Alkali-metal gases in optical lattices: Possible new type of quantum crystals

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Similarities between alkali-metal gases in optical lattices with noninteger occupation of the lattice sites and quantum crystals are explored. The analogy with the vacancy liquid (VL) provides an alternative explanation to the Mott transition for the recent experiment on the phase transition in the lattice. The VL can undergo Bose-Einstein condensation (BEC) with T_c within experimental reach. Direct and vacancy-assisted mechanisms of the band motion for hyperfine impurities are discussed. A large concentration of vacancies can result in the spatial decomposition of the system into pure hyperfine components. Below the vacancy condensation the impurity component resembles ^{3}He in ^{3}He–He II mixtures.

Recently, after the spectacular experimental discovery of Bose condensation, the study of alkali-metal gases in traps has become the focal point in atomic, low temperature, and condensed matter physics. One of the most fascinating features is the possibility of seeing in an experiment some of the phenomena that have been discussed earlier only within theoretical models (see the review [1]). An additional attraction is that the phenomena in ultracold alkali-metal gases are incredibly rich and combine features inherent to diverse condensed matter and low temperature systems (Ref. [2] and references therein). For example, Bose-Einstein condensation (BEC) in trapped gases resembles, but is not quite the same as, the transition in other superfluid or superconducting systems [2]. Another example is the dynamics of the hyperfine components which resembles the spin dynamics of spin-polarized quantum gases [3].

A new example is an ultracold alkali-metal gas in an optical lattice. Alkali-metal atoms are almost localized in microscopically periodic potential wells induced by the Stark effect of interfering laser beams (Ref. [4] and references therein). The tunneling probability t between the wells is determined by the depth and size of the wells, i.e., by the intensity and the wavelength λ of the beams. Since this intensity is adjustable, the atoms can be studied in a wide range of tunneling frequencies t and effective masses $m^* \sim \hbar^2/ta^2$, from an almost free gas with a periodic perturbation to a well-localized "solid" ($a = \lambda/2 = \pi/k$ is the lattice period). Another parameter is the on-site repulsion U for atoms inside the same well.

The standard Hubbard model for electrons predicts [5] that the alkali-metal atoms in an optical lattice should exhibit an analog of the Mott metal-insulator transition at $U/t \approx 5.8z$ (z is the number of nearest neighbors). At $U \gg t$, the system should become an "insulator" without interwell transitions (the particle tunneling between the lattice sites increases the on-site energy by U and is energetically prohibitive). At $U \ll t$, the on-site interaction does not restrict tunneling between the sites and the atoms are in the "metal" phase. Then, at sufficiently low temperature, the system can undergo BEC into a lattice superfluid. The energy parameters U, t, and the potential well V_0 are often measured in units of the recoil energy $E_r = \hbar^2 k^2/2m$. A typical example is [5] $t/E_r \sim 0.07$ and $U/E_r \sim 0.15$ for $V_0/E_r = 15$.

This type of transition has been reported in Ref. [6] for lattices of size $a = \pi/k \sim 426$ nm with recoil energy $E_r = \hbar^2 k^2/2m \sim 1$ kHz. At low beam intensity, i.e., at large t, the experiment revealed a condensate peak in the center of the trap. This peak disappeared at small t (at V_0/E_r between 13 and 22), which might indicate the transition to the Mott insulator (MI) phase. However, the identification of the high-U phase as the MI is not unambiguous. The MI can be observed only when the average number of atoms on the same lattice site is integer. If the average population is fractional, the highest on-site energy states are not fully occupied. The tunneling of the "excessive" particles from a site on which the highest level is occupied to a site with an unoccupied level cannot be banned by the on-site interaction. The tunneling of the "excessive" particle from site $\mathbf{r}_1$ to the empty neighboring site $\mathbf{r}_2$ increases the on-site energy by U on the site $\mathbf{r}_2$ while simultaneously decreasing it by U on the vacated site $\mathbf{r}_1$. Since both sites are translationally equivalent, this opens the way to the band motion of the "excessive" particles and to the existence of a partially filled conduction band. Then the lattice with noninteger occupation stays in the "metal" or "semiconductor" state even at large U with the "excessive" particles in the conduction band. Reference [6] contains experimental proof of a large gap between the filled and conduction bands. However, it is difficult to conclude whether in equilibrium the conduction gap is empty or not. Below we suggest an alternative interpretation for Ref. [6] based not on the analogy with the Mott transition, but on the analogy with quantum crystals (QCs).

There is a strong similarity between the ultracold particles in optical lattices and atoms in QCs, such as solid helium, in which the tunneling is sufficiently high to ensure band motion of atoms unless prohibited by large on-site repulsion (see the review [7] and references therein). In helium crystals, atomic band motion is banned, as for all MIs, when all the lattice sites are occupied by *identical* particles with occupancy equal to 1. If, however, some of the lattice sites are empty, nothing prohibits tunneling of atoms from the occupied onto the vacant sites, leading, as a result of translational symmetry, to the band motion of vacancies, i.e., to the formation of peculiar band quasiparticles—vacancy waves. Similar quasiparticles are formed when some of the atoms occupy interstitial sites and can tunnel through the QC. A

slightly different situation occurs when some of the lattice sites are occupied by atoms of a different kind from the host matrix (impurities). The impurities can also tunnel through the QC despite the fact that each site still has occupancy equal to 1. The tunneling constant for impurities is smaller than for the vacancies since the exchange of places between the impurity and host atoms involves high-energy intermediate states with either double on-site occupancy or the atom in an interstitial position. The impurity-host exchanges could be so low that a more efficient mechanism of impurity motion could be vacancy-assisted diffusion. The behavior of vacancy and impurity waves in QCs is well understood [7]. However, the most exciting possibility in QCs—superfluidity and BEC in a system of vacancy waves—has not been realized for "classical" QCs, namely, solid ^{4}He, despite two decades of intensive effort (Refs. [8,9] and references therein). The reason is that there are no zero-temperature vacancies in solid ^{4}He: with decreasing temperature, the concentration of vacancies drops exponentially, always remaining insufficient for BEC.

The alkali-metal atoms in optical lattices resemble QCs with a very appealing difference: the BEC in the system of vacancy or "impurity" waves could be within reach. When the occupancy of the individual wells is close to an integer, the system resembles a QC with either a small concentration of vacancies or "excessive" atoms. If the occupancy is slightly below the integer K, $K=1+\text{Int}[n/N]$, where n and N are the densities of atoms and lattice sites, then the density of vacancies is $n_v=KN-n\ll N$. If the occupancy slightly exceeds the integer number, then the density of "excessive" atoms $n_e\equiv N-n_v$ is $n_e=n-N\text{Int}[n/N]\ll N$. Since the tunneling probabilities t are the same for vacancies and "excessive" atoms, $t_v=t_e$ (in both cases, an atom tunnels to an empty site), many properties of the system are symmetric with respect to the vacancies and excessive atoms. (This is not so for the usual QC in which the lattice potential is built of the atom interaction and the potential relief is different for a vacancy and an "excessive" atom.)

Below we consider the situation with large on-site interaction U, when the lattice system with integer site occupation would become a MI, making the BEC transition impossible. The analogy with QCs automatically excludes fully occupied lowest on-site states and does not require the concept of countersuperfluidity [10].

In the tight binding approximation for vacancies in a simple cubic lattice,

$$\epsilon_v(\mathbf{p})=\Delta/2-2t_v\sum\cos(p_ia/\hbar), \tag{1}$$

where $\Delta=12t_v$ is the bandwidth. At large U, the fixed chemical potential μ_v is finite, in contrast to $\mu_v=0$ for thermally activated vacancies in solid helium. When n_v is small, the BEC transition temperature for the vacancies can be determined using the standard equations for lattice gases with low band filling:

$$T_c=6.6a^2t_vn_v^{2/3}, \tag{2}$$

and similarly for excessive atoms. A good extrapolation between these two limiting cases is

$$T_c=6.6a^4t_vn_v^{2/3}(N-n_v)^{2/3}. \tag{3}$$

With the above values of E_r and a, the estimate for the BEC transition in the vacancy liquid (VL) is $T_c\sim3\times10^{-7}(t_v/E_r)x_v^{2/3}(1-x_v)^{2/3}$ K, where $x_v=a^3n_v$ is the fraction of unoccupied highest on-site states.

Although T_c for the VL can be quite high, there are two reasons why T_c is lower than the BEC temperature for a free gas. First, the density of participating particles is lower (only the vacancies or the excessive atoms in the highest on-site state are subject to condensation). In the experiment [6] with the occupancy between 2 and 3, this leads, at least, to a factor $5^{-2/3}$ in T_c and even stronger lowering of T_c if the system is close to integer occupancy. Second, the effective mass of vacancy waves or excessive particles, $m^*=\hbar^2/2ta^2=m(E_r/\pi^2t)$, could be much larger than the mass of the free atoms, m. In an experiment, one has limited control over the vacancy concentration. On the other hand, the tunneling frequency depends exponentially on the intensity of the laser beams. This makes m^* a readily adjustable parameter that can make the superfluid transition in the VL (3) observable.

All this suggests a probable alternative to the Mott transition for the experiment [6]. At large t, the experiment confirmed the presence of BEC, probably in the "free" alkali-metal gas rather than in the VL. At small t, the experiment showed the absence of a condensate. However, the experiment, by design, cannot distinguish between the MI and the VL. It is possible that the experiment showed the superfluid-VL transition rather than the superfluid-MI transition.

The analogy with QCs allows one to make several other predictions. First, the role of "impurity waves" can be played by atoms in different hyperfine states. Experimentally, such impurities can be studied by means similar to the NMR methods for ^{3}He diffusion in solid ^{4}He. In principle, impurities become band particles spread across the system with tunneling frequency t_i. However, when the on-site interaction U is large, t_i for direct exchange of impurities with the host atoms and, therefore, the impurity wave bandwidth become very small, of the order of $t_i\sim t_v^2/U\ll t_v$. When U is sufficiently large, such direct tunneling can often be disregarded.

If the number of upper-state vacancies is noticeable, the vacancy-assisted processes dominate the impurity motion with an effective intersite tunneling rate $t_i\sim t_vx_v\gg t_v^2/U$ (in this context, the asymmetry of the vacancy-assisted motion [11] is not important). At $T>T_c$, the vacancy-assisted processes are responsible for independent tunneling transitions between the adjacent sites. This is not a band motion but a more traditional impurity diffusion with an effective diffusion coefficient

$$D_i\sim\frac{t_va^2}{\hbar}\frac{n_v}{N-n_v}. \tag{4}$$

For vacancy-assisted impurity tunneling, in contrast to the pure system (3), t_i and the mean free paths are not symmetric with respect to $n_v \to 0$ and $n_v \to N$. In the former limit, the free paths are atomic while in the latter limit the impurities recover their band properties with the large mean free path determined by impurity-impurity scattering or the scattering by the few remaining upper-state host atoms.

The situation changes dramatically after the vacancy system undergoes the superfluid transition (3). Then the impurity becomes a completely delocalized quasiparticle in a vacancy superfluid background similar to ^{3}He impurities in the superfluid ^{4}He [12]. The effective mass of such quasiparticles at $T=0$ is $m_i^* \sim \hbar^2/2t_v x_v$ and goes up with temperature with a decrease in density of the vacancy condensate. The interaction effects in this quasiparticle gas are negligible, and the properties of the system can be evaluated using the standard equations for an ideal lattice gas of quasiparticles. At low enough temperatures, this impurity component of density n_i will also undergo its own BEC with

$$T_{ci} \simeq 6.62 t_v a^5 n_v n_i^{2/3} = a^3 n_v^{1/3} n_i^{2/3} T_c, \qquad (5)$$

where T_c is the temperature for the vacancy condensation (2). The emerging two-condensate system should exhibit properties similar to those of liquid ^{3}He-^{4}He mixtures with two condensates below the ^{3}He transition [13]. Since this BEC is based on vacancy-assisted tunneling, this two-condensate system is different from the one considered in Ref. [10].

This picture of vacancy-assisted impurity motion works well when the concentration of the hyperfine impurities $x_i = a^3 n_i$ is low. At higher x_i the vacancy motion in this translationally inhomogeneous environment is accompanied by host-impurity permutations suppressing the band motion. This is similar to the vacancy motion in solid ^{3}He with a disordered spin system. Then the vacancies autolocalize within homogeneous domains of size

$$R = \left[\frac{\pi \hbar^2}{2m^* NT[(x_i-1)\ln(1-x_i) - x_i \ln x_i]} \right]^{1/5}, \qquad (6)$$

which are filled by particles in one hyperfine state (Nagaoka polarons). If the density of vacancies is large, $n_v^{1/3} R \gtrsim 1$, this should lead to the decomposition of the system into macroscopic hyperfine domains. The difference between this decomposition and the vacancy-driven spin polarization of solid ^{3}He [14] is that the transition takes place when the concentration of the zero-point vacancies and the "polarization" (the concentration of hyperfine components) are fixed. In contrast to the formation of dynamic, transient domains in experiment [3], this decomposition leads to stationary domains. If the hyperfine impurities are bosons, this decomposition is not always necessary below the vacancy BEC.

One feature of the optical lattices is quite different from more "traditional" QCs such as helium. Since the periodic potential in QCs is built of atomic interactions, the vacancy motion is tied to the deformation of the lattice. For alkali-metal atoms in optical lattices, the lattice is the external potential of the laser beams and the particle displacement is decoupled from the deformation of the lattice. As a result, the low-frequency collective modes above and below the BEC are decoupled from the lattice variables.

An important issue for QCs is the sensitivity of the narrow-band particles to external fields. Since the energy of band particles cannot change by more than the bandwidth Δ, the external field $\Omega(\mathbf{r})$ makes the motion finite and localizes the particles in an area of size $\delta r \sim a\sigma$, $\sigma = \Delta/(\partial\Omega/\partial r)a$. For the usual QC, the important fields are the particle interaction, lattice deformation, and external forces. In the optical lattice, the most important field is the trapping potential $\Omega = \frac{1}{2}\alpha r^2$. In wide traps (small α), this trapping potential does not cause noticeable Umklapp processes and the overall Hamiltonian of a particle (or a vacancy) in the optical lattice, $H = \epsilon(\mathbf{p}) + \frac{1}{2}\alpha r^2$, can be treated quasiclassically. Analysis of this Hamiltonian can be performed in the momentum representation in which $\frac{1}{2}\alpha r^2 = \frac{1}{2}\hbar^2\alpha\nabla_{\mathbf{p}}^2$ and the problem reduces to that for a particle with "mass" $1/\alpha$ in the "potential" $\epsilon(\mathbf{p})$. The quantum problem is simplest near the band minima where the quantized motion is harmonic with the characteristic frequency $\omega_0^* = (2t\alpha)^{1/2}a/\hbar$. Since the effective (tunneling) mass $m^* = \hbar^2/2ta^2$ is larger than the mass of free particles, this frequency is $(m/m^*)^{1/2}$ times lower than for the free particles. The quantization in the trapping potential $\Omega(\mathbf{r})$ is usually not important and the motion is close to classical. At large σ the motion is unrestricted. When $\sigma \to 1$, even the classical motion becomes compressed toward the multiwell shells around the center of the trap , with σ giving the thickness of the shell, to which the particle motion is restricted, in terms of the well size a. In the experiment [6], $\omega_0^* \sim 75(t/E_r)^{1/2}$ Hz and is small, while $\sigma \gtrsim 100(t/E_r)$. The shells narrow to a single well layer at the beam intensity for which $t/E_r \lesssim 0.01$.

The inhomogeneity of the trap also leads to the nonuniform spatial redistribution of particles [5,15]. If the change of the trapping potential from well to well is large in comparison with the temperature ($\Delta/T\sigma \gg 1$), the shells with lower energy are fully filled, have integer population, and become a MI. The rest of the shells (most likely, but not necessarily, the outer ones) will have noninteger population and resemble a VL with a rather large density of vacancies. In the experiment [6], the parameter $\Delta/T\sigma \sim 10^{-10}/T$ with T in Kelvin. If it is small, the redistribution of particles between the shells is insignificant. If this parameter is large, the system represents a thick shell with $\sigma \gtrsim 100(t/E_r)$ of coupled well layers in the quasi-two-dimensional VL state with the rest of the shells in the MI state with filled upper levels. This may actually increase the BEC temperature for the VL since the VL, although restricted to a lower number of shells, can have a higher density of vacancies. To resolve this issue experimentally one should measure the temperature T. To avoid this issue entirely, one can minimize or eliminate completely the overall trapping potential which becomes unnecessary when the atoms are localized within the optical lattice.

In summary, we explored the analogy between alkali-metal gases in optical lattices with noninteger occupation and large on-site interaction and QCs. This analogy provides

an alternative explanation for the experiment [6] as a transition between the BEC and VL states. BEC transition for the VL is predicted. The transition temperature seems to be within experimental reach. The presence of a large number of unoccupied states provides a vacancy-assisted mechanism for diffusion of hyperfine impurities and can sometimes lead to a spatial decomposition of the system into pure hyperfine components. The properties of the hyperfine mixture depend on whether the system is above or below the BEC temperature for the VL. At even lower temperatures one can observe a transition to the state with two—vacancy and impurity—condensates, which is different from Ref. [10]. One of the ways to identify the VL phase is to study the (pseudo)spin diffusion by methods similar to [3].

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