Few interacting fermions in a one-dimensional harmonic trap

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We study spin-1/2 fermions, interacting via a two-body contact potential, in a one-dimensional harmonic trap. Applying exact diagonalization, we investigate their behavior at finite interaction strength and discuss the role of the ground-state degeneracy which occurs for sufficiently strong repulsive interaction. Even low temperature or a completely depolarizing channel may then dramatically influence the system's behavior. We calculate level occupation numbers as signatures of thermalization, and we discuss the mechanisms to break the degeneracy.

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I. INTRODUCTION

Advances in the control and manipulation of ultracold quantum gases have opened up a new avenue to the study of interacting few particle systems [1]. In particular, existing trapping techniques allow for exploring the physics in low dimensions where the quantum-statistical distinction between fermionic and bosonic particles experiences severe modifications. A striking property of one-dimensional systems is that a strongly repulsive bosonic system can be mapped to a noninteracting fermionic system [2–7]. This gives rise to a strongly correlated phase known as the Tonks-Girardeau (TG) gas. For spin-1/2 fermions in a one-dimensional trap, in the strongly repulsive limit, the spin-1/2 fermions may form a ground state which is identical to that of noninteracting fermions without spin [8,9]. High-precision control of such systems has been proven feasible in a recent experiment which allows for preparing the system in a state with a well-defined, small number of particles [10]. In particular, it has become possible to study the ground state and the dynamics of a two-fermion system [11], for which the exact theoretical solution is known in the full interaction parameter range [12–14].

To describe systems with three or more fermions, different analytical and numerical methods have been applied [15–20], suggesting such systems as a tool for studying ferromagnetism and providing some insight into the fermionized nature of the strongly repulsive system. In this paper, we give a theoretical description of few fermions in a one-dimensional harmonic trap based on an exact diagonalization study. This allows us to go beyond the analytic solution of Ref. [15], as we cover the full energy spectrum in the full range of interaction strengths. We focus on the quasidegenerate regime where any small temperature or a completely depolarizing channel may lead to an occupation of several states in the spectrum. As a signature of this effect, we calculate the occupation numbers of the harmonic oscillator levels, which are found to significantly differ from the ground-state expectation value. On the other hand, as the true ground state is protected against mixing with other states by permutation symmetry, such thermalized states require mechanisms to break the degeneracy. While anharmonicities in the trap are found to fail, a small magnetic field gradient is shown to mix the degenerate states, giving rise to a nontrivial spin dynamics.

II. SYSTEM

Our system consists of two-species fermions of mass m confined in a one-dimensional trap with frequency ω. The Hamiltonian has the form

$$H = \sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2} + \frac{m\omega^2}{2}x^2\right] + g_{1D}\sum_{i<j}\delta(x_i - x_j), \quad (1)$$

where g_{1D} is an effective interaction strength between two fermions of different spins. In the following, we refer to the two species as a single species with an internal (pseudo)spin-1/2 degree of freedom. We express all quantities in harmonic oscillator units, i.e., $\hbar\omega$ for energy, $\sqrt{\hbar/m\omega}$ for length, etc. For convenience we introduce the dimensionless interaction strength $g = (m/\hbar^3\omega)^{1/2}\, g_{1D}$. Let us note that the interaction term in Eq. (1) is nonzero only for states having a spatial wave function which is symmetric under particle exchange. For fermions with the same spin the wave function is always antisymmetric, and the interaction term will not contribute. For two fermions with opposite spins, symmetric and antisymmetric wave functions are possible and correspond to states with zero and finite interaction energy.

A convenient basis for studying the many-body problem is given by the eigenstates $\phi_n(x)$ of the single-particle problem, simply being the harmonic oscillator eigenfunctions corresponding to energies $\epsilon_n = n + 1/2$. The Hamiltonian (1) is then diagonalized in blocks with a fixed total number of particles N, and fixed numbers $N_\uparrow$ ($N_\downarrow$) of $\uparrow$ ($\downarrow$) fermions, defining the z component of the spin. We truncate the single-particle basis at a sufficiently large level, $n_{\max} = 20$.

Before turning to our numerical results, let us consider two limiting cases which can be solved analytically. The first case is a noninteracting system, $g = 0$. The ground state is then obtained by simply filling the Fermi sea, defining the Fermi energy E_{F}. The second limiting case is the Girardeau limit of infinitely strong repulsive interaction between the two species, $g \to \infty$. Then, a Fermi-Fermi mapping [4] allows one to treat the repulsive two-species fermions like noninteracting one-species fermions. A spatial wave function for the ground state is then obtained as a Slater determinant of the N lowest levels. It can be rewritten as [8]

$$\Psi \propto \left[\prod_{i=1}^{N} e^{-x_i^2/2}\right] \prod_{1\leqslant j<\ell\leqslant N} (x_j - x_\ell). \tag{2}$$

This spatial wave function is fully antisymmetric and thus corresponds to a fully symmetric spin configuration. It is an eigenfunction of both the single-particle and the interaction part of the Hamiltonian and thus provides an exact eigenfunction for any choice of g. In particular, as the wave function vanishes whenever two particles are at the same position, it describes a state with an energy which is independent from g and which becomes the ground-state energy for $g \to \infty$.

It is possible to symmetrize Eq. (2) with respect to pairs of particles of opposite spin just by including a factor $\mathrm{sgn}(x_\ell - x_k)$. However, as our numerical results suggest, wave functions obtained in that way are eigenfunctions of the Hamiltonian only for $g \to \infty$. More insight is provided by an exact solution of the two-particle problem [12,13] by rewriting the Hamiltonian into the relative motion $r = x_1 - x_2$ and the center-of-mass motion $R = (x_1 + x_2)/2$ coordinates. The relative motion of the two particles is then described by

$$H_{\mathrm{rel}} = -\frac{d^2}{dr^2} + \frac{1}{4}r^2 + g\delta(r). \tag{3}$$

The relative motion part of the wave function (2) is found to be the first-excited state of the Hamiltonian (3) with energy $E - E_{\mathrm{F}} = 1$ for any g. Its center-of-mass motion is in the ground state. In the limit $g \to \infty$, the state (2) becomes degenerate with the ground state which smoothly evolves to the symmetric state $\Psi_0(r,R) \propto |r|e^{-r^2/4}e^{-R^2}$, as we adiabatically increase g. Note that this wave function, despite describing a state of zero interaction energy, is not an eigenstate of Eq. (3) for any finite g.

We thus have seen that in the limit of infinitely strong interactions, the two-particle problem has two degenerate ground states with opposite symmetry of the spatial wave function. One solution is obtained from the other by multiplying $\mathrm{sgn}(x_1 - x_2)$. This operation turns the spatially antisymmetric wave function (2) into a spatially symmetric wave function and thus has to be accompanied with a corresponding change in the symmetry of the spin wave function.

The same mechanism can be applied for larger systems, $N > 2$. Then, for every pair of particles with opposite spin, it is possible to change the symmetry of the spatial wave function in the state (2) and thereby construct new solutions in the Girardeau limit. This has been done in Ref. [15] and leads to a degenerate ground-state manifold, where the number of degenerate ground states D is given by the number of distinct spin configurations. It is counted by the distinct possibilities of dividing N particles into two groups with $N_\uparrow$ and $N_\downarrow$ members; that is, $D = \frac{N!}{N_\downarrow! N_\uparrow!}$. Note that the degeneracy of higher manifolds, corresponding to an excited center-of-mass motion, increases since one also has to take into account excitations in the relative motion.

III. ROLE OF DEGENERACIES

These degeneracies, although known before [15], might play a crucial role in understanding the few-body physics of strongly interacting fermions. Our numerics focuses on the region between the two limiting cases, where, for $N > 2$, exact solutions are not known. In that region, the system makes use of both the possibility of doubly occupying the lowest levels to reduce potential energy and occupying higher levels in order to reduce interactions. Energy spectra as a function of interaction strength g are plotted in Fig. 1 for fixed $N_\uparrow$ and $N_\downarrow$. With this also the total particle number and the z component of spin, $S_z = N_\uparrow - N_\downarrow$, are fixed, but not the total spin. We find different energy manifolds which become degenerate in the limit $g \to \infty$. Each manifold corresponds to different center-of-mass wave functions. The number of degenerate states in the lowest manifold is given by D, the number of different spin configurations. For any S_z, the highest energy state of the lowest manifold is described by the fully antisymmetric wave function of Eq. (2). As explained above, it is an exact solution with zero interaction energy for any g, and its energy function is therefore simply a horizontal line. The degeneracy is lifted at any finite g.

We next consider the population of the different single-particle levels. In the quasidegenerate regime, the vanishing small energy gap does not protect the ground state against mixing with other states from the manifold: If the system's temperature is of the order of the gap, a description in terms of thermal states becomes necessary. In Fig. 2(a) we show, for $N_\uparrow = 4$ and $N_\downarrow = 1$, how temperature strongly affects the

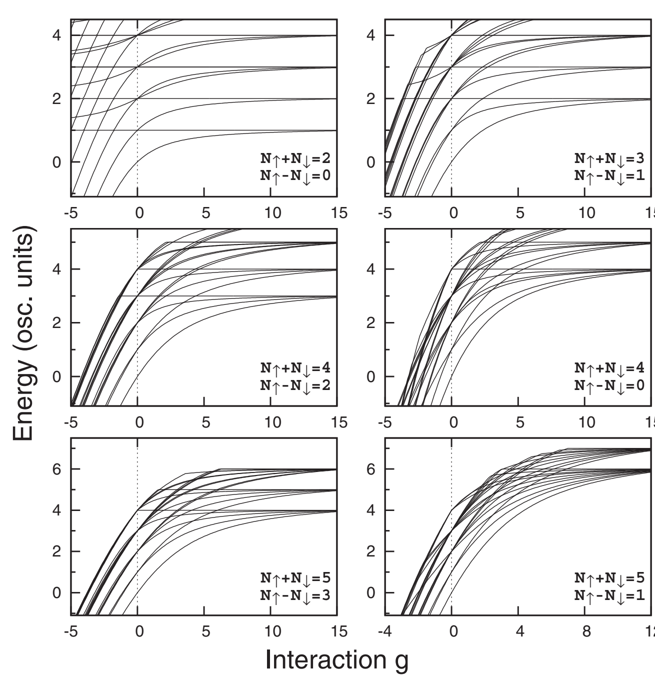

FIG. 1. We plot the energy $E - E_{\mathrm{F}}$ as a function of the dimensionless interaction strength g for different combinations of spin-up and spin-down particles. The energy offset E_{F} is the Fermi energy of the noninteracting system. We find ground-state degeneracies in the limit of strong interactions. We plot first 20 eigenenergies of the Hamiltonian in Hilbert spaces with fixed $S_z = N_\uparrow - N_\downarrow$, but without fixing the total spin.

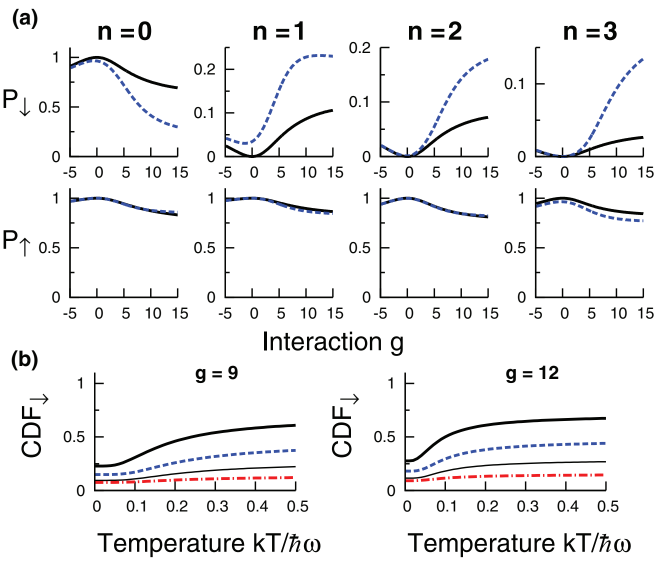

FIG. 2. (Color online) (a) The probabilities $P_\downarrow$ and $P_\uparrow$ for finding $\uparrow$ and $\downarrow$ particles in different orbitals ($n = 0,1,2,3$) as a function of the dimensionless interaction strength g. We consider the effect of temperature using a Boltzman distribution: the solid black and dashed blue lines denote the temperatures $kT/\hbar\omega = 0$ and 0.3, respectively. (b) Temperature dependence of the cumulative distribution function for $g = 9$ (left) and $g = 12$ (right). This function describes the probability of finding the $\downarrow$ particle above the nth harmonic oscillator level, where $n = 0$ is shown by the thick solid line, $n = 1$ by the dashed line, $n = 2$ by the thin solid line, and $n = 3$ by the dash-dotted line. In all plots $N = 5$ and $N_\downarrow = 1$.

occupation probabilities of the $\downarrow$ particle. Taking into account the whole manifold of five quasidegenerate states, we apply a Boltzmann average at different temperatures. For $g \gtrsim 10$, the probability of finding the $\downarrow$ particle in the level $n = 0$ is clearly reduced even by a small temperature, $k_B T \ll \hbar\omega$. To understand this, we note that at zero temperature, as shown by the thick solid line, only the true ground state is occupied. For this state, the probability for the $\downarrow$ particle to be in $n = 0$ ranges between 1 at $g = 0$ down to 0.8 for $g \gg 1$. In contrast, the Girardeau state has an equal population of the five lowest levels, such that the probability of finding the $\downarrow$ particle in $n = 0$ is given by 0.2. This shows that the quasidegeneracy of the ground state enhances the population of the higher energy levels in the limit $g \to \infty$. Interestingly, as shown by the second line of Fig. 2(a), the occupation probabilities for the $\uparrow$ particles are close to unity, independent of temperature and interaction strength g, as a consequence of the Pauli principle.

From the experimental point of view, the probabilities shown in Fig. 2(a) cannot be measured directly. Instead, by tilting the trap potential one can estimate the number of atoms above a certain harmonic oscillator level by the counting atoms that leave the trap [10]. In a series of measurements, this quantity is a counterpart of the cumulative distribution function (CDF). This function describes the probability of a particle to occupy any level above a certain cutoff level n. Measurements of CDFs for different n would allow one to reproduce the probabilities of Fig. 2(a). In Fig. 2(b), we plot the temperature dependence of the CDF of the $\downarrow$ particle in a system with $N_\downarrow = 1$ and $N_\uparrow = 4$ for two different interaction strengths, $g = 9$ and $g = 12$. In both cases, the CDF of the lowest energy levels ($n = 0$ and $n = 1$) is very sensible to small temperatures and more than doubles in the plotted range $0 \leqslant k_B T \leqslant 0.5\hbar\omega$. In the case of $g = 12$, this increase mostly takes place in the interval $0 \leqslant k_B T \leqslant 0.15\hbar\omega$, and the CDF saturates for larger temperatures. This shows that temperature has become large compared to a vanishingly small many-body gap, which exponentially decreases with g. Then, the thermal regime transforms into the scenario where a completely depolarizing channel simply favors the state with maximum entropy according to the Jaynes principle.

IV. EXTERNAL SYMMETRY BREAKING

We now discuss the thermalization mechanisms that are able to bring the system into a superposition of different states from the quasidegenerate manifold. On the basis of our ideal model, neither an adiabatic increase nor a sudden quench of the interaction parameter would lead to occupation of more than *one* state in the degenerate manifold. A mixing with other states is prohibited by the permutation-group symmetry, that is, the conservation of total spin.

Also trap anharmonicities do not change this situation. As shown in Fig. 3(a), they only shift the quasidegenerate energy manifolds without lifting the degeneracy. In fact, the nature of the symmetry dictates that thermalization mechanisms must simultaneously act on spin and spatial degrees of freedom. This could be a spin-orbit coupling, spin-dependent interaction like, for instance, p-wave interaction or the existence of a spatially dependent magnetic field. The latter option is easily implemented as a Zeeman term, $H_Z = \delta \sum_i x_i \sigma_i^z$, in the Hamiltonian. Without loss of generality, we assume that the two internal states have opposite magnetic moments along the z direction and δ is a magnetic field gradient. Such a term can be implemented in a controlled way in the experiment.

To study the effect of a Zeeman term in more detail, we first consider two particles with opposite spins. It is easily seen that the symmetric wave function $|S\rangle \propto |r| e^{-r^2/4} e^{-R^2}$ (which has to be multiplied by an antisymmetric spin wave function $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$) has nonzero transition matrix elements $\langle S| H_Z |A\rangle = 2\sqrt{2/\pi}\,\delta$ with the antisymmetric wave function $|A\rangle \propto r e^{-r^2/4} e^{-R^2}$ (which has to be multiplied by a symmetric spin wave function $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$). This gives rise to a degeneracy splitting Δ which is linear in the magnetic field gradient, $\Delta = 4\sqrt{2/\pi}\,\delta$, and to mixed-symmetry states in the limit of large g. The same effect is found for systems with three or four particles, where we have taken into account the Zeeman term in our exact diagonalization study. The situation is plotted in Fig. 3(b), clearly showing the lifted degeneracy in the large g limit. In particular, we find that for sufficiently small Zeeman energy, $\delta\langle x\rangle \ll \hbar\omega$, only states of the same energy manifold are mixed. Furthermore, since the Zeeman term can be rewritten as a sum of operators acting only on pairs of particles, transition matrix elements of states which differ by more than one unit of total spin are zero. Accordingly, the matrix representation of the Zeeman term has a tridiagonal structure. The mixed symmetry of the eigenstates in the presence of a Zeeman splitting is illustrated by Fig. 3(c). For $N = 4$ and $N_\uparrow = 1$ we consider a system which is prepared in the (maximum

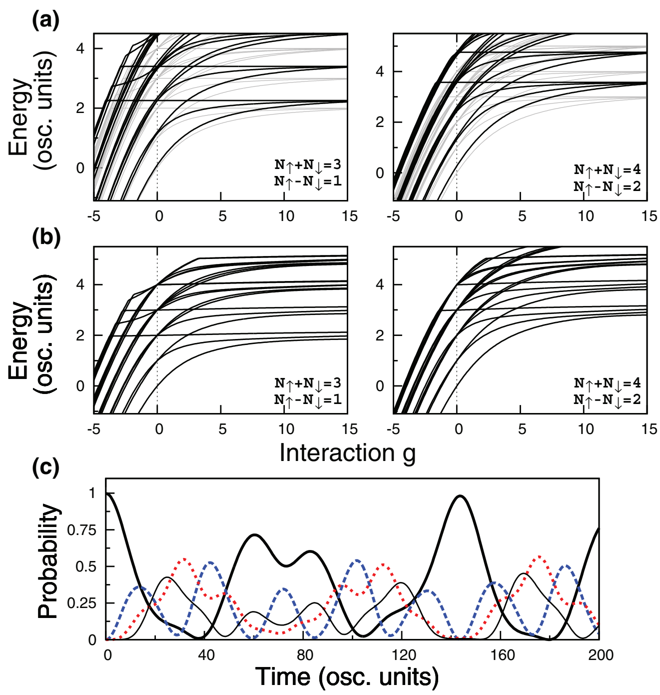

FIG. 3. (Color online) (a) Influence of a symmetric anharmonicity of the trap to the spectrum of the Hamiltonian. Anharmonicity shifts eigenenergies of the Hamiltonian (black lines) relative to the eigenenergies of the Hamiltonian with the harmonic trap (gray lines). It does not lift the degeneracies at large g and provides no mixing between different states in each manifold. (b) Energies as a function of g in the presence of a Zeeman term. No degeneracies occur in the strongly interacting limit. (c) Zeeman breaking of the spin symmetry. For $N = 4$ and $N_\uparrow = 1$, the ground state at $g = 12$ is time-evolved after switching on a Zeeman term, $\delta = 0.05$. The probability for finding the state in one of the four possible spin configurations is plotted. The thick black, dashed blue, dotted red, and thin black lines correspond to the states ordered by energy (increasing).

total spin) ground state of the Hamiltonian for $g = 12$ and $\delta = 0$. Then we switch on the external magnetic field gradient $\delta = 0.05$ and propagate the state for some time t. We then measure the spin symmetry of the state (by projecting back into the spin-conserving basis given by the eigenstates of $\delta = 0$). We then plot the probabilities of finding the system in one of the three different spin sectors as a function of time. The time scale of the dynamics shown in Fig. 3(c) can be controlled by the strength of the field gradient. This could allow for studying the crossover from quantum time evolution to thermalization.

V. CONCLUSIONS

In our study of one-dimensionally trapped spin-1/2 fermions we have focused on the strongly repulsive regime, in which a ground-state degeneracy is exhibited. This quasidegenerate manifold allows one to study thermalization in a small quantum-mechanical system. We have calculated correlation functions and occupation numbers of the harmonic oscillator levels as signatures for distinguishing between pure states and thermal states at finite or even infinite temperature. Since each eigenstate is protected from mixing with other states by its symmetry with respect to the permutation group, mechanisms for thermalization must in general be operators which simultaneously act on spin and spatial degrees of freedom. We have shown that the presence of an additional Zeeman term lifts the degeneracy and may lead to a time-dependent superposition of different states from the quasidegenerate manifold.

Note added in proof. Recently, we became aware of a related work by S. E. Gharashi and D. Blume exploring the degenerate regime of strongly repulsive 1D fermions [21].

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