# Bose-Einstein condensation and heat capacity of two-dimensional spin-polarized atomic hydrogen

M. K. Al-Sugheir,<sup>1,\*</sup> H. B. Ghassib,<sup>2</sup> and M. Awawdeh<sup>3</sup>

<sup>1</sup>Department of Physics, The Hashemite University, Zarqa, Jordan

<sup>2</sup>Department of Physics, The University of Jordan, Amman, Jordan

<sup>3</sup>Department of Physics, Yarmouk University, Irbid, Jordan

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The static fluctuation approximation (SFA) is used to study the condensate fraction and the specific heat capacity of finite two-dimensional spin-polarized atomic hydrogen. It is found that Bose-Einstein condensation occurs in this system. The transition temperature at different densities decreases as the number of particles of the system increases. At low density, a sharp peak in the specific heat capacity is observed at the transition temperature. On the other hand, as the density of the system increases, the transition temperature becomes no longer well-defined, and a hump is observed in the specific heat capacity around the transition temperature. A qualitative comparison of our results to published results for finite Bose systems shows good agreement.

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### I. INTRODUCTION

It is an experimental fact that spin-polarized atomic hydrogen gas condenses in two dimensions [1-3]. Specifically, it condenses on the surface of liquid <sup>4</sup>He to form a two-dimensional Bose system [4,5]. In strictly *infinite* two dimensions, it is well known that no Bose-Einstein condensation (BEC) occurs—unlike the case for a *finite* two-dimensional Bose gas [6–8]. A complete understanding of finite systems remains a challenge [9].

Two-dimensional Bose systems have risen to prominence in condensed-matter physics, especially following the observation of local coherence in hydrogen atoms adsorbed on a liquid-helium surface [3,10]. The hydrogen atoms adsorbed on liquid helium exhibit two-dimensional quantum degeneracy. The hydrogen atom has a small mass and a small S-wave scattering length; these properties affect the behavior of the system quite substantially. The small mass means that BEC occurs at a higher temperature for a given density number, compared to alkali atomic systems.

The properties of a system are dependent on its dimensionality. BEC occurs in three-dimensional spin-polarized atomic hydrogen, but in a uniform two-dimensional system, the thermal fluctuations at any finite temperature destroy the long-range order, which is a characteristic feature of most phase transitions. It has been shown that the theory of BEC used successfully in three dimensions is not valid for two-dimensional atomic gases [11,12], where the long-range order is absent. The Bose gas confined to low dimensions exhibits properties different from those in three dimensions. Since the transition temperature increases with decreasing system dimension [13], it has been suggested that BEC may be achieved more favorably in low-dimensional systems. Therefore, Bose systems in low dimensions have been a subject of intense interest, both experimentally and theoretically. BEC of a charged Bose gas confined in two dimensions may help us to better understand high-temperature superconductivity [14,15]. Many high-temperature superconducting materials have a layered structure. It is expected that bipolarons are

restricted to planes. Therefore, some models have explained high-temperature superconductivity in terms of BEC of bipolarons [14,15].

A homogeneous Bose gas in two dimensions is expected to undergo a phase transition at finite temperatures. Below the critical temperature, the gas is a superfluid. The superfluid phase is characterized by the existence of a so-called quasicondensate. The quasicondensate has been observed in spin-polarized hydrogen gas, and in an ideal Bose gas [3,16]. Kane and Kadanoff [17] were the first to propose that long-range order does not appear in two-dimensional Bose systems. They predicted that, if a phase transition exists in two dimensions, it will have a different character from that in three dimensions. Theoretically, in a low-dimensional Bose gas, BEC cannot take place in a homogeneous one- or two-dimensional system at nonzero temperature, according to the Mermin-Wagner-Hohenberg theorem [18,19], which states that long-wavelength thermal fluctuations destroy long-range order in two dimensions. This theorem is valid only in the thermodynamic limit; it is not valid in finite systems. Therefore, under certain conditions (where the phase is coherent over a distance of the order of the size of the system), BEC in finite low-dimensional Bose gas does occur.

In the semiclassical treatment of the thermodynamic properties of a Bose gas trapped in d dimensions, BEC is not possible [20,21], whereas a quantum-mechanical treatment shows that BEC can occur in low-dimensional systems [20]. A quantum-mechanical analysis shows that the condensate fraction at fixed temperature and number of bosons depends on the trapping potential used [20]. Mean-field theory has been used to study the possibility of BEC occurring in trapped Bose particles [22]. The results of this study show that there is a phase transition at some critical temperature, but this is not a transition to BEC. Hard-core bosons in a finite twodimensional harmonic-oscillator potential has been studied by the path-integral quantum Monte Carlo method [23]. A hump in the heat capacity occurs around the transition temperature. In this study, the effect of the hard-core radius on the transition temperature and on the condensate fraction has been examined; both decrease when the hard-core radius increases. The grand partition function and heat capacity of a finite number of confined bosons have been calculated [24,25]. A peak in the heat capacity in two and three dimensions has been observed. The peak in the heat capacity is taken as an indication of BEC. Also, the functional renormalization method has been used to compute the superfluid density and the condensate density as functions of the temperature for ultracold bosonic atoms in two-dimensional systems. The condensate density vanishes in the infinite-volume limit; for a finite volume, a nonvanishing condensate is observed [26].

This work sets out to study BEC and the heat capacity for a finite number of particles in a two-dimensional spin-polarized atomic hydrogen gas within a quantum framework called the static fluctuation approximation (SFA) [27,28]. This technique has been applied successfully to the three-dimensional spin-polarized atomic hydrogen gas [28]. The good results obtained motivate us to shed further light on the two-dimensional case. The basic input to SFA is the single-particle wave function, which is well defined for the confined two-dimensional spin-polarized atomic hydrogen gas. This has encouraged us to start with this system rather than confined alkali atomic systems.

The rest of this paper is organized as follows. In Sec. II, we introduce the system and SFA. The results and discussion are presented in Sec. III, followed by some concluding remarks in Sec. IV.

#### **II. THEORETICAL FRAMEWORK**

The finite trapped atomic gases and spin-polarized atomic hydrogen have been studied theoretically using different many-body theories: self-consistent mean-field theory [22], quantum Monte Carlo method [23,29], diffusion Monte Carlo [30], variational approach [31], T-matrix theory [32], classical field simulation technique [33], and other theories. A typical theoretical work is interested in calculating the transition temperature, the condensate fraction, and thermodynamic properties. It has been found theoretically that, below the transition temperature, an appreciable number of particles occupy the ground state. This occupation is still under study: Does it represent BEC or quasicondensation?

### A. SFA formalism

In this work we shall use the SFA approach [34] to study spin-polarized atomic hydrogen in two dimensions. This technique has already been used to study several many-body systems, ranging from weakly to strongly interacting systems. This includes a study of the classical two-dimensional Ising model [35]; one-, two-, and three-dimensional Ising model [36]; the strongly interacting systems, liquid helium-4 [37] and liquid helium-3 [38]; <sup>3</sup>He-He II mixtures [39]; hot nuclear matter [40]; three-dimensional spin-polarized atomic hydrogen [41]; and several other systems.

The SFA technique is relatively simple, compared to other many-body approaches, and it is applicable—at least in principle—to any many-body system, although it works better in dilute and weakly interacting systems. The idea of this technique is to replace the square of the local-field operator with its mean value. The physical meaning of this is that the quantum-mechanical spectrum of this operator is replaced with a *distribution* around its mean value. The basic assumption of SFA is that the Hamiltonian of the system can be written as a linear combination of the local-field operator  $\hat{E}_k$  and the occupation operator  $\hat{n}(k)$ :

$$\hat{H} = \sum_{\vec{k}} \hat{E}_k \hat{n}(k);$$

the local-field operator commutes with creation and annihilation operators.

The Hamiltonian describing the system is, in second quantization,

$$\hat{H} = \int \hat{\Psi}^{+}(\vec{r}) \frac{-\hbar^{2}}{2m} \nabla^{2} \hat{\Psi}(\vec{r}) d\vec{r} + \frac{1}{2} \int \hat{\Psi}^{+}(\vec{r}_{1}) \hat{\Psi}^{+}(\vec{r}_{2})$$
$$\times V(|\vec{r}_{1} - \vec{r}_{2}|) \hat{\Psi}(\vec{r}_{2}) \hat{\Psi}(\vec{r}_{1}) d\vec{r}_{1} d\vec{r}_{2}.$$
(1)

The pairwise bare central potential  $V(|\vec{r}_1 - \vec{r}_2|)$  used here is the Silvera potential [42]. The field operator  $\hat{\Psi}(\vec{r})$  is given in terms of annihilation operators  $b_{\vec{k}}$  and the single-particle wave functions  $\psi_{\vec{k}}(\vec{r})$  by

$$\hat{\Psi}(\vec{r}) = \sum_{\vec{k}} \psi_{\vec{k}}(\vec{r}) b_{\vec{k}}.$$
(2)

For a confined spin-polarized atomic hydrogen system, the single-particle wave functions  $\psi(\vec{r})$  are those of a particle in a two-dimensional box. The first term in the Hamiltonian is

$$\hat{T} = \int \hat{\Psi}^{+}(\vec{r}) \frac{-\hbar^{2}}{2m} \nabla^{2} \hat{\Psi}(\vec{r}) d\vec{r} = \sum_{k_{x}k_{y}} \frac{\hbar^{2}}{2m} (k_{x}^{2} + k_{y}^{2}) b_{k_{x}k_{y}}^{+} b_{k_{x}k_{y}},$$
(3)

where  $k_x = \frac{n\pi}{l}$ ,  $k_y = \frac{p\pi}{l}$  are the quantized linear momenta, and the indexes *n* and *p* are integer numbers which run from 1 to  $\infty$ . Here we shall consider the system to be distributed in a square sheet of side *l*. The interacting term in the Hamiltonian is calculated to be

$$\hat{V} = \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} V(k_1, k_2, k_3, k_4) b^+_{\vec{k}_1} b^+_{\vec{k}_2} b^-_{\vec{k}_3} b^-_{\vec{k}_4}.$$
 (4)

The quantized linear momentum is  $\vec{k}_1 = (k_{1x} = \frac{n_1\pi}{l}, k_{1y} = \frac{p_1\pi}{l})$ . The matrix elements of the potential  $V(k_1, k_2, k_3, k_4)$  are given by

$$V(k_1, k_2, k_3, k_4) = \frac{8}{l^4} \int_0^l \int_0^l \int_0^l \int_0^l \sin(k_{1x}x_1) \sin(k_{1y}y_1) \\ \times \sin[k_{2x}(x_1 - x)] \sin[k_{2y}(y_1 - y)] V(x, y) \\ \times \sin[k_{3x}(x_1 - x)] \sin[k_{3y}(y_1 - y)] \\ \times \sin(k_{4x}x_1) \sin(k_{4y}y_1) dx dx_1 dy dy_1.$$
(5)

To proceed further, we follow the technique developed earlier [27,28]; the underlying physics is also explained there. The local-field operator describing a finite spin-polarized atomic hydrogen system is

$$\hat{E}_k = \frac{\hbar^2 k^2}{2m} + \sum_{\vec{k}_1} V(k_1, k) \hat{n}_{k_1}.$$
(6)

 $V(k_1,k)$  is calculated to be

$$V(k_{1},k) = \frac{16}{l^{4}} \int_{0}^{l} \int_{0}^{l} \int_{0}^{l} \int_{0}^{l} \left\{ \sin(k_{1x}x_{1})\sin(k_{1y}y_{1})\sin[k_{x}(x_{1}-x)]\sin[k_{y}(y_{1}-y)]V(x,y) + \sin[k_{1x}(x_{1}-x)]\sin[k_{1y}(y_{1}-y)]\sin(k_{x}x_{1})\sin(k_{y}y_{1})dxdx_{1}dydy_{1} \right\} + \frac{16}{l^{4}} \int_{0}^{l} \int_{0}^{l} \int_{0}^{l} \int_{0}^{l} \int_{0}^{l} \left\{ \sin^{2}(k_{x}x_{1})\sin^{2}(k_{y}y_{1})\sin^{2}[k_{1x}(x_{1}-x)]\sin^{2}[k_{1y}(y_{1}-y)]V(x,y)dxdx_{1}dydy_{1} \right\}.$$
(7)

The distribution function of particles,  $n(k) = \langle \hat{n}_k \rangle$ , is determined to be [27]

$$n(k) = \langle \hat{n}_k \rangle = \frac{1}{2} \left[ \frac{1}{\exp[\beta(\langle \hat{E}_k \rangle + \varphi_k - \mu)] - 1} + \frac{1}{\exp[\beta(\langle \hat{E}_k \rangle - \varphi_k - \mu)] - 1} \right], \quad (8)$$

where  $\beta \equiv \frac{1}{k_BT}$ ,  $k_B$  being Boltzmann's constant. The chemical potential  $\mu$  is evaluated from the condition that the total number of particles *N* is constant:

$$N = \sum_{\vec{k}} n(k), \tag{9}$$

and the fluctuations  $\phi_k$  in the local-field operator are determined from the equation

$$\eta(k)\varphi_k^2 = \sum_{\vec{k}_1} V(k_1,k) \langle \Delta \hat{n}_k \Delta \hat{n}_{k_1} \rangle.$$
(10)

The function  $\eta(k)$  is given by [27]

$$\eta(k) = \frac{1}{2\varphi_k} \left[ \frac{1}{\exp[\beta(\langle \hat{E}_k \rangle + \varphi_k - \mu)] - 1} - \frac{1}{\exp[\beta(\langle \hat{E}_k \rangle - \varphi_k - \mu)] - 1} \right], \quad (11)$$

and the pair correlation function  $\langle \Delta \hat{n}_k \Delta \hat{n}_{k_1} \rangle$  is determined to be [27]

$$\left\langle \Delta \hat{n}_k \Delta \hat{n}_{k_1} \right\rangle_c = \eta(k) \sum_{\vec{k}_2} V(k_2, k) \left\langle \Delta \hat{n}_{k_2} \Delta \hat{n}_{k_1} \right\rangle, \tag{12}$$

the index c denoting the true correlations  $(\vec{k}_1 \neq \vec{k})$  involved. The quadratic fluctuations in the occupation numbers  $\langle \Delta \hat{n}_k \Delta \hat{n}_k \rangle = \langle \Delta \hat{n}_k^2 \rangle$  are evaluated to be [27]

$$\langle (\Delta \hat{n}_k)^2 \rangle = \langle \hat{n}_k \rangle (1 + \langle \hat{n}_k \rangle) + 2\eta(k) \sum_{\vec{k}_1} V(\vec{k}_1, \vec{k}) \langle \Delta \hat{n}_{k_1} \Delta \hat{n}_k \rangle_c.$$
(13)

The closed set of nonlinear equations, (6) and (8)–(11), can be solved numerically along the previous lines [27,28]. In our calculations, the natural system of units is used,  $\hbar = m = 1$ , *m* being the atomic mass of hydrogen.

#### **B.** Numerical scheme

The closed set of nonlinear equations is solved numerically by an iterative method. Initially, we consider the system to be ideal; and the occupation number, n(k), is determined by

$$n(k) = \langle \hat{n}_k \rangle = \frac{1}{\exp\left[\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)\right] - 1}.$$
 (14)

The fixed-point method is used to determine the chemical potential from Eq. (9). Numerically, it is impossible to satisfy the condition  $N - \sum_{\vec{k}} n(k) = 0$  exactly. Through the iteration process, however, we consider the required condition to be satisfied if

$$N - \sum_{\vec{k}} n(k) \leqslant 0.001N. \tag{15}$$

This process is then stopped.

In the second step, we calculate n(k) and  $\langle \hat{E}_k \rangle$  according to the mean-field approximation, by considering the fluctuations in the local-field operator to be zero. The output from the first step for n(k) is used as an input to calculate the expectation value of the local-field operator in Eq. (16). The modified n(k)is then calculated based on the new energy spectrum:

$$\langle \hat{n}_k \rangle = \frac{1}{\exp[\beta(\langle \hat{E}_k \rangle - \mu)] - 1}.$$
 (16)

The modified chemical potential is calculated according to Eq (15). The output distribution, n(k), is reused as an input to recalculate the expectation value of the local-field operator. The function

$$f(k) = \frac{|n(k)_{\text{input}} - n(k)_{\text{output}}|}{n(k)_{\text{output}}},$$
(17)

which measures the error in the number of particles in different states, is calculated in each iteration. The iteration process is stopped when the maximum value of f(k) in all states is <0.001.

In the third step, the output evaluated by the mean-field approximation is plugged as an input into SFA. How do we estimate the initial values of the fluctuations in the local-field operator? To have justified physical values for these fluctuations, we consider the system, to start with, at very low temperatures. Accordingly, we can consider all the particles to be accumulating in the ground state, and the local-field operator can be approximated as

$$\hat{E}_k = \frac{\hbar^2 k^2}{2m} + V(1,k)\hat{n}_1.$$
(18)

The quadratic fluctuations in this field operator are

$$\left\langle \Delta \hat{E}_{k}^{2} \right\rangle = \phi_{k}^{2} = V(1,k)^{2} \left\langle \Delta \hat{n}_{1}^{2} \right\rangle, \tag{19}$$

with  $\langle \Delta \hat{n}_k^2 \rangle$  calculated initially from the first term in Eq. (13). The occupation functions n(k) given in Eq. (8) are calculated based on these fluctuations, and the modified chemical potential is evaluated from Eq. (15). The other functions,  $\eta(k)$ ,  $\langle \Delta \hat{n}_k \Delta \hat{n}_{k_1} \rangle_c$ , the modified  $\langle \Delta \hat{n}_k^2 \rangle$ , and the modified  $\varphi_k$ , are then calculated. The output from the first iteration is reused as an input in the second iteration. At the end of each iteration, the output fluctuations are compared to the input:

$$g(k) = \frac{|\phi(k)_{\text{input}} - \phi(k)_{\text{output}}|}{\phi(k)_{\text{output}}}.$$
(20)

The iteration process is stopped when the maximum value of g(k) in all states is <0.001.

When we calculate these functions at very low temperature T, we use them as input data at higher temperature  $T + \Delta T$ . Also, for  $T + 2\Delta T$ , the output data for  $T + \Delta T$  is used as input data, and so on, until the required temperature has been attained.

### **III. RESULTS AND DISCUSSION**

In this work, we have calculated the number of particles in the ground state within SFA. Does this number represent a quasicondensate or a true condensate? SFA does not provide an answer to this question. Here, we have used the phrase "condensate fraction" to represent the number of particles in the ground state relative to the total number of particles in the system.

The condensate fraction and specific heat capacity  $C_v/Nk_B$ for a finite number of particles in two-dimensional spinpolarized atomic hydrogen have been computed as functions of the temperature at different number densities:  $1 \times 10^{-10}$ ,  $1 \times 10^{-8}$ , and  $1 \times 10^{-6}$  Å<sup>-2</sup>. The bare interaction used in our computations is the Silvera triplet-state potential.

The results obtained for the condensate fraction are presented in Figs. 1–3, and those for the specific heat capacity in Figs. 4–6. The condensate fraction at number density  $1 \times 10^{-10}$  Å<sup>-2</sup> for various particle numbers is shown in



FIG. 1. The condensate fraction of two-dimensional finite-number spin-polarized atomic hydrogen at number density  $1\times10^{-10}$  Å^{-2}.



FIG. 2. The condensate fraction of two-dimensional finite-number spin-polarized atomic hydrogen at number density  $1\times10^{-8}~\text{\AA}^{-2}.$ 

Fig. 1. The transition temperature of the system at this density is  $\sim 0.35 \mu K$ , regardless of the number of particles. For very dilute systems, the number of particles in the system does not play any role in determining the transition temperature.

As the number density of the system increases, the role of the number of particles starts to assert itself. In Figs. 2 and 3, the transition temperature increases as the number of particles decreases. Also, for a large number of particles,  $1 \times 10^5$  in Fig. 2, and  $1 \times 10^5$ ,  $1 \times 10^7$  in Fig. 3, there exists a welldefined transition temperature, whereas for small numbers of particles, the condensate fraction decreases monotonically with temperature at low temperatures, and becomes constant at higher temperatures. Thus, the transition temperature, if present, is not well defined as we shall also see in specific heat capacity calculations. These results agree with those



FIG. 3. The condensate fraction of two-dimensional finite-number spin-polarized atomic hydrogen at number density  $1 \times 10^{-6} \text{ Å}^{-2}$ .



FIG. 4. The specific heat capacity of two-dimensional finite-number spin-polarized atomic hydrogen at number density  $1 \times 10^{-10}$  Å<sup>-2</sup>.

obtained for a Bose gas trapped in a two-dimensional quadratic potential [20].

From Figs. 1–3, it is observed that as the number density increases at a constant number of particles (meaning that the dimension of the box decreases), the transition temperature increases. This result is consistent with published results: In the thermodynamic limit, BEC cannot take place in two-dimensional Bose gases [22]. To probe the effect of the system dimension on the transition temperature, we have determined the transition temperature in Figs. 1–3 at the number of particles  $N = 1 \times 10^5$ . The results are close to 0.35, 4.3, and 220  $\mu$ K at a number density  $1 \times 10^{-10}$ ,  $1 \times 10^{-8}$ , and  $1 \times 10^{-6}$ , respectively. These results show that, as the dimension of the box increases, the transition temperature decreases and might go to zero as the dimension goes to infinity.



FIG. 5. The specific heat capacity of two-dimensional finite-number spin-polarized atomic hydrogen at number density  $1\times10^{-8}$  Å^{-2}.



FIG. 6. The specific heat capacity of two-dimensional finite-number spin-polarized atomic hydrogen at number density  $1 \times 10^{-6} \text{ Å}^{-2}$ .

Our results are qualitatively consistent with those obtained by the path-integral quantum Monte Carlo method for hard-core bosons in a two-dimensional isotropic harmonicoscillator potential [23], where the condensate fraction appears abruptly on increasing the number of particles of the system. The results show that, as the number of particles of the system increases, the transition temperature decreases and may vanish in the thermodynamic limit. This agrees with results observed by Mullin using mean-field theory [22], where he concludes that there is no BEC in a two-dimensional Bose gas in the thermodynamic limit. He finds that, below the transition temperature, the Bose-Einstein condensed state is not a consistent solution of the equations in the thermodynamic limit. In our work, the chemical potential has been calculated self-consistently from Eq. (8).

In Figs. 4–6, the specific heat capacity of the system is shown. In the ideal Bose gas, the heat capacity increases smoothly with temperature; this behavior changes drastically for the interacting system at low densities. For the dilute system, Fig. 4 shows a sharp peak in the heat capacity at the transition temperature, which is consistent with the condensate-fraction results, where the phase changes from the condensed state to the normal state. In Fig. 5, where the number density is  $1 \times 10^{-8}$  Å<sup>-2</sup>, there is a hump around the not-well-defined transition temperature, which indicates that there is an appreciable number of particles in both ground and excited states in this region. Figure 6 shows that the specific heat capacity increases monotonically with temperature towards the classical value. In dense systems, the condensate fraction decreases rapidly with temperature, which means that the number of particles in the excited state grows rapidly.

The specific heat capacity varies smoothly with temperature at high number density; and there is no cusp at number density  $1 \times 10^{-6}$  Å<sup>-2</sup>. This may imply that no BEC occurs at high number density. The cusp in the specific heat is considered to be an indication of BEC, even though the relation between coherence of the quantum state of the condensate and the presence of this peak remains elusive. The position of the peaks, as shown in Figs. 5 and 6, shifts to higher temperature as the number of particles increases. This result is consistent with the results obtained in [24,25].

# **IV. CONCLUSIONS**

SFA has been applied successfully to a finite interacting two-dimensional spin-polarized atomic hydrogen system. Bose-Einstein condensation *can* occur in such a system. The transition temperature in the dilute system is dependent on the number of particles and goes to zero in the thermodynamic limit. A cusp occurs in the specific heat capacity at the transition temperature. The peak becomes broad as the number density of the system increases; at a high number density, no cusp appears.

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