Superfluidity in a 1D disordered Hubbard boson model: numerical spectroscopic analysis

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Superfludity (at $T=0$) and its suppression by disorder are analyzed in a 1D Bose system through an exact diagonalization of a Hamiltonian matrix with a calculation of low-lying excited states. In addition to ordinary phonon excitations in the spectrum, there are some so-called supercurrent states. A sharp change in the splitting of the phonon levels is observed near the theoretical point of the superfluidity/Bose-glass phase transition, which corresponds to the value $K=2/3$ of the universal parameter. A sharp increase in the splitting of the supercurrent levels occurs at a K value of approximately 1/2. This result does not conform to the current understanding of the situation.

Most numerical studies of superfluidity deal with either thermodynamic characteristics of the system[1–4] or properties of the ground state.[5,6] In the 1D case, however, the problem of superfluidity in a large but finite system can be studied by analyzing the spectrum of low-lying excited states. The additional energy associated with a supercurrent state with a topological quantum number M (we are labeling the states with the value of the velocity circulation) in a closed 1D chain of length L can be written

$$E_{SC}^{(M)}=2\pi^2M^2\Lambda_S/L, \tag{1}$$

where Λ_S is the superfluid rigidity. At $|M|\sim 1$ the energy of the supercurrent state has the same macroscopic scale factor L^{-1} as the energy of a phonon with a minimum momentum:

$$E_{\rm ph}^{(1)}=2\pi c/L, \tag{2}$$

where c is the sound velocity. Furthermore, in the most interesting region, in which the disordered system is close to the point at which superfluidity vanishes, these energies are on the same order of magnitude [a transition should occur at $K=2/3$, $K=c/\pi\Lambda_S$ (Ref. 7); from Eqs. (1) and (2) we find $E_{\rm ph}^{(1)}/E_{\rm SC}^{(1)}=K$]. At $K\sim 1$ the low-energy part of the spectrum of a closed boson chain should therefore contain supercurrent levels along with phonon levels. The "superproperties" of these levels should be manifested in the stability with respect to disorder: Their splitting should be small even in a highly disordered system. The splitting of the low-lying phonon levels should also be small, but it might be expected to be greater than that of the supercurrent levels. Accordingly, a study of the splittings can yield qualitative information on the existence of a superfluidity, and the energies of the low-lying states make it possible to find values of macroscopic parameters which characterize the superfluid system: Λ_S, c, and K [see Eqs. (1) and (2)].

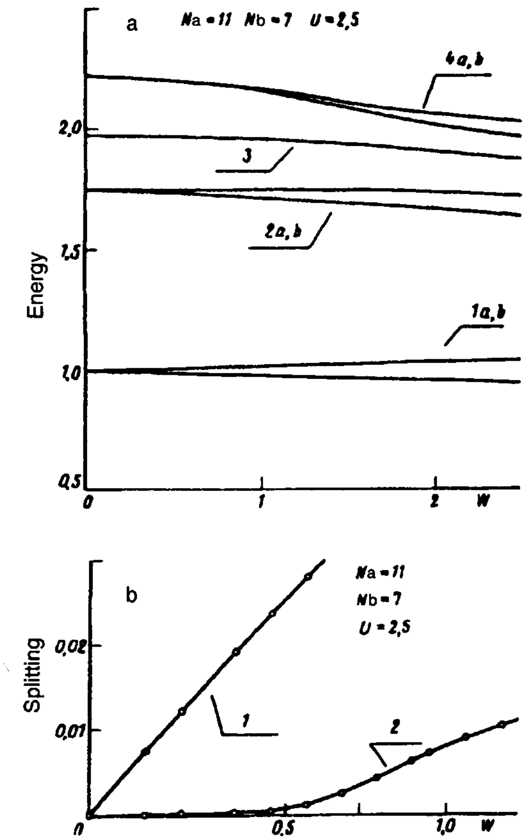

FIG. 1. Evolution of the spectrum with increasing W. a: Overall picture. b: Splitting of the first phonon level (1) and of the first supercurrent level (2).

We turn now to an analysis of the numerical results. We studied a Hubbard boson model with a diagonal disorder:

$$H=\sum_{i=1}^{N_a}\left\{-(a_i^+a_{i+1}+a_{i+1}^+a_i)+\varepsilon_i n_i+\frac{U}{2}n_i(n_i-1)\right\}. \tag{3}$$

The operator a_i annihilates a boson at site i; $n_i=a_i^+a_i$; and ε_i is a random quantity distributed uniformly on the interval from $-W/2$ to $W/2$. Since the chain is closed, we have $a_{N_a+1}\equiv a_1$. Most of the calculations were carried out for a system with $N_a=11$ sites and $N_b=7$ bosons (the dimensionality of the Hilbert space is 19 448). We deliberately selected an incommensurate filling $N_b\neq N_a$ in order to avoid an interference with a Mott transition.

In most cases, the interaction parameter U was chosen on the interval from 2 to 6, since in this case we have $K\sim 1$; i.e., the value of this parameter is near the region of the phase transition. This transition can occur as either W or U (under the condition $W\neq 0$) increases. Figures 1a and 2a show a typical spectrum. Levels 1a and 1b are a superposition of one-phonon states with a minimum momentum $\pm k_0$, $k_0=2\pi/L$. Levels

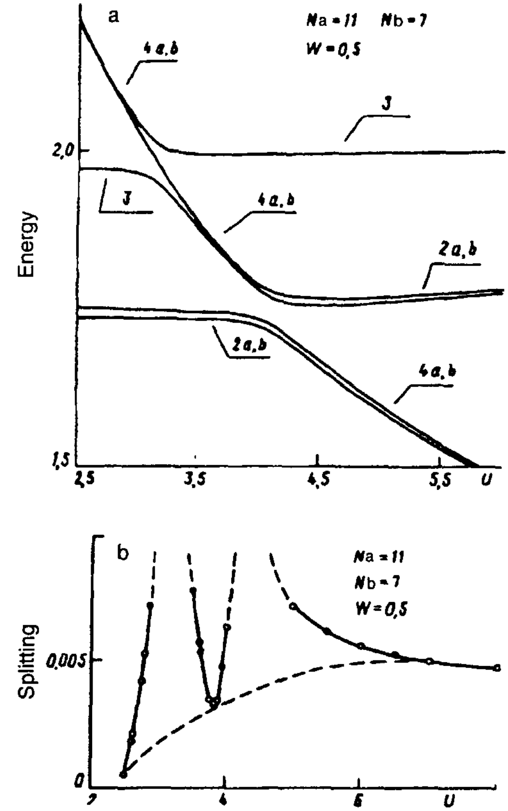

FIG. 2. Evolution of the spectrum with increasing U. a: Overall picture. b: Splitting of the first supercurrent level.

2a and 2b are a superposition of two-phonon states $\{k_0, k_0\}$ and $\{-k_0, -k_0\}$. Level 3 is a two-phonon state $\{k_0, -k_0\}$. Levels 4a and 4b are a superposition of supercurrent levels with $M = \pm 1$. The values of the levels have been normalized in the following way. The levels are counted from the ground state and the system of units is chosen in such a way that the half-sum of levels 1a and 1b is one. In this normalization, the value of the first supercurrent level is the same as $1/K$.

The levels can easily be identified by examining the spectral picture in the limits $U \to \infty$ and $U \to 0$ $(W=0)$. The limit $U \to 0$ is convenient for an identification of phonon lines, since phonons transform into ordinary noninteracting particles, and the supercurrent levels shift upward sharply in the spectrum. In this case the Hamiltonian can be diagonalized analytically, and the levels found numerically can easily be identified by comparing the energy values with the analytic results. As the interaction begins and strengthens, the supercurrent levels descend to elementary quasiparticle excitations (phonons). These supercurrent levels can therefore be demonstrated on the basis of a residual principle. The circumstance that in the limit $U \to 0$ the model in (3) with $W=0$ is equivalent to an ideal Fermi gas can serve as an additional criterion for determining the supercurrent levels. The ground state is always nondegenerate (if there is an even number of particles, an additional gauge phase π is necessary), and the degeneracy of the first excited state is

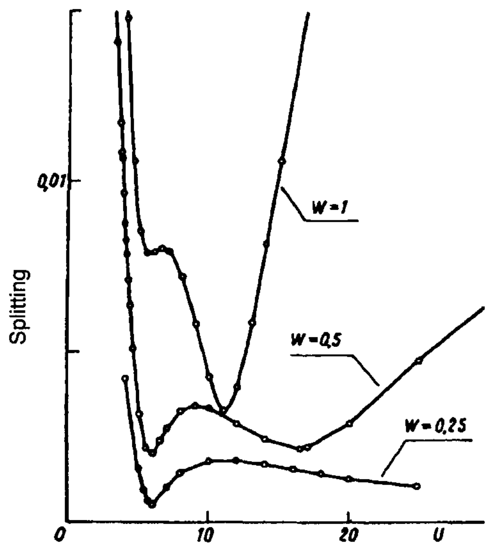

FIG. 3. Splitting of the first phonon level as a function of U for various values of W.

fourfold. Two states of the quartet are the limiting case of a phonon with a minimum momentum $\pm k_0$, while two others are the limiting case of a supercurrent state with $M = \pm 1$ (a slight shift of the Fermi surface as a whole). An alternative way to distinguish supercurrent states from phonon lines is to calculate the density–density correlation function. In supercurrent states, in contrast with phonon excitations, this correlation function behaves in a monotonic way as a function of the distance. Furthermore, the density–density correlation function for supercurrent levels is quantitatively very close to the corresponding correlation function for the ground state, in complete accordance with fundamental principles of superfluidity.

Figure 1a shows the evolution of the spectrum with increasing degree of disorder, W. Figure 1b shows the qualitative difference between the behavior of the supercurrent-level splitting and the phonon splitting. The supercurrent-level splitting is quite nonlinear, while the phonon splitting is directly proportional to W. The supercurrent-level splitting is very small up to $W = 0.6$. At this point, it increases sharply, becoming comparable to the phonon splitting. The effect resembles a phase transition. Interestingly, the value of the parameter K here is close to 1/2; i.e., the system should remain superfluid in this region according to Ref. 7.

Figure 2 shows the evolution of the spectrum with increasing U. Here the picture is more complex, because of a hybridization of supercurrent levels with phonon levels. However, if we put aside the hybridization resonances with levels 2 and 3, the behavior of the supercurrent-level splitting (dashed line in Fig. 2b) is very similar to that in Fig. 1b, and singularities arise at values of K close to 1/2. This splitting of the first phonon level (Fig. 3) exhibits a clearly expressed extremum at $U = 5.8$. This extremum is present at any degree of disorder. The value of K here is very close to 2/3 (Fig. 2a), at which a transition to a state of a Bose glass should occur, according to Ref. 7. This difference between the behavior of the supercurrent-level splitting and the phonon splitting is evidence of a substantial difference in the nature of the supercurrent states and normal excitations.

Let us briefly describe the numerical method. First, working from some initial wave function modified by the Lanczos method,[8] we determine the necessary number of energy levels. We then reconstruct a system of approximate functions from a tridiagonal Rayleigh matrix,[9] and we expand the initial wave function in these functions. We know that the resulting system contains some parasitic states, because of numerical errors. These states can easily be identified, because of their small contribution to the initial function, and they can be eliminated. The system is then reorthogonalized and corrected by Newton's method. The relative errors in the calculation of the energy levels are 10^{-13}–10^{-11} for the ground state and 10^{-9}–10^{-5} for the first ten excited states. (By "relative error" here we mean the ratio of the absolute error of the calculation of the eigenvalues, determined from the wave-vector discrepancy, to the characteristic distance between levels.) The problem of level degeneracy is solved by repeating the procedure with a new initial function, orthogonalized with respect to all the states found previously. The resulting system of states is again reorthogonalized and corrected by Newton's method.

Let us summarize the results. We have presented a numerical analysis of the superfluidity in a 1D Hubbard boson model, studying the low-lying spectral lines and their splitting in the presence of a disorder. We found that the splitting of a supercurrent level increases sharply at $K\sim 1/2$, while singularities appear in the splitting of the phonon level at $K=2/3$. While the behavior of the phonon level conforms to existing theoretical predictions,[7] the behavior of the supercurrent-level splitting is difficult to explain by the existing renormalization analysis. This behavior (and also the singularities in the phonon splitting beyond the phase-transition point, at $U>5.8$, $K>2/3$) can of course be attributed to the finite size of this system. However, a system with $N_a=11$ is already fairly large, as can be seen from the very small splitting of the phonon and supercurrent lines. We might thus expect that the effects observed in it, perhaps even those associated with the finite size, should also occur in vastly larger systems.

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