Finite-Size Studies on the SO(5) Symmetry of the Hubbard Model

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We present numerical evidence for the approximate SO(5) symmetry of the Hubbard model on a 10-site cluster. Various dynamic correlation functions involving the π operators, the generators of the SO(5) algebra, are studied using exact diagonalization, and are found to possess sharp collective peaks. Our numerical results also lend support to the interpretation of the recent resonant neutron scattering peaks in the YBCO superconductors in terms of the Goldstone modes of the spontaneously broken SO(5) symmetry. Perturbations such as longer-ranged hoppings and interactions do not suppress the π resonance in interesting parameter regimes. [S0031-9007(97)04845-X]

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Although the single band Hubbard model has been extensively studied in recent years in connection with high-T_c superconductivity, its low-energy content has so far eluded both analytical and numerical investigations. While being deceptively simple, this model may have many possible competing ground states, and it has proved to be very difficult to organize the low-energy degrees of freedom. Recently, a new analytic approach based on a symmetry principle has been suggested. It was noticed that the Hubbard model enjoys an approximate SO(5) symmetry, unifying antiferromagnetism (AF) with d-wave superconductivity (SC) [1]. This symmetry principle gives a simple description of the transition from an AF ground state to a SC ground state as the chemical potential is varied, and it gives a unified treatment of the low-energy collective degrees of freedom of the Hubbard model.

Motivated by its potential importance to the high-T_c problem, we undertake a numerical finite size study to test this approximate symmetry in the single band Hubbard model. The central object of our study is the so-called π operator defined as follows:

$$\pi_{s/d}^{\dagger} = \sum_{\mathbf{k}} (\cos k_x \pm \cos k_y) c_{\mathbf{k}+\mathbf{Q},\uparrow}^{\dagger} c_{-\mathbf{k},\uparrow}^{\dagger}, \qquad \mathbf{Q} = (\pi, \pi). \tag{1}$$

This operator carries spin 1, charge 2, and total momentum (π, π). Charge conjugation and spin lowering operation gives five other similar operators. Here the subscript $\alpha = s, d$ refers to the internal s-wave or d-wave symmetry of this composite operator. The π operators were first introduced by Demler and Zhang [2] to explain the resonant neutron scattering peaks in the YBCO superconductors [3], and are constructed by following the analogy with the η operators considered by Yang [4]. More recently, it was found [1] that together with the total spin and charge operators, the six π operators form the generators of the SO(5) algebra, and furthermore, they rotate AF and SC order parameters into each other. In Refs. [1,2], it was argued that the π_d operators are approximate eigenoperators of the Hubbard Hamiltonian. This implies that the SO(5) symmetry is an approximate symmetry of the Hubbard model [1], and one can use it to constrain the form of the low-energy effective Hamiltonian. Numerical evidence for an approximate SO(5) symmetry and for superspin multiplets in the t-J model has recently been found by Eoler, Hanke, and Zhang [5].

In this Letter, we present exact numerical diagonalization studies of the dynamic correlation functions involving the π operators and the AF and SC order parameters. We verify that the π operators are approximate eigenoperators of the Hubbard model, and show that the properties of the various mixed correlation functions are consistent with the anticipated pattern of the SO(5) symmetry breaking. Our exact numerical calculation is performed on a $\sqrt{10} \times \sqrt{10}$ site Hubbard cluster, using standard exact diagonalization (ED) methods based on the Lanczos algorithm [6].

Let us first consider the autocorrelation function of the π operators, defined as follows:

$$\pi_{\alpha}^{+}(\omega) = -\frac{1}{\pi} \Im \langle \Psi_0^N | \pi_{\alpha} \frac{1}{\omega - H + E_0^{N+2} + i\eta} \times \pi_{\alpha}^{\dagger} | \Psi_0^N \rangle. \tag{2}$$

Here H is the standard Hubbard Hamiltonian, $|\Psi_0^N\rangle$ its ground state with N electrons, and E_0^N the corresponding ground state energy. $\Im$ takes the imaginary part of a correlation function. Throughout this paper, we measure the energy of a spectral function from the ground state energy of the intermediate state. Since $\pi_{s/d}^{\dagger}$ changes particle number by two, the natural energy scale of the intermediate states is the ground state energy of a $N + 2$ electron system.

Figures 1(a) and 1(b) plot the $\pi_d^{+}(\omega)$ correlation function for $U = 8t$, with electron densities $\langle n \rangle = 0.6$ and 0.8, respectively. We see that these dynamic correlation functions are dominated by a sharp peak, well separated from a higher energy continuum. If $\pi_d^{\dagger}$ was an exact eigenoperator of the Hubbard Hamiltonian, its dynamical

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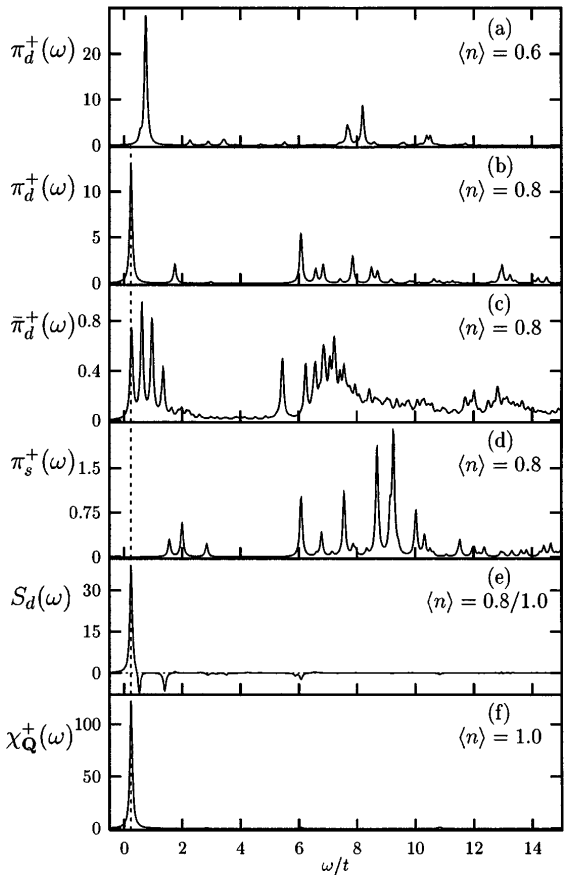

FIG. 1. Dynamic correlation functions of the $\sqrt{10} \times \sqrt{10}$ Hubbard model with $U = 8t$: (a) $\pi_d^+(\omega)$ spectrum at $\langle n\rangle = 0.6$, (b) $\pi_d^+(\omega)$ spectrum at $\langle n\rangle = 0.8$, (c) bubble approximation to $\pi_d^+(\omega)$ as shown in (b), (d) $\pi_s^+(\omega)$ at $\langle n\rangle = 0.8$, (e) off-diagonal correlation function $S_d(\omega)$ at $\langle n\rangle = (0.8/1.0)$, as defined in the text, and (f) spin correlation function $\chi_{\mathbf{Q}}^+(\omega)$.

autocorrelation function should consist of a single peak. Here we see that it is only an approximate eigenoperator in the sense that there is also a high-energy continuum in addition to the resonance peak. The ratio of the spectral weight under the peak to the total spectral weight is found to be 0.63, 0.68 for $U = 4t$ and 0.46, 0.31 for $U = 8t$ in Figs. 1(a) and 1(b), respectively. The separation between the peak and the continuum, and the large relative spectral weight of the peak demonstrate that the $\pi_d^\dagger$ operator is an eigenoperator of the Hubbard model to a good degree of approximation. The energies of these peaks are $1.06t$, $0.66t$ ($U = 4t$), $0.55t$, and $0.24t$ ($U = 8t$), respectively, and *scale inversely with* U.

We see that the qualitative features of our ED agrees with the t-matrix calculation of Ref. [2]. Our ED show that *the* $\pi_d^+(\omega)$ *correlation function is indeed dominated by a single peak whose spectral weight is proportional to the hole density* $1 - n$. *Furthermore, the energy of the* π *resonance peak is also proportional to the hole density, with a scale comparable to the AF exchange* $J = 4t^2/U$.

The π resonance is a composite particle made out of two electrons. Near half-filling, it is very difficult for a single electron or hole to propagate coherently. In view of this fact, it is rather surprising that a two electron Green's function $\pi_d^+(\omega)$ has a coherent peak. To demonstrate that the π peak is a genuine collective behavior, we plot in Fig. 1(c) the bubble approximation to the $\pi_d^+(\omega)$ correlation function. This approximation to $\pi_d^+(\omega)$ consists of a particle-particle bubble with a fully dressed one particle Green's function (of the $\sqrt{10} \times \sqrt{10}$) site cluster inside the bubble. It fully takes into account the single-particle dressing effects, only the vertex correction is neglected. From these figures, we see that the bubble approximation yields a broad spectral distribution, without any identifiable resonance peak. The height of the broad spectral distribution is 1 order of magnitude less than the height of the π peak found in the full calculation. *This calculation demonstrates that the collective behavior, or in other words, the vertex correction, is responsible for the existence of the* π *resonance.*

Figure 1(d) gives the result for $\pi_s^+(\omega)$ at $U = 8t$ at density $n = 0.8$. The spectrum is broadly distributed and no resonance peak can be identified. We interpret this result as evidence that in contrast to $\pi_d^\dagger$, $\pi_s^\dagger$ is not an approximate eigenoperator of the Hubbard model near half-filling. This result is consistent with the conclusion of the t-matrix calculation [2]. The crucial difference between the $\pi_d^+(\omega)$ and $\pi_s^+(\omega)$ correlation function has recently been used by Zhang [1] to argue that *there is an approximate symmetry between AF and d-wave SC, but no symmetry between AF and extended s-wave SC near half-filling.*

In the YBCO superconductors [3], below the superconducting transition temperature T_c, a resonance peak appears in the polarized neutron scattering amplitude with momentum transfer (π, π), and a resonance energy of 25, 33, and 41 meV, depending on doping. Demler and Zhang [2] identified this experimental feature with the π resonance, and showed that the particle-particle π resonance can be mixed into the particle-hole channel below T_c, and therefore appear in the neutron scattering cross section. A number of other theoretical papers [7] explain the experimental feature in terms of a particle-hole threshold behavior near the superconducting gap or possible excitonic states inside the gap. More recently, the π resonance has been interpreted more broadly by Zhang [1] as the Goldstone boson associated with the spontaneous breaking of the SO(5) symmetry below T_c.

In this Letter, we test the ideas of Refs. [1,2] by studying the mixed correlation functions involving the spin-density-wave order parameter

$$S_{\mathbf{Q}}^+ = \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q},\uparrow}^\dagger c_{\mathbf{k},\downarrow}, \qquad S_{\mathbf{Q}}^- = S_{\mathbf{Q}}^{+\dagger}, \tag{3}$$

and the π_d operator, defined by

$$S_d(\omega) = -\frac{1}{\pi}\Im\langle\Psi_0^{N-2}|\left(\pi_d \frac{1}{\omega - (H - E_0^N) + i\eta} S_{\mathbf{Q}}^+ - S_{\mathbf{Q}}^+ \frac{1}{\omega - (H - E_0^{N-2}) + i\eta}\pi_d\right)|\Psi_0^N\rangle, \tag{4}$$

and the dynamical spin correlation function itself, defined by

$$\chi^{+}_{\mathbf{Q}}(\omega) = -\frac{1}{\pi}\Im\langle\Psi_0^N|S^{-}_{\mathbf{Q}}\frac{1}{\omega - (H - E_0^N) + i\eta} \times S^{+}_{\mathbf{Q}}|\Psi_0^N\rangle. \quad (5)$$

The correlation function $S_d(\omega)$ satisfies an important exact sum rule

$$\int_{-\infty}^{\infty} d\omega\, S_d(\omega) = 2\langle\Psi_0^{N-2}|\Delta_d|\Psi_0^N\rangle, \quad (6)$$

where $\Delta_d = \sum_{\mathbf{k}}(\cos k_x - \cos k_y)c_{\mathbf{k},\uparrow}c_{-\mathbf{k},\downarrow}$ is the d-wave superconducting order parameter. This sum rule follows from the fact that the π_d operator is an SO(5) symmetry generator which rotates the AF order parameter into the d-wave SC order parameter [1]. Mixed correlation functions like $S_d(\omega)$, which involve a symmetry generator and an order parameter, are commonly used to prove the Goldstone theorem on the Goldstone bosons associated with spontaneous symmetry breaking [8].

In Fig. 1(e) $S_d(\omega)$ is plotted for $U = 8t$, for electron density between $n = 0.8$ and $n = 1$. We see that the spectrum is dominated by a single peak with relative weight 0.72, located at the same energy as the π resonance. We also verified that the sum rule (6) is satisfied by explicitly computing the d-wave order parameter defined on the right-hand side. Therefore, our result shows that *the 10-site Hubbard cluster at densities between $n = 0.8$ and $n = 1$ possesses considerable d-wave SC fluctuations, and furthermore, there is indeed a Goldstone pole associated with this spontaneous symmetry breaking, consistent with the SO(5) theory [1].* The finite energy of the Goldstone pole results from the fact that the SO(5) is not only broken spontaneously by the SC order parameter, but also broken explicitly by the chemical potential [1]. We also calculated $S_d(\omega)$ between the densities $n = 0.6$ and $n = 0.8$ and found it to be nearly zero. Similarly, the mixed correlation function $S_s(\omega)$ involving the π_s and $S^{+}_{\mathbf{Q}}$ operators vanishes for all densities. This result is consistent with other numerical evidence for d-wave pairing fluctuations in the Hubbard model [9].

Finally, we show our calculation for the spin correlation function $\chi^{+}_{\mathbf{Q}}(\omega)$ in Fig. 1(f) for $U = 8t$ at density $n = 1$. We see that *there is a sharp resonance feature at the same energy as the π resonance.* The fact that all three correlation functions $\pi_d^{+}(\omega)$, $S_d(\omega)$, and $\chi^{+}_{\mathbf{Q}}(\omega)$ have resonance peaks at the same energy demonstrates that the peak in the spin correlation function $\chi^{+}_{\mathbf{Q}}(\omega)$ has a finite overlap with the particle-particle intermediate state $\pi_d^{\dagger}|\Psi_0^{N-2}\rangle$. Because of the finiteness of the mixed correlation function $S_d(\omega)$ and the right-hand side of equation (6), a particle-particle excitation at density $n = 0.8$ makes a finite contribution to the spin correlation function at $n = 1$. This feature confirms the argument of Ref. [2] (see also Ref. [10]).

Work on larger systems (4×4) is in progress to systematically check the finite-size dependence. While the analysis for the 4×4 cluster is rather involved because of multiplet splittings, preliminary results at lower electron density ($n \leq 0.625$) indicate that the overall features are similar: In all systems studied so far, the π_d resonance has a sharply defined low-energy peak, which is well separated from a higher-energy continuum. The separation is large compared to the energy scale of the resonance and, therefore, likely to survive in larger systems.

Recently, Greiter [11] and Baskaran and Anderson [12] raised some questions concerning the compatibility between the Mott-Hubbard gap and the approximate SO(5) symmetry as well as questions concerning the effect of an additional diagonal hopping t' and nearest-neighbor Coulomb interaction V.

Greiter argued that there is no low-energy π resonance. Instead the energy of the π particle should be of order U. Figure 2 displays our ED results for the π resonance as a function of U at various fillings between $\langle n\rangle = 0.2$ to 0.8. We clearly see that the resonance energy scales with $1/U$ and not with U. This result can straightforwardly be understood in strong coupling: because of the spin triplet nature of the π operator, the mutual interaction among the inserted electrons is of order J. If both electrons go into empty sites, there is—in analogy to the quasiparticle band in the doped single-particle spectrum—a finite spectral weight at low energy of the order of J. If, on the other hand, one or both of the inserted electrons go into sites already occupied, the energy of the π-pair will be of order U or $2U$, respectively. Both the low-energy excitations, i.e., the sharp π resonance and also these high-energy excitations with small weight distributed around U, can be detected in Figs. 1(a) and 1(b). However, it is the low-energy π peak which makes a finite contribution to the spin correlation function, and it is the primary object of interest.

Next, we consider the effect of a nearest-neighbor interaction $H_V = V\sum_{\langle i,j\rangle} n_i n_j$, where n_i denotes the electron density at site i, on the approximate SO(5) symmetry [12]. In the left panel of Fig. 3, we compare spectra of the $S_z = 0$ member of the $\pi_d^{\dagger}$ operators with the zero-momentum pair operator $\Delta_d^{\dagger}$ for different values of V, with densities $\langle n\rangle = 0.8$. The energies of the dominant

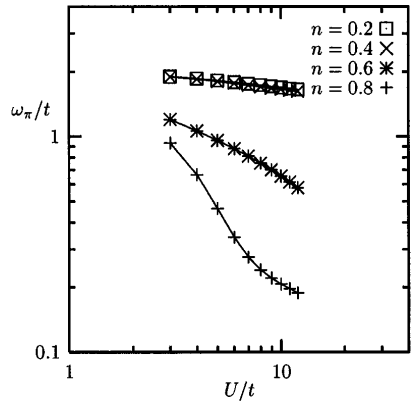

FIG. 2. Energy of the $\pi_d^{\dagger}$-resonance peak in a log-log plot as a function of U at fillings $\langle n\rangle = 0.2$ to 0.8.

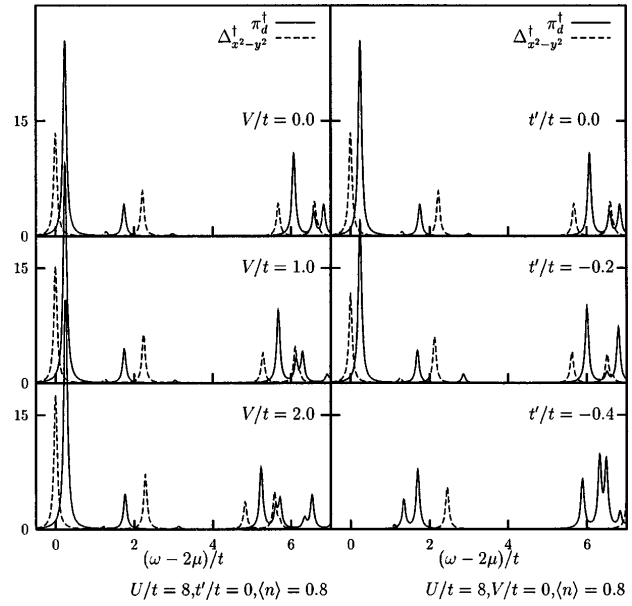

FIG. 3. Spectra at a density $\langle n \rangle = 0.8$ and coupling $U/t = 8$ for the $\pi_d^\dagger$ (solid line) and the $\Delta_d^\dagger$ operator (dashed line) for a series of values V/t (left panel) and t'/t (right panel) (reference energy is E_0^{N+2}).

low-energy peaks are only marginally affected. Most importantly, *the difference of the excitation energies of the Δ and π operators is practically independent of V for the parameter range considered.* This difference gives the energy required to remove a d-wave singlet pair with momentum $(0, 0)$ from the system and reinsert a d-wave triplet pair with momentum (π, π). In a neutron-scattering experiment a Cooper pair from the condensate is turned into a π-pair; we therefore expect the energy difference of the peak energies in Fig. 3 to correspond to the energy of the peak in the inelastic neutron scattering cross section, which is essentially unaffected by V.

In the right panel of Fig. 3, we consider the influence of a next-nearest-neighbor hopping integral t', with the opposite sign as t, and again compare the corresponding spectra of the π and Δ_d operators at a density $\langle n \rangle = 0.8$. For values of $|t'/t| < 0.4$ the overall picture is similar to that seen for the nearest-neighbor interaction, i.e., the difference in excitation energies is nearly independent of t'/t. For values of $|t'/t| > 0.3$ both the low-lying resonances of the Δ-pair and the π-pair are shifted upward in energy. Summarizing both the influence of t' and V perturbations on the approximate SO(5) symmetry, we note that the weight of the peaks are only marginally affected as long as the position is unchanged. This would suggest that as long as d-wave pairing survives the influence of the perturbations, so does the π resonance.

In conclusion, we have numerically verified one of the most fundamental assumptions of the SO(5) theory of the Hubbard model [1], which asserts that the SO(5) symmetry generators, the π_d operators, are approximate eigenoperators of the Hubbard model both near and away from half-filling. Their dynamic autocorrelation function shows well separated resonance peaks with large relative spectral weight and low energy. This behavior is intrinsically collective, and cannot be reproduced by any calculations which neglect vertex corrections. In contrast to the π_d operators, the π_s operators do not show well separated peaks near half-filling. This result shows that there is an approximate SO(5) symmetry only between the AF and the d-wave SC order parameters, and no symmetry between the AF and the s-wave SC order parameters. Close to half-filling, between the densities $n = 0.8$ and $n = 1$, the 10-site Hubbard cluster has finite d-wave superconducting fluctuations, which lead to a nonvanishing mixed correlation function involving the SO(5) symmetry generator and the AF order parameter. Because of the finiteness of this mixed correlation function, there is a contribution to the dynamic spin correlation function from the particle-particle π resonance. These observations are consistent with the proposed explanation of the resonant neutron scattering peaks in the YBCO superconductors [2].

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