Bose-Einstein condensation in the presence of an impurity

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Abstract

It is shown that Bose-Einstein condensation occurs for an ideal gas in two spatial dimensions in the presence of one impurity which is described quantum mechanically in terms of a point-like vortex and a contact interaction. This model is exactly solvable and embodies as a special case the analogous problem in three spatial dimensions.

PACS numbers: 03.75.Fi, 03.65.Bz-Ge, 05.30.Jp
1 Introduction

It is well known [1] that Bose-Einstein condensation, a first order phase transition in momentum space, can not occur for an ideal gas of free particles in two dimensions. In this short note we shall show that, by contrast, the introduction of one point-like impurity on the plane just allows the Bose-Einstein condensation to take place. Furthermore, the general pattern of the above phenomenon will be obtained from a generating Hamiltonian, which encodes a two parameters model to describe the point-like impurity in two and three spatial dimensions. The key point to be gathered is how to treat in quantum mechanics the presence of a point-like, or δ-like, or null support impurity. Formal manipulations involving some kinds of regularized δ-like potentials might drive, in general, to misleading and incorrect conclusions, as the latter ones are mathematically ill-defined. The correct quantum mechanical framework to treat point-like impurities [2] is by means of the analysis of the self-adjoint extensions of the Hamiltonian operator which, in the present case, turns out to be just a symmetric operator. Consequently, its domain has to be suitably defined in order to obtain a self-adjoint Hamiltonian operator which admits a complete orthonormal set of eigenstates. This construction will be referred to in the sequel as the inclusion of contact interaction. To be definite, let us consider as a starting point of our analysis the following classical one-particle Hamiltonian in two spatial dimensions: namely,

$$ H(\phi) = \frac{1}{2m} \left( p - \frac{e}{c} A(r) \right)^2, \quad p, r \in \mathbb{R}^2, $$

(1.1)

$$ A_j(x_1, x_2) = \frac{\phi}{2\pi} \epsilon_{jk} \frac{x_k}{r^2}, \quad r = \sqrt{x_1^2 + x_2^2}. $$

Here the Aharonov-Bohm type [3] vector potential corresponds to the presence of a δ-like vortex of flux \( \phi \), which provides a good classical description of one point-like impurity, as we shall better specify below. Quantization of the classical Hamiltonian (1.1) leads to a symmetric operator and, consequently, one has to face the problem of finding all its self-adjoint extensions. The most general solution has been recently obtained in Ref. [4] and it consists in a four parameter family. However, to our aim, we can restrict ourselves to the one parameter sub-family of the \( O(2) \) rotational invariant self-adjoint Hamiltonians [5, 6]. The corresponding spectral decompositions read

$$ H(\alpha, E_0) = \sum_{l=-\infty}^{+\infty} \int_0^{+\infty} dk \frac{\hbar^2 k^2}{2m} |l,k\rangle \langle k,l| + \vartheta(-E_0) |\psi_B\rangle \langle \psi_B|, $$

(1.2)

$$ \alpha = \frac{e\phi}{\hbar c} \in ]-1, 0[, \quad -\infty \leq E_0 < +\infty $$

\( \vartheta \) being the usual Heaviside’s step distribution, in terms of the eigenfunctions

$$ \langle r, \theta | l, k \rangle = \frac{\exp\{il\theta\}}{\sqrt{2\pi}} \psi_l(k, r; \alpha, E_0), \quad k \geq 0, $$

(1.3)

where the improper eigenfunctions belonging to the continuous part of the spectrum are given by

$$ \psi_l(k, r) = \sqrt{k} J_{|l+\alpha|}(kr), \quad l \in \mathbb{Z} - \{0\}, $$

(1.4)
\[ \psi_0(k, r; E_0) = A(k; \alpha, E_0)J_{|\alpha|}(kr) + B(k; \alpha, E_0)N_{|\alpha|}(kr) , \]  

in which

\[ \frac{B(k; \alpha, E_0)}{A(k; \alpha, E_0)} = \frac{\sin(\pi \alpha)}{\cos(\pi \alpha) + \text{sgn}(E_0) (\hbar^2 k^2 / 2m|E_0|)^{1/2}} , \]  

whereas the normalizable bound state is provided by

\[ \langle r | \psi_B \rangle = \psi_B(\kappa, r) = \kappa \pi \sqrt{\frac{\sin(\pi \alpha)}{\alpha}} K_{|\alpha|}(\kappa r) , \quad \hbar \kappa \equiv \sqrt{2m|E_0|} . \]  

Some remarks are now in order. First, as previously noticed, the above spectral decompositions precisely provides the correct mathematical framework to introduce and properly describe contact interaction in quantum mechanics. As a matter of fact, it turns out that the rotational invariant self-adjoint Hamiltonian operators \( H(\alpha, E_0) \) do represent a one parameter family, which is labeled by the energy scale \( E_0 \). In the range \(-\infty < E_0 < 0\), and only within this range of values, a bound state \( |\psi_B\rangle \) exists, whose energy is just \( E_0 \). More generally, the physical meaning of the characteristic energy scale \( E_0 \) is given by the resonance energy, according to the following pattern: namely,

\[ E_{\text{res}} = \begin{cases} |E_0|(|\sec \pi \alpha|)^{1/|\alpha|} , & \text{if } 0 < |\alpha| < 1/2 , \quad E_0 < 0 ; \\ |E_0| , & \text{if } 1/2 < |\alpha| < 1 , \quad E_0 < 0 ; \\ E_0 |\sec \pi \alpha|^{1/|\alpha|} , & \text{if } 1/2 < |\alpha| < 1 , \quad E_0 \geq 0 . \end{cases} \]  

A further observation is that only the non-integer part of the vortex flux parameter \( \alpha \) is actually observable, as its integer part can always be gauged away by a single valued phase transformation. To sum up, we can say that a general correct quantum mechanical description of one point-like impurity is provided by the two parameters family of self-adjoint Hamiltonians of Eq. (1.2). The existence of the contact interaction just corresponds to the presence of a specific locally square integrable singularity of the wave function at the impurity position - see Eq. (1.5). In the limit \( E_0 \to -\infty \) contact interaction is removed, the domain of the Hamiltonian is that of the regular wave functions on the whole plane and the impurity is described in terms of a pure Aharonov-Bohm vortex of non-integer vorticity \( \alpha \). If we further take the limit \( \alpha \uparrow 0 \), i.e., also the Aharonov-Bohm interaction is turned off, the two dimensional free particle Hamiltonian is truly recovered (Friedrichs’ limit). As we shall discuss in the sequel, it is curious that just in the Friedrichs’ limit the Bose-Einstein condensation disappears in the two spatial dimensional case because, in the presence of contact interaction and no matter how weak it is, a non-vanishing critical temperature for the Bose-Einstein transition always exists.

## 2 One-particle partition function

In order to discuss Bose-Einstein condensation, it is necessary to compute the average number of particles at thermal equilibrium. To this aim, let us first evaluate the diagonal Heat-Kernel and the one-particle partition function. According to the spectral decomposition of Eq. (1.2) and after
separation of the truly free particle Hamiltonian \( H_0 \equiv H(0, -\infty) \) contribution, it is not difficult to verify that the diagonal Heat-Kernel can be cast in the following form: namely,

\[
G(\alpha, \beta, E_0; r) \equiv G_{\text{int}}(\alpha, \beta, E_0; r) + G_0(\beta) \\
= \langle r | \exp \{- \beta H(\alpha, E_0)\} - \exp \{- \beta H_0\} | r \rangle + \lambda_T^{-2} \\
= I(\alpha; r) + I(-\alpha; r) - 2I(0; r) - I_0(\alpha; r) - I_0(-\alpha; r) + I_0(0; r) \\
+ \vartheta(-E_0)e^{-\beta E_0} |\psi_B(\kappa r)|^2 + \mathcal{I}_0(\alpha, E_0; r) + \lambda_T^{-2}, \tag{2.1}
\]

where the translation invariant free particle diagonal Heat-Kernel is nothing but the inverse square thermal wavelength \( \lambda_T \equiv (\hbar/\sqrt{2\pi m k T}) \) and we have set

\[
I(\alpha; r) = \int_0^\infty \frac{dk}{2\pi} k e^{-\beta h^2 k^2/2m} \sum_{l=0}^\infty |J_{l+\alpha}(kr)|^2, \tag{2.2}
\]

\[
I_0(\alpha; r) = \int_0^\infty \frac{dk}{2\pi} k e^{-\beta h^2 k^2/2m} |J_\alpha(kr)|^2, \tag{2.3}
\]

\[
\mathcal{I}_0(\alpha, E_0; r) = \int_0^\infty \frac{dk}{2\pi} \frac{k \exp \{- \beta h^2 k^2/2m\}}{1 + \tan^2[\pi \mu(k)] + 2 \tan[\pi \mu(k)] \cos(\pi)} \\
\times \{ \tan^2[\pi \mu(k)] J_\alpha^2(kr) + J_{\alpha+1}^2(kr) + 2 \tan[\pi \mu(k)] J_{-\alpha}(kr) J_\alpha(kr) \}, \tag{2.4}
\]

\[
\tan[\pi \mu(k)] \equiv \text{sgn}(E_0) \left[ \frac{2m|E_0|}{\hbar^2 k^2} \right]^{[\alpha]}. \tag{2.5}
\]

Now, it is very important to realize that the impurity interaction part of the diagonal Heat-Kernel \( G_{\text{int}}(\alpha, \beta, E_0; r) \) is integrable on the whole plane. This leads to the following result for the one-particle partition function

\[
Z_{2D}(\alpha, \beta, E_0) = \frac{A}{\lambda_T^2} + \frac{\alpha(\alpha + 1)}{2} + \vartheta(-E_0)e^{\beta |E_0|} \\
+ \frac{\alpha \sin(\pi \alpha)}{\pi} \int_0^\infty \frac{dx}{x^{\alpha + 1}} 2\text{sgn}(E_0) e^{-\beta E_0 x} \left[ \frac{e^{-\beta E_0 x}}{x^{[1]} \cos(\pi \alpha) + x^{[2]}} \right], \tag{2.6}
\]

where, as usual, we have denoted by \( A \) the area divergence, due to the presence of the translation invariant part of the free one-particle Heat-Kernel. The above expression for the one-particle partition function can be used as a generating form which encodes different specific notable cases. In particular, the one-particle partition function in two spatial dimensions and in the presence of pure contact interaction can be obtained in the limit \( \alpha \uparrow 0 \) and reads

\[
Z_{2D}(0, \beta, E_B) = \frac{A}{\lambda_T^2} + e^{\beta |E_B|} - \int_0^\infty \frac{dE}{E} \frac{e^{-\beta E}}{\ln^2(-E/E_B) + \pi^2} \tag{2.7}
\]

\[
= \frac{A}{\lambda_T^2} + \nu(\beta |E_B|), \quad E_B < 0, \tag{2.8}
\]

where

\[
\nu(x) \equiv \int_0^\infty \frac{x^t}{\Gamma(t+1)} dt. \tag{2.9}
\]
Notice that in two spatial dimensions the bound state is always present for any $-\infty < E_B < 0$. Another distinguished case that can be read off the basic formula (2.6) is the three dimensions one-particle partition function in the presence of contact interaction. As a matter of fact, thanks to dimensional transmutation [5], the latter case just corresponds to the value $\alpha = -1/2$, up to a suitable redefinition of the free part: namely,

$$Z_{3D}(\beta, E_0) = \frac{V}{\lambda_T^3} + \vartheta(-E_0)e^{\beta|E_0|} + \frac{1}{2}\text{sgn}(E_0)e^{\beta|E_0|}\text{erfc}(\sqrt{\beta|E_0|}) . \quad (2.10)$$

3 Results and Discussion

Now we are ready to discuss the Bose-Einstein condensation for an ideal gas of particles in the presence of one point-like impurity, as generally described by the one-particle Hamiltonian of Eq. (1.2). According to the general form (2.6) of the one-particle partition function, it turns out that the average particles density at thermal equilibrium in two spatial dimensions and in the presence of one point-like impurity is given by

$$\langle n \rangle_{2D} \equiv \langle N \rangle_A = \lambda_T^{-2}g_1(z) + \frac{z\alpha(\alpha + 1)}{2A(1-z)} + \vartheta(-E_0)\frac{z}{A(z_0 - z)}$$

$$+ \vartheta(E_0)\frac{z}{A(1-z)} + \text{sgn}(E_0)\frac{z}{A}\int_0^\infty dE \frac{\varrho(E; \alpha, |E_0|)e^{-\beta E}}{1 - z \exp\{-\beta E\}} , \quad (3.1)$$

where we have set $z_0 \equiv \exp\{\beta E_0\}$ and $g_1(z) = -\ln(1-z)$, whereas

$$\varrho(E; \alpha, |E_0|) = \frac{\alpha \sin(\pi \alpha)E^{\alpha-1}}{\pi |E_0|^\alpha [E^{2\alpha} + |E_0|^{2\alpha} + 2\text{sgn}(E_0)(E|E_0|)^{\alpha} \cos(\pi \alpha)]} . \quad (3.2)$$

It is important to realize that if $E_0 < 0$ the range of the fugacity is $0 \leq z \leq z_0 < 1$, whilst $0 \leq z \leq 1$ if $E_0 \geq 0$. Moreover, it is not difficult to prove that, thanks to analytic continuation, the very last term in Eq. (3.1) admits a finite limit when $z \uparrow 1$ and $E_0 \geq 0$. From the above expression (3.1) for the average particle density in two spatial dimensions, it appears to be manifest that Bose-Einstein condensation occurs only in the presence of the bound state, i.e., only for the sub-family of the self-adjoint extensions of the symmetric Hamiltonian (1.1) in the range $-\infty < E_0 < 0$. In those cases, the critical temperature and/or specific area can be obtained as the unique solutions of the equation

$$\ln \left(1 - e^{\beta E_0}\right) = -\frac{\hbar^2 \beta}{2\pi m} \langle n \rangle_{2D} . \quad (3.3)$$

The three spatial dimensional case can be handled in a quite similar way, as it essentially corresponds to the specific value $\alpha = -1/2$ in Eq. (3.1), up to terms irrelevant in the thermodynamic limit:
namely,
\[
\langle n \rangle_{3D} \equiv \frac{\langle N \rangle}{V} = \lambda T^2 g_{3D}(z) + \vartheta(-E_0) \frac{z}{\sqrt{V(z_0 - z)}} + \vartheta(E_0) \frac{z}{\sqrt{V(1 - z)}} \\
+ \text{sgn}(E_0) \frac{z}{V} \int_{0}^{\infty} dE \frac{\varrho(E; \alpha = -\frac{1}{2}, |E_0|) e^{-\beta E}}{1 - z \exp \{-\beta E\}}.
\]
(3.4)

The above equation clearly indicates that Bose-Einstein condensation always takes place in three spatial dimensions, in the presence as well as in the absence of the impurity. Nonetheless, the actual values of the critical temperature and/or density do depend upon the sign of the parameter characterizing the self-adjoint extension of the Hamiltonian. In fact, for \(E_0 \geq 0\), i.e. in the absence of the bound state, the critical values are the usual ones as given by the solution of the equation \(\lambda_T^3 \langle n \rangle_{3D} = \zeta(3/2)\). At variance, when \(-\infty < E_0 < 0\), i.e. in the presence of the bound state, the critical values can be read off the equation
\[
g_{\frac{3}{2}}(z_0) = \lambda_T^3 \langle n \rangle_{3D}.
\]
(3.5)

The case of pure contact interaction in two spatial dimensions can also be obtained from the basic formula (3.1) taking the limit \(\alpha \uparrow 0\) and treating separately the cases \(E_0 \geq 0\) and \(-\infty < E_0 < 0\). As a matter of fact, the result is
\[
\langle n \rangle_{2D}|_{\alpha=0} = \lambda_T^2 g_1(z) + \vartheta(E_0) \frac{z}{A(1 - z)} + \vartheta(-E_0) \frac{z}{A(z_0 - z)} \\
- \vartheta(-E_0) \frac{z}{A} \int_{0}^{\infty} dE \frac{e^{-\beta E}}{1 - z \exp \{-\beta E\}} \frac{1}{\ln^2(-E/E_0) + \pi^2},
\]
(3.6)

which shows that condensation does not occur when \(E_0 \geq 0\), whereas it appears if \(-\infty < E_0 < 0\), the critical temperature and/or specific volume being always determined by Eq. (3.3) which does not depend upon \(\alpha\). In this latter case, the very same formula can be also obtained directly from Eq. (2.8) as it does.

In conclusion, we have shown in this note that the presence of contact interaction makes it possible the occurrence of Bose-Einstein condensation in two spatial dimensions. This phenomenon is connected to the presence of a bound state in the spectrum of the self-adjoint Hamiltonian. It turns out to be remarkable that the latter circumstance is always there in the pure contact interaction case, that means without Aharonov-Bohm vortex interaction. It is in fact worthwhile to notice that, in the presence of a non-vanishing vorticity \(\alpha\), the half-family without bound state of the self-adjoint extensions does not allow Bose-Einstein condensation, whilst the remaining half-family with bound state leads to Bose-Einstein condensation though the critical temperature is independent from \(\alpha\). Accordingly, only when \(-\infty < E_0 < 0\) a non-vanishing and vorticity-independent critical temperature is allowed in the two spatial dimensional case - see Eq. (3.3)- whereas the critical temperature deviates from its conventional value in the three spatial dimensional case - see Eq. (3.5).

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