRG algorithm as applied to the universal Hamiltonian; more details are available elsewhere [10,11]. Energy levels are added one by one to the system until it obtains its final size. For simplicity, we assume the energy levels to be equally spaced, although none of our methods require this assumption. After adding a level, only a limited number m of basis vectors are kept, such that the size of the Hilbert space remains numerically manageable. These basis vectors are selected in order to represent a number of so-called target states accurately; this is achieved by the DMRG projection described in [8]. By varying m between 60 and 140, we estimate the relative error in the spectral function from the DMRG projection to be of the order of $\sim 10^{-5}$ (for $m = 60$). This accuracy can be improved by increasing m.

In order to calculate the spectral function corresponding to the operator $\hat{O}$ in Eq. (4), we use as target states the ground state and a state representing the No-Gaudino state $|i_1^{-\sigma_1} \cdots j_l^{\sigma'_l}\rangle^0$, with levels $i_1, \ldots, j_l$ singly occupied, in the BCS limit given by Eq. (3). In fact, rather than using the No-Gaudino state itself, we target the state

$$|i_1 \cdots j_l\rangle^0 \equiv \hat{O}^\dagger |i_1^{-\sigma_1} \cdots j_l^{\sigma'_l}\rangle^0, \tag{7}$$

with $\hat{O}$ given by Eq. (4). In Eq. (7), the levels $i_1, \ldots, j_l$, again, do not participate in pair scattering, but levels $i_1, \ldots, i_k$ are now doubly occupied, and levels $j_1, \ldots, j_l$ are empty. The main advantage of this choice is that no singly occupied levels occur at any point in the algorithm; hence only doubly occupied or empty levels have to be considered. Furthermore, it allows the matrix element occurring in the spectral function (2) to be expressed as a simple scalar product:

$$|^0\langle i_1^{-\sigma_1} \cdots j_l^{\sigma'_l}|\hat{O}|\mathrm{gs}\rangle|^2 = |^0\langle i_1 \cdots j_l|\mathrm{gs}\rangle|^2. \tag{8}$$

The sum rule, i.e., the r.h.s. of Eq. (6), is evaluated in a separate run with $|\mathrm{gs}\rangle$ and $\hat{O}^\dagger|\mathrm{gs}\rangle$ as the target states.

Dominance of a single No-Gaudino state.— The fact that the spectral function is dominated by one single No-Gaudino state is displayed in Fig. 1. Here, the expectation value $\langle \mathrm{gs}|c_{i\sigma}c_{i\sigma}^\dagger|\mathrm{gs}\rangle$, which occurs in the sum rule, Eq. (6), with $\hat{O} = c_i^\dagger$, is plotted (for $i = 10$, i.e., ten levels above E_{Fermi}) against the coupling λ. It is practically indistinguishable from the contribution $|^0\langle I|c_{i\sigma}^\dagger|\mathrm{gs}\rangle|^2$ from the No-Gaudino state only.

The lost weight w_L, shown in the inset of Fig. 1, is seen to be less than 0.2% of the total spectral weight throughout the entire parameter regime. The data are shown for $i = 10$ (i.e., the tenth level above the Fermi surface); the plots for other values of i, not shown, look similar. The maximum lost weight somewhat increases as the level i approaches E_{Fermi}, but always remains below 1% of the total weight. The lost weight is seen to be vanishingly small for small λ, as expected in the perturbative regime $\lambda \ll 1/\ln N$. Interestingly, the lost weight also decreases for *large* λ. This is very untypical for interacting systems, and the underlying reason is that the dominance of the No-Gaudino state is protected also in the BCS regime as shown in Eq. (5), which is valid for $\lambda \gg 1/\ln N$. Consequently, the lost weight shown in the inset of Fig. 1 displays a maximum in the intermediate regime around $\lambda \sim 1/\ln N$, indicated by the dotted line, in which neither bulk BCS theory nor perturbation theory in λ are reliable. This peak is a universal feature for all values of i (not shown).

Not shown: We confirmed numerically that the coupling $\lambda_{\max}(N)$, at which the lost weight reaches its maximum, always scales linearly with $1/\ln N$, as expected. The maximum value $w_L[\lambda_{\max}(N), N]$ turns out to be a monotonically decreasing function of N.

Application to tunneling density of states.—The dominance of the No-Gaudino state in the spectral function is not only remarkable by itself, but also has high practical value: it allows us to calculate the spectral function with high precision using the DMRG in what we call the "No-Gaudino approximation," in which only the No-Gaudino state is kept in Eq. (2). From the spectral function, in turn, many important physical quantities can be obtained. The lost weight w_L, defined after Eq. (6), controls the quality of this approximation: when w_L vanishes, the No-Gaudino approximation is exact.

As an application, we calculate the tunneling density of states $\nu(\omega) = \sum_{i\sigma} \mathcal{A}_{c_{i\sigma}^\dagger}(\omega)$ (for $\omega > 0$). Figure 2 illus-

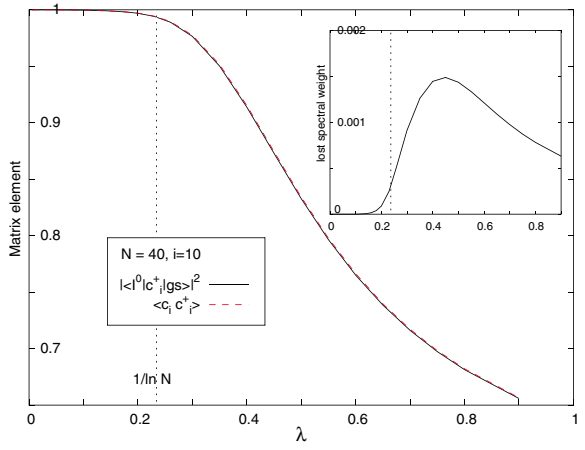

FIG. 1 (color online). The matrix element $\langle c_{i\sigma}c_{i\sigma}^\dagger\rangle$ from Eq. (6) with $\hat{O} = c_{i\sigma}^\dagger$ (dashed line) and the contribution from the No-Gaudino state (solid line) as a function of λ. Here $i = 10$, i.e., the tenth out of a total of $N = 40$ energy levels above E_{Fermi}. The lost weight w_L, i.e., the difference between both, is plotted in the inset. It shows a maximum in the intermediate regime around $\lambda \sim 1/\ln N$ (indicated by dotted line), but even there, w_L is less than 0.2% of the total spectral weight.

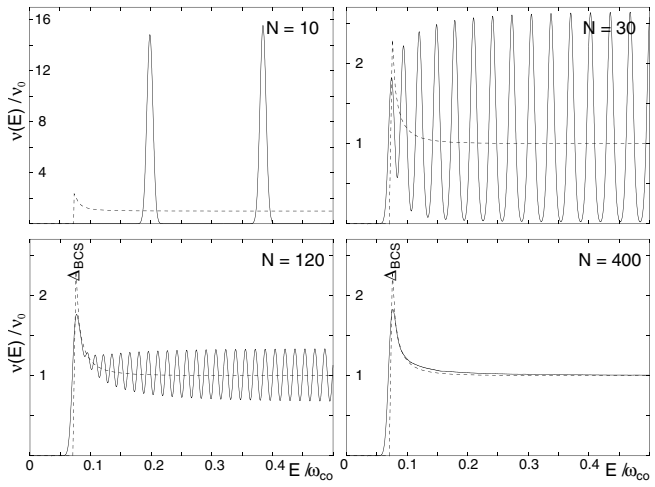

FIG. 2. The tunneling density of states $\nu(E)$ for $\Delta_{\mathrm{BCS}} = 0.07\omega_{\mathrm{co}}$ and $N = 5, 30, 60, 200$ energy levels above E_{Fermi} in the No-Gaudino approximation (solid line; for the sake of better visibility, the delta peaks in Eq. (2) have been replaced by Gaussians of width $0.005\omega_{\mathrm{co}}$). The familiar gap Δ_{BCS} emerges during the crossover from the few-electron ($d \gg \Delta_{\mathrm{BCS}}$) to the bulk limit ($d \ll \Delta_{\mathrm{BCS}}$). In the latter limit, we observe agreement with the BCS result (dashed line).

trates that during the crossover from the few-electron ($d \gg \Delta_{\mathrm{BCS}}$) to the bulk limit ($d \ll \Delta_{\mathrm{BCS}}$), the familiar BCS gap of width Δ_{BCS} emerges together with a strongly pronounced peak at $\omega \approx \Delta_{\mathrm{BCS}}$ as the quasiparticle energies are kept away from the Fermi surface by the pairing interaction and accumulate at Δ_{BCS}. Not shown: As in the inset of Fig. 1, the lost weight again shows a maximum around $\lambda \sim 1/\ln N$ and is found to never exceed fractions of 1%, thus confirming the accuracy of the No-Gaudino approximation.

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