Harmonic Stability Analysis of the 2D Square and Hexagonal Bravais Lattices for a Finite–Ranged Repulsive Pair Potential. Consequence for a 2D System of Ultracold Composite Bosons.

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We consider a classical, two–dimensional system of identical particles which interact *via* a finite–ranged, repulsive pair potential. We assume that the system is in a crystalline phase. We calculate the normal vibrational modes of a two–dimensional square Bravais lattice, first analytically within the nearest–neighbour approximation, and then numerically, relaxing the preceding hypothesis. We show that, in the harmonic approximation, the excitation of a transverse vibrational mode leads to the breakdown of the square lattice. We next study the case of the hexagonal Bravais lattice and we show that it can be stable with respect to lattice vibrations. We give a criterion determining whether or not it is stable in the nearest–neighbour approximation. Finally, we apply our results to a two–dimensional system of composite bosons and infer that the crystalline phase of such a system, if it exists, corresponds to a hexagonal lattice.

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Introduction

Recent developments in atomic Physics, spanning the past decade, have made it possible to observe states of matter which, so far, had only been considered from a theoretical point of view. Bose–Einstein condensation, experimentally achieved in 1995[1,2], is a landmark among these triumphs. More recently, much experimental effort has been directed towards the study of ultracold Fermi gases, allowing for instance an experimental study of the BEC—BCS crossover regime[3].

A stimulating new prospect for atomic physicists is the study of ultracold degenerate Fermi gases containing two *different* types of atomic species, such as ^{6}Li and ^{40}K. In such a gas, it is possible to tune the strength of the interaction between the two species by varying the interspecies scattering length using a Feshbach resonance[4]. For a positive scattering length, bosonic dimers appear, containing one atom of each type[5]. Being in their highest–energy bound states, these composite bosons are stable with respect to collisional relaxation into deeper–bound states. Two–component degenerate Fermi gases have recently been obtained experimentally[6], and interspecies Feshbach resonances have been identified[7].

If the difference between the two atomic masses is large enough, composite bosons interact *via* an effective pair potential which is repulsive. An expression for this pair potential has been derived in the Born–Oppenheimer approximation[8]. In the quasi–two–dimensional regime, this system has been shown to exhibit a crystalline phase for suitable values of the density and of the atomic mass ratio[8].

In this work, we perform an analysis of the stability of the two–dimensional Bravais lattices with high symmetry properties, namely the square lattice and the hexagonal lattice, with respect to classical harmonic vibrations.

We use the nearest–neighbour approximation to derive analytic expressions for the dispersion relations of both lattices. We show that, in the case of a finite–ranged repulsive pair potential, the square lattice is unstable for all values of the density. Still in the nearest–neighbour approximation, we give a criterion determining the range of densities for which the hexagonal lattice is stable. In both cases, we present numerical results which show that taking into account more rings of neighbours does not affect the qualitative behaviour of the system. Applying our results to a two–dimensional system of ultracold composite bosons, we infer that, for values of the mass ratio and density leading to a crystalline phase, the system crystallises into a hexagonal lattice.

I. HARMONIC THEORY OF LATTICE VIBRATIONS FOR PARTICLES INTERACTING *VIA* A PAIR POTENTIAL

For the sake of clarity, we first recall the general method[9] for the calculation of the normal vibrational modes of a two–dimensional crystalline solid.

We consider a two–dimensional system of identical particles which we describe within the framework of classical mechanics. We assume that these particles interact only *via* a finite–ranged pair potential $U(R)$, where R is the distance between two particles. We also assume that the system is in a crystalline phase corresponding to a two–dimensional Bravais lattice generated by two vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$: at classical equilibrium, there is a particle at each lattice site $\boldsymbol{r}_p$ such that

$$\boldsymbol{r}_p = p_1 \boldsymbol{a}_1 + p_2 \boldsymbol{a}_2, \tag{1}$$

where $p = (p_1, p_2)$ is a pair of integers.

In order to characterise the stability of such a lattice, we shall study the propagation of lattice waves. For that

purpose we shall first write the Lagrangian of the system in the harmonic approximation, then derive from it the equations of motion, and finally look for plane–wave solutions to these equations. The lattice is stable if the frequencies of the normal modes thus found are all real; on the contrary, *i.e.* if there is at least one normal mode with an imaginary frequency, the lattice is unstable.

A. Lagrangian of the crystal

The total potential energy of the crystal is

$$U^{\text{tot}}((\boldsymbol{u}_n)) = \frac{1}{2} \sum_{p \neq q} U \left(|\boldsymbol{r}_p + \boldsymbol{u}_p - \boldsymbol{r}_q - \boldsymbol{u}_q| \right), \quad (2)$$

where $\boldsymbol{u}_n$ is the displacement of atom n from the corresponding lattice site $\boldsymbol{r}_n$, and the double sum over p and q spans all pairs of lattice sites. We expand U^{tot} up to second order in the displacements $\boldsymbol{u}_n$. The constant term has no incidence on the dynamics of the crystal lattice and will therefore be dropped in subsequent calculations. The linear term cancels out when the double sum is performed. Consequently, the harmonic approximation to U^{tot} is a quadratic function of the $((\boldsymbol{u}_n))$:

$$U^{\text{tot}}_{\text{harm}}((\boldsymbol{u}_n)) = \frac{1}{2} \sum_{pq} {}^t\boldsymbol{u}_p \Lambda_{pq} \boldsymbol{u}_q, \quad (3)$$

where the real–space dynamical matrices Λ_{pq} are real 2×2 matrices defined by[9]:

$$\Lambda^{ij}_{pq} = \left. \frac{\partial^2 U^{\text{tot}}((\boldsymbol{u}_n))}{\partial u^i_p \, \partial u^j_q} \right|_{(\boldsymbol{u}_n = \boldsymbol{0})}. \quad (4)$$

In the harmonic approximation, the Lagrangian of the crystal is thus:

$$L = \frac{1}{2} m \sum_p \dot{\boldsymbol{u}}_p{}^2 - \frac{1}{2} \sum_{pq} {}^t\boldsymbol{u}_p \Lambda_{pq} \boldsymbol{u}_q, \quad (5)$$

where the first term is the total kinetic energy of the system and the second term is the harmonic approximation to the total potential energy. m is the mass of each particle in the system.

The Λ^{ij}_{pq}'s are endowed with well–documented properties[9,10], among which tensor symmetry, invariance under spatial inversion, and invariance under lattice translations. Additionally, the following expression, valid if only pairwise interactions are considered, greatly simplifies their evaluation:

$$\Lambda^{ij}_{0p} = - \left. \frac{\partial^2 U(|\boldsymbol{r}_p + \boldsymbol{u}|)}{\partial u_i \, \partial u_j} \right|_{\boldsymbol{u} = \boldsymbol{0}}. \quad (6)$$

We now introduce the momentum–space dynamical matrix $\Lambda(\boldsymbol{k})$, defined as the discrete Fourier transform of the Λ_{0p} over the crystal lattice:

$$\Lambda(\boldsymbol{k}) = \sum_p \Lambda_{0p} \, e^{i\boldsymbol{k}\cdot\boldsymbol{r}_p} = -2 \sum_p \Lambda_{0p} \sin^2 \left(\frac{1}{2} \boldsymbol{k} \cdot \boldsymbol{r}_p \right). \quad (7)$$

For a given wavevector $\boldsymbol{k}$, $\Lambda(\boldsymbol{k})$ is a real symmetric matrix. As such, it has two real orthogonal eigenvectors $\boldsymbol{\varepsilon}_{(\boldsymbol{k},1)}$ and $\boldsymbol{\varepsilon}_{(\boldsymbol{k},2)}$.

B. Equations of motion

Using the translational invariance property of the Λ_{pq}'s, the (classical) equation of motion for atom n, resulting from the Lagrangian 5, reads:

$$m\ddot{\boldsymbol{u}}_n = - \sum_p \Lambda_{0p} \boldsymbol{u}_{n+p}. \quad (8)$$

In the harmonic approximation, the motion of the particles in the crystal is thus determined by a set of N coupled linear equations similar to Equation 8, where N is the number of independent particles in the system.

We now determine the normal vibrational modes of the system, *i.e.* we look for a plane–wave solution to the equations of motion :

$$\boldsymbol{u}_n = A\,\boldsymbol{\varepsilon} \exp i \left(\boldsymbol{k} \cdot \boldsymbol{r}_n - \omega t \right), \quad (9)$$

where $\boldsymbol{\varepsilon}$ is the polarisation of the mode, $\boldsymbol{k}$ is its wavevector, and $\frac{\omega}{2\pi}$ is its frequency. A is an arbitrary complex number characterising the amplitude and global phase of the collective vibrational motion. Inserting Equation 9 into Equation 8, we obtain:

$$m\omega^2 \, \boldsymbol{\varepsilon} = \Lambda(\boldsymbol{k}) \, \boldsymbol{\varepsilon}. \quad (10)$$

where $\Lambda(\boldsymbol{k})$ is the momentum–space dynamical matrix defined in Section I A. Equation 10 shows that for a given wavevector $\boldsymbol{k}$, there are two possible polarisations $\boldsymbol{\varepsilon}_{(\boldsymbol{k},1)}$ and $\boldsymbol{\varepsilon}_{(\boldsymbol{k},2)}$ which are the two eigenvectors of the dynamical matrix $\Lambda(\boldsymbol{k})$. The corresponding eigenvalues $m\omega_1^2(\boldsymbol{k})$ and $m\omega_2^2(\boldsymbol{k})$ yield their respectives frequencies $\omega_1(\boldsymbol{k})$ and $\omega_2(\boldsymbol{k})$.

In the harmonic approximation, the classical dynamical properties of the crystal are thus completely determined by the dynamical matrices $\Lambda(\boldsymbol{k})$.

II. THE SPECIFIC CASE OF THE 2D SQUARE LATTICE FOR A PURELY REPULSIVE PAIR POTENTIAL

We now apply the formalism summarised in Section I to the specific case of the square Bravais lattice, generated by two vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ such that:

$$|\boldsymbol{a}_1| = |\boldsymbol{a}_2| = d \quad \text{and} \quad (\widehat{\boldsymbol{a}_1, \boldsymbol{a}_2}) = \frac{\pi}{2}. \quad (11)$$

The wavevectors $\boldsymbol{k}$ are most conveniently described in the reciprocal lattice basis $(\boldsymbol{a}_1^*, \boldsymbol{a}_2^*)$ defined by $\boldsymbol{a}_i^* \cdot \boldsymbol{a}_j = 2\pi \cdot \delta_{ij}$. The reciprocal lattice of a square lattice is also a square lattice:

$$|\boldsymbol{a}_1^*| = |\boldsymbol{a}_2^*| = \frac{2\pi}{d} \quad \text{and} \quad (\widehat{\boldsymbol{a}_1^*, \boldsymbol{a}_2^*}) = \frac{\pi}{2}. \quad (12)$$

A. Analytical expression for the dispersion relation in the nearest–neighbour approximation

We first derive the expression for Λ_{0p}, where the lattice index $p = (p_1, p_2) \in \mathbb{Z}^2$, using Equation 6:

$$\Lambda_{0p} = -\frac{d^2}{r_p^2} \begin{bmatrix} p_1^2 \, U''(r_p) + p_2^2 \, \frac{U'(r_p)}{r_p} & p_1 p_2 \left(U''(r_p) - \frac{U'(r_p)}{r_p} \right) \\ p_1 p_2 \left(U''(r_p) - \frac{U'(r_p)}{r_p} \right) & p_2^2 \, U''(r_p) + p_1^2 \, \frac{U'(r_p)}{r_p} \end{bmatrix}. \tag{13}$$

Next, the momentum–space dynamical matrix $\Lambda(\boldsymbol{k})$ can be calculated from Equation 7. An exact calculation of $\Lambda(\boldsymbol{k})$ would require calculating an infinite series spanning all sites of the two–dimensional Bravais lattice. However, assuming that the range of the pair potential $U(R)$ is small compared to the lattice spac-

ing d, the nearest–neighbour approximation can be used. The right–hand side of Equation 7 then reduces to a sum of five terms, corresponding to the reference lattice site $p = (0,0)$ and to its four nearest neighbours. Letting $\boldsymbol{k} = k_1 \boldsymbol{a}_1^* + k_2 \boldsymbol{a}_2^*$, we thus obtain the following expression for $\Lambda(\boldsymbol{k})$:

$$\Lambda(\boldsymbol{k}) = 4 \begin{bmatrix} U''(d) \sin^2(\pi k_1) + \frac{U'(d)}{d} \sin^2(\pi k_2) & 0 \\ 0 & \frac{U'(d)}{d} \sin^2(\pi k_1) + U''(d) \sin^2(\pi k_2) \end{bmatrix}. \tag{14}$$

In the nearest–neighbour approximation, $\Lambda(\boldsymbol{k})$ is a diagonal matrix. According to the results of Section I, the analytical expressions for the two (acoustic) branches of the dispersion relation can be read off the diagonal elements of $\Lambda(\boldsymbol{k})$:

$$\begin{cases} m\omega_1^2(\boldsymbol{k}) = & 4\left(U''(d) \sin^2(\pi k_1) + \frac{U'(d)}{d} \sin^2(\pi k_2) \right) \\ m\omega_2^2(\boldsymbol{k}) = & 4\left(\frac{U'(d)}{d} \sin^2(\pi k_1) + U''(d) \sin^2(\pi k_2) \right) \end{cases} \tag{15}$$

Because the dynamical matrix is diagonal, the allowed polarisations depend only on the branch of the dispersion relation that is considered (they do not depend on the wavevector). The first branch — $\omega_1^2(\boldsymbol{k})$ — corresponds to the polarisation $\boldsymbol{\varepsilon}_1 = \frac{\boldsymbol{a}_1}{|\boldsymbol{a}_1|}$, whereas the second branch — $\omega_2^2(\boldsymbol{k})$ — corresponds to the polarisation $\boldsymbol{\varepsilon}_2 = \frac{\boldsymbol{a}_2}{|\boldsymbol{a}_2|}$.

Equation 15 is compatible with the four–fold symmetry of the two–dimensional square lattice. Indeed, let $\boldsymbol{k}'$ be the image of $\boldsymbol{k}$ under the vector rotation of angle $\frac{\pi}{2}$: $\boldsymbol{k}' = -k_2 \boldsymbol{a}_1^* + k_1 \boldsymbol{a}_2^*$. Equation 15 yields $\omega_1^2(\boldsymbol{k}') = \omega_2^2(\boldsymbol{k})$ and $\omega_2^2(\boldsymbol{k}') = \omega_1^2(\boldsymbol{k})$.

B. Instability of the square lattice for a purely repulsive pair potential

In the harmonic approximation, a crystal lattice is stable if lattice waves can propagate through the crystal for

all wavevectors $\boldsymbol{k}$ in the first Brillouin zone of the lattice. We now show that this is not the case for the square lattice if the pair potential is purely repulsive.

Nearest–neighbour approximation. Let us consider a wavevector lying along $\boldsymbol{a}_1^*$: $\boldsymbol{k} = k_1 \boldsymbol{a}_1^*$. Equations 15 reduce to:

$$\begin{cases} m\omega_1^2(\boldsymbol{k}) = & 4U''(d) \sin^2(\pi k_1) \\ m\omega_2^2(\boldsymbol{k}) = & 4\frac{U'(d)}{d} \sin^2(\pi k_1) \end{cases} \tag{16}$$

For a purely repulsive potential, $U'(d) < 0$ for all possible values of the lattice spacing d. Consequently, ω_2^2 is negative, and therefore the frequency of the normal mode with wavevector $\boldsymbol{k} = k_1 \boldsymbol{a}_1^*$ and polarisation $\boldsymbol{\varepsilon}_2$ is not defined. Physically, this means that the propagation of a *transverse* normal mode (*i.e.* a normal mode with $\boldsymbol{k} \perp \boldsymbol{\varepsilon}$) with a wavevector along $\boldsymbol{a}_1^*$ would *break* the crystal lattice. Because of the four–fold symmetry of the square lattice, the same results and conclusions are valid for a transverse mode with a wavevector along $\boldsymbol{a}_2^*$.

Consequently, in the particular case of a purely repulsive pair potential, the two–dimensional square lattice is *not stable*.

The variations of $\omega_1^2(\boldsymbol{k})$ and $\omega_2^2(\boldsymbol{k})$, in the nearest–neighbour approximation (*i.e.* as given by the analytical expressions 16), are represented in Figure 1 for wavevectors $\boldsymbol{k}$ whose tips lie on the high–symmetry axes of the Brillouin zone[11], in the case of the pair potential characterising the two–dimensional interactions of composite
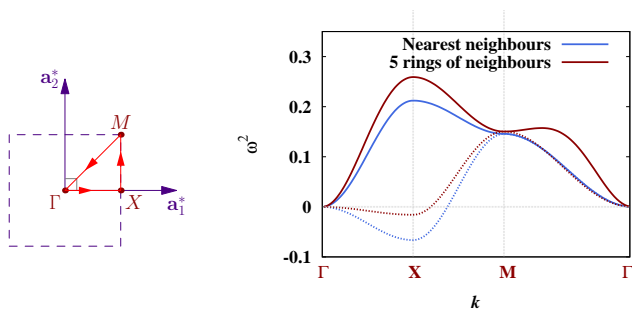
FIG. 1: Left: Brillouin zone of the square Bravais lattice, with the high–symmetry points $\Gamma(0,0)$, $X(\frac{1}{2},0)$, and $M(\frac{1}{2},\frac{1}{2})$. Right: the two branches $\omega_1^2(\boldsymbol{k})$ (solid lines) and $\omega_2^2(\boldsymbol{k})$ (dashed lines) of the dispersion relation of a two–dimensional square lattice, for wavevectors $\boldsymbol{k}$ with origin Γ and whose tips lie on the Γ–X–M–Γ path represented in red on the diagram on the left. The pair potential is the one characterising the interaction of two composite bosons in the two–dimensional case. The lattice spacing is $d = 2.0$ in units of the composite–boson molecular size. The total mass m of the composite bosons is taken to be unity. The blue graphs correspond to the analytical result in the nearest–neighbour approximation; the red graphs are numerical results taking into account five rings of neighbours. Note the lifting of the $\omega_{1,2}^2(\boldsymbol{k})$ degeneracy along the M–Γ branch as soon as next–nearest neighbours are taken into account.

bosons at temperature $T = 0\,\mathrm{K}$[8]. The branch $\omega_2^2(\boldsymbol{k})$ is negative for all wavevectors along $\boldsymbol{a}_1^*$ (Γ–X part of the plot of $\omega^2(\boldsymbol{k})$).

Numerical results including more distant neighbours. In order to go beyond the nearest–neighbour approximation, we have performed numerical calculations including more distant neighbours. For that purpose we have written a Python program which evaluates the lattice sums involved in Equation 7 for a finite–sized square lattice with 100 particles in both the $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ directions. The pair potential is finite–ranged, and the numerical results for $\omega_1^2(\boldsymbol{k})$ and $\omega_2^2(\boldsymbol{k})$ therefore converge quickly as a function of the radius of the disk of neighbours taken into account. The results of these calculations are represented in Figure 1. The branch $\omega_2^2(\boldsymbol{k})$ remains negative for $\boldsymbol{k}$ vectors along $\boldsymbol{a}_1^*$. Consequently, the effect described in the preceding paragraph is not an artefact due to the nearest–neighbour approximation: *in the particular case of a purely repulsive pair potential, and in the harmonic approximation, the two–dimensional square lattice is unstable.*

Geometrical interpretation of the instability. Let us consider the transverse vibrational mode with polarisation $\boldsymbol{\varepsilon}_1$ and wavevector $\frac{1}{2}\boldsymbol{a}_2^*$. Equation 9 shows that the displacement of atom $n = (n_1, n_2)$ from the corresponding lattice site is (omitting the time dependence $e^{i\omega_1 t}$):

$$\boldsymbol{u}_n = A\,\boldsymbol{\varepsilon}_1 \cdot (-1)^{n_2}. \qquad (17)$$

We shall consider the case of a small amplitude A. The positions of the particles for a lattice which is at rest on the one hand, and when the mode described above

is excited on the other hand, are compared on Figure 2. In the absence of vibrations, the distance of atom p to its four nearest neighbours p_1, p_2, p_3, and p_4 is exactly equal to the lattice spacing d (left–hand side of the figure). The mode described above modifies the distances between atom p and some of its neighbours. The distance between p and p_1 remains unchanged (*i.e.* equal to d), as well as the one between p and p_3; however, the distance between p and p_2, as well as the one between p and p_4, are increased to $d\left(1 + \frac{A^2}{d^2}\right)$. All four distances are increased (or remain unchanged), and the pair potential is repulsive, therefore the total interaction energy between atom p and its four nearest neighbours is *decreased*. The slightly distorted lattice represented on the right–hand side of Figure 2 therefore has a lower potential energy than the square lattice represented on the left–hand side, which entails that the square lattice is *not* a stable equilibrium position.

III. THE CASE OF THE 2D HEXAGONAL BRAVAIS LATTICE

In Section II, we showed that, within the framework of the harmonic approximation for crystal vibrations, the two–dimensional square Bravais lattice is not stable. In the present section, we apply the same formalism to the two–dimensional hexagonal lattice and show that, in contrast with the former, the latter is stable in the harmonic approximation.

The two–dimensional hexagonal Bravais lattice is generated by two vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ such that:

$$|\boldsymbol{a}_1| = |\boldsymbol{a}_2| = d \quad \text{and} \quad (\widehat{\boldsymbol{a}_1, \boldsymbol{a}_2}) = \frac{2\pi}{3}. \qquad (18)$$

As for the square lattice, we introduce the reciprocal lattice basis $(\boldsymbol{a}_1^*, \boldsymbol{a}_2^*)$, defined as before by $\boldsymbol{a}_i^* \cdot \boldsymbol{a}_j = \delta_{ij}$. The reciprocal lattice of a hexagonal lattice is also a hexagonal lattice:

$$|\boldsymbol{a}_1^*| = |\boldsymbol{a}_2^*| = \frac{2\pi}{d}\frac{2}{\sqrt{3}} \quad \text{and} \quad (\widehat{\boldsymbol{a}_1^*, \boldsymbol{a}_2^*}) = \frac{\pi}{3}. \qquad (19)$$

Dispersion relation. Equation 6 yields the following expression for Λ_{0p}, where $p = (p_1, p_2) \in \mathbb{Z}^2$:
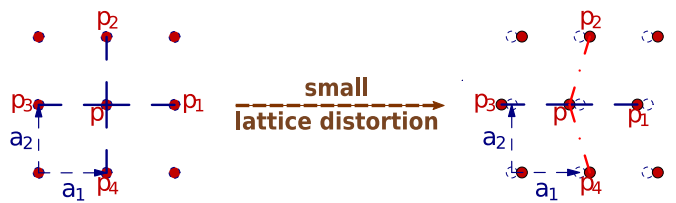

FIG. 2: Distortion of the crystal lattice due to the transverse vibrational mode with polarisation $\boldsymbol{\varepsilon}_1$ and wavevector $\boldsymbol{k} = \frac{1}{2}\boldsymbol{a}_2^*$.

$$\Lambda_{0p} = -\frac{1}{4}\frac{d^2}{r_p^2}\begin{bmatrix} (2p_1-p_2)^2\,U''(r_p) + 3p_2^2\frac{U'(r_p)}{r_p} & \sqrt{3}\,p_2(2p_1-p_2)\left(U''(r_p) - \frac{U'(r_p)}{r_p}\right) \\ \sqrt{3}\,p_2(2p_1-p_2)\left(U''(r_p) - \frac{U'(r_p)}{r_p}\right) & 3p_2^2\,U''(r_p) + (2p_1-p_2)^2\frac{U'(r_p)}{r_p} \end{bmatrix}. \tag{20}$$

Using Equation 7 in the nearest–neighbour approximation, we then derive the expression for $\Lambda(\boldsymbol{k})$:

$$\Lambda(\boldsymbol{k}) = \begin{bmatrix} 4U''(d)s_1^2 + (U''(d)+3\frac{U'(d)}{d})(s_2^2+s_3^2) & \sqrt{3}(U''(d)-\frac{U'(d)}{d})(s_3^2-s_2^2) \\ \sqrt{3}(U''(d)-\frac{U'(d)}{d})(s_3^2-s_2^2) & 4\frac{U'(d)}{d} + (3U''(d)+\frac{U'(d)}{d})(s_2^2+s_3^2) \end{bmatrix}. \tag{21}$$

where $s_1 = \sin\left(\frac{1}{2}\boldsymbol{k}\cdot\boldsymbol{a}_1\right)$, $s_2 = \sin\left(\frac{1}{2}\boldsymbol{k}\cdot\boldsymbol{a}_2\right)$, and $s_3 = \sin\left(\frac{1}{2}\boldsymbol{k}\cdot(\boldsymbol{a}_1+\boldsymbol{a}_2)\right)$. Equation 21 yields the following approximate analytical expression for the two branches of the dispersion relation, which are obtained as the two eigenvalues of $\Lambda(\boldsymbol{k})$:

$$m\omega_{1,2}^2(\boldsymbol{k}) = 2\left(U''(d)+\frac{U'(d)}{d}\right)(s_1^2+s_2^2+s_3^2)$$
$$\pm 2\left(U''(d)-\frac{U'(d)}{d}\right)s_0^2, \tag{22}$$

where $s_0^2 = \sqrt{(s_1^2+s_2^2+s_3^2)^2 - 3(s_1^2s_2^2+s_2^2s_3^3+s_3^2s_1^2)}$. Equation 22 is symmetrical in s_1, s_2, and s_3, and is thus compatible with the six–fold symmetry of the two–dimensional hexagonal lattice.

The polarisations corresponding to $\omega_{1,2}$ are $\boldsymbol{\varepsilon}_{1,2} = \varepsilon_{1,2}^x\boldsymbol{e}_x + \varepsilon_{1,2}^y\boldsymbol{e}_y$, where $(\boldsymbol{e}_x,\boldsymbol{e}_y)$ is the two–dimensional direct orthonormal basis with $\boldsymbol{e}_x$ along $\boldsymbol{a}_1$, and

$$\begin{cases} {\varepsilon_{1,2}^x}^2(\boldsymbol{k}) = \frac{3(s_3^2-s_2^2)^2}{3(s_3^2-s_2^2)^2+(2s_1^2-s_2^2-s_3^2\mp 2s_0^2)^2} \\ {\varepsilon_{1,2}^y}^2(\boldsymbol{k}) = \frac{(2s_1^2-s_2^2-s_3^2\mp 2s_0^2)^2}{3(s_3^2-s_2^2)^2+(2s_1^2-s_2^2-s_3^2\mp 2s_0^2)^2} \end{cases} \tag{23}$$

The frequencies $\omega_{1,2}(\boldsymbol{k})$ of the normal vibrational modes depend on the first and second derivatives of the pair potential, whereas the corresponding polarisations are independent of the particular shape $U(x)$ of this potential. However, in contrast to the case of the square lattice, the polarisations $\boldsymbol{\varepsilon}_{1,2}(\boldsymbol{k})$ for the hexagonal lattice do depend on the considered wavevector $\boldsymbol{k}$.

The variations of $\omega_{1,2}^2(\boldsymbol{k})$ are represented in Figure 3 in the case of the pair potential characterising the interaction of two composite bosons in the fully two–dimensional situation[8], for wavevectors $\boldsymbol{k}$ whose tips lie on the high–symmetry axes of the Brillouin zone[11]. The analytical results obtained in the nearest–neighbour approximation (Equation 22) are compared to numerical calculations taking into account five rings of neighbours on a finite–sized hexagonal lattice with 100 independent particles in both the $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ directions. Both calculations have been performed for the lattice parameter $d = 2.0$ (in units of the composite–boson molecular size). In both cases, the two branches $\omega_{1,2}^2(\boldsymbol{k})$ of the dispersion relation are positive for all wavevectors $\boldsymbol{k}$ in the Brillouin zone. Consequently, contrary to the results presented in Section II B for the square Bravais lattice, there is a range
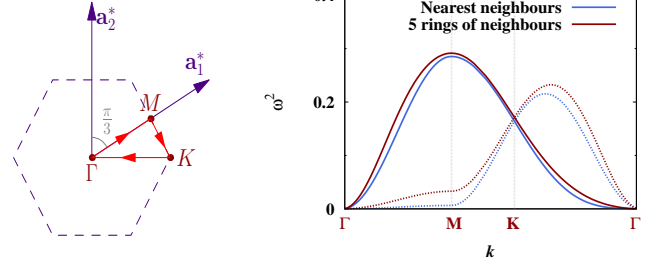

FIG. 3: Left: Brillouin zone of the two–dimensional hexagonal Bravais lattice, with the high–symmetry points $\Gamma(0,0)$, $M(\frac{1}{2},0)$, and $K(\frac{1}{3},\frac{1}{3})$. Right: the two branches $\omega_{1,2}(\boldsymbol{k})^2$ of the dispersion relation for the hexagonal lattice, for wavevectors $\boldsymbol{k}$ with origin Γ and whose tips lie on the Γ–M–K–Γ path represented in red on the diagram on the left. The pair potential is the one characterising the interaction of two composite bosons in the two–dimensional case. The blue graphs correspond to the analytical result in the nearest–neighbour approximation; the red graphs are numerical results taking into account five rings of neighbours. As in Figure 1, the lattice spacing is $d = 2.0$ and the total mass is $m = 1$, in the same units.

of densities ρ for which the two–dimensional hexagonal Bravais lattice of composite bosons is stable with respect to harmonic lattice vibrations.

Stability criterion for the hexagonal lattice. We now derive, in the nearest–neighbour approximation, a simple criterion on the relative values of $U''(d)$ and $U'(d)/d$ determining whether the hexagonal lattice is stable or not.

A two–dimensional hexagonal Bravais lattice with a given lattice spacing d (*i.e.* a given density $\rho = \frac{2}{d^2\sqrt{3}}$) is stable with respect to (harmonic) vibrations if the frequencies of all normal modes are real. Using Equation 22, and assuming $U'(d) < 0$ (repulsive potential), the stability condition becomes:

$$\frac{U''(d)}{-U'(d)/d}\left(s_1^2+s_2^2+s_3^2+\eta s_0^2\right) \geq \left(s_1^2+s_2^2+s_3^2-\eta s_0^2\right), \tag{24}$$

for all $\boldsymbol{k}$ in the Brillouin zone and $\eta = \pm 1$. Noting that $0 \leq s_1^2+s_2^2+s_3^2-s_0^2 \leq s_1^2+s_2^2+s_3^2+s_0^2$, the preceding

condition can be rewritten as:

$$\frac{U''(d)}{-U'(d)/d} \geq \max_{\boldsymbol{k} \in \mathrm{BZ}} \frac{s_1^2 + s_2^2 + s_3^2 + s_0^2}{s_1^2 + s_2^2 + s_3^2 - s_0^2}. \quad (25)$$

An analysis of the function of $\boldsymbol{k}$ on the right–hand side of Equation 25 shows that the sought maximum is 3, and that it is achieved for all wavevectors lying along the $\boldsymbol{a}_1^*$, $\boldsymbol{a}_2^*$, or $(\boldsymbol{a}_2^* - \boldsymbol{a}_1^*)$ axes of the Brillouin zone (*cf.* Figure 3). The locus of the maximum is thus compatible with the six–fold symmetry of the reciprocal lattice. The preceding inequality therefore reduces to:

$$\frac{U''(d)}{-U'(d)/d} \geq 3. \quad (26)$$

For a given repulsive pair potential $U(x)$, Equation 26 determines the values of the density ρ for which the hexagonal Bravais lattice is stable with respect to harmonic vibrations, in the nearest–neighbour approximation.

IV. CONSEQUENCE FOR THE TWO–DIMENSIONAL CRYSTAL OF COMPOSITE BOSONS

We now a consider a two–dimensional system of composite bosons obtained in an ultracold mixture containing two different types of Fermionic atoms. These composite bosons interact *via* an effective pair potential which is purely repulsive. An analytic expression for this pair potential has been derived in the Born–Oppenheimer approximation:

$$U_{2\mathrm{D}}(R) = U_0 \cdot \left[\kappa_0 R \, \mathrm{K}_0(\kappa_0 R) \, \mathrm{K}_1(\kappa_0 R) - \mathrm{K}_0^2(\kappa_0 R) \right] \quad (27)$$

where K_0 and K_1 are Bessel functions, U_0 is a constant, and κ_0^{-1} is the composite–boson molecular size. This system has been shown to exhibit a crystalline phase if the ratio of the two different atomic masses is sufficiently large[8]. The results presented in Sections II and III provide a simple argument as to which two–dimensional lattice, if any, the system crystallises into.

This ultracold system of composite bosons cannot be completely described using classical mechanics. Indeed, the particles in the system are not at rest, even at $T = 0\,\mathrm{K}$: their positions exhibit quantum zero–point fluctuations. However, if the system is in a crystalline phase, this zero–point motion can be interpreted as a vibration of the particles around the corresponding lattice sites. Therefore, this (quantum) crystal can only be stable if the corresponding crystal lattice is stable from a classical point of view.

There are five types of two–dimensional Bravais lattices[12]. Among these, only two exhibit high symmetry properties: the square lattice (four–fold symmetry) and the hexagonal lattice (six–fold symmetry). The unit cells of both of these lattices are represented in Figure 4.

All particles in the system are identical (they are all composite bosons). It is therefore reasonable to assume
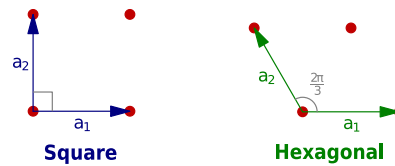

FIG. 4: Direct–lattice bases of the two 2D Bravais lattices with high symmetry properties: the square lattice (four–fold symmetry) and the hexagonal lattice (six–fold symmetry).

that its crystal phase will be highly symmetrical, and thus that the system crystallises in either the square lattice or the hexagonal lattice. However, the interaction between two composite bosons is characterised by a pair potential which is repulsive for all relative distances. Therefore, the results of Section II B imply that the square lattice is not a stable equilibrium position for this system. Consequently, for values of the mass ratio and density leading to a crystalline phase, the system will crystallise in a hexagonal lattice. This prediction is confirmed by Quantum Monte Carlo calculations[8].

The range of densities for which the hexagonal lattice is stable is determined, in the nearest–neighbour (NN) approximation, by the criterion stated in Section III. The relevant function $\frac{U''(d)}{-U'(d)/d}$ is represented in Figure 5 in the case of the pair potential 27 (left–hand plot). The criterion for stability (Equation 26) is satisfied for all densities lower than $\rho_{\max}^{\mathrm{NN}} = 0.31$. For $\rho > \rho_{\max}^{\mathrm{NN}}$, neither the square lattice nor the hexagonal lattice are stable in the nearest–neighbour approximation. Numerical calculations of $\rho_{\max}$ taking into account farther rings of neighbours on a 100×100 hexagonal lattice (Figure 5, right–hand plot) show that the corrections due to the next neighbours do not affect the qualitative behaviour of the system: starting from the eighth ring of neighbours, the critical density saturates to $\rho_{\max} = 0.499(1)$. We therefore predict that, for densities greater than $\rho_{\max}$, the system can exhibit no crystalline phase: it is in a disordered phase regardless of the value of the mass ratio.

Note that the numerical value of $\rho_{\max}$ that has just been obtained must be considered with caution, since the expression of the pair potential U_{2D} (Equation 27) that has been used to derive it results from approximations that may not be strictly valid in the present case. Nevertheless, it remains straightforward, using our suggested procedure, to confirm the existence of a critical density, and possibly refine its value given a more accurate pair potential.

Discussion

Observability. The composite bosons are obtained in a trapped bipartite Fermi mixture which has been cooled to degeneracy. The quasi–two–dimensional regime can be
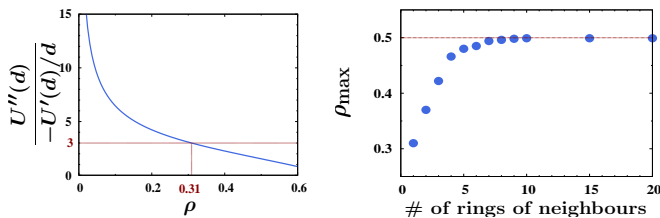
FIG. 5: Stability of the hexagonal lattice in the case of the pair potential between composite bosons. Left: plot of $\frac{U''(d)}{-U'(d)/d}$ as a function of the density $\rho = \frac{2}{d^2\sqrt{3}}$. In the nearest–neighbour approximation, the hexagonal lattice is stable for $\frac{U''(d)}{-U'(d)/d} > 3$, *i.e.* for $\rho < \rho_{max}^{NN} = 0.31$. Right: critical density ρ_{max} above which the hexagonal lattice is not stable, as a function of the number of rings of neighbours taken into account. Starting from the eighth ring of neighbours the critical density saturates to $\rho_{max} = 0.499(1)$. As in Figures 1 and 3, the unit of length is the composite–boson molecular size κ_0^{-1}.

reached by confining both types of atoms to the antinodes of an optical lattice. The crystalline or liquid phase of the composite boson system may be characterised through absorption–imaging techniques[6,13].

Applicability. General theorems[14] have been stated, concerning a specific — albeit large — class of pair potentials, which imply that no crystalline order can be observed in infinite two-dimensional systems. However, the composite-boson systems conceivable in experiments are trapped, and hence finite-sized, systems, to which these theorems do not apply, regardless of the specific shape of the pair potential[14]. The experimental observation of a two-dimensional crystalline phase of composite bosons will therefore not contradict the theorems mentioned above. Furthermore, hexagonal lattices have already been observed in numerous other systems, such as vortices in superconductors[15] and rotating Bose-Einstein condensates[16], C_{60} molecules on a substrate[17], and colloidal suspensions[18]. In all four preceding cases, the observed two-dimensional lattice is the hexagonal one, which corresponds to our present prediction for the composite-boson system.

Conclusion

The interactions of composite bosons in a two–dimensional ultracold system are remarkable inasmuch as they are described by a finite–ranged repulsive pair potential. In this context, we have shown the square Bravais lattice to be unstable with respect to harmonic vibrations, first through an analytic expression of its dispersion relation derived using the nearest–neighbour approximation, and then through numerical calculations taking into account farther rings of neighbours. Again using the nearest–neighbour approximation, we have derived an analytic expression of the dispersion relation for the hexagonal lattice. We have stated a criterion determining the range of densities for which this lattice is stable. In the particular case of the interaction between composite bosons, this criterion yields a maximum density above which no crystalline phase can be observed. Numerical calculations have shown that taking into account farther rings of neighbours does not qualitatively change the behaviour of the system. We thus conclude that, for all values of the density and mass ratio yielding a crystalline phase, the system of composite bosons crystallises into the hexagonal lattice.

Acknowledgments

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