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# Quasiparticles, coherence, and nonlinearity: Exact simulations of rf spectroscopy of strongly interacting one-dimensional Fermi gases

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We consider rf spectroscopy of ultracold Fermi gases by exact simulations of the many-body state and the coherent dynamics in one dimension. Deviations from the linear response sum rule result are found to suppress the pairing contribution to the rf line shifts. We compare the coherent rotation and quasiparticle descriptions of rf spectroscopy which are analogous to NMR experiments in superfluid <sup>3</sup>He and tunneling in solids, respectively. We suggest that rf spectroscopy in ultracold gases provides an interesting crossover between these descriptions that could be used for studying decoherence in quantum measurement, in the context of many-body quantum states.

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## I. INTRODUCTION

The excitation spectrum of a quantum state can be measured by outcoupling particles and creating quasiparticles. In ultracold Fermi gases, rf spectroscopy [1–8] realizes such outcoupling. One of the two interacting (pseudo)spin components is coupled by a rf field to a third component. This can be viewed as a quasiparticle creation process [9–18] analogous to tunneling. It can also be viewed as a coherent rotation in (pseudo)spin space [19–22], analogous to NMR experiments in superfluid <sup>3</sup>He [23–25]. The picture that applies depends on the coherence of the time evolution [22]. We compare the coherent rotation and quasiparticle descriptions, and study nonlinear effects, by exact simulations of the dynamics in one dimension (1D), using the matrix product state (MPS) method [26].

In this paper, we suggest that the amount of decoherence, not the final state interactions directly, is the crucial issue determining which kind of theoretical description for rf spectroscopy should be applied. We discuss the difference between the coherent and quasiparticle pictures from this viewpoint, and make a connection between rf spectroscopy and the quantum measurement problem [27,28], with discussion of possible experiments. We give exact numerical results on how deviations from the linear response lead to a reduced pairing contribution to the rf line shifts. These predictions are directly relevant for coming 1D experiments and should be a good estimate for the coherent 3D case as well.

## II. COHERENT AND QUASIPARTICLE PICTURES

The system considered is described by the Hamiltonian

$$\begin{aligned}
 H = \int d\mathbf{r} \left[ \sum_{\sigma=1,2,f} \Psi_{\sigma}^{\dagger}(\mathbf{r}) \left( -\frac{\nabla^2}{2m} - \mu_{\sigma} \right) \Psi_{\sigma}(\mathbf{r}) + \Psi_1^{\dagger}(\mathbf{r}) \right. \\
 \times [U_{12}n_2(\mathbf{r}) + U_{1f}n_f(\mathbf{r})] \Psi_1(\mathbf{r}) + \Omega \Psi_f^{\dagger}(\mathbf{r}) \Psi_2(\mathbf{r}) + \text{H.c.} \\
 \left. + \frac{\delta}{2} [n_2(\mathbf{r}) - n_f(\mathbf{r})] \right], \quad (1)
 \end{aligned}$$

where  $U_{12}$  and  $U_{1f}$  are the interaction strengths ( $U_{2f}$  interaction is neglected),  $\mu_1 = \mu_2 \equiv \mu$  the chemical potentials,  $m$  is the mass,  $n_i(\mathbf{r}) = \Psi_i^{\dagger}(\mathbf{r}) \Psi_i(\mathbf{r})$ , and  $\Omega$  is the field (effective) Rabi frequency. For a noninteracting system ( $U_{12} = U_{1f} = 0$ ), the spectrum of transferring particles to the (initially empty) final state  $f$  has a peak at frequency  $\omega_{\text{free}}$ . For an interacting system, the maximum transfer of atoms from state 2 to state  $f$  takes place at a certain rf frequency  $\omega_{\text{rf}}$  that can differ from  $\omega_{\text{free}}$  by some detuning  $\delta = \omega_{\text{rf}} - \omega_{\text{free}}$ .

In the quasiparticle picture, assuming a BCS state with excitation energy  $E_k$ , gap  $\Delta$ , and linear response for the field, the detuning is bound by the energy conservation relation [9]  $\delta = E_k + \epsilon_k - \mu = \sqrt{(\epsilon_k - \mu)^2 + \Delta^2} + \epsilon_k - \mu$ , which gives the threshold detuning  $\delta_{\text{th}} = \sqrt{\mu^2 + \Delta^2} - \mu \approx \Delta^2/2\mu \approx \Delta^2/2E_F$  (the minimum  $\delta_{\text{th}}$  is obtained for the noninteracting case with single particle energy  $\epsilon_k = 0$ ). Including the Hartree interactions gives

$$\begin{aligned}
 \delta_{\text{th}} &= \sqrt{(-\mu + U_{12}n_1)^2 + \Delta^2} - \mu + U_{1f}n_1 \\
 &\approx (U_{1f} - U_{12})n_1 + \frac{\Delta^2}{2(\mu - U_{12}n_1)} \\
 &\approx (U_{1f} - U_{12})n_1 + \frac{\Delta^2}{2E_F}, \quad (2)
 \end{aligned}$$

where  $E_F$  is the Fermi energy and  $n_{\sigma}$  denotes the densities for different components. For the BCS state the threshold  $\delta_{\text{th}}$  corresponds well to the maximum peak position. Equation (2) gives also the molecular binding energy  $\delta_{\text{th}} \sim 2|\mu|$ , for  $\mu < 0$  and  $|\mu| \gg \Delta$ .

In the coherent rotation picture, within the linear response regime, the mean value for the frequency shift  $\bar{\delta}$  can be obtained from the sum rules [20,21]

$$\bar{\delta} = \frac{\int d\delta \delta \chi''(\delta)}{\int d\delta \chi''(\delta)} = (U_{1f} - U_{12}) \frac{\langle \int d\mathbf{r} \Psi_1^{\dagger}(\mathbf{r}) \Psi_2^{\dagger}(\mathbf{r}) \Psi_2(\mathbf{r}) \Psi_1(\mathbf{r}) \rangle}{n_2}, \quad (3)$$

which in the BCS limit becomes [20]

$$\bar{\delta} = (U_{1f} - U_{12})n_1 + (U_{1f} - U_{12}) \frac{\Delta^2}{U_{12}^2 n_2}. \quad (4)$$

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The Hartree term  $(U_{1f}-U_{12})n_1$  is the same in Eqs. (2) and in (4). Neglecting it, one obtains for  $U_{1f}=0$  that

$$\delta_{\text{th}} \approx \frac{\Delta^2}{2E_F}, \quad \bar{\delta} = \frac{-\Delta^2}{U_{12}n_2}.$$

Both the quasiparticle and coherent rotation pictures predict that the frequency shift is proportional to  $\Delta^2$ , but for different reasons. For the coherent rotation, the term  $\Delta^2/|U_{12}|$  is the difference between the total energy of the final and initial many-body states, and dividing it by  $n_2$  gives the energy difference per particle. In the quasiparticle picture, the suppression of pairing by the Fermi energy,  $\delta_{\text{th}} \approx \Delta^2/E_F$ , appears because the particles that can be excited with the smallest energy are at the bottom of the Fermi sea ( $\epsilon_k=0$ ). Note that in some other contexts (e.g., tunneling in metals), the states at the bottom of the Fermi sea are Pauli blocked, whereas here the final state is initially empty. In fact, by having initial occupation of the final state, the dependence of  $\delta_{\text{th}}$  on  $\Delta$  could be brought toward  $\delta_{\text{th}} \sim \Delta$  [9,10,29] in the quasiparticle picture, whereas in the coherent rotation picture the  $\Delta^2$  dependence would be unchanged. For the coherent rotation, the term  $(U_{12}-U_{1f})$  multiplying  $\Delta^2$  leads to the zero shift  $\bar{\delta}=0$  if the interaction strengths are the same, i.e., the interaction is SU(2) invariant in spin space [25]. In contrast, in the simplest quasiparticle picture [Eq. (2)] the term proportional to  $\Delta^2$  does not depend on the final state interactions. This can be valid for many-body pairing with weak interactions: a single outcoupled particle does not form a Cooper pair because there is no Fermi sea for the particles in the final state. For strong final state interactions and/or if bound states exist, pairing can take place without the Fermi sea. Such a  $1f$  bound state can be added to the quasiparticle picture to describe bound-bound transitions [13,18].

The shape of the spectra in the coherent rotation and quasiparticle pictures allows them to be distinguished in experiment. In the quasiparticle picture, the spectral peak is asymmetric with a long tail. In the coherent rotation description, the spectra are symmetric and not broadened by interactions [20,22]. We will now compare the coherent and quasiparticle pictures in a one-dimensional system, paying particular attention to the validity of the linear response. All the previous work in the literature on rf spectroscopy has assumed linear response (only in [30] was an approximate nonlinear model considered). We here present results with no approximations in the field-matter interaction.

### III. METHODS AND RESULTS

We consider the Hamiltonian (1) within the one-dimensional, one-band Hubbard model with nearest neighbor hopping and on-site interaction, assuming the tight binding approximation:

$$\begin{aligned} H = & -J\sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + U_{12}\sum_i c_{i1}^\dagger c_{i2}^\dagger c_{i2} c_{i1} + U_{1f}\sum_i c_{i1}^\dagger c_{i1}^\dagger c_{if} c_{if} c_{i1} \\ & + \sum_{i\sigma} \mu_\sigma c_{i\sigma}^\dagger c_{i\sigma} + \sum_i (\delta/2)(c_{i2}^\dagger c_{i2} - c_{if}^\dagger c_{if}) \\ & + \Omega \sum_i (c_{if}^\dagger c_{i2} + c_{i2}^\dagger c_{if}), \end{aligned}$$

where  $c_{i\sigma}^\dagger$  creates a particle  $\sigma$  at site  $i$ . No renormalization is needed for the interaction strengths due to the natural cutoff

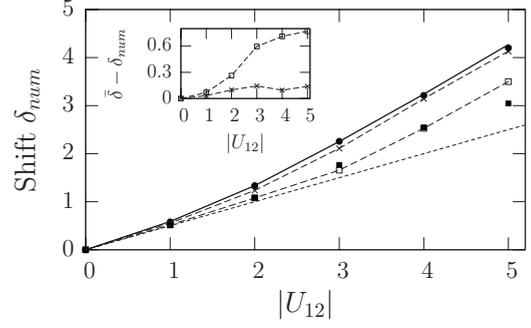


FIG. 1. Frequency shifts  $\delta_{\text{num}}$  for different interaction strengths  $U_{12} \leq 0$  ( $U_{1f}=0$ ). The circles represent 1.0%, crosses 10%, and open squares 50% particle transfer, also in the inset. The linear response–sum rule result  $\bar{\delta}$  (solid line) works well for weak interactions or if the amount of transferred particles is small. The results given by Fermi golden rule (filled squares) and the Hartree term  $U_{12}n_1$  (dotted line) are also presented. The inset shows the difference between sum rule and numerical results,  $\bar{\delta} - \delta_{\text{num}}$ .

by the first band. We set the hopping  $J=1$  in calculations; all other quantities are in units of  $J$ . The relation between  $J, U$ , and the parameters for atoms in an optical lattice are as in [31]. The chemical potentials  $\mu_\sigma$  are chosen so that the density takes a value corresponding to half filling. The final state is initially empty.

For calculating the ground state and simulating the dynamics we use the matrix state product method as described in [26,32]. This formalism is especially suited for simulating time evolution in sufficiently regular systems. All interaction strengths, i.e., the BCS to Bose-Einstein condensate (BEC) crossover, can be considered, provided the single-band approximation stays valid. The ground state (when  $\Omega = \delta=0$ ) is obtained by operating on the initial state with imaginary time evolution operator which we approximate by the Forest-Ruth formula [33]. After calculating the ground state, we simulate the dynamics by applying a square pulse. For each detuning, we calculate the expectation value for the number of atoms in the final state after having applied the pulse and thus obtain the spectrum. The numerically obtained rf line shift is denoted as  $\delta_{\text{num}}$ .

The errors due to the numerical method are controlled and very small: we have varied the Schmidt number in the MPS method from 5 to 12, and the results start to converge around 5 (depending on the interaction). The error still left in the results fits within the data point symbols. The simulations are double checked using two computer codes (one in C++, the other in FORTRAN).

Figure 1 shows the shift  $\delta_{\text{num}}$  as a function of the interaction strength  $U_{12}$  when  $U_{1f}=0$ . In Fig. 2, we vary  $U_{1f} \neq 0$  and keep  $U_{12}$  fixed. For comparison, we show the shift of the peak  $\bar{\delta}$  as given by the sum rule within the linear response theory, Eq. (3), where we calculate

$$\langle \int d\mathbf{r} \Psi_1^\dagger(\mathbf{r}) \Psi_2^\dagger(\mathbf{r}) \Psi_2(\mathbf{r}) \Psi_1(\mathbf{r}) \rangle$$

numerically. Having the BCS result Eq. (4) in mind, we also plot the Hartree mean field contribution  $U_{12}n_1$ , and extract

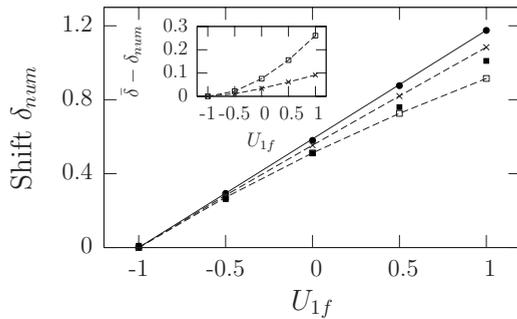


FIG. 2. Frequency shifts  $\delta_{\text{num}}$  for different final state interaction strengths  $U_{1f}$  ( $U_{12} = -1.0$ ). The circles represent 1.0%, crosses 10%, and open squares 50% particle transfer, also in the inset. The sum rule result  $\bar{\delta}$  is shown with the solid line and the Fermi golden rule result with filled squares (at  $U_{1f} = -1$  the former is 0 and latter 0.01). The inset shows the differences between sum rule and numerical results,  $\bar{\delta} - \delta_{\text{num}}$ .

the quantity  $\Delta$  from Eqs. (3) and (4) via  $\langle c_{i1}^\dagger c_{i2}^\dagger c_{i2} c_{i1} \rangle \approx U n_1 n_2 + \Delta^2 U^{-1}$ . Using  $\Delta$  obtained in this way we apply the standard BCS description to present results given by the simplest quasiparticle picture (Fermi golden rule).

As Fig. 1 shows, the numerical result deviates from the linear response sum rule result [Eq. (3)] by an increasing amount for increasing interactions, if the number of particles transferred is, e.g., 50%, or even 10%, of the particle number in state 2. Only when as little as  $\sim 1\%$  of the atoms are transferred is the linear response strictly valid. For  $U_{12} > 0$ , the deviation is found to be similar. Figure 2 shows the effect of nonzero  $U_{1f}$ , i.e., the simple amplification by the factor  $(U_{1f} - U_{12})$  in Eq. (3). As expected for a coherent process, the spectra are symmetric and the width depends only on  $\Omega$  as seen in Fig. 3.

We checked whether the simulated time evolution corresponds to simple Rabi oscillations with some effective detuning caused by interactions: we fitted to the numerical oscillations the maximum peak height  $4\Omega^2/(\delta'^2 + 4\Omega^2)$  and the period  $2\pi(\delta'^2 + 4\Omega^2)^{-1/2}$  with  $\delta'$  as the fitting parameter. The fitting was found to fail hand in hand with the failure of linear response approximation for increasing interactions. This is in accordance with the observation (see Fig. 1) that nonlinear effects show up when the pairing contribution starts to become considerable compared to the Hartree term (for Hartree shifts alone, the simple Rabi picture should be valid). For 50% of transferred particles, the suppression of the remaining pairing contribution (i.e., other than Hartree) by nonlinearity ranges from 30% to 100% for the values used in Fig. 1. In the simplest quasiparticle picture, the nonlinear shift is not necessarily this dramatic since higher-order processes might produce primarily subthreshold weight rather than a shift of the peak.

The results shown here are for densities close to half filling. For  $U_{12} = -1$ , we have done simulations also for low densities (filling 0.25) which correspond to the continuum 1D case, and found that the nonlinear deviation for 50% particle transfer was  $\sim 10\%$  of the total shift (cf. 2% for half filling and  $U_{12} = -1$ ). We have mainly used 20 lattice sites but also bigger lattices give the same results; see Fig. 3.

#### IV. QUANTUM MEASUREMENT AND EXPERIMENTS

It is now interesting to compare the coherent and quasiparticle pictures from the point of view of a quantum measurement. In the former, the system decoheres only after the pulse. In the latter, the measurement instantaneously projects the system into the total final state which can be, e.g., one free particle in state  $f$  and one quasiparticle in the superfluid. The starting point for both descriptions (within the linear response) is the imaginary part of the correlation function  $D_{f2} = -i \int d\mathbf{r} \langle T[\psi_2^\dagger(\mathbf{r}, t) \psi_f(\mathbf{r}, t) \psi_f^\dagger(0, 0) \psi_2(0, 0)] \rangle$  which, as well as the sum rules, corresponds to the coherent Hamiltonian evolution. On the other hand, the Fermi golden rule corresponds to instantaneous projection (the Fermi golden rule result is often obtained in an experiment for a long, weak excitation, but formally it describes an instantaneous projection). The Fermi golden rule follows by dividing the final and initial state contributions by  $D_{f2}$ . The measurement done is thus defined by the way the correlation function is calculated. It is possible to calculate  $D_{f2}$  by including final state interactions in a fully self-consistent way [20], corresponding to coherent rotation of all particles. In contrast, the simplest quasiparticle picture [Eq. (2)] is obtained by a straightforward factorization of  $D_{f2}$ . Then the spectrum obtained no longer satisfies the  $f$ -sum rule, i.e., it does not describe coherent evolution but a projection measurement to the chosen final state. If the final state is likely to have bound states or strong interactions, they should be included in the quasiparticle description [16,18].

Some of the spectra obtained in the early rf experiments on pairing [3,6,7] are symmetric although this could be partly due to broadening by inhomogeneous density in Ref. [3,6]. However, the spectral shapes depend on the interaction strength, density, and temperature, and the quasiparticle picture can be applied to describe qualitative features such as the double-peak structure [12,14,17]. Exact modeling of the intermediate cases between the coherent and simple quasiparticle pictures—or realizing the experiment in such a way that one picture is strictly valid—becomes crucial in high-precision measurements of the pairing gap. The recently obtained spectra [8] in the case where final state interactions have been reduced show a clearly asymmetric shape.

For strong initial state and weak final state interactions the eigenstate wave functions of the initial and final states are very different: the rf field then couples one state to a continuum of states. The decoherence is strongest when a state is coupled to a large number of other states, which enforces a projection measurement. This is obviously the case for the molecule continuum dissociation process. If the final state resembles the initial state, the process is more likely to stay coherent. This can happen, e.g., for stronger final state interactions. The extreme case is the Hartree mean fields which do not affect the wave function in a homogeneous system; fully coherent rotation was observed in measurements of the Hartree shifts [2,19]. The experimental observation of both quasiparticle and coherent rotation type results for ultracold Fermi gases and the possibility of a tunable crossover between them suggest that rf spectroscopy in these systems may be suited for studying the long-standing problem of quantum measurement and the question of how decoherence

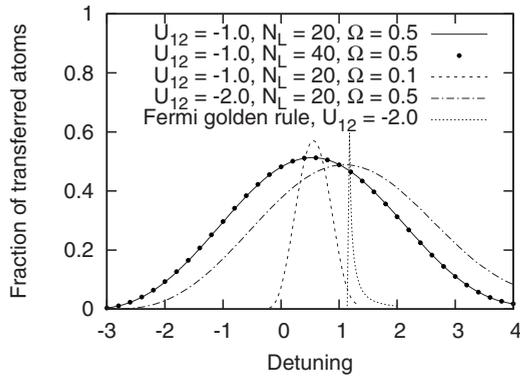


FIG. 3. Spectra for different values of the coupling  $\Omega$ , the interaction strength  $U_{12}$ , and the number of lattice sites  $N_L$ . The shape of the Fermi golden rule result is also shown (in arbitrary units). The width of the spectrum depends only on  $\Omega$ . Here  $U_{1f}=0$  and the duration of the pulse is  $0.8\Omega^{-1}$ .

sets in in the measurement process, in the context of many-body states. Our 1D results give predictions for the fully coherent and the fully decoherent (quasiparticle + Fermi golden rule) values of the rf line shift. Another experimental indicator of the amount of decoherence is the asymmetry of the peak. One could investigate how these two observable quantities (peak position and asymmetry) evolve—smoothly or abruptly—when the amount of decoherence is changed, either by the length of the pulse or by the strength of the final state interactions. One could further repeat such experiments throughout the BCS-BEC crossover to find out whether many-body and single-particle paired states are vulnerable to decoherence in a different way.

## V. CONCLUSIONS

We have compared the exact coherent dynamics of the rf spectroscopy of interacting fermions in one dimension to the quasiparticle picture within the BCS formalism. We have also pointed out a potential connection with quantum measurement and decoherence. Large suppression of the pairing shift from the linear response prediction was found when the number of transferred particles was more than  $\sim 1\%$ . The main difference between the 1D and 3D physics is the absence of long-range order in 1D. Since rf spectroscopy does not measure the long-range coherence of the many-body state, our results should give a good estimate of the relative effect of nonlinearity also in the 3D coherent case. Therefore, in 3D experiments where more than 1% of particles were transferred and final state effects were considerable (the nearly coherent case), it is likely that the rf shifts have been suppressed by amounts similar to the ones presented here. In the future, it would be especially interesting to consider 1D systems where exact theory and modeling is possible, to understand both coherent and incoherent processes in rf spectroscopy. The deviations from the linear response for strong interactions found here also indicate that such systems could display other interesting nonlinear phenomena in the field-matter interaction.

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