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Superfluid Fermi Gas in a 1D Optical Lattice

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We calculate the superfluid transition temperature for a two-component 3D Fermi gas in a 1D tight optical lattice and discuss a dimensional crossover from the 3D to quasi-2D regime. For the geometry of finite size discs in the 1D lattice, we find that even for a large number of atoms per disc the critical effective tunneling rate for a quantum transition to the Mott insulator state can be large compared to the loss rate caused by three-body recombination. This allows the observation of the Mott transition, in contrast to the case of Bose-condensed gases in the same geometry.

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The observation of a BCS superfluid transition remains a challenging goal in the studies of ultracold Fermi gases. It was recently suggested that gases confined to low dimensions are promising candidates for achieving superfluidity as the confinement enhances interaction effects [1]. Adding a tunable periodic potential allows one to combine the benefit of the reduced dimensionality with the advantage of working with large yet coherent samples. Importantly, in the presence of a 1D periodic potential plus a superimposed weak harmonic trapping, the superfluid transition is signaled by a marked change in the behavior of the center of mass oscillations of the atomic cloud along the lattice direction [2].

In this Letter, we obtain the BCS transition temperature \(T_c\) for a two-component 3D Fermi gas in a 1D optical lattice. We reveal how the presence of the lattice renormalizes the effective coupling constant, leading to a density-dependent coupling and introducing a crossover to the quasi-2D regime. These findings form a basis for studying superfluid transport for atomic fermions in 1D lattices. For the geometry of finite size discs in the 1D lattice, we also discuss the possibility of achieving the superfluid-Mott insulator quantum transition by tuning the lattice depth above a critical value [3]. In this peculiar phase, the gas is superfluid in each separate disc, but the coherence along the lattice direction is completely lost. We show that for Fermi superfluids the critical effective tunneling rate can be large compared to the loss rate of all inelastic processes and therefore the Mott transition can be achieved. This result is a direct consequence of the Fermi statistics and is in marked contrast with the case of Bose-Einstein condensates in the same geometry, where the Mott transition can be hardly observed [4] unless the number of atoms per disc is very small.

We consider a two-component atomic Fermi gas in the presence of a 1D optical potential [5]:

\[
V_{\text{opt}} = sE_R \sin^2 q_B z,
\]  

where \(s\) is a dimensionless factor fixed by the intensity of the laser beam and \(E_R = \hbar^2 q_B^2 / 2m\) is the recoil energy, with \(\hbar q_B\) being the Bragg momentum and \(m\) the atom mass. The potential (1) has periodicity \(d = \pi / q_B\) along the \(z\) axis. The weak attraction between atoms in different internal states is modeled by a \(s\)-wave pseudo-potential \(U(r) = g \delta(r) \delta(r')\) with coupling constant \(g = 4\pi\hbar^2 a / m\), where \(a < 0\) is the 3D scattering length.

We will discuss the situation where the laser intensity is sufficiently large \((s \approx 5)\) and the Fermi energy \(\epsilon_F\) is small compared to the interband gap \(\epsilon_\perp\). We thus confine ourselves to the lowest Bloch band where the physics is governed by the ratio of the Fermi energy to the bandwidth \(4t\), where \(t\) is the hopping rate between neighboring wells. For \(\epsilon_F < 4t\) the Fermi surface is closed and the system retains a 3D behavior, whereas in the case of \(\epsilon_F > 4t\) the Fermi surface is open and the system undergoes a dimensional crossover. Hence, one has two distinct regimes: an anisotropic 3D regime \((\epsilon_F \ll \epsilon_\perp)\) and a quasi-2D regime \((\epsilon_\perp \gg \epsilon_F \gg t)\). This is clearly different from the case of a 3D lattice [6] where the Fermi energy scales with the bandwidth and can therefore be much smaller than the corresponding value in free space for a given atom density.

The mean field transition temperature \(T_c^0\) is the highest temperature at which the Gorkov equation for the gap parameter has a nontrivial solution [7]. This gives

\[
\frac{1}{g_{\text{eff}}} = \mathcal{P} \int \frac{d^3q}{(2\pi)^3} \frac{1}{\xi_q} \exp(\xi_q/T_c^0) + 1 \bigg|_{\xi_q},
\]  

where \(g_{\text{eff}}\) is an effective coupling constant. The symbol \(\mathcal{P}\) stands for the principal value and \(\xi_q = \hbar^2 q_\perp^2 / 2m + \epsilon(q_z) - \mu\), where \(q_\perp\) is the momentum in the direction perpendicular to the lattice, \(\epsilon(q_z)\) is the band dispersion, and \(\mu \approx \epsilon_F\) is the chemical potential. A straightforward integration of Eq. (2) yields

\[
T_c^0 = \frac{2\gamma}{\pi} \mu \exp\left(\frac{1}{g_{\text{eff}}} \frac{1}{\nu(\mu)} - F(\mu)\right),
\]
with $\gamma = 1.781$ and $\nu(\mu) = \int \delta(x_q)dq/(2\pi)^3$ being the density of states per internal state at the Fermi level. The function $F$ is defined as

$$F = -\frac{\int_{q_0}^{q_0} dq_2 \ln(1 - e(q_2)/\mu)\Theta(\mu - e(q_2))}{\int_{q_0}^{q_0} dq_2 \Theta(\mu - e(q_2))},$$

(4)

where $\Theta(x)$ is the unit-step function.

The effective coupling constant is related to the scattering amplitude $f(E)$ for Cooper pairs by $g_{\text{eff}}^{-1} = (m/4\pi^2h^2)\text{Re}[1/f(E = 2\mu)]$ [8]. This requires us to solve the two-body problem for finding the scattering amplitude in the presence of the 1D lattice. In this case the expression for $f(E)$ is given by

$$f(E) = a \int dZ\phi_1^*(Z, 0)\partial_r(\Psi(Z, r))_{r=0},$$

(5)

where $\phi_1(E, r) = \phi_{t_{q_0}}(z_1)\phi_{-q_0}(-z_2)e^{iq_1r_1}$ is the incoming wave function for two atoms undergoing Cooper pairing. The center of mass and relative coordinates are $Z = (z_1 + z_2)/2$ and $r = r_1 - r_2$, and $E = h^2q_1^2/2m + 2\epsilon_1(q_1)$ is the total energy. The two-particle wave function $\Psi(Z, r)$ obeys the Schrödinger equation

$$\left(-\frac{\hbar^2}{m}\frac{\partial^2}{\partial Z^2} + V(Z, z) + g\delta(r)\frac{\partial}{\partial r}r - E\right)\Psi = 0,$$

(6)

and retain only the contribution of the lowest Bloch band. In the tight binding limit, these states can be written in terms of Wannier functions as $\phi_{t_{q_0}}(z) = \sum_i e^{iq_0d_iw(z - \ell d)}$, where $w(z) = (1/\sqrt{\pi\sigma}^{1/2})\exp(-z^2/2\sigma^2)$ is a variational Gaussian ansatz. By minimizing the energy of noninteracting lattice atoms with respect to $\sigma$, one finds $d/\sigma = \pi\sigma^{1/4} \exp(-1/4\sqrt{\pi})$ [9].

We now insert the ansatz $Y(Z) = A\sum_i w_i^2(Z - \ell d)$ into Eq. (8) and take into account that the relation $\int dZ'K_{E=0}(Z, Z')Y(Z')dZ' = Y(Z)m/4\pi^2a$ gives a critical value of the scattering length $a = a_c$ needed to form a two-body bound state in the lattice [10]. Then, using the dispersion relation $\epsilon_1(q_1) = 2[1 - \cos(q_1d)]$ and obtaining the kernel $K_{E}(Z, Z')$ on the basis of Eq. (9), we find the coefficient $A$ in the expression for $Y(Z)$. Equation (5) then leads to the scattering amplitude

$$f(E) = \frac{aC}{1 - a/a_c + (a/\sqrt{2\pi}\sigma)\alpha(E/4\pi)},$$

(10)

where $C = d/\sqrt{2\pi}\sigma$. The function $\alpha$ is defined as $\alpha(x) = \arccos(1 - x)$ for $x < 2$ and $\alpha(x) = -\ln[x(1 + \sqrt{1 - 2/x^2})/2] + i\pi$ for $x \geq 2$.

Equation (10) is one of the key results of this Letter. It shows that the scattering amplitude undergoes a dimensional crossover as a function of energy. In the anisotropic 3D regime ($E \ll 8t$), we have $f = aC/(1 - a/a_c + iaC\sqrt{Em}/\hbar)$, where $m^*$ is the effective mass at the bottom of the band. In the quasi-2D regime ($E \gg 8t$), the tunneling between wells is irrelevant and the two atoms are in the ground state of an effective harmonic potential of frequency $\omega_0 = h/m^*\sigma$. The scattering amplitude of Eq. (10) should then reduce to $f = f_{2D}$, where $f_{2D} = (a_0(C^2/2\pi\sigma)(1 + (a_0/\sqrt{2\pi}\sigma)(\ln[\lambda\omega_0/2\pi]) + (a_0^2/2\pi\sigma)^2))$ and $\lambda = 0.915/\pi$ [11]. This provides us with the asymptotic behavior of the critical value of the scattering length

$$a_c = -\sqrt{2\pi\sigma}\ln^{-1}(\lambda\omega_0/2t),$$

(11)

which agrees with numerics of Ref. [10] already for $s \approx 5$.

We see that the 1D lattice affects $f(E)$ and the coupling constant $g_{\text{eff}}$ in a nontrivial way. For $\epsilon_F < 4t$, the coupling is density independent and from Eq. (3) we get

$$T_0 = \frac{2\gamma}{\pi} e^{-\epsilon_F} \epsilon_F \exp\left[-\frac{\pi}{2q_F^2C}\left(\frac{1}{|a|} - 1/|a_c|\right)\right].$$

(12)

where the function $F$ is given by Eq. (4), and $q_F = \arccos(1 - \epsilon_F/2t)/d$ is the Fermi wave vector along the $z$ axis. Equation (12) is valid provided $T_0 \ll \epsilon_F$, which
implies $|a| < |a_{\text{ref}}|$. In the low density limit $\epsilon_F \ll 4t$, the temperature $T^0_c$ reduces to the mean field transition temperature [12] for a homogeneous gas of atoms with an anisotropic quadratic dispersion and a renormalized 3D inverse scattering length $a_{\text{ref}}^{-1} = C^{-1}(|a|^{-1} - |a_{\text{ref}}|^{-1})$.

The presence of the lattice causes an effective shift of the resonance from $1/a = 0$ to $1/a = 1/a_{\text{ref}} < 0$, which in turn gives rise to a sharp increase in $T^0_c$ at a fixed value of the 3D scattering length.

For $\epsilon_F > 4t$, the coupling constant $g_{\text{eff}}$ becomes density dependent. Equation (4) yields $F(\mu) = 2\ln[2/(1 + \sqrt{1 - 4t/\mu})]$, and from Eq. (3) we find

$$T^0_c = \frac{\gamma}{2\pi} \left[ 1 + \sqrt{1 - \frac{4t}{\epsilon_F}} \right] \epsilon_F \exp \left[ \sqrt{\frac{2}{\pi}} \left( \frac{\sigma}{a} - \frac{\sigma}{a_{\text{ref}}} \right) \right].$$

Note that the exponent on the right-hand side of Eq. (13) does not depend on the Fermi energy, the density of states being constant for $\epsilon_F > 4t$.

Finally, for $\epsilon_F \gg 4t$ and values of the scattering length $|a| > |a_{\text{ref}}|$, but still $|a| \ll \sigma$, the BCS temperature reduces to the value $T^0_c = \gamma/2\epsilon_F \epsilon_b / \pi$ found for isolated discs, where $\epsilon_b$ is the energy of the two-body bound state. In this limit one has $t \ll T^0_c$ and the system behaves as a stack of quasi-2D superfluids weakly coupled by Josephson junctions. We emphasize that the low-energy collective excitations of the isolated disc are Bogolubov-Anderson phonons, so each pancake is superfluid below the Kosterlitz-Thouless temperature $T_{\text{KT}} \ll \epsilon_F$. Despite the fact that there is no real condensation of pairs in two dimensions at finite temperatures [13], BCS theory provides a rather good estimate for $T_{\text{KT}}$, namely, $T_c/T_{\text{KT}} \sim 1 - T_c/\epsilon_F \ll 1$ [14]. The inclusion of a small interplanar coupling changes the nature of the superfluid transition from Kosterlitz-Thouless to the continuous (second order) type, leading to a critical temperature $T_c$ slightly larger than $T_{\text{KT}}$. This upward shift has been calculated for layered systems [15].

We next proceed to evaluate Gorkov’s correction to the transition temperature due to the polarization of the medium [12]. Following Ref. [16], we introduce the static Lindhard function

$$L(p) = \frac{1}{(2\pi)^3} \int \frac{df(E_q) - f(E_{q+p})}{\xi_{q+p} - \xi_q},$$

where $f(x) = \Theta(-x)$ is the Fermi distribution at $T = 0$. Since $L(p = 0) = n(\mu)$, we write $L(p) = n(\mu) B(p)$, where $B$ is a dimensionless positive function sensitive to the geometry of the Fermi surface. The critical temperature is then given by $T_c = T^0_c e^{-\delta_{\text{eff}}}$, where

$$\delta_{\text{eff}} = \frac{i B(q + q') \delta(E_q) \delta(E_{q+p}) dq dq'}{\int \delta(E_q) \delta(E_{q+p}) dq dq'}.$$

The integration in (15) is done numerically and the corresponding Gorkov correction $T_c/T^0_c$ is shown in Fig. 1. For $\epsilon_F \ll 4t$, the system has an anisotropic quadratic dispersion and we recover the result for the homogeneous case $T_c = T^0_c/(4\epsilon)^{1/3} = 0.45T^0_c$. In the limit $\epsilon_F \gg 4t$, the band dispersion $\epsilon(k)$ can be neglected in Eq. (14) and we find $T_c/T^0_c = e^{-1}$, in agreement with Ref. [11]. The cusp at $\epsilon_F = 4t$ is expected as this is the point of the Van Hove singularity [17] where the derivative of the density of states, $\partial \nu/\partial \epsilon$, diverges.

So far we have discussed the BCS superfluid transition in a 1D optical lattice. In the second part of the Letter we assume that the superfluid gas is at zero temperature and it is confined in the $x, y$ directions by a trapping potential. Then, as the tunneling rate between neighboring discs is tuned below a critical value $t_c$, the system undergoes the superfluid-Mott insulator quantum transition. For a large number of atoms per well ($N \gg 1$), the critical hopping rate can be evaluated within the hydrodynamic approach [18]. Neglecting the coupling with radial degrees of freedom and the particle loss due to inelastic processes, the proper dynamical variables are the particle number fluctuations $N^e_\ell$ and the phase $\Phi_\ell$ of the order parameter in each disc. The hydrodynamic equations are equivalent to the classical equations of motion of the 1D phase Hamiltonian

$$H_p = \frac{1}{2} (E_c/2) N^2_\ell - E_J \cos(\Phi_{\ell+1} - \Phi_\ell),$$

where $E_c = 2\mu/N$ and $E_J = t^2 N/\mu$ are the charging and Josephson energies, respectively, and $hN^e_\ell$ and $\Phi_\ell$ are considered as conjugated variables.

Quantization of the classical Hamiltonian (16) is achieved by replacing these variables with operators $h\hat{N}^e_\ell$ and $\hat{\Phi}_\ell$ satisfying the commutation relation $[h\hat{N}^e_\ell, \hat{\Phi}_\ell] = i\hbar$. The quantized Hamiltonian is known to exhibit a phase transition at the critical value $E_c = \eta E_J$, with $\eta \approx 0.81$ [19]. The superfluid phase occurs for $E_c < \eta E_J$ and is characterized by an algebraic decay of the phase correlation function $\langle \cos(\Phi_{\ell+1} - \Phi_\ell) \rangle$ at large distances $|\ell - k| \gg 1$. The decay becomes exponential for $E_c > \eta E_J$ where one enters the Mott regime, characterized by large phase fluctuations which suppress interwell tunneling. The ground state is an insulator with a fixed number of atoms.
per disc and a finite gap in the excitation spectrum. By comparing the values of the charging and the Josephson energies, we find that for BCS superfluids one has

$$
\frac{t_c}{\mu} = \frac{1}{N} \sqrt{\frac{2}{\eta}}.
$$

(17)

This result differs from the corresponding value for Bose condensates in the same geometry, $t_c^B/\mu^B \sim 1/N^2$, where $\mu^B = n g_{2D}$ is the chemical potential and $g_{2D}$ is the 2D coupling constant. This is because the Josephson energy in the Hamiltonian (16) for the bosonic case is $E_J^B = t N^2$.

Equation (17) has been derived under the assumption that the effective tunneling rate $\nu_c = t_c^2/\hbar \mu = \mu^2/N^2$ is large compared to the loss rate $\tilde{\nu}$. The most severe losses come from three-body recombination. For an array of Bose-condensed atomic gases in the same geometry the corresponding loss rate is always large compared to the critical tunneling rate [4], unless the number of atoms per disc is very small as in the experiment of Ref. [3]. For Fermi superfluids the situation is completely different because the inelastic processes are strongly inhibited by quantum statistics. In the quasi-2D geometry, in analogy with the 3D case [20], for the 3-body loss rate one can write $\tilde{\nu} = -\tilde{n}/n = \ln^2(k_F R_c)^2$, where $L$ is the quasi-2D recombination coefficient and the small factor $(k_F R_c)^2 \ll 1$ comes from Pauli blocking, with $R_c$ being a characteristic radius of the interatomic potential. For the ratio of the loss to critical tunneling rate, which should be small for consistency, we then find

$$
\tilde{\nu}/\nu_c = (h \ln^2/\mu)(k_F R_c)^2 N^2.
$$

(18)

Note that compared to the case of bosons, where the coefficient $L$ has the same order of magnitude but the statistics-induced inhibition of 3-body losses is absent, the ratio $\tilde{\nu}/\nu_c$ has an extra small factor $(k_F R_c)^2 \sim n R_c$. For a weakly interacting gas the quantity $(h \ln^2/\mu)$ is small, and already a crude dimensional estimate $(h \ln^2/\mu) \sim n R_c^2$ indicates wide possibilities to have a small ratio (18) for a large number $N$ of atoms per pancake. For example, let us consider $N = 10^3$ fermionic potassium atoms ($R_c = 5$ nm) in each disc, with density $n = 10^9$ cm$^{-2}$ corresponding to a chemical potential $\mu = \epsilon_F = 380$ nK $k_B$. From Eq. (17) we find $t_c/\hbar \sim 70$ s$^{-1}$ corresponding to $s \sim 25$ for a lattice period $d = 400$ nm, and $\sigma \approx 60$ nm. This leads to $\nu_c \sim 0.1$ s$^{-1}$. Then, taking into account that $L \approx L_{3D}/\sigma^2$ and assuming the 3D recombination $L_{3D} \approx 10^{-28}$ cm$^3$/s, from Eq. (18) we obtain $\tilde{\nu}/\nu_c \sim 1$. Hence, owing to quantum statistics, in Fermi superfluids one can easily have $\tilde{\nu} \ll \nu_c$ and achieve the Mott insulator transition. It is important to emphasize that, in the given example, the suppression of recombination processes by a factor of $(k_F R_c)^2 \sim 10^{-3}$ originating from the Pauli principle is crucial to keep the ratio (18) small even for $N \sim 10^3$.

In conclusion, we have found the superfluid transition temperature for a two-component Fermi gas in a 1D optical lattice and revealed that the effective coupling constant depends in a nontrivial way on both the atom density and the parameters of the optical field. For an array of finite size discs with a large number of atoms per disc, we have shown that the critical effective tunneling rate for the Mott insulator quantum transition can be larger than the rate of particle losses. Thus, the Mott phase transition in a chain of weakly coupled 2D Fermi superfluids can be observed for ultracold gases.

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