Scanning tunneling microscopy for ultracold atoms

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We propose a versatile experimental probe for cold atomic gases analogous to the scanning tunneling microscope (STM) in condensed matter. This probe uses the coherent coupling of a single particle to the system. Depending on the measurement sequence, our probe allows us to obtain either the *local* density and spatial density correlations, with a resolution on the nanometer scale, or the single particle correlation function in real time. We discuss applications of this scheme to the various possible phases for a two dimensional Hubbard system of fermions in an optical lattice.

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I. INTRODUCTION

Recent advances in the field of ultracold atoms have led to a close connection between quantum gases and condensed matter physics. The achievement of strongly correlated systems and their remarkable tunability open the possibility to realize "quantum simulators" for quantum many-body phenomena. To name one example, ultracold fermionic systems clarified the crossover between a BCS state of paired fermions to a Bose-Einstein condensate of ultracold bosonic molecules [1–5]. Further investigations of strongly correlated systems were initialized by the successful loading of ultracold bosonic [6] and fermionic [7] atoms into three-dimensional optical lattices. In these periodic lattice potentials created by counterpropagating laser beams the physics of various lattice models can be mimicked [8,9]. In particular, the fermionic Hubbard model, which plays an important role in the way of understanding high-temperature superconductivity, can be realized naturally given the short range nature of the interactions between the neutral atoms.

Whereas achieving the exotic quantum phases experimentally appears feasible with today's technology, their clear identification remains an obstacle. Compared to condensed matter the neutrality of the cold atoms is both an advantage and a drawback since the atoms cannot be perturbed as easily as electrons in a solid. Possible probes are thus more sophisticated than their condensed matter counterparts. In addition, for ultracold atomic gases an inhomogeneous confining potential causes the coexistence of different spatially separated quantum phases [8,10,11]. This makes their realization and observation in the presence of a trapping potential very involved and creates a need for a method of probing the systems locally. However, the existing probes [10,11] still involve an averaging over regions of various densities and new techniques which allow for a local detection need to be developed.

In condensed matter physics, a remarkable local probe was provided by the scanning tunneling microscope (STM) [12]. It was used to explore and image the surface topography with atomic resolution, paving the way to control and analyze quantum phenomena on solid surfaces [13]. In addition to the density analysis, the STM has also become a spectroscopic tool probing the local density of states. This spectroscopic method had a major impact on the understanding of the physical properties of strongly correlated systems for which the local density of states provides unique information on the physics of the system. In particular, the STM has made significant contributions to the field of high temperature superconductors [14].

In this work we propose and analyze a versatile experimental setup to locally probe cold atomic systems in an approach similar to and as versatile as the STM. The probe relies on the coupling of a single particle to the system. Different "operating modes" yield either a measurement of the local density and spatial density correlations or of the single particle Green's function in time. The realization of such a probe will open the possibilities to investigate exotic quantum phases in great detail as we show in the example of the Hubbard model. In extension to the conventional STM in condensed matter physics, our scheme would allow for measurements in a three-dimensional sample.

II. COLD ATOM TUNNELING MICROSCOPE

The key idea for the realization of an STM-like scheme with cold atoms, the "cold atom tunneling microscope" is sketched in Fig. 1. A single trapped particle is used as a probe of local quantities by inducing a controlled interaction

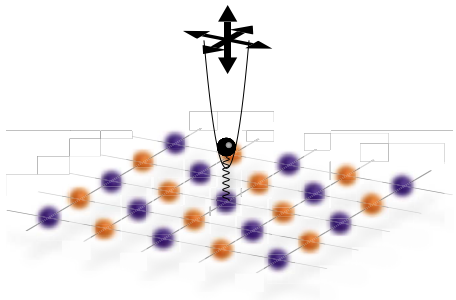

FIG. 1. (Color online) Sketch of the cold atom tunneling microscope. As an example the application to an antiferromagnetic state with alternating spin states labeled by different colors is shown.

between the probe particle and the quantum many-body state. To allow for a precise control over the motion of the probe and to facilitate a convenient readout mechanism, we suggest employing a single atomic ion trapped in the vibrational ground state of a radio-frequency Paul trap [15]. In this case the spatial resolution of the microscope relies on the excellent control over the position and motion of trapped ions on the submicron scale [16]. However, the working principle of the microscope does not depend on the charge of the probe particle and it also applies to a neutral atomic quantum dot [17] provided that the trapping potential of the dot has only a negligible influence on the quantum many-body system [18]. The controlled interaction between the probe particle (the ion) and the quantum many-body system could be provided by a two-photon Raman coupling.

As we show below, the cold atom tunneling microscope facilitates a local detection of the density and of density correlations on individual lattice sites and, quite remarkably, it even allows us to perform a spin-resolved detection. The realization of a spin-resolved STM is a long-sought goal in condensed matter systems but has not yet been achieved. The cold atom tunneling microscope also allows us to perform spectroscopy by observing the local single particle Green's function $\langle c^{\dagger}_{\sigma,j}(t_0)c_{\sigma,j}(0)\rangle_F$ in time. Here $c_{\sigma,j}$ is the annihilation operator for the neutral atom on a site j with spin $\sigma=\{\uparrow,\downarrow\}$ and $\langle\cdot\rangle_F$ stands for taking the expectation value with respect to the atomic system only. The temporal decay of this function reflects the nature of the excitations and thus gives direct information on the quantum phases present in the system.

We first show how a measurement of the local density and density correlations (scanning mode) can be achieved. We take the example of fermionic atoms in two different spin states $\uparrow$ and $\downarrow$ in an optical lattice. It is facilitated by a two-photon Raman coupling between the ion $|i\rangle$ and an atom $|a_j\rangle$ in a lattice well j by which a weakly bound molecular ion $|i+a_j\rangle$ can be created (see Fig. 2). This coupling can be described by the expression $[\Sigma_\sigma \Omega_\sigma(t) M^{\dagger}_{\sigma} I c_{\sigma,j} + \text{H.c.}]$. Here M_σ and I are the annihilation operators for the molecular ion and the atomic ion, respectively. The coupling strength $\Omega_\sigma(t)$ can be controlled experimentally. By choosing the correct frequency and polarization of the laser fields, the coupling is dependent on the atomic "spin" state paving the way for the spin-resolved microscopy.

III. "SCANNING MODE": LOCAL DENSITY MEASUREMENT

The experimental sequence to detect the local density is as follows: At time $t=0$ the atomic many-body system is prepared in its ground state $|\Psi_0\rangle$. By a sudden increase of the lattice potential the density profile of the state is frozen to ease the measurement process. The ion is introduced into the lattice well j in state $|i\rangle$ and a $\pi/2$-Raman pulse is applied over a time δt, i.e., $\Omega_\sigma \delta t = \pi/2$. Detecting the probability (i.e., the average of the outcome of several quantum measurements) for molecule formation after the application of the Raman pulse measures the local density of

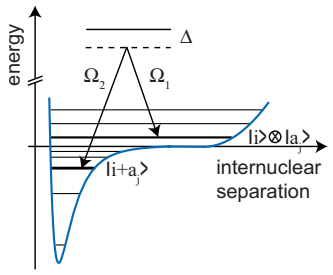

FIG. 2. (Color online) Two-photon Raman coupling of the ion $|i\rangle$ and an atom $|a_j\rangle$ in a harmonic potential well to a molecular ion bound state $|i+a_j\rangle$. The single photon coupling is detuned by Δ from a resonant transition to suppress spontaneous emission from the intermediate excited state. The effective two-photon Rabi frequency Ω_0 is proportional to the coefficients of the single photon transitions and inversely proportional to the detuning Δ, i.e., $\Omega_0 \propto \Omega_1 \Omega_2 / \Delta$.

atoms in the lattice well j by the relation $\langle \Sigma_\sigma M^{\dagger}_{\sigma} M_\sigma \rangle = \Sigma_\sigma \sin^2(\Omega_\sigma \delta t) \langle n_{\sigma,j} \rangle_F$ with $\langle n_{\sigma,j} \rangle$ the local atomic density. The outcome of the photoassociation process can be detected by measuring the changed oscillation frequency of the heavier molecular ion in the Paul trap or by observing the absence of resonant light scattering of the molecular ion and its reappearance after photodissociation [19]. Since the time scale of one single measurement (a $\delta t = 100$ μs Raman pulse into a deeply bound molecular state followed by state sensitive optical detection of the ion for ~ 100 μs) is short compared to the relaxation of the frozen system (~ 0.1 s) several tens of different lattice sites could be measured sequentially for each preparation of the system. From the single shot measurements of the densities at various lattice sites higher order correlation functions such as $\langle n_i n_j \rangle$ can be directly extracted [20]. In order to obtain an accuracy of the local density of 15%, approximately 100 measurements on newly prepared systems are required. This number of averages is comparable with recent noise correlations measurements [21], however, now resulting in a measurement of the *local* density and density-density correlations.

IV. "TUNNELING MODE": PROBING THE LOCAL SINGLE PARTICLE GREEN'S FUNCTION

Using the cold atom tunneling microscope with a different sequence, the tunneling mode allows us to perform spectroscopy and to measure time dependent correlations locally. The working principle of the tunneling mode relies on the coherent coupling of a single particle to the quantum many-body system. The experimental sequence is sketched in Fig. 3. We start at $t=0$ in the state $|\Psi_0\rangle \otimes |i\rangle$, i.e., the ground state $|\Psi_0\rangle$ of the atomic system and a single atomic ion. A two-photon Raman process is applied over a short time interval δt_1 to couple the ion with an atom present in the lattice well. Subsequently, the superposition state of the atomic and the molecular ion $|i\rangle + \alpha |i+a_j\rangle$ is removed from the system such that they are noninteracting with the remaining quantum many-body system, for example, their center-of-mass position can

be shifted by applying a small dc voltage. After a variable time of free evolution t_0 in this isolated position they return into the addressed lattice well and the application of the two-photon Raman process is repeated for a time interval δt_2. The coherent preparation of superpositions of atomic and molecular states using Raman coupling has already been demonstrated for pairs of neutral atoms [22]. The outcome of the molecule formation is detected afterwards:

$$\langle M^\dagger M\rangle = A(\delta t_1,\delta t_2) + \sin^2(\delta t_2\Omega)[\cos(\delta t_1\Omega)-1]\{[\cos(\delta t_1\Omega)-1]\langle n_j(0)n_j(t_0)n_j(0)\rangle + \langle n_j(t_0)n_j(0)\rangle\}$$
$$+ [\sin^2(\delta t_2\Omega)+\sin^2(\delta t_1\Omega)]\langle n_j(t_0)\rangle + \sin^2(\delta t_1\Omega)[\cos(\delta t_2\Omega)-1]\langle c_j^\dagger(0)c_j(t_0)c_j^\dagger(t_0)c_j(0)\rangle,$$

$$A(\delta t_1,\delta t_2) = 2\sin(\delta t_1\Omega)\sin(\delta t_2\Omega)\cos(\delta t_2\Omega)\mathrm{Re}\left\{e^{-i(\varepsilon_M-\varepsilon_I)t_0/\hbar}[\underbrace{\langle c_j^\dagger(t_0)c_j(0)\rangle}_{=:A_1} + [\cos(\delta t_1\Omega)-1]\underbrace{\langle n_j(0)c_j^\dagger(t_0)c_j(0)\rangle}_{=:A_2}]\right\}. \quad (1)$$

We suppressed the spin index and on the right hand side additionally the index F. Most of the terms do only appear if the system under consideration is a quantum many-body system.

Using appropriate measurement sequences different correlation functions can be extracted. To obtain the temporal correlation function $\langle c_{\sigma,j}^\dagger(t_0)c_{\sigma,j}(0)\rangle_F$ the described measurement procedure is applied sequentially: first, using $\delta t_1=\delta t_2=\delta t$ for both pulses, second, using $\delta t_1=\delta t$ for the first pulse and $\delta t_2=2\pi/\Omega_\sigma-\delta t$ for the second pulse. For example, first a sequence of two $\pi/4$ pulses and then a sequence of a $\pi/4$ and a $7\pi/4$ pulse can be applied. Subtracting the outcome for the molecule formation of the two measurements gives $\Delta\langle M_\sigma^\dagger M_\sigma\rangle=2A(\delta t,\delta t)$. For the proposed pulse sequence the prefactor of the second term A_2 is suppressed by a factor 0.3 smaller than the prefactor of the summand A_1. Since additionally in many systems the decay of the correlation function $\langle n_{\sigma,j}(0)c_{\sigma,j}^\dagger(t_0)c_{\sigma,j}(0)\rangle$ is faster or comparable to the decay of the single particle correlation function, the second term can safely be neglected.

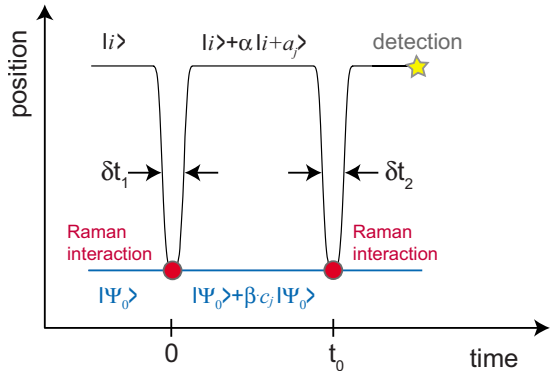

FIG. 3. (Color online) Schematics of the experimental sequence for the tunneling mode. The atomic ion $|i\rangle$ is introduced at the lattice site j into the many-body system in state $|\Psi_0\rangle$. The two-photon Raman process (red) couples an atom at this lattice site $|a_j\rangle$ to the ion with a certain amplitude. Subsequently, the ion and the many-body system are separated for the probe time t_0 during which they evolve individually. After recombination, the Raman interaction is applied again and the molecule formation is detected.

The expression $(\varepsilon_I-\varepsilon_M)t_0/\hbar$ represents the phase difference the atomic ion and the molecular ion collect during the time t_0. In principle this quantity could be zeroed by choosing a suitable combination of the optical lattice field and the ion trapping fields. However, this cancellation is not necessary if $\varepsilon_I-\varepsilon_M \gg U,J$ (i.e., energy scales set by the atom-atom interaction U and the kinetic energy of the atoms J) because then the temporal evolution of the correlation function is encoded simply in the envelope of the detection signal.

V. DETECTION OF CORRELATED QUANTUM PHASES

The cold atom tunneling microscope can be used to identify the quantum many-body phases in many different systems. One direct application would be the identification of the phases of the two dimensional Hubbard model. In addition to the normal (Fermi liquid) quantum fluid of fermions, this model can lead to broken symmetry phases such as an antiferromagnet, and a strongly correlated (Mott) insulator. An important and yet open question is whether other more exotic phases can exist in this model, such as inhomogeneous distribution of the density (stripes and checkerboards) or even superconducting phases with d-wave symmetry for the pairing. The scanning mode of the proposed local probe directly detects symmetry broken phases such as the antiferromagnet in which the spin density and spin density correlations are modulated (cf. Fig. 1) and even more inhomogeneous phases with a modulation of the density (stripes and checkerboards [23]).

Additionally, the tunneling mode reveals the nature of the excitations even in systems with a homogeneous number and spin density by probing the single particle density of states. This, for example, allows us to characterize an s-wave or a d-wave superconductor. In Fig. 4 we plot the Fourier transform of the correlation function $\langle c_{\sigma,j}^\dagger(t_0)c_{\sigma,j}(0)\rangle_F$ for both an s-wave superconducting and a d-wave superconducting phase on a two-dimensional lattice. Both are obtained using

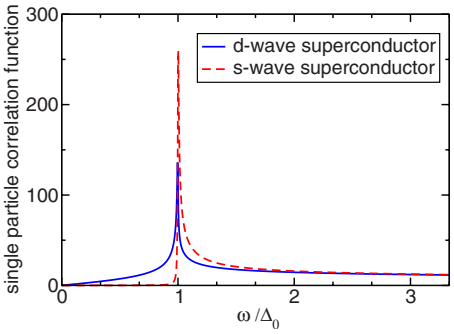

FIG. 4. (Color online) The Fourier transform of the temporal correlation function in an *s*-wave and a *d*-wave superconducting state is shown for a gap value of $\Delta_0=0.3J$.

the phenomenological BCS approach using the energy dispersion on the lattice $-2J[\cos(k_x a)+\cos(k_y a)]$. In the *s*-wave superconducting phase, the gap $\Delta_s(k)\equiv\Delta_0$, clearly leads to a strong divergence of the correlation signal and a zero response in the gap below Δ_0. For the *d*-wave superconducting phase with $\Delta_d(k)=\frac{\Delta_0}{2}[\cos(k_x a)-\cos(k_y a)]$ [24], one observes a different signal having a spectral weight below the gap energy. Thereby the structure of the superconducting order parameter and the size of the gap can be extracted from the proposed measurement.

VI. EXPERIMENTAL IMPLEMENTATION

The independent control over the single particle and the neutral atomic quantum gas lies at the heart of the cold atom tunneling microscope. To good approximation the ion experiences only the ion trapping potential, the atom only the optical lattice potential, and the weakly bound molecular ion both potentials. This can be achieved using a red-detuned optical lattice, e.g., operating at a wavelength of 1 μm. The relevant optical transition for a neutral alkali atom (e.g., ^{40}K) is in the near infrared (767 nm) and thus the atom experiences a trapping potential of up to $\approx$100 kHz oscillation frequency in a lattice well for a deep lattice. In contrast, an earth-alkali ion (e.g., Yb^+) with a resonance in the UV (370 nm) experiences for the same infrared laser intensity a weaker trapping potential (corresponding to a trapping frequency of $\approx$20 kHz). Thus the optical potential for the ion is weak as compared to the electrical trapping potentials which typically give rise to trapping frequencies in the MHz range. Additionally, the comparatively low static dipole polarizability of a neutral atom causes the atom to be practically insensitive to the electric fields generated by the ion trap at the MHz frequencies at which these traps are typically operated [25]. The rapidly oscillating electric field gives rise to a weak antitrapping potential for the neutral which may affect the overall confinement but not on length scales comparable to the lattice spacing. This makes the single ion a particularly attractive choice for shuttling the atomic and the molecular ion in and out of the lattice without influencing the neutral atomic quantum many-body state. In particular, a spatial resolution on the order of 20 nm has been reported [26–28] as well as very quick displacements over 1.2 mm within 50 μs without exciting vibrational quanta [29]. Note that the experimental control over the ion's position is considerably better than the effective range of the atom-ion interaction potential [30].

One challenge for the proposed experiment is to generate molecules that are stable enough to be shuttled in and out of the lattice. The binding energies of the weakly bound states of the atom-ion interaction potential (see Fig. 2) are determined by its asymptotic behavior scaling as $-C_4/r^4$. Here C_4 is proportional to the electric dipole polarizability of the neutral atom and r is the internuclear separation. The atom-ion scattering length can for alkali atoms be estimated to be $a_{ai}\approx 10^3 a_0$ with a_0 being the Bohr radius [31]. Thus the binding energy of the most weakly bound molecular state is two orders of magnitude less than for typical neutral atom interactions [30]. To ensure a stable molecule with respect to shuttling the binding energy should exceed the optical potential depth. Thus it is preferable to use more deeply bound states whose binding energies can be estimated by the LeRoy-Bernstein approach [32]. Several bound states exist in the 10–100 MHz range which is still easily accessible for Raman photoassociation. The generation of weakly bound molecules using two-photon Raman coupling in optical lattices has already been demonstrated for pairs of neutral atoms [33] realizing sufficiently large molecular binding energies. Moreover, even the coherent coupling of free atomic and bound molecular states has been observed [22] which is crucial for the tunneling mode.

In order to probe the quantum many-body state in the tunneling mode without perturbing it, the time scales set by the parameters of the atomic system should be larger than the time intervals of the Raman pulses. To realize a strongly correlated phase in the lattice, the atom-atom scattering length a_{aa} needs to be enhanced by a Feshbach resonance. Assuming $a_{aa}\approx a_{ai}\approx 10^3 a_0$ results in $U\simeq U_{ai}\simeq 20$ kHz for the fermionic isotope ^{40}K, whereas J is typically one order of magnitude smaller. These conditions for the tunneling mode can be fulfilled using an effective Raman coupling $\Omega_\sigma=2\pi\times 100$ kHz, i.e., $\delta t_i\approx 1-10$ μs. The shortness of the photoassociation pulse has other direct benefits: first, the level shift due to the interaction U_{ai} is not resolved and thus the measurement is independent of the occupation of the lattice well by an atom in the second hyperfine state which is not probed in the spin-resolved mode. Second, the short pulse and the subsequent removal of the molecular ion from the quantum many-body system ensures also the stability of the microscope scheme against three-body recombination in a lattice well. Using 200 measurements the correlation function for a certain time t_0, i.e., $\langle c^\dagger_{\sigma,j}(t_0)c_{\sigma,j}(0)\rangle$ could be determined to an accuracy of 20%. Here we assume the value of the correlation function to be approximately 0.5.

In conclusion, we have proposed a versatile experimental setup, the cold atom tunneling microscope, to observe *locally* the (spin-resolved) density and the single particle Green's function. In contrast to previous work this measurement procedure does not average over spatially different regions of the system with coexisting quantum phases, but can resolve single lattice wells. This opens the prospect to investigate exotic quantum phases appearing in condensed matter simu-

lations with cold atomic gases in great detail. In particular it would give the possibility to identify the phases of the Hubbard model and thereby make a major contribution to the understanding of the phenomenon of high-T_c superconductivity. In addition, a modification of the proposed scheme would also give access to *nonlocal* single particle correlation functions. The required modification consists of moving the probe particle during the tunneling mode scheme to a different lattice well, say m, before the second Raman pulse is applied. The outcome of the molecule formation then will be related to the correlation function $\langle c^{\dagger}_{\sigma,m}(t_0)c_{\sigma,j}(0)\rangle_F$ of the atomic system.

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