# **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  $D \le 2$  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  $D \le 2$  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  $D \le 2$  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,  $n \ge 5$ , that are characteristic of quasicrystals and incompatible with translational periodicity.

### 2. Crystals

The Hamiltonian for the interacting Bose gas is

$$\hat{H} = \int d\mathbf{r}\hat{\psi}^{\dagger}(\mathbf{r})(\frac{-\hbar^{2}}{2m}\nabla^{2})\hat{\psi}(\mathbf{r}) + \int d\mathbf{r}\hat{\psi}^{\dagger}(\mathbf{r})V_{ext}(\mathbf{r})\hat{\psi}(\mathbf{r}) 
+ \int d\mathbf{r}_{1}\int d\mathbf{r}_{2}\int d\mathbf{r}_{3}\int d\mathbf{r}_{4}\hat{\psi}^{\dagger}(\mathbf{r}_{1})\hat{\psi}^{\dagger}(\mathbf{r}_{2})V(\mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{3},\mathbf{r}_{4})\hat{\psi}(\mathbf{r}_{4})\hat{\psi}(\mathbf{r}_{3}),$$
(1)

where  $V_{ext}(\mathbf{r})$  is an arbitrary, external potential,  $V(\mathbf{r}_1; \mathbf{r}_2; \mathbf{r}_3; \mathbf{r}_4)$  is a general two-particle interaction potential, and  $\hat{\psi}(\mathbf{r})$  and  $\hat{\psi}^{\dagger}(\mathbf{r})$  are bosonic field operators that destroy or create a particle at spatial position  $\mathbf{r}$ , respectively.

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

$$\hat{\psi}(\mathbf{r}) = \psi(\mathbf{r}) + \hat{\varphi}(\mathbf{r}), \tag{2}$$

where

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$$\hat{\varphi}(\mathbf{r}) = \sqrt{\frac{1}{V(D)}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{\mathbf{k} \cdot \mathbf{r}}$$
(3)

with the condensate wavefunction

$$\psi(\mathbf{r}) = \sqrt{\frac{N_0}{V(D)}} \sum_{\mathbf{k}'} \xi_{\mathbf{k}'} e^{i\mathbf{k}' \cdot \mathbf{r}},\tag{4}$$

and normalization

$$\sum_{\mathbf{k}'} |\xi_{\mathbf{k}'}|^2 = 1,\tag{5}$$

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

$$\hat{H}_{symm} = \int d\mathbf{r}_1 \hat{\varphi}^{\dagger}(\mathbf{r}_1) \int d\mathbf{r}_2 \int d\mathbf{r}_3 \int d\mathbf{r}_4 \psi^*(\mathbf{r}_2) [V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) + V(\mathbf{r}_2, \mathbf{r}_1, \mathbf{r}_3, \mathbf{r}_4)] \psi(\mathbf{r}_3) \psi(\mathbf{r}_4) + h.c.$$

$$\equiv \int d\mathbf{r}_1 \hat{\varphi}^{\dagger}(\mathbf{r}_1) \chi(\mathbf{r}_1) + h.c.$$
(6)

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  $\mathbf{k}$ ,  $\mathbf{k} \pm \mathbf{q}_1$ , and  $\mathbf{k} \pm \mathbf{q}_2$ , where  $\mathbf{q}_1 \ge \mathbf{q}_2 \neq \mathbf{0}$ , gives rise to additional macroscopic occupation in the single-particle momenta states  $\mathbf{k} + n_1\mathbf{q}_1 + n_2\mathbf{q}_2$ , with  $n_1$ ,  $n_2 = 0$ ,  $\pm 1$ ,  $\pm 2$ ,  $\bullet \bullet \bullet$  owing to the symmetry breaking term  $\hat{H}_{symm}$ .

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

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sqrt{\frac{N_0}{V(D)}} \sum_{n_1, n_2 = -\infty}^{\infty} \xi_{\mathbf{k}+n_1 \mathbf{q}_1 + n_2 \mathbf{q}_2} e^{i(\mathbf{k}+n_1 \mathbf{q}_1 + n_2 \mathbf{q}_2) \cdot \mathbf{r}}$$

$$\equiv e^{i\mathbf{k} \cdot \mathbf{r}} u_{\mathbf{k}}(\mathbf{r}), \qquad (7)$$

with  $u_{\mathbf{k}}(\mathbf{r} + \mathbf{r}_0) = u_{\mathbf{k}}(\mathbf{r})$ , where

$$\mathbf{r}_{0} = 2\pi \left[ \frac{(q_{2}^{2} - \mathbf{q}_{1} \cdot \mathbf{q}_{2})\mathbf{q}_{1} + (q_{1}^{2} - \mathbf{q}_{1} \cdot \mathbf{q}_{2})\mathbf{q}_{2}}{q_{1}^{2}q_{2}^{2} - (\mathbf{q}_{1} \cdot \mathbf{q}_{2})^{2}} \right].$$
(8)

#### 3. Quasicrystals

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

$$\hat{H}_{symm}^{(ext)} = \int \mathrm{d}\mathbf{r}\hat{\varphi}^{\dagger}(\mathbf{r}) V_{ext}(\mathbf{r})\psi(\mathbf{r}) + h.c.$$
(9)

Consider the local, finite two-dimensional quasicrystal lattice potential,

$$V_{ext}(\mathbf{r}) = \frac{1}{(2\pi)^2} \sum_{\mathbf{k}} g(\mathbf{k}) \sum_{m_1 \cdots m_n = -M_1 \cdots - M_n}^{M_1 \cdots M_n} e^{-i\mathbf{k} \cdot \left(\mathbf{r} - \sum_{i=1}^n m_i(\alpha_i \mathbf{a} + \beta_i \mathbf{b})\right)}$$
(10)

where  $g(\mathbf{k})$  is the Fourier transform, **a** and **b** are arbitrary two-dimensional vectors in the xy plane with  $\mathbf{a} \times \mathbf{b} \neq 0$ ,  $(\alpha_i \mathbf{a} + \beta_i \mathbf{b}) \times (\alpha_j \mathbf{a} + \beta_j \mathbf{b}) \neq 0$ ,  $\alpha_i$  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 twodimensional crystals, respectively. One obtains that

$$\hat{H}_{symm}^{(ext)} = \int d\mathbf{r} \hat{\varphi}^{\dagger}(\mathbf{r}) V_{ext}(\mathbf{r}) \psi(\mathbf{r}) + h.c.$$

$$= \frac{\sqrt{N_0}}{V(D)} \sum_{\mathbf{k}_1, \mathbf{k}_2 \neq \mathbf{k}_1} \hat{a}_{\mathbf{k}_1}^{\dagger} \xi_{\mathbf{k}_2} g(\mathbf{k}) \prod_{i=1}^n \frac{\sin\left[\mathbf{k} \cdot (\alpha_i \mathbf{a} + \beta_i \mathbf{b})(M_i + 1/2)\right]}{\sin\left[\mathbf{k} \cdot (\alpha_i \mathbf{a} + \beta_i \mathbf{b})/2\right]} + h.c.,$$
(11)

where  $\mathbf{k} \equiv \mathbf{k}_2 - \mathbf{k}_1$ , which follows with the aid of (3), (4), and (10). Recall that

$$\sum_{m=-M}^{M} e^{imx} = \frac{\sin[x(M+1/2)]}{\sin[x/2]} \to 2\pi\delta(x) \quad (M \to \infty).$$
(12)

Note that  $\mathbf{k_1} \neq \mathbf{k_2}$ , that is,  $\mathbf{k} \neq \mathbf{0}$ , since  $\mathbf{k_2}$  is in the condensate and  $\mathbf{k_1}$  is not in the condensate. Therefore,  $\hat{H}_{symm}^{(ext)}$  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  $T \ge 0$  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  $k = 2\pi (m + m'\tau)\sqrt{5}$ , where  $\tau = (1 + \sqrt{5})/2$  is the golden mean and *m* and *m'* are integers [9]. Expressed in terms of Fourier transforms (9) becomes

$$\hat{H}_{symm}^{(ext)} = \frac{\sqrt{N_0}}{V(D)} \sum_{\mathbf{k}'\mathbf{k}} \hat{a}_{\mathbf{k}}^{\dagger} \xi_{\mathbf{k}'} \, \tilde{V}_{ext}(\mathbf{k}' - \mathbf{k}) + h.c.$$
(13)

where

$$\tilde{V}_{ext}(\mathbf{k}' - \mathbf{k}) = \int \mathrm{d}\mathbf{r} \, V_{ext}(\mathbf{r}) \, e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}}.$$
(14)

Consider the case where  $\tilde{V}_{ext}(\mathbf{k'} - \mathbf{k})$  is given by a sum of Dirac  $\delta$ -functions, which is the case for the Fibonacci tiling [9]. Now the vector  $\mathbf{k'} - \mathbf{k}$  must lie either in the condensate or outside the condensate. In either case,  $\hat{H}_{symm}^{(ext)}$  vanishes for arbitrary BEC since the vector  $\mathbf{k}$  is not in the condensate while the vector  $\mathbf{k'}$  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 **0**, **q**<sub>1</sub>,  $\alpha_1$ **q**<sub>1</sub>, **q**<sub>2</sub>, and  $\alpha_2$ **q**<sub>2</sub>, where  $\alpha_1$  and  $\alpha_2$  are irrational numbers and **q**<sub>1</sub> x **q**<sub>2</sub>  $\neq$  **0**, gives rise to additional macroscopic occupation in the single-particle momenta states  $(m_1 + \alpha_1 m_2)$ **q**<sub>1</sub> +  $(n_1 + \alpha_2 n_2)$ **q**<sub>2</sub>, with  $m_1$ ,  $m_2$ ,  $n_1$ ,  $n_2 = 0$ ,  $\pm 1$ ,  $\pm 2$ , ••• owing to the symmetry breaking term  $\hat{H}_{symm}$  and the linear momentum conservation of the interparticle potential.

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

$$\psi(\mathbf{r}) = \sqrt{\frac{N_0}{V(D)}} \sum_{m_1, m_2, n_1, n_2 = -\infty}^{\infty} \xi_{(m_1 + \alpha_1 m_2)\mathbf{q}_1 + (n_1 + \alpha_2 n_2)\mathbf{q}_2} e^{i[(m_1 + \alpha_1 m_2)\mathbf{q}_1 + (n_1 + \alpha_2 n_2)\mathbf{q}_2] \cdot \mathbf{r}},$$
(15)

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

## 5. Summary and Discussion

We have established that supersolids in  $D \le 2$  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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