Bose-Einstein Condensation and Quasicrystals

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Abstract. We consider interacting Bose particles in an external local potential. It is shown that large class of external quasicrystal potentials cannot sustain any type of Bose-Einstein condensates. Accordingly, at spatial dimensions $D \leq 2$ in such quasicrystal potentials a supersolid is not possible via Bose-Einstein condensates at finite temperatures. The latter also hold true for the two-dimensional Fibonacci tiling. However, supersolids do arise at $D \leq 2$ via Bose-Einstein condensates from infinitely long-range, nonlocal interparticle potentials.

1. Introduction

In a recent paper [1], the question of the existence of a Bose-Einstein condensate (BEC) in a supersolid was investigated. It was shown that an external crystalline lattice potential could not by itself sustain a condensate and so a crystalline lattice potential cannot give rise to a supersolid via a BEC. In addition, it was found that for spatial dimensions $D \leq 2$ self-crystallization occurs if the interparticle interaction between bosons is nonlocal and of infinitely long-range. In what following, we consider the same issues but now addressing quasicrystals, as well as, the 2-dimensional square Fibonacci tiling, which does not posses one of the “forbidden” $n$-fold rotational symmetries, $n \geq 5$, that are characteristic of quasicrystals and incompatible with translational periodicity.

2. Crystals

The Hamiltonian for the interacting Bose gas is

\begin{equation}
\hat{H} = \int dr \hat{\psi}^\dagger(r) \left( \frac{-\hbar^2}{2m} \nabla^2 \right) \hat{\psi}(r) + \int dr \hat{\psi}^\dagger(r) V_{\text{ext}}(r) \hat{\psi}(r) \\
+ \int dr_1 \int dr_2 \int dr_3 \int dr_4 \hat{\psi}^\dagger(r_1) \hat{\psi}^\dagger(r_2) V(r_1, r_2, r_3, r_4) \hat{\psi}(r_3) \hat{\psi}(r_4),
\end{equation}

where $V_{\text{ext}}(r)$ is an arbitrary, external potential, $V(r_1, r_2; r_3, r_4)$ is a general two-particle interaction potential, and $\hat{\psi}(r)$ and $\hat{\psi}^\dagger(r)$ are bosonic field operators that destroy or create a particle at spatial position $r$, respectively.

Macroscopic occupation in the single-particle state $\psi(r)$ result in the non-vanishing [2] of the quasi-average $\langle \hat{\psi}(r) \rangle = \langle \psi(r) \rangle$ and so the boson field operator

\begin{equation}
\hat{\psi}(r) = \psi(r) + \hat{\psi}(r),
\end{equation}

where
\[ \hat{\phi}(r) = \sqrt{\frac{1}{V(D)}} \sum_k \hat{\phi}_k e^{i k \cdot r} \]  

with the condensate wavefunction

\[ \psi(r) = \sqrt{\frac{N_0}{V(D)}} \sum_{k'} \xi_{k'} e^{i k' \cdot r}, \]  

and normalization

\[ \sum_{k'} |\xi_{k'}|^2 = 1, \]  

where \( N_0 \) is the number of atoms in the condensate, \( V(D) \) is the D-dimensional “volume,” \( \hat{\phi}_k, \hat{\phi}_k^\dagger \) are the creation (annihilation) operators with commutation relations \( [\hat{\phi}_k, \hat{\phi}_{k'}^\dagger] = \delta_{k,k'} \), and \( \langle \hat{\phi}(r) \rangle = 0 \). The operator \( \hat{\phi}(r) \) has no Fourier components with momenta \( \{k'\} \) that are macroscopically occupied and so \( \int d r \hat{\phi}^\dagger(r) \psi(r) = 0 \). The separation of \( \hat{\psi}(r) \) into two parts gives rise to the following (gauge invariance) symmetry breaking term [2] associated with the interparticle potential in the Hamiltonian (1)

\[ \hat{H}_{\text{symm}} = \int d r_1 \hat{\phi}^\dagger(r_1) \int d r_2 \int d r_3 \int d r_4 \psi^\dagger(r_1) [V(r_1, r_2, r_3, r_4) + V(r_2, r_1, r_3, r_4)] \psi(r_2) \psi(r_3) \psi(r_4) + h.c. \]  

Recall that the interaction potential between bosons indicates that macroscopic occupation in a single-particle linear momentum state, viz., a spatially uniform condensate, does not give rise to additional macroscopic occupation in any other single-particle linear momentum states owing to the conservation of linear momentum by the interaction [1]. However, macroscopic occupation in two or more single-particle linear momentum states give rise to a denumerably infinite, macroscopically occupied states. For instance, macroscopic occupation in the single-particle momenta states \( k, k \pm q_1, \) and \( k \pm q_2, \) where \( q_1 \times q_2 \neq 0, \) gives rise to additional macroscopic occupation in the single-particle momenta states \( k + n_1 q_1 + n_2 q_2, \) with \( n_1, n_2 = 0, \pm 1, \pm 2, \cdots \) owing to the symmetry breaking term \( \hat{H}_{\text{symm}}. \)

Accordingly, the condensate wave function gets augmented and is of the Block form given by

\[ \psi_k(r) = \sqrt{\frac{N_0}{V(D)}} \sum_{n_1,n_2=-\infty}^{\infty} \xi_{k+n_1 q_1 + n_2 q_2} e^{i(k+n_1 q_1 + n_2 q_2) \cdot r} \]  

with \( u_k(r + r_0) = u_k(r), \) where

\[ r_0 = 2\pi \left[ \frac{(q_2^2 - q_1 \cdot q_2) q_1 + (q_1^2 - q_1 \cdot q_2) q_2}{q_1^2 q_2^2 - (q_1 \cdot q_2)^2} \right]. \]  

3. Quasicrystals

We now consider the replacement (2) in the term in (1) associated with the external, local potential \( V_{\text{ext}}(r) \). One obtains the symmetry breaking Hamiltonian

\[ \hat{H}_{\text{symm}}^{(\text{ext})} = \int d r \hat{\phi}^\dagger(r) V_{\text{ext}}(r) \hat{\psi}(r) + h.c. \]
Consider the local, finite two-dimensional quasicrystal lattice potential,

\[ V_{\text{ext}}(r) = \frac{1}{(2\pi)^2} \sum_{k} g(k) \sum_{m_1,\ldots,m_n=-M_1,\ldots,-M_n}^{M_1,\ldots,M_n} e^{-ik \cdot (r-\sum_{i=1}^{n} m_i (\alpha_i a + \beta_i b))} \]  

(10)

where \( g(k) \) is the Fourier transform, \( a \) and \( b \) are arbitrary two-dimensional vectors in the x-y plane with \( a \times b \neq 0 \), \((\alpha_i a + \beta_i b) \times (\alpha_j a + \beta_j b) \neq 0\), \( \alpha_i \) and \( \beta_i \) are irrational numbers, and \( n \geq 3 \). In (10), we have projected a periodic structure in \( n \)-dimensional space into a \( D \)-dimensional quasicrystal space \((n > D)\). Cases \( n = 1,2 \) reduce to a one- and two-dimensional crystals, respectively. One obtains that

\[ \hat{H}^{(\text{ext})}_{\text{symm}} = \int \! dr \hat{\varphi}^\dagger(r) V_{\text{ext}}(r) \hat{\varphi}(r) + h.c. \]

\[ = \frac{\sqrt{N_0}}{V(D)} \sum_{k_1,k_2 \neq k_1} \hat{a}^\dagger_{k_1} \hat{\zeta}_{k_2} g(k) \prod_{i=1}^{n} \frac{\sin [k \cdot (\alpha_i a + \beta_i b)(M_i + 1/2)]}{\sin [k \cdot (\alpha_i a + \beta_i b)/2]} + h.c., \]

(11)

where \( k \equiv k_2 - k_1 \), which follows with the aid of (3), (4), and (10). Recall that

\[ \sum_{m=-M}^{M} e^{imx} = \frac{\sin [x(M + 1/2)]}{\sin [x/2]} \rightarrow 2\pi \delta(x) \quad (M \rightarrow \infty). \]

(12)

Note that \( k_1 \neq k_2 \), that is, \( k \neq 0 \), since \( k_2 \) is in the condensate and \( k_1 \) is not in the condensate. Therefore, \( \hat{H}^{(\text{ext})}_{\text{symm}} \) vanishes for arbitrary BEC in the macroscopically large aperiodic lattice limit whichever order the limits are taken. Therefore, one cannot generate a two-dimensional supersolid via a BEC at temperatures \( T \geq 0 \) from an external aperiodic lattice potential. However, a two-dimensional supersolid at finite temperatures can be generated via long-range, nonlocal potentials provided by the interparticle interaction which results in self-organization [1], much as Wigner crystallization or Wigner lattice, electrons moving in a uniform background of positive charge that restore electric neutrality [3].

The embedded spaces of \( D \)-dimensional quasiperiodic structures are abstract spaces whose dimensions are more than three. The dimensions of the embedded space are dependent on the symmetry of the quasicrystal \((D > 1)\) [4, 5]. For example, the quasicrystals with 5, 8-, 10-, and 12-fold symmetry need to be embedded into four-dimensional space, \( n = 4 \). While for the quasiperiodic structures with 7-, 9-, 18-fold symmetry, the dimension of the embedding spaces increases [4-6] to six, \( n = 6 \).

The Fibonacci tiling [7, 8] does not fall in the above class of lattice potentials given by (10). However, the Fourier transform of the Fibonacci sequence has \( \delta \)-function peaks at \( k = 2\pi (m + m')/\sqrt{5} \), where \( r = (1 + \sqrt{5})/2 \) is the golden mean and \( m \) and \( m' \) are integers [9]. Expressed in terms of Fourier transforms (9) becomes

\[ \hat{H}^{(\text{ext})}_{\text{symm}} = \frac{\sqrt{N_0}}{V(D)} \sum_{k' \neq k} \hat{a}^\dagger_{k'} \hat{\zeta}_{k'} \hat{V}_{\text{ext}}(k' - k) + h.c. \]

(13)

where

\[ \hat{V}_{\text{ext}}(k' - k) = \int \! dr \hat{V}_{\text{ext}}(r) e^{i(k' - k) \cdot r}. \]

(14)

Consider the case where \( \hat{V}_{\text{ext}}(k' - k) \) is given by a sum of Dirac \( \delta \)-functions, which is the case for the Fibonacci tiling [9]. Now the vector \( k' - k \) must lie either in the condensate or outside the condensate. In either case, \( \hat{H}^{(\text{ext})}_{\text{symm}} \) vanishes for arbitrary BEC since the vector \( k \) is not in the condensate while the vector \( k' \) is in the condensate.
4. Quasicrystal condensate

The necessity that a BEC has the Bloch form and represents a self-organized supersolid for \( D \leq 2 \) requires that the interaction between the atoms be nonlocal and of infinitely long-range [10]. This proof also applies for the existence of an aperiodic condensate. For instance, macroscopic occupation in the single-particle momenta states \( \mathbf{0}, \mathbf{q}_1, \alpha_1 \mathbf{q}_1, \mathbf{q}_2, \) and \( \alpha_2 \mathbf{q}_2, \) where \( \alpha_1 \) and \( \alpha_2 \) are irrational numbers and \( \mathbf{q}_1 \times \mathbf{q}_2 \neq \mathbf{0}, \) gives rise to additional macroscopic occupation in the single-particle momenta states \( (m_1 + \alpha_1 m_2)\mathbf{q}_1 + (n_1 + \alpha_2 n_2)\mathbf{q}_2, \) with \( m_1, m_2, n_1, n_2 = 0, \pm 1, \pm 2, \cdots \) owing to the symmetry breaking term \( H_{symm} \) and the linear momentum conservation of the interparticle potential.

Accordingly, the condensate wave function gets augmented and is given by

\[
\psi(r) = \sqrt{\frac{N_0}{V(D)}} \sum_{m_1,m_2,n_1,n_2=-\infty}^{\infty} \xi((m_1+\alpha_1 m_2)q_1 + (n_1+\alpha_2 n_2)q_2) e^{i((m_1+\alpha_1 m_2)q_1 + (n_1+\alpha_2 n_2)q_2) \cdot r},
\]

where \( \mathbf{q}_1 \) and \( \mathbf{q}_2 \) are crystallographic directions.

5. Summary and Discussion

We have established that supersolids in \( D \leq 2 \) cannot be generated via Bose-Einstein condensates in a wide class of quasicrystal potentials that includes the Fibonacci tiling. However, supersolids do arise via Bose-Einstein condensates from infinitely long-range, nonlocal interparticle potentials.

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