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 \textsuperscript{1}. Adding a tunable periodic potential allows one to combine the benefit of the reduced dimensionality with the advantage to work with large yet coherent samples. In particular, it has recently been shown that the study of the center of mass oscillations of the cloud in a 1D lattice plus a superimposed weak harmonic potential allows one to probe the superfluid transition \textsuperscript{2}. Importantly, the presence of periodic potential introduces a much richer physics related to a possibility of observing a variety of quantum phase transitions \textsuperscript{3}.

In this Letter we obtain the BCS transition temperature $T_c$ for a two-component Fermi gas in a 1D optical lattice, assuming that the Fermi energy is small compared to the interband gap and, hence, superfluid pairing occurs only in the lowest band. This requires us to reveal how the presence of the 1D lattice renormalizes the effective coupling constant at the Fermi level. 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. 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 as pointed out by Hadzibabic et al. \textsuperscript{4}, unless the number of atoms per disc is very small.

We consider a two component atomic Fermi gas in the presence of a one dimensional (1D) optical potential

$$V_{opt} = s E_R \sin^2 q_B z,$$  \hspace{1cm} (1)

where $s$ is a dimensionless parameter coming from the intensity of the laser beam, $E_R = \hbar^2 q_B^2 / 2m$ is the recoil energy, with $\hbar q_B$ being the Bragg momentum and $m$ the atom mass. The potential 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 pseudopotential $U(r) = g\delta(r)d(r)$ 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 ($s \gtrsim 5$) and the Fermi energy $\epsilon_F$ is small compared to the interband gap $\epsilon_g$. We thus confine ourselves to the lowest Bloch band where the physics is governed by the ratio of the Fermi energy to the band-width $4t$, where $t$ is the hopping rate between neighboring wells. For $\epsilon_F < 4t$ the Fermi surface is closed and the system retains a 3D behaviour, 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 ($\epsilon_F \ll t$) and a quasi-2D regime ($\epsilon_g \gg \epsilon_F \gg t$). This is clearly different from the case of a 3D lattice \textsuperscript{5} 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 $T^0_c$ is the highest temperature at which the Gorkov equation for the gap parameter has a non-trivial solution \textsuperscript{6}. This gives

$$\frac{1}{g_{eff}} = \int \frac{d^3 q}{(2\pi)^3} \frac{1}{\xi q \exp(\xi q/T^0_c)} + 1,$$  \hspace{1cm} (2)

where $g_{eff}$ is an effective coupling constant. The symbol P stands for Principal value and $\xi q = \hbar^2 q^2 / 2m + \epsilon_1(q_z) - \mu$, where $q_z$ is the momentum in the direction perpendicular to the lattice, $\epsilon(q_z)$ is the band dispersion and $\mu \simeq \epsilon_F$ is the chemical potential. A straightforward integration of Eq.\,(2) yields

$$T^0_c = \frac{2\gamma}{\pi} \mu \exp \left( \frac{1}{g_{eff}} \nu(\mu) - F(\mu) \right),$$  \hspace{1cm} (3)

with $\gamma = 1.781$ and $\nu(\mu) = \int \delta(\xi q) dq/(2\pi)^3$ being the density of states per internal state at the Fermi level.
The function $F$ is defined as
\[
F = \frac{\int_{-\infty}^{\infty} dq \, dq_z \, \ln(1 - \epsilon(q_z)/\mu) \Theta(\mu - \epsilon(q_z))}{\int_{-\infty}^{\infty} dq \, dq_z \, \Theta(\mu - \epsilon(q_z))},
\] (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 $g_{eff} = \langle m/4\pi\hbar^2 \rangle \text{Re}[1/f(E = 2\mu)]$. 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
\[
f(E) = a \int dZ \phi_0^*(Z, 0) \partial_r (r \Psi(Z, r))_{r=0}
\] (5)
where $\phi_0(Z, r) = \phi_{1q_1}(z) \phi_{1q_2}(z) e^{i q_1 \cdot r_1}$ is the incoming wavefunction 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 $E = \hbar^2 q_1^2 / m + \epsilon_1(q_z)$ is the total energy. The two-particle wavefunction $\Psi(Z, r)$ obeys the Schrödinger equation
\[
\left( \frac{\hbar^2}{m} \Delta - \frac{\hbar^2}{4m} \frac{\partial^2}{\partial Z^2} + V(Z, z) + g\sigma(r) \frac{\partial}{\partial r}(r - E) \right) \Psi = 0,
\] (6)
where $V(Z, z) = V_{opt}(z_1) + V_{opt}(z_2)$. The solution of Eq. (6) can be written as
\[
\Psi(Z, r) = \phi_0(Z, r) + g \int dZ^2 K_{E}(Z, Z') Y(Z').
\] (7)
where $G_E(Z, r)$ is the Green function of Eq. (6) with $g = 0$. The behavior of the Green function at short distances $r$ is governed by the Laplacian term in Eq. (6), yielding $G_E(Z, Z') = -\delta(Z - Z')/m + \hbar^2 \gamma r + K_E(Z, Z')$, where $K_E(Z, Z')$ is a regular function. Then, from Eq. (7) we immediately obtain an equation for the function $Y(Z) = \partial_r (r \Psi(Z, r))_{r=0}$ appearing in Eq. (5):
\[
Y(Z) = \phi_0(Z, 0) + g \int dZ^2 K_{E}(Z, Z') Y(Z').
\] (8)
Writing the kernel of the integral equation in the form $K_E(Z, Z') = [G_E(Z, r; 0, Z') - G_{E=0}(Z, 0, Z')]_{r=0} + K_{E=0}(Z, Z')$, we expand the Green function $G_E$ in eigenstates of non-interacting atoms:
\[
G_E(Z, 0, Z') = \sum_{n_1, n_2} \int \frac{d\mathbf{q}_1}{(2\pi)^3} \int \frac{dq_1}{2\pi} \frac{dq_2 e^{i q_2 \cdot r}}{2\pi} \frac{\phi_{n_1 q_1}(z) \phi_{n_2 q_2}(z) \phi_{n_1 q_2}(Z') \phi_{n_2 q_1}(Z')}{E + i\epsilon - \epsilon_{n_1}(q_1) - \epsilon_{n_2}(q_2) - \hbar^2 \gamma^2 / m},
\] (9)
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 $\phi_{n_1 q_1}(z) \sim \sum_t e^{i q_1 \cdot d t} w(z - td)$, where $w(z) = (1/\pi)^{1/2} \sigma(z^2/2\sigma^2) \exp(-z^2/2\sigma^2)$ is a variational Gaussian ansatz. By minimizing the energy of non-interacting lattice atoms with respect to $\sigma$, one finds $d/\sigma = \pi s^{1/4} \exp(-1/4\sqrt{s})$.[8]

We now insert the ansatz $Y(Z) = A \sum t w^2(Z - td)$ into Eq. (5) and take into account that the relation $f(E) K_E(Z, Z') Y(Z') dZ' = Y(Z) m/4\hbar^2a$ gives a critical value of the scattering length $a = a_{cr}$ needed to form a two-body bound state in the lattice.[9] Then, using the dispersion relation $\epsilon(q_z) = 2(1 - \cos(q_z a))$ 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 (10) then leads to the scattering amplitude
\[
f(E) = \frac{a G}{1 - a/a_{cr} + (a/\sqrt{2\pi} \sigma) \alpha(E/4t)},
\] (10)
where $C = d/\sqrt{2\pi} \sigma$. The function $\alpha(x) = \text{arccos}(1-x)$ for $x < 2$, and $\alpha(x) = -\ln[x(1 + \sqrt{1-4x^2})/2] + \pi i$ for $x \geq 2$.

Equation (10) is one of the key results of this paper. 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 $f = aC/(1 - a/a_{cr} + iaC \sqrt{\hbar m^*/\hbar})$ 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 $\omega_0 = h/m^*$. The scattering amplitude of Eq. (10) should then reduce to $f = f_{2D}d$ where $f_{2D} = (a/\sqrt{2\pi} \sigma) \text{ln}[4\hbar \omega_0 (E + i\pi)]$ and $\lambda = 0.915/(\sqrt{2t})$. This provides us with the asymptotic behaviour of the critical value of the scattering length
\[
a_{cr} = -\sqrt{2\pi} \sigma \text{ln}^{-1}(\lambda \omega_0 / 2t),
\] (11)
which agrees with numerics of Ref.[10] already for $s > 5$.

We see that the 1D lattice affects $f(E)$ and the coupling constant $g_{eff}$ in a non-trivial way. For $E < 4t$, the coupling is density independent and from Eq. (10) we get
\[
T_c^0 = \frac{2\pi e^{-F} e^{-\epsilon_F}}{\epsilon_F} \text{exp}\left[\frac{-\pi}{2d_2C} \left(\frac{1}{|a|} - \frac{1}{|a_{cr}|}\right)\right],
\] (12)
where the function $F$ is given by Eq. (4), and $q_{2F} = \text{arccos}(1 - \epsilon_F/2d)/d$ is the Fermi wavevector along the z-axis. Equation (12) is valid provided $T_c^0 < \epsilon_F$, which implies $|a| < |a_{cr}|$. In the low density limit $\epsilon_F \ll 4t$, $T_c^0$ reduces to the mean field transition temperature $T_0$ for a homogeneous gas of atoms with an anisotropic quadratic dispersion and a renormalized 3D inverse scattering length $a_{cr} = C^{-1}|a|^{-1} - |a_{cr}|^{-1}$.[11] The presence of the lattice causes an effective shift of the resonance from $1/a = 0$ to $1/a = 1/a_{cr} < 0$, which in turn gives rise to a sharp increase in $T_c^0$ at a fixed value of the 3D scattering length.

For $\epsilon_F > 4t$, the coupling constant $g_{eff}$ becomes density dependent. Equation (4) yields $F(\mu) = 2 \ln[2/(1 + \sqrt{1 - 4t/\mu})]$, and from Eq. (10) we find
\[
T_c^0 = \frac{\gamma}{2\pi} \left(1 + \sqrt{1 - 4\frac{d_2}{\epsilon_F}}\right) \sqrt{\epsilon_F / 4t} \text{exp}\left[\frac{\pi}{2} \left(\frac{\sigma}{\alpha} - \frac{\sigma}{a_{cr}}\right)\right].
\] (13)
Note that the exponent in the rhs of Eq. (13) does not depend on the Fermi energy, the density of states being constant for $\epsilon_F > 4t$. For $\epsilon_F \gg 4t$, the ratio $\sqrt{\mu/\epsilon_F}$ plays the role of a small parameter ensuring the inequality $T_c/\epsilon_F \ll 1$ also for values of the scattering length larger than $a_s$, but still $|a| \ll \sigma$. In this regime, the system behaves as a stack of quasi-2D superfluid gases weakly coupled by Josephson junctions. The transition temperature in each disc takes the form $T_c = \gamma \sqrt{2F_0 E_k/\pi}$ [12], where in our case $E_k$ is the binding energy of the two-body bound state in the 1D optical lattice. In the absence of coupling between the discs ($t = 0$), the gas in each disc is two-dimensional and the transition is therefore of the Kosterlitz-Thouless type. However, for 2D BCS superfluids a standard calculation of the Kosterlitz-Thouless transition temperature gives a value that is lower than $T_c$ by an amount $\sim T_c^2/\epsilon_F \ll T_c$ [12] and thus lies inside a narrow region of critical fluctuations in the neighborhood of $T_c$. Therefore the mean field approach leads to a correct result for the transition temperature.

We next proceed to evaluate Gorkov’s correction to the transition temperature due to the polarization of the medium [11]. Following Ref. [13], we introduce the static Lindhard function

$$L(p) = \int \frac{d\mathbf{q}}{(2\pi)^3} \frac{f(\xi_q) - f(\xi_{q+p})}{\xi_{q+p} - \xi_q}, \quad (14)$$

where $f(x) = \Theta(-x)$ is the Fermi distribution at $T = 0$. The induced interaction between two states $\mathbf{q}$ and $\mathbf{q}'$ on the Fermi surface is given by $U_{\text{ind}}(\mathbf{p}) = gCL(\mathbf{p})$, with $\mathbf{p} = \mathbf{q} + \mathbf{q}'$ and $C$ defined as above. Since $L(\mathbf{p} = 0) = \nu(\mu)$, we write $L(\mathbf{p}) = \nu(\mu)B(p)$, where $B$ is a dimensionless positive function sensitive to the geometry of the Fermi surface. The critical temperature is then given by $T_c = T_c^0 e^{-C/B} r_s$, where

$$\langle B \rangle_{FS} = \int B(q + q') \delta(q_\xi) \delta(q_{\xi'}) dq dq'. \quad (15)$$

The integration in (13) is done numerically and the corresponding Gorkov correction $T_c/T_c^0$ 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 $\langle B \rangle_{FS} = (1 + 2 \ln 2)/3$, yielding $T_c^0 = T_c^0(4\epsilon_F)^{1/3} = 0.45 T_c$. In the limit $\epsilon_F \gg 4t$, the band dispersion $\epsilon(k_z)$ can be neglected in Eq. (13) and we find $T_c/T_c^0 = e^{-1}$, in agreement with Ref. [11]. The cusp at $\epsilon_F = 4t$ is expected as this is the point of the Van Hove singularity [12] 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 [12]. Neglecting the coupling with radial degrees of freedom and the particle loss due to inelastic processes, the proper dynamical variables are the particle number fluctuation $N_p$ and the phase $\Phi$ of the order parameter in each disc. The hydrodynamic equations are equivalent to the classical equations of motion of the 1D phase Hamiltonian

$$H_P = \sum_\ell \left( E_c/2 \right) N_p^2 - E_J \cos(\Phi_{\ell+1} - \Phi_{\ell}), \quad (16)$$

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

Quantization of the classical Hamiltonian (16) is achieved by replacing these variables with operators $\hbar N_p'$ and $\Phi$ satisfying the commutation relation $[\hbar N_p', \Phi] = i\hbar$. The quantized Hamiltonian is known to exhibit a phase transition at the critical value $E_c = \eta E_J$, with $\eta \approx 0.81$ [17]. 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 phase, 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

$$\frac{t_c}{\mu} = \frac{1}{N} \sqrt{\frac{2}{\eta}}. \quad (17)$$

This result differs from the corresponding value for Bose condensates in the same geometry, $\nu_c^B/\mu^B \sim 1/N^2$ where $\mu^B = \eta g_{2D}$ is the chemical potential and $g_{2D}$ is the 2D
coupling constant. This is because the Josephson energy in the Hamiltonian for the bosonic case is \( E_0^2 = tN \).

Equation \( \text{14} \) has been derived under the assumption that the effective tunneling rate \( \nu = \frac{\mu}{\sigma^2} \) is large compared to the loss rate \( \bar{\nu} \). 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 \( \text{2} \), unless the number of atoms per disc is very small as in the experiment of Ref. \( \text{3} \). For Fermi superfluids the situation is completely different because the inelastic processes are strongly inhibited by quantum statistics. In the quasi2D geometry, in analogy with the 3D case \( \text{17} \), for the 3-body loss rate one can write \( \bar{\nu} = -\dot{n}/n = \mp n^2(k_F R_e)^2 \), where the small factor \( (k_F R_e)^2 \) comes from the Pauli principle, \( R_e \) is a characteristic radius of the interatomic potential, and \( L \) is the quasi2D recombination coefficient. This coefficient is related to the corresponding quantity of a 3D gas as \( L \sim L_{3D}/\sigma^2 \). Within an order of magnitude, \( L_{3D} \) coincides with the recombination rate constant for bosonic isotopes of the same atom, which ranges from \( 10^{-27} \) to \( 10^{-30} \text{cm}^3/\text{s} \) for alkali atoms. The ratio of the loss to the effective tunneling rate is then given by

\[
\frac{\bar{\nu}}{\nu_c} \approx \frac{\hbar L_{3D}^2 (k_F R_e)^2 N^2}{\mu \sigma^2} \approx \left( \frac{2mL_{3D}}{hR_e^2 \sigma^2} \right) (nR_e^2)^2 N^2 \tag{18}
\]

and should be much smaller than unity for consistency.

Note that in the case of bosons the effective tunneling rate is \( \nu_b^e = \nu_b/h \sim n_{3D}/N^2 \). For a given \( N \), it is smaller than the one for fermions by a factor of \( (n_{3D}/\pi \hbar^2) \), which is a small parameter of the theory for the 2D weakly interacting gas. The bosonic 3-body loss rate is \( \bar{\nu}_b \sim (L_{3D}/\sigma^2)n^2 \) and it exceeds the fermionic loss rate by a factor of \( (k_F R_e)^{-2} \). Thus, we have \( \bar{\nu}/\nu_c \sim (m_{3D}/\pi \hbar^2)(k_F R_e)^2 \bar{\nu}_b/\nu_b^e \). For realistic densities the fermionic ratio \( \bar{\nu}/\nu_c \) is smaller than the bosonic ratio \( \nu_b^e/\nu_b \) by 4 or 5 orders of magnitude. This is a consequence of Fermi statistics and it is crucial for the observation of the Mott transition.

For example, considering \( N = 10^3 \) fermionic potassium atoms \( (R_e \approx 5 \text{ nm}) \) in each disc, with density \( n = 10^9 \text{cm}^{-2} \) corresponding to a Fermi energy (chemical potential) \( \epsilon_F \approx \mu = 380 \text{nK} \), from Eq. \( \text{17} \) we find \( \nu_c/(\pi) \sim 70 \text{s}^{-1} \) corresponding to \( s \sim 25 \) for a lattice period \( d = 400 \text{ nm} \), and \( \sigma \approx 60 \text{ nm} \). This leads to \( \nu_c \sim 0.1 \text{s}^{-1} \) and, assuming \( L_{3D} \lesssim 10^{-28} \text{cm}^{3}/\text{s} \), from Eq. \( \text{18} \) we obtain \( \bar{\nu}/\nu_c \lesssim 0.1 \). Hence, owing to quantum statistics, in Fermi superfluids one can easily have \( \bar{\nu} \ll \nu_c \) 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 \( (k_F R_e)^2 \sim 10^{-3} \) originating from the Pauli principle is crucial to keep the ratio \( \text{15} \) 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 non-trivial 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 particles losses. Thus, the Mott phase can be observed for Fermi superfluids in this geometry.

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