Macroscopic Distinguishability Between Quantum States Defining Different Phases of Matter: Fidelity and the Uhlmann Geometric Phase

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We study the fidelity approach to quantum phase transitions (QPTs) and apply it to general thermal phase transitions (PTs). We analyze two particular cases: the Stoner-Hubbard itinerant electron model of magnetism and the BCS theory of superconductivity. In both cases we show that the sudden drop of the mixed state fidelity marks the line of the phase transition. We conduct a detailed analysis of the general case of systems given by mutually commuting Hamiltonians, where the non-analyticity of the fidelity is directly related to the non-analyticity of the relevant response functions (susceptibility and heat capacity), for the case of symmetry-breaking transitions. Further, on the case of BCS theory of superconductivity, given by mutually non-commuting Hamiltonians, we analyze the structure of the system's eigenvectors in the vicinity of the line of the phase transition showing that their sudden change is quantified by the emergence of a generically non-trivial Uhlmann mixed state geometric phase.

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One of the main characteristics of quantum mechanics that makes it different from any classical physical theory is that in quantum mechanics two different quantum states, being either pure or mixed, are in general not fully distinguishable. By fully distinguishable we mean that it is possible, upon a result of a *single-shot* measurement of a suitable observable, to infer with probability one in which of the two given quantum states the observed system has been prepared. In particular, two pure quantum states are fully distinguishable if and only if they are orthogonal to each other. Otherwise, the maximal probability to unambiguously distinguish between two non-orthogonal pure quantum states is always strictly smaller than one. The reason for this lies in the fact that, while the outcomes of measurements on classical systems are, at least in principle, given with certainty, quantum measurements in general generate non-trivial probability distributions. This feature of quantum mechanics has found numerous applications within the field of quantum information and computation, in particular in quantum cryptography, quantum communication complexity, designing novel quantum algorithms, etc. (for an overview, see [1]).

Within the field of quantum information, the function widely used to quantify the distinguishability between two quantum states $\hat{\rho}_1$ and $\hat{\rho}_2$ is *fidelity* [2], given by the expression:

$$F(\hat{\rho}_1, \hat{\rho}_2) = \mathrm{Tr}\sqrt{\sqrt{\hat{\rho}_1}\hat{\rho}_2\sqrt{\hat{\rho}_1}}. \tag{1}$$

Note that in the case of pure states $\hat{\rho}_1 = |\psi_1\rangle\langle\psi_1|$ and $\hat{\rho}_2 = |\psi_2\rangle\langle\psi_2|$, the above expression reduces to $F(|\psi_1\rangle\langle\psi_1|, |\psi_2\rangle\langle\psi_2|) = |\langle\psi_1|\psi_2\rangle|$, which is nothing but the square root of the probability for a system in state $|\psi_2\rangle$ to pass the test of being in state $|\psi_1\rangle$. The fidelity (1) between two quantum states, given for two systems 1 and 2, quantifies the statistical distinguishability between them, in a sense of *classical* statistical distinguishability between the probability distributions obtained by measuring an *optimal* observable in states $\hat{\rho}_1$ and $\hat{\rho}_2$. In other words, for every observable $\hat{A}$, we have $F(\hat{\rho}_1, \hat{\rho}_2) \leq F_c(\{p_1(i|\hat{A})\}, \{p_2(i|\hat{A})\}) \equiv \sum_i \sqrt{p_1(i|\hat{A})p_2(i|\hat{A})}$, where $\{p_\alpha(i|\hat{A})\}$, $\alpha \in \{1, 2\}$, is a probability distribution obtained measuring the observable $\hat{A}$ in the state $\hat{\rho}_\alpha$, and $F_c(\{p_1(i|\hat{A})\}, \{p_2(i|\hat{A})\})$ is the classical fidelity between the two probability distributions $\{p_1(i|\hat{A})\}$ and $\{p_2(i|\hat{A})\}$. For an overview of the results on distinguishability between quantum states and its applications to the field of quantum information, see [3] and the references therein.

Quantum mechanics was originally developed to describe the behavior of microscopic systems. Therefore, most of its applications are focused on the study of the properties and dynamics of quantum states referring to such systems, where quantum features dominate. On the other hand, it is a common assumption that classical behavior emerges in the thermodynamical limit, when the number of degrees of freedom of the system becomes large (in the limit of a large number of microscopic sub-systems). Yet, there is no special objection why quantum mechanics should not be generally applicable, even to macroscopic systems. Indeed, macroscopic phenomena such as magnetism, superconductivity or superfluidity, to name just a few, can only be explained by using the rules of quantum mechanics. As in these, as well as in many other, highly physical relevant cases, the macroscopic features of matter are given through the features of its quantum states, the question of quantifying those macroscopic properties given by many-body quantum states arises as a relevant problem in physics.

In this study, we are interested in those macroscopic features of matter that define its thermodynamical phase. Different phases of matter are separated by the so-called *regions of criticality*, regions in parameter space where the system's free energy becomes non-analytic. As the free energy is a function of the system's states, it is precisely the features of its states that determine the phase the system is in. Indeed, different phases have different values of the *order parameter*, given by the expectation value of a certain observable. As in the case of general quantum states, here as well, fidelity can be used as a function whose behavior can mark the regions of criticality (and therefore the phase transitions).

In the case of quantum phase transitions (QPTs) [4], which occur at zero temperature and are driven by purely quantum fluctuations, the study of the ground state fidelity has been first conducted on the examples of the Dicke and XY models [5]. Note that in this case, the ground states are pure quantum states, so the fidelity is given by a simple overlap between two pure states. It was shown that approaching the regions of criticality the fidelity between two neighboring ground states exhibits a dramatic drop [26]. Subsequently, the fidelity approach to QPTs was applied to free Fermi systems and graphs [6] and to the Bose-Hubbard model [7]. The connection between fidelity, scaling behavior in QPTs and the renormalization group flows was introduced in [8] and further discussed in [9]. Also, it was shown that the fidelity can mark the regions of criticality in systems whose QPTs can not be described in terms of Landau-Ginzburg-Wilson (LGW) theory: when the ground states are given by the matrix product states [10], in the case of a topologically ordered QPT [11], and in the Kosterlitz-Thouless type of transition [12] as well. The formal differential-geometry description of the fidelity approach to QPTs was first introduced in [13] and subsequently developed in [14], where the connection to the Berry phase approach to QPTs (see [15]) was also established. Further, on the example of the spin one-half XXZ Heisenberg chain, it was shown that the fidelity does not necessarily exhibit a dramatic drop at the critical point, but that the proper finite-size scaling analysis allows for correct identification of the QPT, see [14]. An interesting example of a Heisenberg chain where the fidelity approach fails when applied to the ground states, but does mark the point of criticality when applied to the first excited states, was discussed in [16] (note that the numerical results were obtained for up to 12 spins only, which leaves open the question of the ground state fidelity behaviour in the thermodynamic limit). Introducing the temperature as an additional parameter, QPTs were studied in [17] and it was shown that extending the fidelity approach to general mixed (thermal) states can still mark the regions of criticality as well as the cross-over regions at finite temperatures. Finally, the genuine thermal PTs were discussed in [13] and [18], where the connection between the singularities in fidelity and specific heat or magnetic susceptibility was explicitly shown for the cases of systems given by mutually commuting Hamiltonians and symmetry-breaking PTs of LGW type.

In this paper, we apply the fidelity approach to general thermal phase transitions [27]. We analyze in detail two particular examples given by the Stoner-Hubbard model for magnetism and the BCS theory of superconductivity. In general, a system is defined by a Hamiltonian $\hat{H}(U)$ which is a function of a set of parameters representing the interaction coupling constants generically denoted as U. In thermal equilibrium, a system's state is given by a density operator $\hat{\rho}(T, U)$. Thus, in discussing the general, thermal as well as quantum phase transitions, we can consider the coupling constant(s) U and the temperature T to form a "generalized" parameter $q = (T, U)$. We consider the behavior of the fidelity $F(\hat{\rho}(q), \hat{\rho}(\tilde{q}))$ between two equilibrium thermal states $\hat{\rho}(q)$ and $\hat{\rho}(\tilde{q})$ defined by two close parameter points $q = q(T, U)$ and $\tilde{q} = q + \delta q = (T + \delta T, U + \delta U)$. We show that in both models considered, the PTs are marked by the sudden drop of fidelity in the vicinity of regions of criticality - a signature of enhanced distinguishability between two quantum states defining two different phases of matter, based on both short-range microscopic as well as long-range macroscopic features. For the general case of mutually commuting Hamiltonians, we analytically prove in detail that the same holds for PTs which fall within the symmetry-breaking paradigm described by the LGW theory (see also [13] and [18]). Further, for the case of mutually non-commuting Hamiltonians, on the example of BCS theory of superconductivity we show that the non-analyticity of the fidelity is accompanied by the emergence of a generically non-trivial Uhlmann geometric phase [19], the mixed-state generalization of the Berry geometric phase (for the relation between QPTs and Berry phases, see [15], [13] and [14]).

STONER-HUBBARD ITINERANT ELECTRON MODEL FOR MAGNETISM

First, we discuss the case of the Stoner-Hubbard model for itinerant electrons on a lattice given by the Hamiltonian [20]:

$$\hat{H}_{SH} = \sum_k \varepsilon_k \left(\hat{c}^\dagger_{k\uparrow}\hat{c}_{k\uparrow} + \hat{c}^\dagger_{k\downarrow}\hat{c}_{k\downarrow}\right) + U\sum_l \hat{c}^\dagger_{l\uparrow}\hat{c}_{l\uparrow}\hat{c}^\dagger_{l\downarrow}\hat{c}_{l\downarrow}. \tag{2}$$

The anti-commuting fermionic operators $\hat{c}^\dagger_{k\sigma}$ represent the free-electron momentum Bloch modes ($\sigma \in \{\uparrow,\downarrow\}$), while the on-site operators $\hat{c}^\dagger_{l\sigma} = V^{-1/2}\sum_k e^{-ikx_l}\hat{c}^\dagger_{k\sigma}$ are given by their Fourier transforms, where x_l represents the position of the l-th lattice site. The coupling constant $U > 0$ defines the on-site electron Coulomb repulsion. There are in total N electrons and they occupy the volume V (such that in the thermodynamic limit, when $N, V \to \infty$, we have $N/V \to$ const). Finally, we assume for simplicity that the kinetic energy is given by $\varepsilon_k = \hbar^2k^2/(2m)$, while the number operators are $\hat{n}_{k\sigma} = \hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma}$ and $\hat{n}_{l\sigma} = \hat{c}^\dagger_{l\sigma}\hat{c}_{l\sigma} = V^{-1}\sum_{qk} e^{iqx_l}\hat{c}^\dagger_{k\sigma}\hat{c}_{k+q\sigma}$. Thus,

$$\hat{H}_{SH} = \sum_{k\sigma}\varepsilon_k\hat{n}_{k\sigma} + U\sum_l \hat{n}_{l\uparrow}\hat{n}_{l\downarrow}. \tag{3}$$

In order to obtain the mean-field effective Hamiltonian, we neglect the term quadratic in the fluctuations $\delta\hat{n}_{l\sigma} = \hat{n}_{l\sigma} - n_{l\sigma}$, where $n_{l\sigma} = \langle\hat{n}_{l\sigma}\rangle$, in the potential written as $\hat{n}_{l\uparrow}\hat{n}_{l\downarrow} = \delta\hat{n}_{l\uparrow}\delta\hat{n}_{l\downarrow} + n_{l\uparrow}\hat{n}_{l\downarrow} + n_{l\downarrow}\hat{n}_{l\uparrow} - n_{l\uparrow}n_{l\downarrow}$. Expressing the number operators in terms of the Bloch momentum operators, and using $\langle\hat{c}^\dagger_{k\sigma}\hat{c}_{k'\sigma}\rangle = \delta_{kk'}\langle\hat{n}_{k\sigma}\rangle$ (which expresses the translational invariance in a ferromagnetic ground state), the mean-field linearized effective Hamiltonian becomes:

$$\hat{H}^{eff}_{SH} = \sum_k \left(E_{k\uparrow}\hat{n}_{k\uparrow} + E_{k\downarrow}\hat{n}_{k\downarrow}\right) - VUn_\uparrow n_\downarrow. \tag{4}$$

Here, $n_\sigma = N_\sigma/V$ is the density of electrons with spin projection along z-axis given by $\sigma \in \{\uparrow,\downarrow\}$ ($N_\sigma = \sum_k\langle\hat{n}_{k\sigma}\rangle$ being the total number of electrons with spin σ). The one-particle electron energies in this effective model are obtained by shifting the free-electron energies ε_k by an amount depending on the particle's spin:

$$\begin{aligned} E_{k\uparrow} &= \varepsilon_k + Un_\downarrow, \\ E_{k\downarrow} &= \varepsilon_k + Un_\uparrow. \end{aligned} \tag{5}$$

Since the one-particle energy modes are decoupled, the overall ground state is obtained by filling the electrons up to the Fermi level ε_F:

$$|g\rangle = \otimes_{k\leq k_{F\uparrow}}\hat{c}^\dagger_{k\uparrow}\otimes_{k\leq k_{F\downarrow}}\hat{c}^\dagger_{k\downarrow}|0\rangle, \tag{6}$$

where $|0\rangle$ represents the vacuum state with no electrons and $k_{F\uparrow}$ the maximal value of the momentum for spin up electrons, given by $E_{k_{F\uparrow}} = \varepsilon_F$ (and analogously for $k_{F\downarrow}$) [28]. Note that, due to the different dispersion formulas (5) for particles with spin up and spin down, in general the values of $k_{F\uparrow}$ and $k_{F\downarrow}$ that minimize the ground state energy, and therefore define the state (6) itself, are different and consequently the number of up and down electrons will be different. This is precisely the reason for the existence of magnetism in this model. As soon as the energy of the "biased" (magnetic) state, for which for example $k_{F\uparrow} > k_{F\downarrow}$, becomes lower than the energy of the "balanced" (paramagnetic) state ($k_{F\uparrow} = k_{F\downarrow}$), a magnetic phase transition will occur. Obviously, for reasons of symmetry, the magnetic state can be reversed with the $k_{F\uparrow} > k_{F\downarrow}$ and $k_{F\uparrow} < k_{F\downarrow}$ cases having the same energy, in the absence of an external symmetry breaking field $\vec{H}$. The qualitative picture of the emergence of magnetic features can be seen already from looking at the original Hamiltonian (2): in the $U \to 0$ limit, when the Coulomb interaction is negligible, the Hamiltonian represents a system of free electrons that exhibits no magnetic order (all Bloch states are doubly occupied); in the opposite $U \to \infty$ limit, the second term of the Hamiltonian becomes the dominant one and is minimized by one of two possible states for which either $N_\uparrow = 0$ or $N_\downarrow = 0$.

The quantitative analysis of the zero-temperature critical behavior of the effective Hamiltonian (4) can be done by looking at the divergence of the magnetic susceptibility, using the one-particle energy dispersion relations (5). At $T = 0$ it leads to the well known Stoner criterion for the emergence of magnetism [20]:

$$D_F U_c = 1, \tag{7}$$

where U_c is the critical value of the coupling constant above which the system is in a magnetic phase and $D_F = D(\varepsilon_F)$ is the density of states around the Fermi energy. From this, one can obtain (see Appendix 1) the critical value U_c of the coupling constant [29]:

$$U_c = \frac{4}{3}\,\varepsilon_F \frac{V}{N}, \tag{8}$$

where N is the total number of electrons, V is the volume of the system and m is the electron mass.

Alternatively, the above result can be derived by minimizing the overall ground state energy, thus obtaining the explicit dependencies $k_{F\uparrow} = k_{F\uparrow}(U)$ and $k_{F\downarrow} = k_{F\downarrow}(U)$ which determine the ground state (6) and U_c in particular (the maximum value of U for which $k_{F\uparrow} = k_{F\downarrow}$) [30]. The total number of electrons in the system is given by $N = N_\uparrow + N_\downarrow$, and thus:

$$\frac{N}{V} = \frac{1}{6\pi^2}[(k_{F\uparrow})^3 + (k_{F\downarrow})^3], \tag{9}$$

since the up and down electrons occupy spheres of radius $k_{F\uparrow}$ and $k_{F\downarrow}$, with volumes $V(k_{F\uparrow})$ and $V(k_{F\downarrow})$, in momentum space, with a density of states $V/(2\pi)^3$, as follows from the periodic boundary conditions for the Bloch functions. From $E_{k_{F\uparrow}} = E_{k_{F\downarrow}}$ (see Appendix 1), using the energy dispersion formulas (5), we obtain the second equation that determines the Fermi momenta $k_{F\uparrow}$ and $k_{F\downarrow}$ (with $\alpha = \frac{3}{2}k_F U_c$):

$$(k_{F\uparrow} - k_{F\downarrow})[(k_{F\uparrow} + k_{F\downarrow}) - \frac{U}{\alpha}(k^2_{F\uparrow} + k_{F\uparrow}k_{F\downarrow} + k^2_{F\downarrow})] = 0. \tag{10}$$

We see that the above two equations always have the trivial solution $k_{F\uparrow} = k_{F\downarrow} \equiv k_F$, which from (9) is $k_F = \left(3\pi^2 \frac{N}{V}\right)^{1/3}$. Yet, it is not necessarily the only possible solution, as the quadratic term in equation (10) can also be satisfied, $(k_{F\uparrow} + k_{F\downarrow}) - \frac{U}{\alpha}(k^2_{F\uparrow} + k_{F\uparrow}k_{F\downarrow} + k^2_{F\downarrow}) = 0$. It turns out that precisely for $U > U_c$ this term has non-trivial, "non-balanced" solutions that are energetically more favorable than the "balanced" one and that give rise to magnetic order (see Appendix 1).

Thus, equations (9) and (10) define $k_{F\uparrow} = k_{F\uparrow}(U)$ and $k_{F\downarrow} = k_{F\downarrow}(U)$ functions which, via (6), give the ground state as a function of the external parameter U, $|g\rangle = |g(U)\rangle$. This enables us to analyze the fidelity between two ground states $|g\rangle \equiv |g(U)\rangle$ and $|\tilde{g}\rangle = |g(U + \delta U)\rangle$ in two close parameter points U and $U + \delta U$. The fidelity is then $F(|g\rangle\langle g|, |\tilde{g}\rangle\langle\tilde{g}|) = |\langle g|\tilde{g}\rangle|$, and for $U < U_c$ (and δU sufficiently small, i.e. $\delta U < U_c - U$) we see that the fidelity is identical to 1. This is a simple consequence of our mean-field approximation based on a simplified description in terms of single particle energy states. On the magnetic side of the phase diagram, the ground states are indeed different from each other, which follows from the relation $k_{F\uparrow}(U) \neq k_{F\downarrow}(U)$. In fact, from equation (6) it follows that *any* two ground states with different numbers $N_\uparrow$ and $N_\downarrow$ are *orthogonal* to each other. Since this is precisely the case in the thermodynamic limit, the fidelity between any two different ground states (in two different parameter points) is identically equal to zero. This is the famous Anderson orthogonality catastrophe, discussed in more detail in [5]. For systems with infinitely many degrees of freedom, such as those taken in the thermodynamic limit are, every two ground states are generally orthogonal to each other. Therefore, in order to infer the points of criticality, we are forced to either analyze the finite-size scaling behavior (see [5]), or to introduce the fidelity per lattice site and work directly in the thermodynamic limit (see [8], [9] and [21]).

In our case though, even for finite systems the ground state is discontinuous at the point of criticality. This is due to the fact that the unperturbed and the symmetry-breaking perturbation Hamiltonian commute with each other, which results in a first-order quantum phase transition at the point of level-crossing between the ground and the first excited state. In other words, in the case of finite systems ($N, V < \infty$), the small enough changes of the parameter $U \to U + \delta U$ will result in small changes of volumes $V(k_{F\uparrow}) \to V(k_{F\uparrow}) + \delta V(k_{F\uparrow})$ such that $|\delta V(k_{F\uparrow})| < V_0 = (2\pi)^3/V$ (V_0 is the volume occupied by each one-particle state in momentum space): infinitesimal changes of the volumes $V(k_{F\uparrow})$ and $V(k_{F\downarrow})$ are small enough to cause a change in the numbers $N_\uparrow$ and $N_\downarrow$, and thus in the ground state. Therefore, for finite systems, the fidelity between two ground states is either one or zero – it is not a continuous function of and its rate of change can not be analyzed directly.

Yet, we can use the rate of change of $V(k_{F\uparrow})$, the derivative $\frac{dV(k_{F\uparrow})}{dU}$, to quantify the change of fidelity itself (note that, due to the fixed total number of electrons N, we have that $\frac{dV(k_{F\downarrow})}{dU} = -\frac{dV(k_{F\uparrow})}{dU}$). Lengthy, but elementary algebra (see Appendix 1) shows that precisely at $U = U_c$, the derivative $\frac{dV(k_{F\uparrow})}{dU}$ diverges to infinity, thus marking the *macroscopic* distinguishability between the states from paramagnetic and magnetic phase (see Fig. 1).

Next, we discuss the general case of $T \neq 0$ phase transitions. First, we transform the Hamiltonian $\hat{H}^{eff}_{SH}$ to a form with the explicit symmetry breaking term that drives the phase transition. Using $M = (N_\uparrow - N_\downarrow)/2 = \langle \hat{S}^z \rangle = \sum_k \langle \hat{S}^z_k \rangle$,

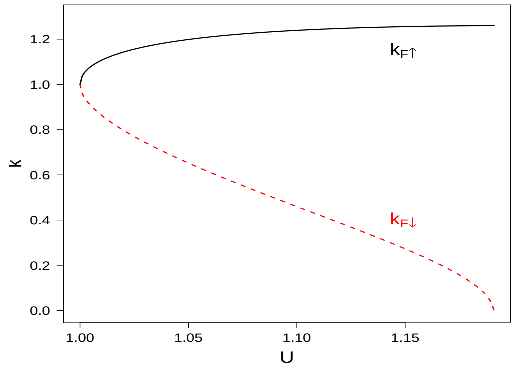

FIG. 1: (color online) The explicit dependencies $k_{F\uparrow} = k_{F\uparrow}(U)$ (black, solid line) and $k_{F\downarrow} = k_{F\downarrow}(U)$ (red, dashed line) determining the ground state (6). Note that at the point of QPT, given by $U_c = 1$, the two derivatives $\frac{dk_{F\uparrow}}{dU}$ and $\frac{dk_{F\downarrow}}{dU}$ become infinite, marking the non-analyticity in the ground state fidelity. The plot is given in rescaled quantities $U \to D_F U$ and $k_{F\sigma} \to k_{F\sigma}/k_F$.

with $N_\sigma = \langle \hat{N}_\sigma \rangle = \sum_k \langle \hat{n}_{k\sigma} \rangle$, $\hat{n}_k = \hat{n}_{k\uparrow} + \hat{n}_{k\downarrow}$ and $\hat{S}^z_k = \frac{1}{2}(\hat{n}_{k\uparrow} - \hat{n}_{k\downarrow}) = \hat{\Psi}^\dagger \frac{\sigma^z}{2} \hat{\Psi}$, where $\hat{\Psi}^\dagger_k = [\hat{c}^\dagger_{k\uparrow} \; \hat{c}^\dagger_{k\downarrow}]$ and σ^z is the z-component of the vector $\vec{\sigma}$ of Pauli matrices, we get:

$$\hat{H}^{eff}_{SH} = \sum_k \left[\left(\varepsilon_k + \frac{UN}{2V} \right) \hat{n}_k - 2\frac{UM}{V} \hat{S}^z_k \right] - \frac{U}{V} \left(\frac{N^2}{4} - M^2 \right). \tag{11}$$

In thermal equilibrium, the state of the system is given by $\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H}^{eff}_{SH} - \mu \hat{N})}$, where $Z = \mathrm{Tr}[e^{-\beta(\hat{H}^{eff}_{SH} - \mu \hat{N})}]$ is the grand canonical partition function, $\beta = 1/(k_B T)$, with k_B being the Boltzmann constant and T the absolute temperature and $\mu = \mu(T)$ is the chemical potential. Using the above expression for the Hamiltonian $\hat{H}^{eff}_{SH}$, we can write:

$$-\beta(\hat{H}^{eff}_{SH} - \mu \hat{N}) = \sum_k \left(\alpha_k \hat{n}_k + h_z \hat{S}^z_k \right) + C. \tag{12}$$

Here, $\alpha_k = -\beta E_k$ (with $E_k = \bar{\varepsilon}_k + \frac{UN}{2V}$ and $\bar{\varepsilon}_k = \varepsilon_k - \mu$), $h_z = 2\beta \frac{U}{V} M$ and $C = \beta \frac{U}{V} (\frac{N^2}{4} - M)$. Note that the coefficients α_k, h_z and C are functions of both the coupling constant U and, through β and the chemical potential $\mu = \mu(T)$, of the temperature T as well, so that the "generalized" parameter is $q = (T, U)$. Using the obvious commutation relations $[\hat{n}_k, \hat{n}_{k'}] = [\hat{n}_k, \hat{S}^z_{k'}] = [\hat{S}^z_k, \hat{S}^z_{k'}] = 0$ (for $k \neq k'$), the equilibrium state can be expressed as:

$$\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H}^{eff}_{SH} - \mu \hat{N})} = \frac{e^{\sum_k \left(\alpha_k \hat{n}_k + h_z \hat{S}^z_k \right) + C}}{\mathrm{Tr}\left[e^{\sum_k \left(\alpha_k \hat{n}_k + h_z \hat{S}^z_k \right) + C} \right]} = \frac{\prod_k \left(e^{\alpha_k \hat{n}_k} e^{h_z \hat{S}^z_k} \right)}{\prod_k \mathrm{Tr}\left[e^{\alpha_k \hat{n}_k} e^{h_z \hat{S}^z_k} \right]}. \tag{13}$$

We next choose two parameter points $q_a = (T_a, U_a)$ and $q_b = (T_b, U_b)$ defining the Hamiltonians $\hat{H}_a = \hat{H}^{eff}_{SH}(U_a)$ and $\hat{H}_b = \hat{H}^{eff}_{SH}(U_b)$ and the corresponding equilibrium states $\hat{\rho}_a = \hat{\rho}(q_a)$ and $\hat{\rho}_b = \hat{\rho}(q_b)$ respectively. The fidelity between the two states is then given by:

$$F(\hat{\rho}_a, \hat{\rho}_b) = \mathrm{Tr}[(\hat{\rho}_a^{1/2} \hat{\rho}_b \hat{\rho}_a^{1/2})^{1/2}] = \mathrm{Tr}[\sqrt{\hat{\rho}_a \hat{\rho}_b}] = \frac{\mathrm{Tr}\left[e^{\frac{\beta_a \hat{H}_a + \beta_b \hat{H}_b}{2}} \right]}{\sqrt{Z(\hat{H}_a) Z(\hat{H}_b)}}. \tag{14}$$

Using (13) and the expression $\mathrm{Tr}[e^{(\alpha_k \hat{n}_k + h_z \hat{S}^z_k)}] = 2e^{\alpha_k} (\cosh \alpha_k + \cosh \frac{h_z}{2})$ (for the proof, see Appendix 2), the fidelity between two different equilibrium states $\hat{\rho}_a$ and $\hat{\rho}_b$ finally becomes:

$$F(\hat{\rho}_a, \hat{\rho}_b) = \prod_k \frac{\cosh \bar{\alpha}_k + \cosh \frac{\bar{h}_z}{2}}{\sqrt{\left[\cosh(\bar{\alpha}_k + \frac{\Delta \alpha_k}{2}) + \cosh(\frac{\bar{h}_z}{2} + \frac{\Delta h_z}{2}) \right] \left[\cosh(\bar{\alpha}_k - \frac{\Delta \alpha_k}{2}) + \cosh(\frac{\bar{h}_z}{2} - \frac{\Delta h_z}{2}) \right]}}, \tag{15}$$

with $\bar{\alpha}_k = (\alpha_k(q_a) + \alpha_k(q_b))/2$, $\Delta\alpha_k = \alpha_k(q_a) - \alpha_k(q_b)$, and similarly for $\bar{h}_z$ and Δh_z. If we choose the two points to be close to each other, $\Delta\alpha_k << 1$ and $\Delta h_z << 1$, then the fidelity can be seen as a function of $\bar{\alpha}_k$ and $\bar{h}_z$, with a fixed parameter difference.

In order to evaluate the fidelity (15), we need to determine the magnetization $M = M(T, U)$ and the chemical potential $\mu = \mu(T, U)$, given by the pair of self consistent integral equations:

$$
\begin{aligned}
N &= VD_F \int_0^{+\infty} d\varepsilon \sqrt{\frac{\varepsilon}{\varepsilon_F}} \left[f(E_{k\uparrow}) + f(E_{k\downarrow}) \right], \\
M &= VD_F \int_0^{+\infty} d\varepsilon \sqrt{\frac{\varepsilon}{\varepsilon_F}} \frac{1}{2} \left[f(E_{k\uparrow}) - f(E_{k\downarrow}) \right],
\end{aligned}
\tag{16}
$$

where $f(E_{k\sigma}) = [\exp(\beta E_{k\sigma}) + 1]^{-1}$ is the usual Fermi distribution. We used the subroutine hybrd.f from MINPACK [22] to solve the above system numerically. In the $T \to 0$ limit, the above system reduces to equations (9) and (10) that determine the $T = 0$ ground state. The result for the magnetization is given on Fig. 2. The line of the phase transition $U_c = U_c(T)$ is clearly marked, and is plotted on Fig. 3. Finally, using the numerical results for M and μ, we obtain the fidelity, depicted on Fig. 4. We clearly see the same line of the phase transition as the line of a sudden drop of F. Note that all the plots are given in rescaled quantities $T \to k_B T$, $U \to D_F U$ and $M \to M/N$, with $\delta T = 0, \delta U = 2\times10^{-3}$. We have evaluated the fidelity for $\delta T = 2\times10^{-3}$ and $\delta U = 0$, as well as for $\delta T = \delta U = 2\times10^{-3}$ and the results are qualitatively the same.

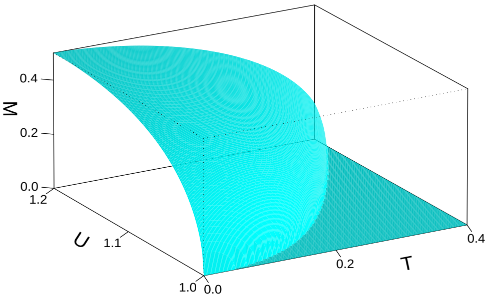

FIG. 2: (color online) Magnetization $M = M(T, U)$ as a function of the temperature T and the coupling constant U. The plot is given in rescaled quantities $T \to k_B T$, $U \to D_F U$ and $M \to M/N$.

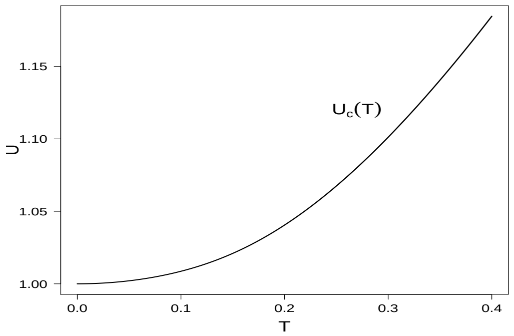

FIG. 3: The critical line of the magnetic phase transition $U_c = U_c(T)$. The plot is given in rescaled quantities $T \to k_B T$ and $U \to D_F U$.

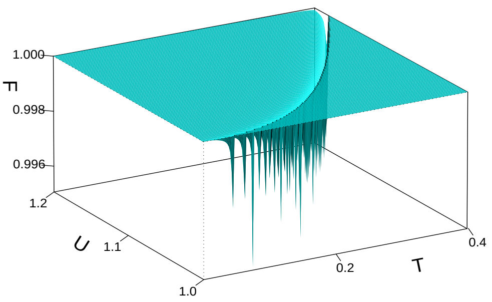

FIG. 4: (color online) The fidelity $F = F(T, U)$. The plot is given in rescaled quantities $T \to k_B T$ and $U \to D_F U$, with $\delta T = 0, \delta U = 2 \times 10^{-3}$.

THE GENERAL CASE OF MUTUALLY COMMUTING HAMILTONIANS

The above singular behavior of the fidelity indeed marks the regions of phase transitions, not only for the case of the Stoner-Hubbard model but also for the broad class of systems given by a set of mutually commuting Hamiltonians $\hat{H}(q)$ and whose critical behavior is explained by the LGW theory, as can be seen by the following analysis. Using the mean Hamiltonian $\bar{\hat{H}} = (\hat{H}_a + \hat{H}_b)/2$ and the difference $\Delta\hat{H} = \hat{H}_a - \hat{H}_b$, from equation (14) the fidelity can be written as:

$$F(\hat{\rho}_a, \hat{\rho}_b) = \frac{Z(\bar{\hat{H}})}{\sqrt{Z(\bar{\hat{H}} + \frac{\Delta\hat{H}}{2}) Z(\bar{\hat{H}} - \frac{\Delta\hat{H}}{2})}}. \tag{17}$$

Within the LGW theory, PTs occur as a consequence of the emergence of a symmetry-breaking term in the Hamiltonian, given by an operator $\hat{S}$. Thus, we can write the overall Hamiltonian as a sum of unperturbed and symmetry-breaking terms, $\hat{H} = \hat{H}_0 - h\hat{S}$, with $h = h(q)$. Using [31] $Z(\hat{H}) = \mathrm{Tr}[e^{-\beta(\hat{H}_0 - h\hat{S})}]$ (note the implicit dependence of partition function Z on temperature T, through β), for the first and the second derivative we obtain $\frac{\partial \ln Z}{\partial h} = \beta \mathrm{Tr}[\hat{\rho}(\hat{H})\hat{S}] = \beta\langle\hat{S}\rangle = \beta M$ and $\frac{\partial^2}{\partial h^2}(\ln Z) = \beta\chi$. Here, $M = M(h)$ and $\chi = \chi(h) = \beta(\langle\hat{S}^2\rangle - \langle\hat{S}\rangle^2)$ are the generalized "magnetization" and "susceptibility" respectively. Thus, for the logarithm of the partition function (free energy) we obtain $\ln Z(\hat{H})|_{h+\Delta h} = \ln Z(\hat{H})|_h + \beta M(h)\Delta h + \frac{1}{2}\beta\chi(h)\Delta h^2 + o(\Delta h^2)$. Finally, in the vicinity of the points of parameter space where the self-consistent field h vanishes, the fidelity (17) reads as:

$$F|_{h=\Delta h} \simeq e^{-\frac{1}{2}\beta\chi(0)\Delta h^2}. \tag{18}$$

According to the LGW theory, at the phase transition, the zeroth-field "susceptibility" $\chi(0)$ becomes non-analytic and diverges. Thus it follows that the fidelity F will itself become nonanalytic and experience a sudden drop.

When interested in the system's behavior at PTs, we usually simplify the problem by taking the unperturbed Hamiltonian to be constant. Yet, in general, the unperturbed Hamiltonian is also a function of the parameters, $\hat{H}_0 = \hat{H}_0(q)$. This gives the correction to the above formula for the fidelity which, introducing $\bar{\hat{H}} = \bar{\hat{H}}_0 - \bar{h}\hat{S}$ and $\Delta\hat{H} = \Delta\hat{H}_0 - \Delta h\hat{S}$, reads as:

$$F|_{h=\Delta h} \simeq \frac{Z(\bar{\hat{H}}_0)}{\left[Z(\bar{\hat{H}}_0 + \frac{\Delta\hat{H}_0}{2}) Z(\bar{\hat{H}}_0 - \frac{\Delta\hat{H}_0}{2})\right]^{1/2}} \; e^{-\frac{1}{2}\beta\chi(0)\Delta h^2}. \tag{19}$$

The "correction" term in the above product is responsible for "short-range" local correlations, while the second one quantifies the global "long-range" correlations giving rise to macroscopic phase distinguishability. Note though that even within a single phase, a system can be in different macroscopically distinguishable states – phase distinguishability is not the only form of macroscopic distinguishability. Yet, it is in some sense the “extreme” version of it, which clearly affects the behavior of fidelity.

Finally, we note that in the above discussion we focused on PTs driven by the local order parameter $\hat{S}$. Therefore, we analyzed the Taylor expansion of F with respect to Δh deviations only, which at the second order are given by the generalized susceptibility $\chi(h)$. In the general case, considering the temperature deviations as well, one would include additional terms involving the specific heat $C = C(q)$, again resulting in a singular behavior of the fidelity.

BCS SUPERCONDUCTIVITY

Next, we discuss the BCS theory for superconductivity [20], providing us with an example of a model with mutually non-commuting Hamiltonians. The one-electron Bloch momentum modes are given by the fermionic anti-commuting operators $\hat{c}_{k\sigma}$ (label $\sigma \in \{\uparrow, \downarrow\}$ represents spins with projections up and down along, say z-axis), with the one-particle kinetic energies taken to be, again for simplicity, $\varepsilon_k = \hbar^2 k^2/(2m)$. The BCS superconducting Hamiltonian that represents the sum of one-particle kinetic and Cooper-pair interaction energies can be written in the following way ($V_{k'k} = V^*_{kk'}$ are the coupling constants):

$$\hat{H}_{BCS} = \sum_{k\sigma} \varepsilon_k \hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma} + \sum_{kk'} V_{kk'} \hat{c}^\dagger_{k'\uparrow}\hat{c}^\dagger_{-k'\downarrow}\hat{c}_{-k\downarrow}\hat{c}_{k,\uparrow}. \tag{20}$$

By $\hat{n}_{k\sigma} = \hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma}$ we denote the one-particle number operators, while by $\hat{b}^\dagger_k = \hat{c}^\dagger_{k\uparrow}\hat{c}^\dagger_{-k\downarrow}$ and $\hat{b}_k = \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow}$ we define the Cooper-pair creation and annihilation operators respectively. Analogously to the previous case, using $\hat{b}_k = \langle \hat{b}_k \rangle + \delta\hat{b}_k$ and neglecting the term quadratic in the fluctuations, we obtain the effective mean-field BCS Hamiltonian:

$$\hat{H}^{eff}_{BCS} = \sum_k \varepsilon_k(\hat{n}_{k\uparrow} + \hat{n}_{-k\downarrow}) - \sum_k (\Delta_k \hat{b}^\dagger_k + \Delta^*_k \hat{b}_k - \Delta^*_k b_k), \tag{21}$$

with $\Delta_k = -\sum_{k'} V_{kk'} b_{k'}$ and $b_k = \langle \hat{b}_k \rangle$. We will use the usual assumption that the lattice-mediated pairing interaction is constant and non-vanishing between electrons around the Fermi level only, i.e. $V_{kk'} = -V$ for $|\bar{\varepsilon}_k|$ and $|\bar{\varepsilon}_{k'}| < \hbar\omega_D$, and zero otherwise ($\omega_D$ is the Debye frequency). Using the Nambu operators [20] $\hat{\vec{T}}_k = \hat{\psi}^\dagger_k \frac{\vec{\sigma}}{2} \hat{\psi}_k$, where $\hat{\psi}^\dagger_k = [\hat{c}^\dagger_{k\uparrow}\ \hat{c}_{-k\downarrow}]$ and $\vec{\sigma}$ is the vector of Pauli matrices [32], the operators are given by $\hat{T}^+_k = \hat{b}^\dagger_k$, $\hat{T}^-_k = \hat{b}_k$ and $2\hat{T}^0_k + 1 = (\hat{n}_{k\uparrow} + \hat{n}_{-k\downarrow})$ and form a su(2) algebra (see the Appendix 3). Using this notation, the Hamiltonian takes the form:

$$\hat{H}^{eff}_{BCS} = \sum_k (2\varepsilon_k \hat{T}^0_k - \Delta_k \hat{T}^+_k - \Delta^*_k \hat{T}^-_k) + \sum_k (\varepsilon_k + \Delta^*_k b_k). \tag{22}$$

As before, the thermal equilibrium state is given by $\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H}^{eff}_{BCS} - \mu\hat{N})}$ and, using the above expression for the Hamiltonian $\hat{H}^{eff}_{BCS}$, we can write:

$$-\beta(\hat{H}^{eff}_{BCS} - \mu\hat{N}) = \sum_k \vec{\tilde{h}}_k \hat{\vec{T}}_k + K, \tag{23}$$

where $\vec{\tilde{h}}_k = (\tilde{h}^+_k, \tilde{h}^-_k, \tilde{h}^0_k) = (2\beta\Delta^*_k, 2\beta\Delta_k, -2\beta\bar{\varepsilon}_k)$, $\hat{\vec{T}}_k = (\hat{T}^+_k, \hat{T}^-_k, \hat{T}^0_k)$, $K = -\beta\sum_k(\bar{\varepsilon}_k + \Delta^*_k b_k)$ and $\bar{\varepsilon}_k = \varepsilon_k - \mu(T)$. The norms of the vectors $\vec{\tilde{h}}_k$ are given by $\tilde{h}_k = 2\beta E_k$, with $E_k = \sqrt{\bar{\varepsilon}^2_k + |\Delta_k|^2}$. Similarly to what we had before, the coefficients $\vec{\tilde{h}}_k = \vec{\tilde{h}}_k(T, V)$ are functions of both the coupling constant V and the temperature T, through the gap parameters $\Delta_k = \Delta_k(T, V)$ and the chemical potential $\mu = \mu(T)$. Thus, we can talk of the “generalized” parameter $q = (T, V)$. Since $[\hat{\vec{T}}_k, \hat{\vec{T}}_{k'}] = 0$, for $k \neq k'$, we have:

$$\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H}^{eff}_{BCS} - \mu\hat{N})} = \frac{e^{\sum_k \vec{\tilde{h}}_k \hat{\vec{T}}_k + K}}{\mathrm{Tr}[e^{\sum_k \vec{\tilde{h}}_k \hat{\vec{T}}_k + K}]} = \frac{\prod_k e^{\vec{\tilde{h}}_k \hat{\vec{T}}_k}}{\prod_k \mathrm{Tr}[e^{\vec{\tilde{h}}_k \hat{\vec{T}}_k}]}. \tag{24}$$

We wish to evaluate the fidelity between two thermal states $\hat{\rho}_a$ and $\hat{\rho}_b$, given for two different parameter points $q_a = (T_a, V_a)$ and $q_b = (T_b, V_b)$. Using definition (1) and $\vec{a}_k = \vec{\tilde{h}}_k(q_a)$ and $\vec{b}_k = \vec{\tilde{h}}_k(q_b)$, we have:

$$F(\hat{\rho}_a, \hat{\rho}_b) = \mathrm{Tr}[(\hat{\rho}^{1/2}_a \hat{\rho}_b \hat{\rho}^{1/2}_a)^{1/2}] = \frac{\mathrm{Tr}[(\prod_k e^{\frac{\vec{a}_k}{2}\hat{\vec{T}}_k} e^{\vec{b}_k \hat{\vec{T}}_k} e^{\frac{\vec{a}_k}{2}\hat{\vec{T}}_k})^{1/2}]}{\prod_k (\mathrm{Tr}[e^{\vec{a}_k \hat{\vec{T}}_k}]\mathrm{Tr}[e^{\vec{b}_k \hat{\vec{T}}_k}])^{1/2}}. \tag{25}$$

As for every k the operators $\hat{\vec{T}}_k$ form a su(2) algebra, and therefore by exponentiation define a Lie group, we can write $e^{\frac{\vec{a}_k}{2}\hat{\vec{T}}_k}e^{\vec{b}_k\hat{\vec{T}}_k}e^{\frac{\vec{a}_k}{2}\hat{\vec{T}}_k} = e^{2\vec{c}_k\hat{\vec{T}}_k}$. Also (see Appendix 3), we have that $\mathrm{Tr}[e^{\vec{a}_k\hat{\vec{T}}_k}] = 2(1+\cosh\frac{a_k}{2})$. Therefore, we finally have (see Appendix 3) that $F(\hat{\rho}_a,\hat{\rho}_b) = \prod_k F_k(\hat{\rho}_a,\hat{\rho}_b)$ with [33]:

$$F_k(\hat{\rho}_a,\hat{\rho}_b) = \frac{\mathrm{Tr}[e^{\vec{c}_k\hat{\vec{T}}_k}]}{\sqrt{\mathrm{Tr}[e^{\vec{a}_k\hat{\vec{T}}_k}]\mathrm{Tr}[e^{\vec{b}_k\hat{\vec{T}}_k}]}} = \frac{1+\sqrt{\frac{1}{2}(1+\cosh c_k)}}{\sqrt{(1+\cosh\frac{a_k}{2})(1+\cosh\frac{b_k}{2})}}, \qquad \text{and} \tag{26}$$

$$\cosh c_k = \cosh(\beta^a E_k^a)\cosh(\beta^b E_k^b)\left\{1+\tanh(\beta^a E_k^a)\tanh(\beta^b E_k^b)\frac{\bar{\varepsilon}_k^a\bar{\varepsilon}_k^b + \mathrm{Re}[\Delta_k^a(\Delta_k^b)^*]}{E_k^a E_k^b}\right\}. \tag{27}$$

Here, we used the relation $\bar{\varepsilon}_k^a = \varepsilon_k^a - \mu^a$ and $a_k = 2\beta^a E_k^a$, $E_k^a = \sqrt{(\bar{\varepsilon}_k^a)^2 + |\Delta_k^a|^2}$, so that $\cosh\frac{a_k}{2} = \cosh(\beta^a E_k^a)$ (and analogously for $q_b = (V_b, T_b)$). Note the explicit dependence of all the quantities on the temperature and the coupling strength, given through the superscripts a and b, denoting two parameter points $q_a = (T_a, V_a)$ and $q_b = (T_b, V_b)$.

Assuming that the chemical potential is also constant ($\mu = \varepsilon_F$) in the region of interest, where the phase transition takes place, the gap parameter reduces to $\Delta_k = \Delta$, for $|\bar{\varepsilon}| < \hbar\omega_D$ (and zero otherwise). Thus, the self consistent equation for the gap $\Delta_k = -\sum_{k'} V_{kk'}\frac{1-2f(E_{k'})}{2E_{k'}}\Delta_{k'}$ reads as ($1-2f(E_{k'}) = \tanh\frac{\beta E_{k'}}{2}$):

$$1 = D_F V \int_{-\hbar\omega_D}^{\hbar\omega_D} d\varepsilon\, \frac{\tanh\frac{\beta}{2}\sqrt{\varepsilon^2+\Delta^2(T,V)}}{2\sqrt{\varepsilon^2+\Delta^2(T,V)}}, \tag{28}$$

with $f(E)$ being the Fermi distribution.

In the $T \to 0$ limit, we obtain the expression for the ground state fidelity $F(|g_a\rangle\langle g_a|, |g_b\rangle\langle g_b|) = |\langle g_a|g_b\rangle|$. At zero temperature, the chemical potential is equal to the Fermi energy ε_F, $\mu(T=0) = \varepsilon_F$. Further, the gap equation reduces to $\Delta(V) = \hbar\omega_D/(\sinh\frac{2}{D_F V}) \simeq 2\hbar\omega_D\exp(-2/D_F V)$, where D_F is the density of states around the Fermi level. The zero temperature ground state fidelity is $F(|g_a\rangle\langle g_a|, |g_b\rangle\langle g_a|) = \prod_k \frac{1}{\sqrt{2}}\left(1+\frac{(\varepsilon_k-\varepsilon_F)^2+\Delta(V_a)\Delta(V_b)}{\sqrt{(\varepsilon_k-\varepsilon_F)^2+\Delta(V_a)^2}\sqrt{(\varepsilon_k-\varepsilon_F)^2+\Delta(V_b)^2}}\right)^{1/2}$, which matches the expression one obtains for $T=0$. In other words, we see that, as in the case of the Stoner-Hubbard model, the point of criticality of the $T=0$ QPT can be inferred from the mixed state fidelity between the thermal states. The phase transition from superconductor to normal metal happens at $V=0$. Thus, for $V_a \to 0_+$ and $V_b = V_a + \delta V \to \delta V > 0$, the fidelity between the corresponding ground states of Fermi sea $|g_F\rangle$ and the BCS superconductor $|g_{BCS}\rangle$ becomes: $|\langle g_F|g_{BCS}\rangle| = \prod_k \frac{1}{\sqrt{2}}\left(1+\frac{|\varepsilon_k-\varepsilon_F|}{\sqrt{(\varepsilon_k-\varepsilon_F)^2+\Delta(\delta V)^2}}\right)^{1/2}$. We see that the BCS model at $T=0$ features the Anderson orthogonality catastrophe, just as the Stoner-Hubbard model.

As in the previous case, in obtaining the numerical results for the fidelity, we used the subroutine hybrd.f from MINPACK [22]. Again, all the numerical results are given in rescaled quantities $T \to k_B T/(\hbar\omega_D)$, $V \to D_F V$ and $\Delta \to \Delta/(\hbar\omega_D)$. The result for the gap is given on Fig. 5. The line of the phase transition is clearly marked as the line along which the gap becomes non-trivial, and is presented on Fig. 6. Finally, the fidelity, with $\delta T = 0, \delta V = 10^{-3}$, is plotted on Fig. 7. We varied the parameter differences δT and δV, and all the results obtained show the same qualitative picture – the fidelity exhibits a sudden drop from $F=1$ precisely along the line of the phase transition.

As already discussed, in the case of mutually commuting Hamiltonians, the fidelity reduces to the quantity

$$C(\hat{\rho}_a,\hat{\rho}_b) = \frac{Z(\hat{\bar{H}})}{\sqrt{Z(\hat{\bar{H}}+\frac{\Delta\hat{H}}{2})Z(\hat{\bar{H}}-\frac{\Delta\hat{H}}{2})}} \tag{29}$$

which, through relation (18), establishes the connection between the singular behavior of the fidelity and the corresponding susceptibility (or the heat capacity, etc.). In the non-commuting case, the same relation between $C(\hat{\rho}_a,\hat{\rho}_b)$ and χ is still valid (see Appendix 4), yet the fidelity is in general *not* identically equal to C.

If we approach a line of the phase transition along a curve $q = q(\alpha)$, $\alpha \in \mathbb{R}$, we find: $F = C(1+\mathcal{F}d\alpha^2)$, where $d\alpha$ defines the difference δq. For reasons of simplicity, we omit here the explicit, lengthy expression for $\mathcal{F}$. Although relatively complicated and difficult to study directly, it is evident that, apart from the Hamiltonian's eigenvalues, it is also explicitly given by the rate of change, with respect to α, of the Hamiltonian's eigenbasis. This is also evident from the fact that for the case of mutually commuting Hamiltonians, when the eigenbasis is common, $C \equiv F$ and thus $\mathcal{F} \equiv 0$. In the commuting case, the change of state is given by the change of the Hamiltonian's eigenvalues

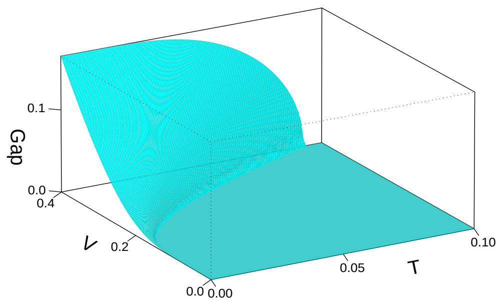

FIG. 5: (color online) The gap $\Delta = \Delta(T, V)$ as a function of the temperature T and the coupling constant V. The plot is given in rescaled quantities $T \rightarrow k_B T/(\hbar\omega_D)$, $V \rightarrow D_F V$ and $\Delta \rightarrow \Delta/(\hbar\omega_D)$.

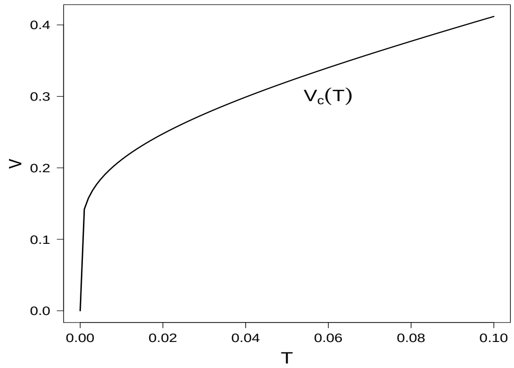

FIG. 6: (color online) The critical line $V_c = V_c(T)$ as a function of the temperature T. The plot is given in rescaled quantities $T \rightarrow k_B T/(\hbar\omega_D)$ and $V \rightarrow D_F V$.

only, while in the non-commuting case, the overall change of state is given by the change of *both* the eigenvalues and the eigenvectors. Thus, the singularity of $\mathcal{F}$ can on its own mark the drastic change in the structure of the system's eigenbasis, thus bringing about the finite difference between C and F. This is indeed the case for BCS superconductors, where the difference $C - F$ becomes non-trivial precisely along the line of the phase transition, where $C < F$, see Fig. 8. We see that, as intuitively expected, the state of a system exhibits an abrupt change in its structure along the line of the phase transition both in terms of its eigenvalues, as well as in terms of its eigenstates (for the structural analysis of the system's eigenstates given by a parametrized Hamiltonian $\hat{H}(q)$, see for example [23] and [24]).

Another way to quantify the structural change of the eigenvectors is through the Uhlmann connection and the corresponding mixed-state geometric phase [19], the mixed-state generalization of the Berry connection and phase. The fidelity $F(\hat{\rho}_a, \hat{\rho}_b) = \mathrm{Tr}\sqrt{\sqrt{\hat{\rho}_a}\hat{\rho}_b\sqrt{\hat{\rho}_a}}$ can also be expressed as $F(\hat{\rho}_a, \hat{\rho}_b) = \mathrm{Tr}\left[|\sqrt{\hat{\rho}_a}\sqrt{\hat{\rho}_b}|\right]$, where $|\hat{A}| = (\hat{A}\hat{A}^\dagger)^{1/2}$ represents the modulus of the operator $\hat{A}$ (see [25]). The Uhlmann parallel transport condition (i.e. the connection) is given by the unitary operator $\hat{U}_{ab}$, such that $F(\hat{\rho}_a, \hat{\rho}_b) = \mathrm{Tr}\left[\sqrt{\hat{\rho}_a}\sqrt{\hat{\rho}_b}\hat{U}_{ab}\right]$ (see equation (9) from [25]). In other words, the connection operator defining the parallel transport is the inverse of the unitary $\hat{V}_{ab}$, given by the polar decomposition [1] $\sqrt{\hat{\rho}_a}\sqrt{\hat{\rho}_b} = |\sqrt{\hat{\rho}_a}\sqrt{\hat{\rho}_b}|\hat{V}_{ab}$, i.e. $\hat{U}_{ab} = \hat{V}_{ab}^\dagger$. Note that the parallel transport condition (the connection), given by $\hat{U}_{ab}$, induces both the local Uhlmann curvature two-form, as well as the global mixed-state geometric phase

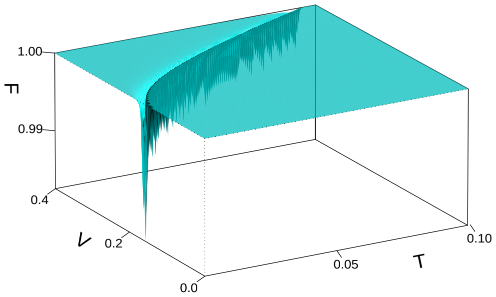

FIG. 7: (color online) The fidelity $F = F(T, V)$ as a function of the temperature T and the coupling constant V. The plot is given in rescaled quantities $T \to k_B T/(\hbar\omega_D)$ and $V \to D_F V$, with $\delta T = 0, \delta V = 10^{-3}$.

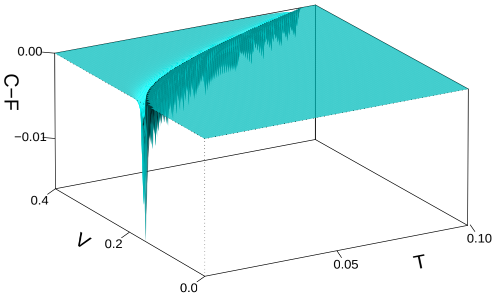

FIG. 8: (color online) The difference $C(T, V) - F(T, V)$ as a function of the temperature T and the coupling constant V. The plot is given in rescaled quantities $T \to k_B T/(\hbar\omega_D)$ and $V \to D_F V$, with $\delta T = 0, \delta V = 10^{-3}$.

(see equations (11) and (12) from [25]). Let us define

$$H(\hat{\rho}_a, \hat{\rho}_b) = \mathrm{Tr}\left[\sqrt{\hat{\rho}_a}\sqrt{\hat{\rho}_b}\right]. \tag{30}$$

Obviously, in the case of mutually commuting Hamiltonians $H = F(= C)$ and the Uhlmann connection is trivial, $\hat{U}_{ab} = \hat{I}$. In the case of the BCS model, we have evaluated the quantity $H - F$, and the result is qualitatively the same as for $C - F$. In other words, along the line of the phase transition we have found the strict inequality $H - F = \mathrm{Tr}\left[|\sqrt{\hat{\rho}_a}\sqrt{\hat{\rho}_b}|(\hat{U}_{ab} - \hat{I})\right] < \mathrm{const} < 0$. From the Cauchy-Schwarz inequality it follows then that $\hat{U}_{ab} - \hat{I} \neq 0$, or $\hat{U}_{ab} \neq \hat{I}$ – a clearly abrupt change of the connection operator $\hat{U}_{ab}$ occours and it becomes non-trivial in the vicinity of the line of the phase transition. Since the two parameter points q_a and q_b are taken to be close to each other, such a behavior implies the non-analyticity of the local Uhlmann curvature form along the line of the phase transition, which in turn results in generally non-trivial global Uhlmann mixed-state geometric phase (see for example the discussions in [13] and [14]). This can be seen as a mixed thermal state generalization of recent results [15] on the relation between QPTs and Berry geometric phases. Further, we have that along the line of the phase transition we have $C < H < F$, while $C \simeq H \simeq F \simeq 1$ otherwise.

CONCLUSION

In this paper we analyzed the fidelity approach to both zero temperature (quantum) as well as finite temperature phase transitions. It is based on the notion of quantum state distinguishability, applied to the case of macroscopic many-body systems whose states determine the global order of the system and its phase. We focused on the two particular cases of the Stoner-Hubbard model for itinerant electron magnetism and the BCS theory of superconductivity, as representatives of two distinct classes of physical systems: those defined by a set of mutually commuting Hamiltonians and those defined by mutually *non*-commuting Hamiltonians, with respect to a given parameter space. We found that in both cases the fidelity can mark the regions of PTs by its sudden drop in the vicinity of the transition line. We discussed in detail the general case of mutually commuting Hamiltonians, where in the case of symmetry-breaking LGW type of transitions the non-analyticity of fidelity is a direct consequence of the non-analyticity of the corresponding "generalized" susceptibility. The case of mutually non-commuting Hamiltonians is more complex as there the structure of the Hamiltonian's eigenvectors directly affects the system's thermal state thus introducing a novel feature relevant for the macroscopic phase distinguishability. On the example of the BCS superconductivity we showed that the phase transition is accompanied by the abrupt change of the Hamiltonian's eigenvectors, quantified by the differences $C-F$ and $H-F$. The second one is of particular interest as it determines the Uhlmann connection and the associated mixed-state geometric phase, which generically becomes non-trivial in the vicinity of the phase transition only – a mixed state generalization of the emergence of non-trivial Berry geometric phase in the vicinity of criticality for QPTs.

There are two main extensions of this work. First, the study of more general phase transitions that fall outside the standard symmetry-breaking LGW paradigm. Second, the general study of the structural analysis of the system's eigenstates in the case of mutually non-commuting Hamiltonians, given within the framework of the mixed state fidelity and the Uhlmann geometric phase.

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APPENDIX 1

In this Appendix we prove various technical statements relevant for the analysis of the ground state fidelity in the Stoner-Hubbard model.

- **Proving the relation $\varepsilon_F = \tilde{\varepsilon}_{k_{F\uparrow}} = \tilde{\varepsilon}_{k_{F\downarrow}}$:**

  Using $N_\sigma = \int_0^{N_\sigma} dN_\sigma$, the ground state energy can be written as:

$$E_g = \int_0^{N_\uparrow} E_{k\uparrow} dN_\uparrow + \int_0^{N_\downarrow} E_{k\downarrow} dN_\downarrow - U\frac{N_\uparrow N_\downarrow}{V} = \int_0^{N_\uparrow} \varepsilon_k dN_\uparrow + \int_0^{N_\downarrow} \varepsilon_k dN_\downarrow + U\frac{N_\uparrow N_\downarrow}{V}. \tag{31}$$

  Since it is the local minima, for given $N = N_\uparrow + N_\downarrow$ we have that:

$$\begin{aligned} \frac{\partial(E_g - \mu N)}{\partial N_\uparrow} &= \varepsilon_{k_F\uparrow} - \mu + U\frac{N_\downarrow}{V} = 0, \\ \frac{\partial(E_g - \mu N)}{\partial N_\downarrow} &= \varepsilon_{k_F\downarrow} - \mu + U\frac{N_\uparrow}{V} = 0, \end{aligned} \tag{32}$$

  and we immediately get $E_{k_{F\uparrow}} = \varepsilon_{k_F\uparrow} + Un_\downarrow = \varepsilon_{k_F\downarrow} + Un_\uparrow = E_{k_{F\downarrow}} = \varepsilon_F$, with $\mu = \varepsilon_F$, for $T = 0$.

- **Deriving U_c from Stoner criterion:**

  The density of states is defined as $D(\varepsilon) = \frac{1}{V}\frac{dN_\sigma}{d\varepsilon}$ in the paramagnetic phase, where ε is the one-particle energy and $N_\sigma(\varepsilon)$ is the number of states for each spin direction whose energy is smaller or equal than ε. For each spin projection, we have $N_\sigma/V = k_F^3/(6\pi^2)$, while from $\varepsilon(k) = \frac{\hbar^2}{2m}k^2$ we have that $k = (\frac{2m}{\hbar^2}\varepsilon)^{1/2}$. Thus, $\frac{N_\sigma(\varepsilon)}{V} = \frac{1}{6\pi^2}(\frac{2m}{\hbar^2}\varepsilon)^{3/2}$ and:

$$D(\varepsilon) = \frac{1}{V}\frac{dN_\sigma(\varepsilon)}{d\varepsilon} = \frac{3}{2}\frac{1}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon} = \frac{3}{2\varepsilon}\frac{N_\sigma}{V} = \frac{3}{4\varepsilon}\frac{N}{V}. \tag{33}$$

The difference between the up and down single particle energies $E_{k\uparrow}$ and $E_{k\downarrow}$ defines the self consistent magnetic field $\Delta = 2U\frac{M(\Delta)}{V}$. The phase transition occurs when Δ becomes non-zero, leading to the equation $1 = \frac{2U_c}{V}\frac{\partial M}{\partial \Delta}|_{\Delta=0}$, which also gives the vanishing of the susceptibility denominator in the random phase approximation (Stoner enhancement factor) [20]. One has then $U_c D_F = 1$, and therefore we find $U_c = \frac{1}{D_F} = \frac{4}{3}\varepsilon_F\frac{V}{N}$.

- **Deriving U_c from (9) and (10):**

  Using $x = k_{F\uparrow}$, $y = k_{F\downarrow}$, equation (9) can be rewritten as $f(x,y) \equiv x^3 + y^3 - a = 0$, with $a = 6\pi^2\frac{N}{V} \equiv 2k_F^3$. Also, the quadratic term from equation (10) that is for $U > U_c$ responsible for non-trivial magnetic solutions reads as $g(x,y;U) \equiv (x+y) - \frac{U}{\alpha}(x^2 + xy + y^2) = 0$, with $\alpha = 3\pi^2\frac{\hbar^2}{m} \equiv \frac{3}{2}k_F U_c$.

  First, we show that for $U > U_c$ (see equation (8)), curves f and g have intersection in two points, symmetric with respect to the $y = x$ line, while for $U = U_c$ they touch precisely in the point $(x,y) = (k_F, k_F)$. In the coordinate system $(\bar{x},\bar{y})$, rotated by the angle $\varphi = \pi/4$ and translated by the vector (A,0) from the system (x,y), the curve $g(\bar{x},\bar{y};U) = 0$ becomes [34]:

$$\frac{\bar{x}^2}{A^2} + \frac{\bar{y}^2}{B^2} = 1, \tag{34}$$

  with $A = \frac{\sqrt{2}}{3}\frac{k_F}{U}$ and $B = \sqrt{\frac{2}{3}\frac{k_F}{U}}$ – a real ellipse with the main axes $A = A(U)$ and $B = B(U)$. As the parameter U increases from 0 (when $A, B \to \infty$), the main axes A and B decrease and eventually the ellipse g touches the curve f in the point $(\bar{x},\bar{y}) = (2A, 0)$, which in the original coordinate system correspond to the point $(x,y) = (k_F, k_F)$. In other words, $2A = \sqrt{2}k_F$ and $U = U_c$. Further increase of U beyond U_c results in even smaller ellipses that intersect the curve f in two symmetric points (note that the curve f is itself symmetric along the $y = x$ line).

  To show that for $U > U_c$ the "balanced" solutions of (9) and (10) are indeed the physical ones, we calculate the total ground state energy E_g of the system:

$$E_g = V\int_{E_{0\uparrow}}^{E_{F\uparrow}} \tilde{\varepsilon}_{k\uparrow} D(E_{k\uparrow})dE_{k\uparrow} + V\int_{E_{0\downarrow}}^{E_{F\downarrow}} E_{k\downarrow}D(E_{k\downarrow})dE_{k\downarrow} - VUn_\uparrow n_\downarrow. \tag{35}$$

  Upon evaluating the above integrals, using $M = (N_\uparrow - N_\downarrow)/2$, the total ground state energy reads:

$$E_g = \frac{V}{20\pi^2}\frac{\hbar^2}{m}\left(3\pi^2\frac{N}{V}\right)^{5/3}\left[\left(1 + \frac{2M}{N}\right)^{5/3} + \left(1 - \frac{2M}{N}\right)^{5/3}\right] + \frac{UN^2}{4V}\left[1 - \left(\frac{2M}{N}\right)^2\right]. \tag{36}$$

  From the above expression, we see that for every value of the coupling constant U, $\frac{\partial E_g}{\partial M}(U, M = 0) = 0$, while $\frac{\partial^2 E_g}{\partial M^2}(U, M = 0)$ changes the sign from positive to negative precisely in $U = U_c$. Thus, we indeed have that for $U > U_c$ the "balanced" magnetic solutions with $M \neq 0$ have lower energy.

- **Deriving the maximum fidelity, i.e. the maximum derivative dk_F/dU for $U = U_c$, from (9) and (10):**

  From $df = 0$ and $dg = 0$, we get ($\frac{\partial f}{\partial x} = f_x$, $\frac{dx}{dU} = \dot{x}$, etc.):

$$\begin{aligned} f_x\dot{x} + f_y\dot{y} &= 0, \\ g_x\dot{x} + g_y\dot{y} &= -g_u. \end{aligned} \tag{37}$$

  Solving it for $\dot{x}$ and $\dot{y}$, we obtain:

$$\begin{bmatrix} \dot{x} \\ \dot{y} \end{bmatrix} = \frac{g_u}{f_x g_y - f_y g_x}\begin{bmatrix} f_y \\ -f_x \end{bmatrix}. \tag{38}$$

Finally:

$$\begin{bmatrix} \dot{x} \\ \dot{y} \end{bmatrix} = \frac{3}{4}\frac{k_f}{D_F V^2}\frac{x+y}{x-y}\frac{1}{xy}\begin{bmatrix} y^2 \\ -x^2 \end{bmatrix}. \tag{39}$$

Thus, in the limit $U \to U_{c+}$ (note that $g(x, y; U) = 0$ is valid for $U \geq U_c$), we have that $x \to k_{F+}$, $y \to k_{F-}$ and $\dot{x} \to +\infty$, $\dot{y} \to -\infty$ (or vice versa, for the $x < y$ solution branch). In other words, $\frac{dV(k_{F\downarrow})}{dU} = 4\pi(k_{F\downarrow})^2 \frac{d(k_{F\downarrow})}{dU} = 4\pi x^2 \dot{x} \to +\infty$ and $\frac{dV(k_{F\uparrow})}{dU} \to -\infty$, or vice versa.

APPENDIX 2

Below, the basic identities of the su(2) algebra of the electron spin operators leading to equation (15) are proven. We discuss operators having a fixed momentum and drop the index k for convenience.

- **$\hat{\vec{S}}$-algebra identities:**

  In general, operators defined by $\hat{S}^a = \hat{c}^\dagger_\alpha S^a_{\alpha\beta}\hat{c}_\beta$, where $\hat{c}^\dagger_\alpha$ and $\hat{c}_\beta$ are either bosonic or fermionic operators and $S^a_{\alpha\beta}$ is a matrix representation of a spin S algebra, i.e. satisfying $[S^a, S^b]_{\alpha\beta} = i\varepsilon^{abc}S^c_{\alpha\beta}$, define a su(2) algebra. This is the case of the electron spin operators defined by $\hat{\vec{S}} = \hat{\Psi}^\dagger \frac{\vec{\sigma}}{2}\hat{\Psi}$, where $\hat{\Psi}^\dagger = [\hat{c}^\dagger_\uparrow \; \hat{c}^\dagger_\downarrow]$ and $\vec{\sigma}$ is the vector of Pauli matrices, and given by $\hat{S}^z = \frac{1}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow)$, $\hat{S}^+ = \hat{c}^\dagger_\uparrow \hat{c}_\downarrow$ and $\hat{S}^- = \hat{c}^\dagger_\downarrow \hat{c}_\uparrow$ (with $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$).

  Using the anti-commutation relations for the one-electron modes $\hat{c}^\dagger_\sigma$, one can easily obtain the following commutation and anti-commutation identities:

  $$\begin{aligned} [\hat{S}^z, \hat{S}^\pm] &= \pm\hat{S}^\pm, \quad [\hat{S}^+, \hat{S}^-] = 2\hat{S}^z, \\ \{\hat{S}^z, \hat{S}^\pm\} &= 0, \quad \{\hat{S}^+, \hat{S}^-\} = \hat{I}_s. \end{aligned} \tag{40}$$

  with $\hat{I}_s \equiv \hat{n}_\uparrow + \hat{n}_\downarrow - 2\hat{n}_\uparrow\hat{n}_\downarrow = (2 - \hat{n})\hat{n}$, $\hat{n} = \hat{n}_\uparrow + \hat{n}_\downarrow$, the projector onto the subspace of the single-occupied states, being an identity operator for this algebra, since $\hat{I}_s^2 = \hat{I}_s$, $\hat{I}_s\hat{\vec{S}} = \hat{\vec{S}}\hat{I}_s = \hat{\vec{S}}$ and $(\hat{\vec{S}})^2 = \frac{3}{4}\hat{I}_s$. One of the immediate consequences of the above commutation relations is that $\{\hat{S}^x, \hat{S}^y, \hat{S}^z\}$ form a su(2) algebra.

  Further, we can obtain the traces: $\mathrm{Tr}[\hat{I}] = 4$, $\mathrm{Tr}[\hat{I}_s] = 2$ and $\mathrm{Tr}[\hat{\vec{S}}] = \vec{0}$.

- **Evaluating $e^{\vec{h}\hat{\vec{S}}}$ and $\mathrm{Tr}[e^{\vec{h}\hat{\vec{S}}}]$:**

  $$e^{\vec{h}\hat{\vec{S}}} = \sum_{n=0}^{+\infty} \frac{1}{n!}(\vec{h}\hat{\vec{S}})^n = \hat{I} + \sum_{n=1}^{+\infty} \frac{1}{n!}(\vec{h}\hat{\vec{S}})^n. \tag{41}$$

  For $(\vec{h}\hat{\vec{S}})^2$, we have:

  $$\begin{aligned} (\vec{h}\hat{\vec{S}})^2 &= [\frac{1}{2}(h^+\hat{S}^- + h^-\hat{S}^+) + h_z\hat{S}^z]^2 \\ &= \frac{1}{4}(h^+)^2(\hat{S}^-)^2 + \frac{1}{4}(h^-)^2(\hat{S}^+)^2 + h_z^2(\hat{S}^z)^2 + \frac{1}{4}(h^+h^-)\{\hat{S}^-, \hat{S}^+\} + \frac{1}{2}(h_z h^+)\{\hat{S}^z, \hat{S}^-\} + \frac{1}{2}(h_z h^-)\{\hat{S}^z, \hat{S}^+\}. \end{aligned} \tag{42}$$

  Using the $\hat{\vec{S}}$-algebra identities (40), we get:

  $$(\vec{h}\hat{\vec{S}})^2 = \frac{1}{4}(h_z)^2\hat{I}_s + \frac{1}{4}(h^+h^-)\hat{I}_s = \frac{1}{4}|h|^2\hat{I}_s, \tag{43}$$

  where [35] $|h|^2 = (h_z)^2 + h^+h^- \equiv h^2$. Thus, we obtain:

  $$e^{\vec{h}\hat{\vec{S}}} = \hat{I} + \sum_{n=1}^{+\infty} \frac{1}{(2n)!}\left(\frac{h}{2}\right)^{2n}\hat{I}_s + \sum_{n=0}^{+\infty} \frac{1}{(2n+1)!}\left(\frac{h}{2}\right)^{2n}(\vec{h}\hat{\vec{S}})$$

$$
\begin{aligned}
&= (\hat{I}-\hat{I}_s) + \left[\sum_{n=0}^{+\infty}\frac{1}{(2n)!}\left(\frac{h}{2}\right)^{2n}\right]\hat{I}_s + \left[\sum_{n=0}^{+\infty}\frac{1}{(2n+1)!}\left(\frac{h}{2}\right)^{2n+1}\right]\frac{2}{h}(\vec{h}\hat{\vec{S}}),\\
e^{\vec{h}\hat{\vec{S}}} &= (\hat{I}-\hat{I}_s) + \cosh\left(\frac{h}{2}\right)\hat{I}_s + 2\sinh\left(\frac{h}{2}\right)\frac{(\vec{h}\hat{\vec{S}})}{h}.
\end{aligned}
\tag{44}
$$

Using the trace formulas, we finally obtain:

$$
\mathrm{Tr}[e^{\vec{h}\hat{\vec{S}}}] = 2\left(1+\cosh\frac{h}{2}\right). \tag{45}
$$

- **Evaluating $e^{\alpha\hat{n}}$ and $\mathrm{Tr}[e^{\alpha\hat{n}}]$:**

  Enlarging the su(2) algebra of the $\hat{\vec{S}}$ operators to the operator $\hat{n} = \hat{n}_\uparrow + \hat{n}_\downarrow$ it is useful to know its algebraic properties and their relation to the other operators. We first evaluate $\hat{n}^k$. Since $\hat{n}_\sigma^2 = \hat{n}_\sigma$ and $\hat{n}^2 = (\hat{n}_\uparrow + \hat{n}_\downarrow)^2 = \hat{n} + 2\hat{n}_\uparrow\hat{n}_\downarrow$ we find that $\hat{n}^3 = -2\hat{n} + 3\hat{n}^2$ and in general $\hat{n}^k = -a_k\hat{n} + b_k\hat{n}^2$, where a_k and b_k satisfy the recurrence equations $a_{k+1} = 2b_k$ and $b_{k+1} = 3b_k - a_k$, leading to: $\hat{n}^k = -(2^{k-1}-2)\hat{n} + (2^{k-1}-1)\hat{n}^2$. The exponential $e^{\alpha\hat{n}}$ is given by:

$$
e^{\alpha\hat{n}} = \hat{I} - \left(\frac{e^{2\alpha}}{2} - 2e^{\alpha} + \frac{3}{2}\right)\hat{n} + \left(\frac{e^{2\alpha}}{2} - e^{\alpha} + \frac{1}{2}\right)\hat{n}^2 = \hat{I} + u\hat{n} + v\hat{n}^2, \tag{46}
$$

  which can be easily verified since $\hat{n} = \hat{n}_\uparrow + \hat{n}_\downarrow$ can only take the values $n = 0, 1, 2$.

  Using the obvious trace relations $\mathrm{Tr}[\hat{n}] = 4$ and $\mathrm{Tr}[\hat{n}^2] = 6$, we also get $\mathrm{Tr}[e^{\alpha\hat{n}}] = 4 + 4u + 6v$, or:

$$
\mathrm{Tr}[e^{\alpha\hat{n}}] = (e^{\alpha}+1)^2. \tag{47}
$$

The number operator commutes with the $\hat{\vec{S}}$ operators, and one has $\hat{n}\hat{I}_s = \hat{I}_s\hat{n} = \hat{I}_s$ and $\hat{n}\hat{\vec{S}} = \hat{\vec{S}}\hat{n} = \hat{\vec{S}}$. Finally, one obtains:

$$
\mathrm{Tr}\left[e^{(\alpha\hat{n}+\vec{h}\hat{\vec{S}})}\right] = \left(1+e^{\alpha+\frac{h}{2}}\right)\left(1+e^{\alpha-\frac{h}{2}}\right) = 2\,e^{\alpha}\left(\cosh\alpha + \cosh\frac{h}{2}\right). \tag{48}
$$

APPENDIX 3

In the following, we obtain the basic formulas for the su(2) algebra of the Nambu operators $\hat{\vec{T}}$ used in evaluating equation (26) for the fidelity between two states of a BCS superconductor in thermodynamical equilibrium.

- **$\hat{\vec{T}}$-algebra identities:**

  We now consider the operators defined by $\hat{\vec{T}} = \hat{\psi}^\dagger\frac{\vec{\sigma}}{2}\hat{\psi}$, where $\hat{\psi}^\dagger = [\hat{c}_\uparrow^\dagger\ \hat{c}_\downarrow]$ and $\vec{\sigma}$ is the vector of Pauli matrices, and given by $\hat{T}^z = \frac{1}{2}(\hat{n}_\uparrow + \hat{n}_\downarrow - 1)$, $\hat{T}^+ = \hat{c}_\uparrow^\dagger\hat{c}_\downarrow^\dagger$ and $\hat{T}^- = \hat{c}_\downarrow\hat{c}_\uparrow$ (with $\hat{T}^\pm = \hat{T}^x \pm i\hat{T}^y$). These operators $\hat{T}^a$ are of the form considered before, since the fermion anti-commutation relations are invariant under the electron-hole transformation, i.e. under the interchange $\hat{c} \leftrightarrow \hat{c}^\dagger$. Similarly to the previous case of the $\hat{\vec{S}}$-algebra, we obtain the commutation and anti-commutation relations:

$$
\begin{aligned}
[\hat{T}^0, \hat{T}^\pm] = \pm\hat{T}^\pm, &\quad [\hat{T}^+, \hat{T}^-] = 2\hat{T}^0,\\
\{\hat{T}^0, \hat{T}^\pm\} = 0, &\quad \{\hat{T}^+, \hat{T}^-\} = \hat{I}_t.
\end{aligned}
\tag{49}
$$

  with $\hat{I}_t \equiv 2\hat{n}_\uparrow\hat{n}_\downarrow - (\hat{n}_\uparrow + \hat{n}_\downarrow) + 1 = (n-1)^2$, the projector onto the subspace of the empty and doubly occupied states, being an identity operator for this algebra, since $\hat{I}_t^2 = \hat{I}_t$, $\hat{I}_t\hat{\vec{T}} = \hat{\vec{T}}\hat{I}_t = \hat{\vec{T}}$ and $(\hat{\vec{T}})^2 = \frac{3}{4}\hat{I}_t$. One of the immediate consequences of the above commutation relations is that $\{\hat{T}^0, \hat{T}^+, \hat{T}^-\}$ form a su(2) algebra. Further, simple algebra gives:

$$
\mathrm{Tr}[\hat{\vec{T}}] = 0, \qquad \mathrm{Tr}[\hat{I}_t] = 2. \tag{50}
$$

Note that in the above definition of $\hat{\psi}^\dagger$, the operators $\hat{c}_\uparrow^\dagger$ and $\hat{c}_\downarrow$ have the opposite momenta, k and $-k$, respectively. Had the momenta been defined to be the same, the two sets of operators $\hat{\vec{S}}$ and $\hat{\vec{T}}$ would commute with each other, i.e. $[\hat{S}^a, \hat{T}^b] = 0$. Also, one would have $\hat{I}_s + \hat{I}_t = \hat{I}$.

- **Evaluating $e^{\vec{a}\hat{\vec{T}}}$ and** $\mathrm{Tr}[e^{\vec{a}\hat{\vec{T}}}]$**:**

$$e^{\vec{a}\hat{\vec{T}}} = \sum_{n=0}^{+\infty} \frac{1}{n!} (\vec{a}\hat{\vec{T}})^n = \hat{I} + \sum_{n=1}^{+\infty} \frac{1}{n!} (\vec{a}\hat{\vec{T}})^n. \tag{51}$$

Similarly to the previous case, for $(\vec{a}\hat{\vec{T}})^2$, we have:

$$(\vec{a}\hat{\vec{T}})^2 = [a_z \hat{T}^0 + \frac{1}{2}(a^+ \hat{T}^- + a^- \hat{T}^+)]^2 = \frac{1}{4}|a|^2 \hat{I}_t, \tag{52}$$

where $|a|^2 = (a_z)^2 + a^+ a^- \equiv a^2$. Thus, we obtain ($\hat{Z}_t = \hat{I} - \hat{I}_t$):

$$\begin{aligned}
e^{\vec{a}\hat{\vec{T}}} &= \hat{I} + \sum_{n=1}^{+\infty} \frac{1}{(2n)!} \left(\frac{a}{2}\right)^{2n} \hat{I}_t + \sum_{n=0}^{+\infty} \frac{1}{(2n+1)!} \left(\frac{a}{2}\right)^{2n} (\vec{a}\hat{\vec{T}}) \\
&= (\hat{I} - \hat{I}_t) + \left[\sum_{n=0}^{+\infty} \frac{1}{(2n)!} \left(\frac{a}{2}\right)^{2n}\right] \hat{I}_t + \left[\sum_{n=0}^{+\infty} \frac{1}{(2n+1)!} \left(\frac{a}{2}\right)^{2n+1}\right] \frac{2}{a} (\vec{a}\hat{\vec{T}}), \\
e^{\vec{a}\hat{\vec{T}}} &= \hat{Z}_t + \cosh\left(\frac{a}{2}\right) \hat{I}_t + 2\sinh\left(\frac{a}{2}\right) \frac{(\vec{a}\hat{\vec{T}})}{a}.
\end{aligned} \tag{53}$$

Using the trace formulas (50), we finally obtain:

$$\mathrm{Tr}[e^{\vec{a}\hat{\vec{T}}}] = 2\left(1 + \cosh\frac{a}{2}\right). \tag{54}$$

- **Evaluating $e^{2\vec{c}\hat{\vec{T}}} = e^{\frac{\vec{a}}{2}\hat{\vec{T}}} e^{\vec{b}\hat{\vec{T}}} e^{\frac{\vec{a}}{2}\hat{\vec{T}}}$ and** $\mathrm{Tr}[e^{\vec{c}\hat{\vec{T}}}]$**:**

From the above formula (54) and the known trigonometric relation $(\cosh\frac{\alpha}{2})^2 = \frac{1}{2}(1 + \cosh\alpha)$, we have that $\mathrm{Tr}[e^{\vec{c}\hat{\vec{T}}}] = 2\left(1 + \cosh\frac{c}{2}\right) = 2\left(1 + \sqrt{\frac{1}{2}(1 + \cosh c)}\right)$. Thus, by evaluating $e^{2\vec{c}\hat{\vec{T}}}$ we obtain the result for $\cosh c$ and therefore $\mathrm{Tr}[e^{\vec{c}\hat{\vec{T}}}]$. First, we obtain the general expression for $e^{\vec{a}\hat{\vec{T}}} e^{\vec{b}\hat{\vec{T}}}$. Using the result (53) for $e^{\vec{a}\hat{\vec{T}}}$ (and analogously for $e^{\vec{b}\hat{\vec{T}}}$), we get:

$$e^{\vec{a}\hat{\vec{T}}} e^{\vec{b}\hat{\vec{T}}} = \hat{Z}_t + \left(\cosh\frac{a}{2}\cosh\frac{b}{2}\right)\hat{I}_t + 2\left[\left(\cosh\frac{a}{2}\sinh\frac{b}{2}\right)\frac{\vec{b}}{b} + \left(\sinh\frac{a}{2}\cosh\frac{b}{2}\frac{\vec{a}}{a}\right)\right]\hat{\vec{T}} + 4\left(\sinh\frac{a}{2}\sinh\frac{b}{2}\right)\frac{\vec{a}\hat{\vec{T}}}{a}\frac{\vec{b}\hat{\vec{T}}}{b}. \tag{55}$$

In deriving the above expression, we have used the above identities (50). As in (52), using (49) we obtain:

$$(\vec{a}\hat{\vec{T}})(\vec{b}\hat{\vec{T}}) = \frac{1}{4}\left[(\vec{a}\vec{b})\hat{I}_t + 2i(\vec{a} \times \vec{b})\hat{\vec{T}}\right]. \tag{56}$$

Therefore, we have:

$$\begin{aligned}
e^{\vec{a}\hat{\vec{T}}} e^{\vec{b}\hat{\vec{T}}} = \hat{Z}_t &+ \left[\left(\cosh\frac{a}{2}\cosh\frac{b}{2}\right) + \left(\sinh\frac{a}{2}\sinh\frac{b}{2}\right)\frac{(\vec{a}\vec{b})}{ab}\right]\hat{I}_t \\
&+ 2\left[\left(\sinh\frac{a}{2}\cosh\frac{b}{2}\right)\frac{\vec{a}}{a} + \left(\cosh\frac{a}{2}\sinh\frac{b}{2}\right)\frac{\vec{b}}{b} + i\frac{(\vec{a}\times\vec{b})}{ab}\right]\hat{\vec{T}}.
\end{aligned} \tag{57}$$

Applying the above result twice, we finally obtain the expression for $e^{2\vec{c}\hat{\vec{T}}}$:

$$
\begin{aligned}
e^{2\vec{c}\hat{\vec{T}}} &= e^{\frac{\vec{a}}{2}\hat{\vec{T}}}e^{\vec{b}\hat{\vec{T}}}e^{\frac{\vec{a}}{2}\hat{\vec{T}}} = \hat{Z}_t + \left[\left(\cosh\frac{a}{2}\cosh\frac{b}{2}\right) + \left(\sinh\frac{a}{2}\sinh\frac{b}{2}\right)\frac{(\vec{a}\vec{b})}{ab}\right]\hat{I}_t \\
&+ \left[\left(\sinh\frac{a}{2}\cosh\frac{b}{2}\right)\frac{\vec{a}}{a} + 2\left(\sinh\frac{b}{2}\right)^2\frac{\vec{b}}{b} + \left(\cosh\frac{a}{2} - 1\right)\left(\sinh\frac{b}{2}\right)\frac{(\vec{a}\vec{b})\vec{a}}{a^2 b}\right]\hat{\vec{T}}.
\end{aligned} \tag{58}
$$

Comparing the above result with the expression (53), we eventually end up with the expression for $\cosh c$:

$$
\cosh c = \left(\cosh\frac{a}{2}\cosh\frac{b}{2}\right) + \left(\sinh\frac{a}{2}\sinh\frac{b}{2}\right)\frac{(\vec{a}\vec{b})}{ab} \tag{59}
$$

which reduces to (27) for particular values of $\vec{a}_k = \vec{\tilde{h}}_k(q_a)$ and $\vec{b}_k = \vec{\tilde{h}}_k(q_b)$.

APPENDIX 4

In this Appendix we prove that in the case of mutually non-commuting Hamiltonians a relation analogous to (18) holds between C, given by equation (29), and the susceptibility χ. As in the commuting case, for simplicity, we consider a Hamiltonian $\hat{H} = \hat{H}_0 - h\hat{S}$ with the symmetry-breaking term $\hat{S}$, and $h = h(q)$. Note that in this case, the two terms in the Hamiltonian *do not commute* with each other, $[\hat{H}_0, \hat{S}] \neq 0$. Thus, we have the following imaginary time Dyson expansion around the point $h = 0$ [36]:

$$
e^{-\beta(\hat{H}_0 - h\hat{S})} \simeq \left\{ e^{-\beta\hat{H}_0} + h\int_0^\beta d\tau e^{-\beta\hat{H}_0}\hat{S}(\tau) + h^2\int_0^\beta d\tau\int_0^\tau d\tau_1 e^{-\beta\hat{H}_0}\hat{S}(\tau)\hat{S}(\tau_1)\right\}, \tag{60}
$$

with $\hat{S}(\tau) = e^{\tau\hat{H}_0}\hat{S}e^{-\tau\hat{H}_0}$. From the above equation, we obtain the expressions for the magnetization $M = \langle\hat{S}\rangle$ and the susceptibility $\chi = \frac{\partial M}{\partial h}$ given by derivatives of the partition function Z. First, the magnetization can be expressed as (using the commutativity between the partial derivative and the trace, $\frac{\partial}{\partial h}\mathrm{Tr}[\cdot] = \mathrm{Tr}\frac{\partial}{\partial h}[\cdot]$):

$$
M = \frac{1}{\beta}\frac{\partial \ln Z}{\partial h} = \frac{1}{\beta}\frac{1}{Z}\frac{\partial Z}{\partial h} = \frac{1}{\beta}\frac{1}{Z}\frac{\partial}{\partial h}\mathrm{Tr}[e^{-\beta\hat{H}}] = \frac{1}{\beta}\frac{1}{Z}\int_0^\beta d\tau\mathrm{Tr}[e^{-\beta\hat{H}_0}e^{\tau\hat{H}_0}\hat{S}e^{-\tau\hat{H}_0}] = \frac{1}{\beta}\int_0^\beta d\tau\mathrm{Tr}[\frac{e^{-\beta\hat{H}_0}}{Z}\hat{S}] = \langle\hat{S}\rangle. \tag{61}
$$

The susceptibility is then:

$$
\chi = \frac{\partial M}{\partial h} = \frac{\partial}{\partial h}\left(\frac{1}{\beta}\frac{1}{Z}\frac{\partial Z}{\partial h}\right) = \frac{1}{\beta}\frac{1}{Z}\frac{\partial^2 Z}{\partial h^2} - \frac{1}{\beta}\frac{1}{Z^2}\left(\frac{\partial Z}{\partial h}\right)^2. \tag{62}
$$

The second term is obviously equal to $\beta M^2 = \beta\langle\hat{S}\rangle^2$, while the first term can be transformed as follows [37]:

$$
\frac{1}{\beta}\frac{1}{Z}\left(\frac{\partial^2 Z}{\partial h^2}\right)_0 = \frac{1}{\beta}\frac{1}{Z}\left(\frac{\partial}{\partial h}\int_0^\beta d\tau\mathrm{Tr}[e^{-\beta\hat{H}}\hat{S}]\right)_0 = \frac{1}{Z}\mathrm{Tr}[\left(\frac{\partial e^{-\beta\hat{H}}}{\partial h}\right)_0\hat{S}] = \frac{1}{Z}\int_0^\beta d\tau\mathrm{Tr}[e^{-\beta\hat{H}_0}\hat{S}(\tau)\hat{S}] = \int_0^\beta d\tau\langle\hat{S}(\tau)\hat{S}\rangle. \tag{63}
$$

Thus, the susceptibility is given by $\chi = \int_0^\beta d\tau[\langle\hat{S}(\tau)\hat{S}\rangle - \langle\hat{S}\rangle^2]$. From this, the Taylor expansion for Z,

$$
Z \simeq Z_0\left\{1 + \beta Mh + \frac{1}{2}\beta^2 M^2 h^2 + \frac{1}{2}\beta\chi h^2\right\}, \tag{64}
$$

is identical to the one obtained for the case of mutually commuting Hamiltonians, and therefore a relation analog to equation (18) holds between C and the susceptibility χ.

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[26] Fidelity is closely related to various distance measures on the set of quantum states: the closer two states are, the more similar (less distinguishable) they are (for an overview of different distance measures induced by the fidelity, see [3]).
[27] The use of the fidelity approach to thermal phase transitions was also suggested in [8].
[28] For the proof of the relation $\varepsilon_F = E_{k_{F\uparrow}} = E_{k_{F\downarrow}}$ see Appendix 1.
[29] In the following, we discuss the case of a 3-dimensional spatial lattice. This treatment could be easily generalized to a different lattice dimensionality.
[30] Strictly speaking, for $U > U_c$ we speak of multi (two-fold) valued functions $k_{F\uparrow}(U)$ and $k_{F\downarrow}(U)$.
[31] For reasons of simplicity, we use formulas for canonical rather than grand canonical ensemble. Introducing chemical potential results only in a "shift" of the one-particle energies from the unperturbed Hamiltonian $\hat{H}_0$.
[32] Note the similarity, and the difference, to the previously introduced operators $\hat{\Psi}_k$.
[33] We use the well known identity $\cosh \frac{c_k}{2} = \sqrt{\frac{1}{2}(1 + \cosh c_k)}$.
[34] Alternatively, we could first translate the coordinate system by the vector $(\sqrt{2}A, \sqrt{2}A)$ and then rotate it by the angle $\varphi = \pi/4$ to obtain the same system $(\bar{x}, \bar{y})$.
[35] Using $A^{\pm} = A_x \pm iA_y$ and $A^0 = A_z$, we can write $\vec{A} = A_x\vec{e}_x + A_y\vec{e}_y + A_z\vec{e}_z = A^+\vec{e}_+ + A^-\vec{e}_- + A^0\vec{e}_0$, where $\vec{e}_{\pm} = \vec{e}_x \pm i\vec{e}_y$ and $\vec{e}_0 = \vec{e}_z$ (and analogously for $\vec{B}$). The scalar product between two vectors is then $\vec{A} \cdot \vec{B} = A_xB_x + A_yB_y + A_zB_z = \frac{1}{2}(A^+B^- + A^-B^+) + A^0B^0$. Therefore, $A_k^2 = A^+A^- + (A^0)^2$.
[36] We consider the particular case of the $h = 0$ expansion, but all the results obtained can be easily generalized for the $h \neq 0$ case.
[37] In order to avoid a possible confusion, here we explicitly denote that the derivatives are taken for $h = 0$.