High-Temperature Superfluidity of Fermionic Atoms in Optical Lattices

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Fermionic atoms confined in a potential created by standing wave light can undergo a phase transition to a superfluid state at a dramatically increased transition temperature. Depending upon carefully controlled parameters, a transition to a superfluid state of Cooper pairs, antiferromagnetic states or d-wave pairing states can be induced and probed under realistic experimental conditions. We describe an atomic physics experiment that can provide critical insight into the origin of high-temperature superconductivity in cuprates.

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The experimental realizations of degenerate Bose [1] and Fermi [2–5] atomic samples have stimulated a new wave of studies of quantum many-body systems in the dilute and weakly interacting regime. The intriguing prospective of extending these studies into the domain of strongly correlated phenomena is hindered by the apparent relative weakness of atomic interactions. For example, an active search is now under way to implement a BCS transition of degenerate fermionic gases to a superfluid (SF) state analogous to superconductivity [6,7]. However, in free-space or weakly confining atom traps the transition temperature to the SF state scales exponentially with interaction strength, $k_B T_c^{\text{free}} \approx 0.3 E_F^{\text{free}} \times \exp[-\pi/(2k_F|a_s|)]$, with E_F^{free} the Fermi energy. For a dilute atomic gas the product of Fermi momentum and scattering length $k_F|a_s| \ll 1$, which makes the transition temperature exceedingly low. Efforts are presently being directed toward increasing the atomic interaction strength by means of Feshbach resonances [8–11]. However, departure from the dilute regime often comes at the price of enhanced losses [12] and/or instabilities which may have particularly severe consequences for fermionic systems [13].

The effects due to interactions can, however, be enhanced if the atoms are confined in optical potentials created by standing light waves [14–16]. Very recently, fascinating experiments involving bosonic atoms in optical lattices [15] revealed a quantum phase transition from a SF to Mott insulating state [14,17]. Fermionic atoms confined in an optical lattice can undergo a phase transition to a SF state at a temperature that exceeds that of weakly confined atoms by several orders of magnitude. Attractive atomic interactions result in s-wave pairing in which case fermionic atoms can undergo a BCS-type transition [18]. In what perhaps is the even more intriguing prospective, fermionic atoms with repulsive interactions correspond to an experimental realization of a Hubbard model that is widely discussed for strongly correlated electron systems such as high-T_c cuprates [19,20]. In particular, d-wave superconducting states [21] have been conjectured to exist in such systems, but so far this conjecture eluded rigorous confirmation. We show that atomic systems with carefully controllable parameters and a variety of precise tools to detect the resulting phases can be used to provide a critical insight into this outstanding problem. In essence, this approach can be viewed as an implementation of the pioneering ideas due to Feynman [22] for simulations of one quantum system by another.

Consider an ensemble of fermionic atoms illuminated by several orthogonal, standing wave laser fields tuned far from atomic resonance. These fields produce a periodic potential for atomic motion in two (or three) dimensions of the form $V(x) = V_0 \sum_{i=1}^{2(3)} \cos^2(kx_i)$ with k the wave vector of the light. The potential depth V_0 is typically expressed in the units of the atomic recoil energy $E_R = \hbar^2 k^2/2m$. We will be interested in the situation in which there is roughly one atom per lattice site. Such atomic densities correspond to free-space Fermi energies on the order of $E_F^{\text{free}} = (3/\pi)^{2/3} E_R$. We assume that two kinds of atoms are present, differing by angular momentum or generalized spin ($\sigma = \{\uparrow, \downarrow\}$). For sufficiently low temperatures the atoms will be confined to the lowest Bloch band, and the system can be described by a Hubbard Hamiltonian [14,20]

$$H = -t \sum_{\{i,j\},\sigma} (c_{i,\sigma}^{+} c_{j,\sigma} + c_{j,\sigma}^{+} c_{i,\sigma}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \quad (1)$$

where $c_{i,\sigma}$ are fermionic annihilation operators for localized atom states of spin σ onsite i, $n_{i,\sigma} = c_{i,\sigma}^{+} c_{i,\sigma}$. The parameter t corresponds to the tunneling matrix element between adjacent sites, $t = E_R (2/\sqrt{\pi}) \xi^3 \exp(-2\xi^2)$, and the parameter $U = E_R a_s k \sqrt{8/\pi}\, \xi^3$ characterizes the strength of the onsite interaction with $\xi = (V_0/E_R)^{1/4}$.

Consider first the attractive case ($U < 0$). The effect of the lattice on the superfluid transition can be best understood starting from the limit of large tunneling $t \gg |U|$. Here, similar to the free-space transition, the interaction strength is much weaker than the kinetic energy and the ground state of the system is then given by a ''standard'' BCS wave function, with an energy gap and transition temperature T_c that depend upon t and U [23]. BCS theory can be applied to predict a critical temperature T_c that for a 3D situation scales as $k_B T_c \approx 6t \exp(-7t/|U|)$ [23]. An increase in the depth of the optical potential results in stronger atom localization and hence an increased interaction strength U. At the same time, the tunneling t becomes weaker. The combined effect of these two factors is a dramatic increase in T_c.

As the tunneling becomes comparable to the onsite interaction, the BCS picture is no longer valid. Because of strong attraction, atoms form pairs within single lattice sites. The entire system can then be considered as an ensemble of composite bosons. They can tunnel together at a rate $\sim t^2/|U|$, by virtual transitions via intermediate singly occupied states. In this regime nonordered pairs exist at high temperatures, whereas the superfluid state — a condensate of composite bosons — appears below $k_B T_c \sim t^2/|U|$. Clearly, in this limit the increase in the potential depth will lead to a reduced mobility of pairs and hence a decrease in T_c. The maximal critical temperature $T_c^{\max}$ is achieved at the crossover between the two regimes, when interaction and tunneling are comparable (more precisely at $U \sim 10t$), which corresponds to a potential depth $\xi^2 \approx 1/2\log[5\sqrt{2}/k|a_s|]$ and

$$k_B T_c^{\max} \approx 0.3 E_F^{\text{free}} k|a_s|. \tag{2}$$

That is, the critical temperature for atomic fermions trapped in a lattice scales only *linearly* with the small parameter $k|a_s|$. Our accurate results for the critical temperature are based on nonperturbative Monte-Carlo simulations of the fermionic Hubbard model [23].

Several specific approaches to achieve the SF state can be considered. For example, the optical potential can be adiabatically turned on, starting from a weakly confined Fermi-degenerate mixture of the two atomic states of appropriately chosen density. In this procedure the atomic quasimomentum is approximately conserved but the band structure associated with the periodic potential changes, resulting in a nonequilibrium distribution, with an effective temperature different from the initial T_{in}. The final temperature T_f after thermalization can easily be estimated from the relation $\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} f(\epsilon^0_{\mathbf{k}}/T_{\text{in}}) = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} f(\epsilon_{\mathbf{k}}/T_f)$, where $f(x) = 1/(e^x + 1)$ is the Fermi-Dirac distribution function, $\epsilon^0_{\mathbf{k}} = k^2/2m - \mu^0$ is the original dispersion of atoms in free space, and $\epsilon_{\mathbf{k}} = -2t[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)] - \mu$ is the dispersion in a tight-binding model with $a = \pi/\lambda$ the lattice period. Two important processes determine T_f. First of all, the presence of the lattice makes the system anisotropic and hence changes the shape of the Fermi surface. This results in an effective heating of the system as V_0 increases from zero to about E_R. As V_0 is increased even further the shape of the Fermi surface remains approximately the same and only the Fermi velocity (or effective atomic mass) changes, leading to a reduction of the effective temperature within the lowest Bloch band (see Fig. 1). This suggests that it is optimal to turn on a weak lattice potential while the fermionic sample is in contact with a cooling reservoir (e.g., atomic BEC), thus avoiding the heating which is present at the initial stages of creating an optical lattice. When $V_0 \sim E_R$ (point C in Fig. 1(b)) the system is decoupled from the reservoir and the lattice potential is increased until the transition to the SF phase is reached.

To control precisely the resulting quantum phase, an accurate manipulation of the filling fraction may be important. This can be achieved, for example, if atoms with three internal states are used. If a dense, degenerate ensemble is prepared in a state that is not affected by the optical lattice, a laser driven Raman transition into a pair of trapped spin states can be used to produce exactly one atom (or its fraction) per each lattice site. The essential idea of this approach is that the energy shifts associated with atom interactions and the Pauli principle can be used to block the transitions into states with more than one atom per lattice site. In this case an effective $\nu\pi$-pulse will result in a filling fraction of ν with an uncertainty that scales with the inverse size of the lattice.

Let us now consider the implications of these results in the light of present experimental possibilities. The relevant critical temperature calculated numerically for Li^6 [3] and K^{40} [2] atoms is shown in Fig. 1. In this figure we consider a Li^6 atomic sample of a very modest density corresponding to a unity filling in an optical lattice produced by a CO_2 laser ($\lambda = 10\ \mu$m). For such densities, a dramatic increase in the critical temperature is possible.

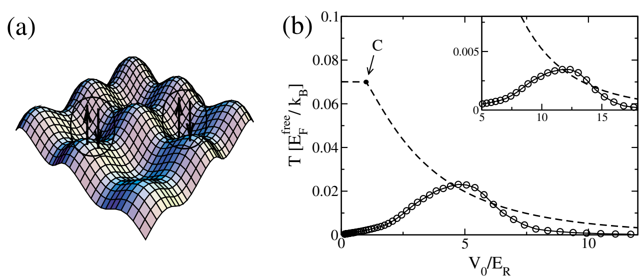

FIG. 1 (color online). (a) Attractive fermionic atoms in optical lattices. (b) Critical temperature for the SF transition of Li^6 atoms (circles) as a function of the optical lattice depth in a 3D CO_2 lattice. Li atoms in the states $|\downarrow(\uparrow)\rangle = |F = 1/2, m_F = \mp 1/2\rangle$ are considered at a magnetic field of $\sim$0.1 T corresponding to $a_s \sim -2.5 \times 10^3 a_0$. The absolute energy scale is given by $t/\hbar \approx 0.5$ kHz at the phase transition. For the same density and scattering length, the free-space BCS formula yields $T_c^0 = 1.6 \times 10^{-12} E_F^{\text{free}}/k_B$ for Li^6. Inset: analogous plot for K^{40} atoms in a Nd:YAG lattice at half filling at a magnetic field above a Feshbach resonance and $a_s \sim -2. \times 10^2 a_0$. Dashed curve: the adiabatic cooling effect described in the text.

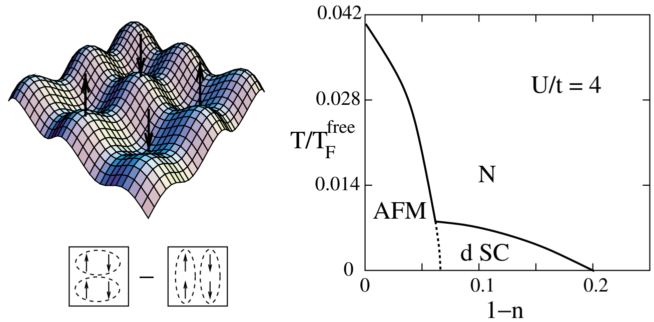

FIG. 2 (color online). In the case of repulsive interactions one finds either antiferromagnetic (AFM, upper left) or d-wave SF phases (lower left), depending upon the filling fraction n. Right: phase diagram for repelling Li^6 atoms in a 2D lattice (obtained in the fluctuation-exchange approximation). Adiabatic cooling due to switching on of the lattice has been taken into account. Note: the repulsive Hubbard model may also have phase separation for some filling factors, which corresponds to immiscibility of the two spin species of the atoms.

Note, in particular, that a phase transition can be achieved starting from an initial temperature of about $0.1E_f^{\text{free}}$. The CO_2 lattice has the additional advantage of exceptionally long lifetimes, which should be sufficient to achieve the transition even for relatively low energy scales involved. Another scenario is to trap Li atoms in an optical lattice created by a Nd:YAG laser $\lambda \sim 1.06\ \mu$m. Although in this case the densities of 10^{12}–10^{13} cm^{-3} will correspond to a filling fraction slightly less than unity, the resulting critical temperature can still be in the range of $0.1E_F^{\text{free}}$. The inset shows a diagram for K^{40} atoms trapped in a similar lattice. As indicated by the two cases presented in Fig. 1 the transition to a SF state is expected to occur for the same initial temperature if adiabatic cooling is taken into account. Therefore, the maximal initial temperature at which a phase transition can occur is *almost independent of the scattering length* and corresponds to about one tenth of the free-space Fermi energy.

We emphasize that in contrast to the approaches that are based on increasing the scattering length or the atom density, which result in an interesting regime of BCS-BEC crossover [9–11], the critical temperature for the lattice filled with attractive atoms (Fig. 1) can be predicted very accurately even in the most interesting, intermediate, regime $t \sim |U|$, since the behavior of the Hubbard model for this case is by now very well understood. While the free-space ensembles at densities $n|a_s|^3 > 1$ can no longer be considered as a weakly interacting gas [9,10], the Hubbard model remains a valid description for the lattice even in the regime of very strong confinement.

It is intriguing to consider possible extensions of the above ideas to a situation in which different atoms repel each other ($a_s > 0$). This is realized for atomic K^{40} at zero magnetic field [2]. In this case it is energetically unfavorable for two atoms to be on the same lattice site.

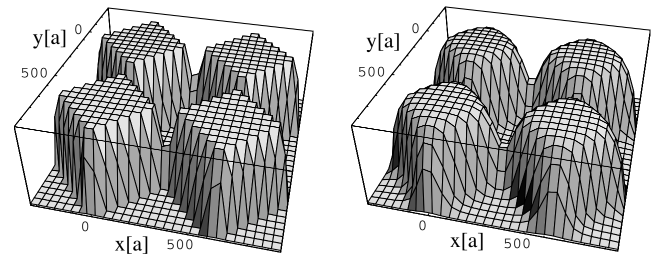

FIG. 3. Central part of the atomic interference pattern after a free expansion for a time $t = 500 \times (\hbar/E_R)$ and a 10×10 optical lattice (with lattice constant a). Left: normal state at half filling. The sharp edges of the interference peaks reflect the atomic momentum distribution. Right: BCS state at half filling, with a gap $\Delta/t = 0.6$ corresponding to $U/t \approx -2.5$.

However, adjacent atoms can virtually tunnel to the same site. This process lowers the total energy of two atoms in adjacent wells, thereby creating effective hard-core attractive interactions of different spins. When the filling fraction of the lattice is close to 1, this leads to a ground state in which adjacent sites are always occupied by atoms with alternating spins (see Fig. 2), i.e., an antiferromagnetic phase.

For filling fractions smaller than 1 it has been conjectured [21] that anisotropic d-wave pairs can be formed, which can result in a d-wave SF phase capable of explaining many of the observed properties in high-temperature superconducting cuprates. So far the existence of d-wave superconductivity in the repulsive Hubbard model has eluded rigorous confirmation. We propose that these ideas can now be tested experimentally in ensembles of fermionic atoms. For example, Fig. 2 shows a phase diagram for the system of repulsive atoms in two dimensions [21] calculated within the fluctuation-exchange approximation [24]. Although the resulting T_c is believed to be somewhat lower than in the s-wave case, this calculation suggests the existence of the d-wave phase for feasible atomic temperatures and densities.

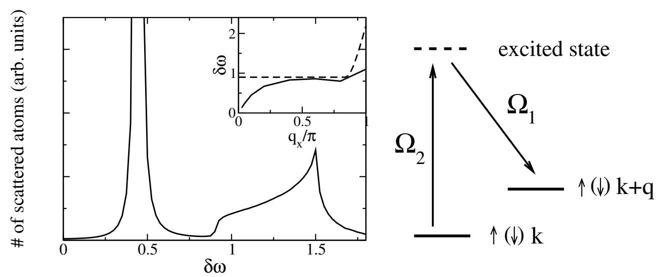

FIG. 4. Left: Bragg scattering of atoms off laser beams with frequency difference $\delta\omega$ and wave-vector difference $q_x = q_y = 0.1\pi$ for attractive fermions at filling $n = 0.6$ and $U/t = -2.5$, corresponding to an s-wave gap $\Delta/t \approx 0.45$. Inset: dispersion of the collective mode (solid line) and the onset frequency of the continuum (dashed line). Right: schematic picture of the two-photon process involved with $\Omega_{1,2}$ Rabi frequencies.

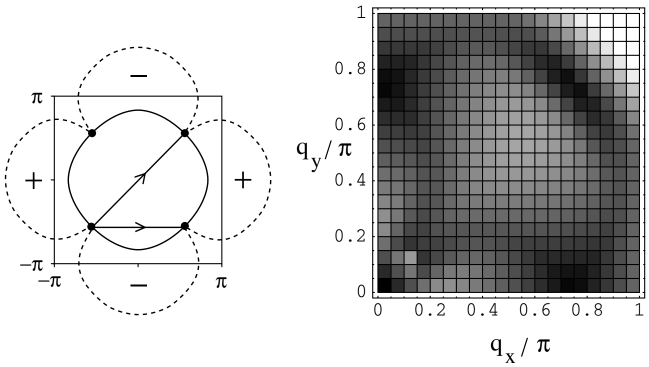

FIG. 5. Probing d-wave pairing at filling $n < 1$ via Bragg scattering. Left: schematic diagram of the Fermi surface (solid line) and the q dependence of the gap $\Delta(q_x, q_y)$ (dashed line). At the four nodal points shown by black dots, the wave function and the quasiparticle excitation energy vanishes. For the special wave vectors connecting these points, the density response is gapless (black spots in the right figure). Right: onset frequency $\omega_{\min}(q_x, q_y)$ of the quasiparticle continuum, dark regions corresponding to low frequencies (vanishing gap).

We next consider several approaches that can be used to detect and accurately probe the resulting quantum phases. Interference of atoms released from the lattice has been used to probe the superfluidity of bosons [15]. In the degenerate regime, atomic interference patterns for each momentum state will be superimposed due to the exclusion principle, resulting in real-space interference peaks which reflect the shape of the Fermi surface, see Fig. 3. Broadening of these peaks is mainly due to finite temperature and the finite diameter of the harmonic trap. With the appearance of pairing, the atomic momentum in the pairs becomes on the order of Planck's constant divided by the size of the pair. As a result, the momentum distribution will be additionally broadened, which is reflected in the interference pattern. At the temperatures currently available, this diagnostic method may be more difficult than the detection of the collective mode discussed below.

In order to detect superfluidity of the pairs, photoassociation spectroscopy [25] can be used. Weakly bound Cooper pairs can be converted into molecules by using a laser-induced transition into a bound molecular state. The interference pattern of the released bosonic molecules will then provide extremely sharp peaks due to the presence of a SF fraction, in direct analogy to [15].

The spectrum of elementary excitations also provides an accurate probe for the nature of the quantum phase. It can be measured in a system of cold atoms by exciting the motional states of atoms using laser pulses. For example, atoms can experience Bragg scattering off two noncollinear laser beams, provided that the frequency difference $\delta\omega$ of the lasers matches the resonance frequency of elementary excitation with momentum q determined by the angle between two lasers (Fig. 4) [26]. This technique provides a direct measurement of the density-density correlation function. By monitoring the number of Bragg-scattered atoms as a function of $\delta\omega$, the presence of a SF phase can be detected unambiguously: One observes a sharp peak due to a collective Bogoliubov mode, which is slightly broadened as a result of the finite trap size. It is separated from a broad feature, corresponding to quasiparticle excitations, by an energy gap (see Fig. 4). In the normal state, on the other hand, the continuum excitations are gapless and the collective mode is not visible due to strong damping. With this technique, it is also possible to detect d-wave superfluidity considering, for example, the onset frequency of the quasiparticle continuum corresponding to the d-wave SF phase (see Fig. 5). A strong anisotropy, together with a vanishing gap for certain momenta can provide unambiguous evidence for the presence of such a phase.

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