Bose–Einstein condensation of atomic hydrogen Feynman path integral approach

2004 J. Phys. A: Math. Gen. 37 5251

(http://iopscience.iop.org/0305-4470/37/19/012)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **37** (2004) 5251–5259 PII: S0305-4470(04)66273-1

Bose–Einstein condensation of atomic hydrogen Feynman path integral approach

Wattana Lim and Virulh Sa-yakanit

Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

Received 9 July 2003, in final form 9 February 2004
Published 27 April 2004
Online at stacks.iop.org/JPhysA/37/5251
DOI: 10.1088/0305-4470/37/19/012

Abstract

We study the ground state properties of Bose–Einstein condensation of atomic hydrogen in the Ioffe–Pritchard magnetic trap using many-body Feynman path integral theory, which leads to the calculation of the ground state energy and the wavefunction. We also calculate the size, peak condensate density and the value of the ground state energy, which are in good agreement with the experimental results obtained by laser spectroscopy of the 1S–2S transition.

PACS numbers: 31.15.Kb, 03.75.Nt

1. Introduction

In 1998, the first observation of Bose–Einstein condensation (BEC) in spin-polarized hydrogen was reported by Fried at the Massachusetts Institute of Technology [1–3]. They used dilution refrigerators, magnetic trapping and RF evaporative cooling. The hydrogen condensate was detected by laser spectroscopy. That is an important result because hydrogen condensates are huge, compared with other alkali metal atoms. Moreover, hydrogen has small mass, so the transition temperature occurs at a higher temperature than for other atoms. Hydrogen is a very interesting element to study BEC, due to its small scattering length making it an almost ideal Bose gas.

In this paper, we use Feynman path integral theory to study BEC in hydrogen. By this method, we can study the properties of the hydrogen condensate from the experimental data such as ground state energy, wavefunction, size of the condensate, peak condensate density and distribution of the probability which give useful information for the prediction and study of the BEC.

2. Feynman path integral theory of BEC in hydrogen

We calculate the ground state properties of atomic hydrogen using Feynman path integral theory with the assistance of the variational principle. In the experiment, the magnetic trap shape that was used to confine hydrogen atoms is called the Ioffe–Pritchard trap with axial coordinate z and radial coordinate ρ. The potential energy is

$$V(\rho, z) = \sqrt{(\alpha\rho)^2 + (\gamma z^2 + \theta)^2} - \theta. \tag{1}$$

Here α, γ and θ are radial potential energy gradient, axial potential energy curvature and bias potential energy, respectively. In the limit of $\rho \ll \theta/\alpha$, the Ioffe–Prithchard potential is harmonic in the radial coordinate [1], as may be seen by expanding the potential in power series.

$$V_{\mathrm{IP}}(\rho, z) = \gamma z^2 + \frac{1}{2}\frac{\alpha^2}{\gamma z^2 + \theta}\rho^2 + \frac{1}{8}\frac{\alpha^3}{(\gamma z^2 + \theta)^2}\rho^3 + \cdots. \tag{2}$$

First we consider N hydrogen atoms in the Ioffe–Pritchard trap, retaining only the first two terms of the expansion from equation (2) and treating the interaction among hydrogen atoms are mean field energy, which is repulsive for s-wave scattering lengths $a > 0$. The interaction between condensate and thermal atoms is totally neglected in the present treatment because this interaction is quite small. Therefore, the Lagrangian for the entire system is written as

$$L = \frac{m}{2}\sum_{i=1}^{N}\left(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2\right) - \sum_{i=1}^{N}\left[\gamma z_i^2 + \frac{\alpha^2}{2\left(\gamma z_i^2 + \theta\right)}\left(x_i^2 + y_i^2\right)\right] - \left(\frac{4\pi\hbar^2 a}{m}\right)\sum_{ij}\delta(\mathbf{r}_i - \mathbf{r}_j) \tag{3}$$

where the action associated with this Lagrangian is defined as $S = \int L\,\mathrm{d}t$. To solve the density matrix ρ exactly, we choose the trial action

$$S_0 = \int_0^{\beta}\left(\frac{m}{2}\sum_{i=1}^{N}\left(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2\right) - \sum_{i=1}^{N}\left[\omega_z^2 z_i^2 + \omega_\rho^2\left(x_i^2 + y_i^2\right)\right]\right)\mathrm{d}t \tag{4}$$

where ω_z and ω_ρ are treated as variational parameters. Thus, we can calculate the density matrix by using the first cumulant expansion as shown below

$$\begin{aligned}\rho &= \rho_0\left\langle \mathrm{e}^{-\frac{1}{\hbar}(S-S_0)}\right\rangle_{S_0} \simeq \rho_0\,\mathrm{e}^{\langle -\frac{1}{\hbar}(S-S_0)\rangle_{S_0}} \\ &\simeq \rho_0 \exp\left[\int_0^{\beta}\mathrm{d}t\left(\begin{array}{l}\sum_{i=1}^{N}\left(\frac{m}{2}\omega_z^2 - \gamma\right)\left\langle z_i^2\right\rangle_{S_0} + \sum_{i=1}^{N}\frac{m}{2}\omega_\rho^2\left(\left\langle x_i^2\right\rangle_{S_0} + \left\langle y_i^2\right\rangle_{S_0}\right) \\ -\sum_{i=1}^{N}\frac{\alpha^2}{2}\left\langle\frac{\left(x_i^2 + y_i^2\right)}{\gamma z_i^2 + \theta}\right\rangle_{S_0} - \frac{4\pi\hbar^2 a}{m}\sum_{ij}\left\langle\delta(\mathbf{r}_i - \mathbf{r}_j)\right\rangle_{S_0}\end{array}\right)\right]\end{aligned} \tag{5}$$

where the average $\langle A\rangle_{S_0}$ is defined as $\langle A\rangle_{S_0} = \frac{\int_{\mathbf{r}_N(0)}^{\mathbf{r}_N(\beta)} D^N(\mathbf{r}_N(t))A\exp\left[-\frac{S_0}{\hbar}\right]}{\int_{\mathbf{r}_N(0)}^{\mathbf{r}_N(\beta)} D^N(\mathbf{r}_N(t))\exp\left[-\frac{S_0}{\hbar}\right]}$. The path integral $\int_{\mathbf{r}_N(0)}^{\mathbf{r}_N(\beta)} D^N(\mathbf{r}_N(t))$ symbol is given as

$$\int_{\mathbf{r}_N(0)}^{\mathbf{r}_N(\beta)} D^N(\mathbf{r}_N(t)) = \int_{\mathbf{r}_N(0)}^{\mathbf{r}_N(\beta)} D^1(\mathbf{r}_1(t))\int_{\mathbf{r}_N(0)}^{\mathbf{r}_N(\beta)} D^2(\mathbf{r}_2(t))\ldots..\int_{\mathbf{r}_N(0)}^{\mathbf{r}_N(\beta)} D^N(\mathbf{r}_N(t)). \tag{6}$$

To evaluate the exponent in equation (5), we proceed as follows. We first evaluate averages $\langle x^2\rangle_{S_0}$, $\langle y^2\rangle_{S_0}$, $\langle z^2\rangle_{S_0}$ as well as $\left\langle\frac{(x^2+y^2)}{\gamma z^2+\theta}\right\rangle_{S_0}$ by using the generating functional [4].

$$\left\langle \exp\left[\frac{\mathrm{i}}{\hbar}\int f(t)x(t)\,\mathrm{d}t\right]\right\rangle_{S_0} = \left\{\exp\left[\frac{\mathrm{i}}{\hbar}\left(S'_{0_{\mathrm{cl}}} - S_{0_{\mathrm{cl}}}\right)\right]\right\} \tag{7}$$

where $S_{0_{\mathrm{cl}}}$ is classical action associated with the trial action S_0 and $S'_{0_{\mathrm{cl}}}$ is defined as $S_{0_{\mathrm{cl}}} + \int f(t)x(t)\,\mathrm{d}t$. The averages $\langle x(t)\rangle$ and $\langle x(t)^2\rangle$ can be obtained from

$$\langle x(t)\rangle = \left[\frac{\delta S'_{\mathrm{Cl}}}{\delta f(t)}\right]_{f(t)=0} \tag{8}$$

$$\langle x(t)^2\rangle = \left[-\frac{\mathrm{i}}{\hbar}\frac{\delta^2 S'_{\mathrm{Cl}}}{\delta f(t)^2} + \left(\frac{\delta S'_{\mathrm{Cl}}}{\delta f(t)}\right)^2\right]_{f(t)=0} \tag{9}$$

where classical force harmonic action S'_{Cl} is given by Feynman and Hibbs [4].

$$S'_{\mathrm{Cl}} = \frac{m\omega}{2\sin\omega T}\begin{bmatrix}\cos\omega T\left(x_2^2+x_1^2\right) - 2x_1x_2 + \frac{2x_2}{m\omega}\int_0^T f(t)\sin\omega t\,\mathrm{d}t \\ +\frac{2x_1}{m\omega}\int_0^T f(t)\sin\omega(T-t)\,\mathrm{d}t \\ -\frac{1}{m^2\omega^2}\int_0^T\int_0^T f(t)f(s)\sin\omega(T-t)\sin\omega s\,\mathrm{d}s\,\mathrm{d}t\end{bmatrix}. \tag{10}$$

Substituting equation (10) into equations (8) and (9) and replacing t by $-\mathrm{i}\hbar t$, we obtain

$$\langle x(t)\rangle_{S_0} = \frac{x_2\sinh\omega_\rho\hbar t + x_1\sinh\omega_\rho\hbar(\beta-t)}{\sinh\omega_\rho\hbar\beta} \tag{11}$$

and

$$\langle x(t)^2\rangle_{S_0} = \frac{\hbar}{m\omega_\rho}\frac{\sinh\omega_\rho\hbar(\beta-t)\sinh\omega_\rho\hbar t}{\sinh\omega_\rho\hbar\beta} + \left(\frac{x_2\sinh\omega_\rho\hbar t + x_1\sinh\omega_\rho\hbar(\beta-t)}{\sinh\omega_\rho\hbar\beta}\right)^2. \tag{12}$$

Similarly we can calculate $\langle y(t)\rangle_{S_0}$, $\langle y^2(t)\rangle_{S_0}$, $\langle z(t)\rangle_{S_0}$ and $\langle z^2(t)\rangle_{S_0}$. To find the density matrix we have to integrate equation (12) over t which can be solved exactly as shown below.

$$\begin{aligned}\int_0^\beta \langle x^2(t)\rangle_{S_0}\,\mathrm{d}t &= \frac{\hbar\beta}{2\omega_\rho m}\coth\omega_\rho\hbar\beta - \frac{1}{2\omega_\rho^2 m} + \frac{\left(x_1^2+x_2^2\right)}{2\omega_\rho\hbar}\coth(\omega_\rho\hbar\beta)\\ &\quad - \frac{x_1x_2}{\omega_\rho\hbar}\mathrm{cosech}(\omega_\rho\hbar\beta) - \frac{1}{2}\left(x_1^2+x_2^2\right)\mathrm{cosech}^2(\omega_\rho\hbar\beta)\beta\\ &\quad + x_1x_2\coth(\omega_\rho\hbar\beta)\mathrm{cosech}(\omega_\rho\hbar\beta)\beta.\end{aligned} \tag{13}$$

The next step is to evaluate $\left\langle\frac{x^2}{\gamma z^2+\theta}\right\rangle_{S_0}$ by using the identity $\frac{1}{x} = \int_0^\infty \mathrm{e}^{-xq}\,\mathrm{d}q$ and using the first cumulant expansion. Thus we may write

$$\left\langle\frac{x^2}{\gamma z^2+\theta}\right\rangle_{S_0} \simeq \langle x^2\rangle_{S_0}\int_0^\infty \mathrm{e}^{-(\gamma\langle z^2\rangle_{S_0}+\theta)q}\,\mathrm{d}q = \frac{\langle x^2\rangle_{S_0}}{\gamma\langle z^2\rangle_{S_0}+\theta}. \tag{14}$$

Substituting the results for $\langle x^2\rangle_{S_0}$ and $\langle z^2\rangle_{S_0}$ into equation (14) and using the relation $\sinh\omega_\rho\hbar(\beta-t)\sinh\omega_\rho\hbar t = (\cosh\omega_\rho\hbar\beta - \cosh(2\omega_\rho\hbar t - \omega_\rho\hbar\beta))/2$ and $\frac{1}{1-x} = 1+\sum_{n=1}^\infty x^n$, as well as retaining only the first two terms of the expansion, we obtain

$$\begin{aligned}\int_0^\beta \frac{\langle x^2\rangle}{\gamma\langle z^2\rangle+\theta}\,\mathrm{d}t &= \frac{\omega_z\hbar\beta\coth\omega_\rho\hbar\beta}{\omega_\rho(\gamma\hbar\coth\omega_z\hbar\beta + 2m\omega_z\theta)}\\ &\quad + \frac{2m\omega_z}{(\gamma\hbar\coth\omega_z\hbar\beta+2m\omega_z\theta)}\left(\frac{\left(x_1^2+x_2^2\right)}{2\omega_\rho\hbar}\coth(\omega_\rho\hbar\beta) - \frac{x_1x_2}{\omega_\rho\hbar}\mathrm{cosech}(\omega_\rho\hbar\beta)\right)\\ &\quad - \frac{2\gamma m\hbar\omega_z^2}{\omega_\rho(\gamma\hbar\coth\omega_z\hbar\beta+2m\omega_z\theta)^2}\left(\frac{\left(z_1^2+z_2^2\right)}{2\omega_z\hbar}\coth(\omega_z\hbar\beta) - \frac{z_1z_2}{\omega_z\hbar}\mathrm{cosech}(\omega_z\hbar\beta)\right)\\ &\quad + \cdots.\end{aligned} \tag{15}$$

Our next task is to calculate the average of the delta function. In order to manipulate the delta function within the path integral, we express it by its Fourier transform,

$$\langle\delta(\mathbf{r}_i-\mathbf{r}_j)\rangle = \int_{-\infty}^{\infty}\mathrm{d}\mathbf{k}\frac{1}{(2\pi)^3}\left\langle\mathrm{e}^{\mathbf{ik}\cdot(\mathbf{r}_i-\mathbf{r}_j)}\right\rangle_{S_0}. \tag{16}$$

We can write

$$\langle \exp[\mathrm{i}\mathbf{k}\cdot(\mathbf{r}_i(t)-\mathbf{r}_j(t))]\rangle_{S_0} = \langle \exp[\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i(t)]\rangle_{S_0}\langle \exp[-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j(t)]\rangle_{S_0}. \tag{17}$$

Expanding the first factor in the first and second cumulants,

$$\langle \exp[\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i(t)]\rangle_{S_0} = \exp\left[\mathrm{i}\mathbf{k}\cdot\langle\mathbf{r}_i(t)\rangle_{S_0} - \mathbf{k}^2\tfrac{1}{2}\left(\langle\mathbf{r}_i(t)^2\rangle_{S_0} - \langle\mathbf{r}_i(t)\rangle_{S_0}^2\right)\right]. \tag{18}$$

Similarly the second factor

$$\langle \exp[\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j(t)]\rangle_{S_0} = \exp\left[\mathrm{i}\mathbf{k}\cdot\langle\mathbf{r}_j(t)\rangle_{S_0} - \mathbf{k}^2\tfrac{1}{2}\left(\langle\mathbf{r}_j(t)^2\rangle_{S_0} - \langle\mathbf{r}_j(t)\rangle_{S_0}^2\right)\right]. \tag{19}$$

The Green function $g(t,t)$ can be defined as

$$\begin{aligned} g(t,t) &= \langle\mathbf{r}_i(t)^2\rangle_{S_0} - \langle\mathbf{r}_i(t)\rangle_{S_0}^2 \\ &= \frac{\hbar}{m\omega_\rho}\frac{\sinh\omega_\rho\hbar(\beta-t)\sinh\omega_\rho\hbar t}{\sinh\omega_\rho\hbar\beta}. \end{aligned} \tag{20}$$

Note that the Green function is independent of the particle index. We can write

$$\langle\delta(\mathbf{r}_i-\mathbf{r}_j)\rangle = \int_{-\infty}^{\infty}\frac{1}{(2\pi)^3}\,\mathrm{d}\mathbf{k}\exp\left[\mathrm{i}\mathbf{k}\cdot\left(\langle\mathbf{r}_i(t)\rangle_{S_0} - \langle\mathbf{r}_j(t)\rangle_{S_0}\right)\right]\exp[-\mathbf{k}^2 2(g(t,t))]. \tag{21}$$

Considering the x coordinate, we can solve equation (21) by substituting equations (11) and (12) into equation (21). Using the formula $\int_{-\infty}^{\infty}\mathrm{d}x\,\mathrm{e}^{-ax^2+bx} = \sqrt{\frac{\pi}{a}}\,\mathrm{e}^{b^2/4a}$ and replacing t by $-\mathrm{i}\hbar t$ we obtain

$$\begin{aligned} \delta(x_i-x_j) &= \sqrt{\frac{m\omega_\rho}{4\pi\hbar}\frac{\sinh\omega_\rho\hbar\beta}{\sinh\omega_\rho\hbar(\beta-t)\sinh\omega_\rho\hbar t}} \\ &\quad\times\exp\left[-\frac{m\omega_\rho}{4\hbar}\frac{\begin{pmatrix} x_{i_2}\sinh\omega_\rho\hbar t + x_{i_1}\sinh\omega_\rho\hbar(\beta-t) \\ -x_{j_2}\sinh\omega_\rho\hbar t + x_{j_1}\sinh\omega_\rho\hbar(\beta-t)\end{pmatrix}^2}{\sinh\omega_\rho\hbar(\beta-t)\sinh\omega_\rho\hbar t\sinh\omega_\rho\hbar\beta}\right]. \end{aligned} \tag{22}$$

Using the relation $\mathrm{e}^{-x} = \sum_{n=0}^{\infty}\frac{(-x)^n}{n!} = 1 - x + \frac{1}{2}x^2 + \cdots$ we can write the delta function in three dimensions as

$$\begin{aligned} \langle\delta(\mathbf{r}_i-\mathbf{r}_j)\rangle_{S_0} &= \left(\frac{m\omega_\rho\sinh\omega_\rho\hbar\beta}{4\pi\hbar\sinh\omega_\rho\hbar(\beta-t)\sinh\omega_\rho\hbar t}\right)\left(\frac{m\omega_z\sinh\omega_z\hbar\beta}{4\hbar\sin\omega_z\hbar(\beta-t)\sin\omega_z\hbar t}\right)^{1/2} \\ &\quad\times\left(1-\begin{pmatrix} \frac{m\omega_\rho\left(\left(x_{i_2}-x_{j_2}\right)\sinh\omega\hbar t+\left(x_{i_1}-x_{j_1}\right)\sinh\omega\hbar(\beta-t)\right)^2}{4\hbar\sinh\omega\hbar(\beta-t)\sinh\omega\hbar t\sinh\omega\hbar\beta} \\ +\frac{m\omega_\rho\left(\left(y_{i_2}-y_{j_2}\right)\sinh\omega_\rho\hbar t+\left(y_{i_1}-y_{j_1}\right)\sinh\omega_\rho\hbar(\beta-t)\right)^2}{4\hbar\sinh\omega_\rho\hbar(\beta-t)\sinh\omega_\rho\hbar t\sinh\omega_\rho\hbar\beta} \\ +\frac{m\omega_z\left(\left(z_{i_2}-z_{j_2}\right)\sinh\omega_z\hbar t+\left(z_{i_1}-z_{j_1}\right)\sinh\omega_z\hbar(\beta-t)\right)^2}{4\hbar\sinh\omega_z\hbar(\beta-t)\sinh\omega_z\hbar t\sinh\omega_z\hbar\beta}\end{pmatrix}+\cdots\right). \end{aligned} \tag{23}$$

Integrating equation (23) by using the same method of calculating $\langle x^2\rangle/(\gamma\langle z^2\rangle+\theta)$ and keeping only the first order of the expansion ,we obtain

$$\begin{aligned} \int_0^\beta\langle\delta(\mathbf{x}_i-\mathbf{x}_j)\rangle\,\mathrm{d}t &= \left(\frac{m\omega_\rho}{2\pi\hbar}\tanh\omega_\rho\hbar\beta\right)\left(\frac{m\omega_z}{2\pi\hbar}\tanh\omega_z\hbar\beta\right)^{1/2}\beta \\ &\quad+\left(\frac{m\omega_\rho}{2\pi\hbar}\right)\left(\frac{m\omega_z}{2\pi\hbar}\right)^{1/2}\left(\frac{m}{2\hbar^2}\left(\left(x_{i_1}-x_{j_1}\right)^2+\left(x_{i_2}-x_{j_2}\right)^2\right)\right) \\ &\quad-\left(\frac{m\omega_\rho}{2\pi\hbar}\right)\left(\frac{m\omega_z}{2\pi\hbar}\right)^{1/2}\left(\frac{m}{\hbar^2}\left(x_{i_1}-x_{j_1}\right)\left(x_{i_2}-x_{j_2}\right)\right)\mathrm{sech}(\omega_\rho\hbar\beta) \end{aligned}$$

$$
\begin{aligned}
&-\left(\frac{m\omega_\rho}{2\pi\hbar}\right)\left(\frac{m\omega_z}{2\pi\hbar}\right)^{1/2}\left(\frac{\omega_\rho m\beta}{\hbar}\left(\left(x_{i_1}-x_{j_1}\right)^2+\left(x_{i_2}-x_{j_2}\right)^2\right)\right)\operatorname{cosech}(2\omega_\rho\hbar\beta)\\
&+\left(\frac{m\omega_\rho}{2\pi\hbar}\right)\left(\frac{m\omega_z}{2\pi\hbar}\right)^{1/2}\left(\frac{\omega_\rho m\beta}{\hbar}\left(x_{i_1}-x_{j_1}\right)\left(x_{i_2}-x_{j_2}\right)\right)\operatorname{cosech}(\omega_\rho\hbar\beta)\\
&+\cdots.
\end{aligned}
\tag{24}
$$

In the case of Bose–Einstein condensation in which all particles are confined in a small region, we may make the assumption that all particles are approximately at the same point in space. Using equations (13), (15) and (24), we obtain our approximated result for the density matrix of the system of N particles undergoing Bose–Einstein condensation in the Ioffe–Pritchard trap as

$$
\begin{aligned}
\rho_N =& \left(\frac{m\omega_\rho}{\pi\hbar}\right)^N\left(\frac{m\omega_z}{\pi\hbar}\right)^{N/2}\\
&\times\exp\left[-N\begin{pmatrix}\omega_\rho\hbar+\frac{1}{2}\omega_z\hbar-\frac{1}{2}\omega_\rho\hbar\coth\omega_\rho\hbar\beta-\frac{1}{4}\omega_z\hbar\coth\omega_z\hbar\beta\\ +\frac{\alpha^2\omega_z\hbar\coth\omega_\rho\hbar\beta}{\omega_\rho(\gamma\hbar\coth\omega_z\hbar\beta+2m\omega_z\theta)}+\frac{\hbar\gamma}{2m\omega_z}\coth\omega_z\hbar\beta\\ +a\hbar\,(N-1)\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\tanh\omega_\rho\hbar\beta\sqrt{\omega_z\tanh\omega_z\hbar\beta}\end{pmatrix}\beta\right]\\
&\times\exp\left[\begin{aligned}&-\left(\tfrac{Nm\omega_\rho}{4\hbar}+\tfrac{N\alpha^2m\omega_z}{2\hbar\omega_\rho(\gamma\hbar\coth\omega_z\hbar\beta+2m\omega_z\theta)}-N(N-1)\pi a\left(\tfrac{m\omega_\rho}{2\pi\hbar}\right)\left(\tfrac{m\omega_z}{2\pi\hbar}\right)^{1/2}\right)\\ &\quad\times\left(\rho_1^2+\rho_2^2\right)\coth(\omega_\rho\hbar\beta)\\ &\quad-\left(\tfrac{Nm\omega_z}{4\hbar}+\tfrac{N\gamma}{2\omega_z\hbar}-N(N-1)\pi a\left(\tfrac{m\omega_\rho}{2\pi\hbar}\right)\left(\tfrac{m\omega_z}{2\pi\hbar}\right)^{1/2}\right)\left(z_1^2+z_2^2\right)\coth(\omega_z\hbar\beta)\end{aligned}\right]\\
&+\cdots.
\end{aligned}
\tag{25}
$$

The density matrix for one particle can be written as

$$
\begin{aligned}
\rho_1 =& \left(\frac{m\omega_\rho}{\pi\hbar}\right)\left(\frac{m\omega_z}{\pi\hbar}\right)^{1/2}\\
&\times\exp\left[-\begin{pmatrix}\omega_\rho\hbar+\frac{1}{2}\omega_z\hbar-\frac{1}{2}\omega_\rho\hbar\coth\omega_\rho\hbar\beta-\frac{1}{4}\omega_z\hbar\coth\omega_z\hbar\beta\\ +\frac{\alpha^2\omega_z\hbar\coth\omega_\rho\hbar\beta}{\omega_\rho(\gamma\hbar\coth\omega_z\hbar\beta+2m\omega_z\theta)}+\frac{\hbar\gamma}{2m\omega_z}\coth\omega_z\hbar\beta\\ +a\hbar(N-1)\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\tanh\omega_\rho\hbar\beta\sqrt{\omega_z\tanh\omega_z\hbar\beta}\end{pmatrix}\beta\right]\\
&\times\exp\left[\begin{aligned}&-\left(\tfrac{m\omega_\rho}{4\hbar}+\tfrac{\alpha^2m\omega_z}{2\hbar\omega_\rho(\gamma\hbar\coth\omega_z\hbar\beta+2m\omega_z\theta)}-(N-1)\pi a\left(\tfrac{m\omega_\rho}{2\pi\hbar}\right)\left(\tfrac{m\omega_z}{2\pi\hbar}\right)^{1/2}\right)\\ &\quad\times\left(\rho_1^2+\rho_2^2\right)\coth(\omega_\rho\hbar\beta)\\ &\quad-\left(\tfrac{m\omega_z}{4\hbar}+\tfrac{\gamma}{2\omega_z\hbar}-(N-1)\pi a\left(\tfrac{m\omega_\rho}{2\pi\hbar}\right)\left(\tfrac{m\omega_z}{2\pi\hbar}\right)^{1/2}\right)\left(z_1^2+z_2^2\right)\coth(\omega_z\hbar\beta)\end{aligned}\right]\\
&+\cdots.
\end{aligned}
\tag{26}
$$

3. Ground state energy and wavefunction

When BEC occurs, the temperature goes to nearly absolute zero temperature and $\beta = \frac{1}{kT} \to \infty$ where k is the Boltzmann constant and T is the temperature. Thus $\coth\omega_\rho\hbar\beta$, $\coth\omega_\rho\hbar\beta$, $\tanh\omega_\rho\hbar\beta$ and $\tanh\omega_\rho\hbar\beta \to 1$. To obtain the ground state energy we need only the diagonal parts of the propagator, therefore taking the trace is equivalent to setting $\overrightarrow{r}(\beta) = \overrightarrow{r}(0)$.

$$Z[\beta] = \mathrm{Tr}[\rho(\mathbf{r}(\beta), \mathbf{r}(\beta))] = \left(\frac{m\omega_\rho}{\pi\hbar}\right)^N \left(\frac{m\omega_z}{\pi\hbar}\right)^{N/2}$$
$$\times \exp\left[-N\begin{pmatrix}\frac{1}{2}\omega_\rho\hbar + \frac{1}{4}\omega_z\hbar + \frac{\alpha^2\omega_z\hbar}{\omega_\rho(\gamma\hbar+2m\omega_z\theta)} \\ +\frac{\hbar\gamma}{2m\omega_z} + a\hbar(N-1)\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z}\end{pmatrix}\beta\right]$$
$$\times \exp\left[\begin{matrix}-\left(\frac{Nm\omega_\rho}{4\hbar} + \frac{N\alpha^2 m\omega_z}{\hbar\omega_\rho(\gamma\hbar+2m\omega_z\theta)} - N(N-1)\pi a\left(\frac{m\omega_\rho}{2\pi\hbar}\right)\left(\frac{m\omega_z}{2\pi\hbar}\right)^{1/2}\right)\rho^2 \\ -\left(\frac{Nm\omega_z}{2\hbar} + \frac{N\gamma}{\omega_z\hbar} - N(N-1)\pi a\left(\frac{m\omega_\rho}{2\pi\hbar}\right)\left(\frac{m\omega_z}{2\pi\hbar}\right)^{1/2}\right)z^2\end{matrix}\right]. \tag{27}$$

This means that the ground state energy of the entire system has the energy

$$E_0 = N\hbar\left(\frac{1}{2}\omega_\rho + \frac{1}{4}\omega_z + \frac{\gamma}{2\omega_z m} + \frac{\alpha^2\omega_z}{\omega_\rho(\hbar\gamma + 2m\omega_z\theta)} + a\,(N-1)\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z}\right). \tag{28}$$

This result agrees with Baym and Pethick [5]. Using the relation $\int_{-\infty}^{\infty}\phi_0(\mathbf{r})^*\phi_0(\mathbf{r})\,\mathrm{d}^3\mathbf{r} = N$, we obtain the normalized ground state wavefunction in three dimensions from equation (26).

$$\phi_0(\mathbf{r}) = \sqrt{N}\left(\frac{m}{\pi\hbar}\left(\frac{\omega_\rho}{2} + \frac{\alpha^2\omega_z}{\omega_\rho\,(\gamma\hbar + 2m\omega_z\theta)} - (N-1)a\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z}\right)\right)^{1/2}$$
$$\times\left(\frac{m}{\pi\hbar}\left(\frac{\omega_z}{2} + \frac{\gamma}{m\omega_z} - (N-1)a\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z}\right)\right)^{1/4}$$
$$\times\exp\left[-\frac{m}{2\hbar}\begin{pmatrix}\frac{\omega_\rho}{2} + \frac{\alpha^2\omega_z}{\omega_\rho(\gamma\hbar+2m\omega_z\theta)} \\ -(N-1)a\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z}\end{pmatrix}\rho^2\right]$$
$$\times\exp\left[-\frac{m}{2\hbar}\left(\frac{\omega_z}{2} + \frac{\gamma}{m\omega_z} - (N-1)a\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z}\right)z^2\right]. \tag{29}$$

4. Calculation results and discussions

We minimize the ground state energy by solving partial derivative $E(\omega_\rho, \omega_z)$ from equation (28) with respect to $\omega_\rho\ \partial E(\omega_\rho, \omega_z)/\partial\omega_\rho = 0$. The parameters α, γ and θ for the trap shape A [1] are $\gamma = 25\times k$ (J cm^{-2}), $\theta = 35\times k$ (J) and $\alpha = 15.9\times 10^3\times k$ (J cm^{-1}). A condensate containing 1.2×10^9 atoms is observed in this trap. For hydrogen in the ground state, the s-wave scattering length $a = 0.648\times 10^{-10}$ (m) and the mass of hydrogen is 1.6746×10^{-27} kg. If we fix the value of ω_z and vary the value of ω_ρ, then we find two curves that have maximum and minimum points; in the case of ω_ρ negative (positive) the curve has a maximum (minimum) point. If we plot energy against ω_z, we find one curve which has a minimum point. See figure 1.

Physically, the frequency cannot be negative, thus we are interested only in the case of positive ω_ρ. From the result of the calculation, we obtain the values, $\omega_\rho = (2\pi)\,607.078$ Hz, $\omega_z = (2\pi)\,0.004\,342\,48$ Hz and the ground energy is $2.467\,51\times 10^{-20}$ J.

We can also calculate the size of the condensate in the IP trap from the full expression in equation (29). We have to use high significant digit $\omega_\rho = (2\pi)\,607.078\,045\,237$ Hz and $\omega_z = (2\pi)\,0.004\,342\,477\,118\,54$ Hz because the magnitude of the frequency in the z axis is very small compared to the ρ axis frequency ($\omega_\rho/\omega_z = 1.4\times 10^5$). Substituting ω_ρ and ω_z into

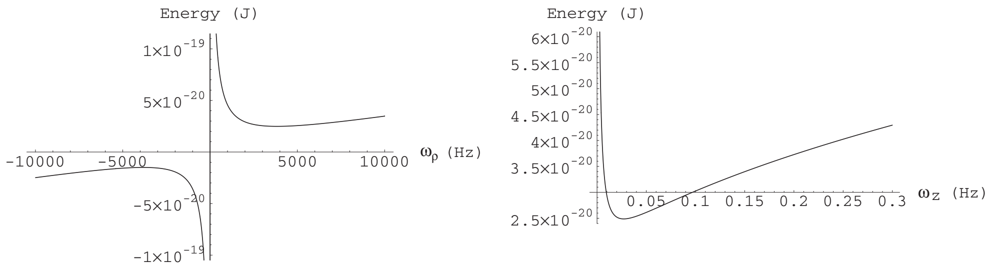

Figure 1. Energy plotted in various ω_ρ and ω_z, respectively.

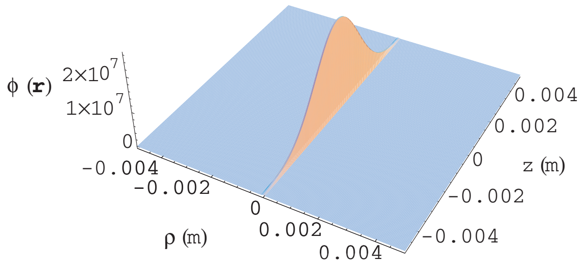

Figure 2. Ground state wavefunction plotted in three dimensions.

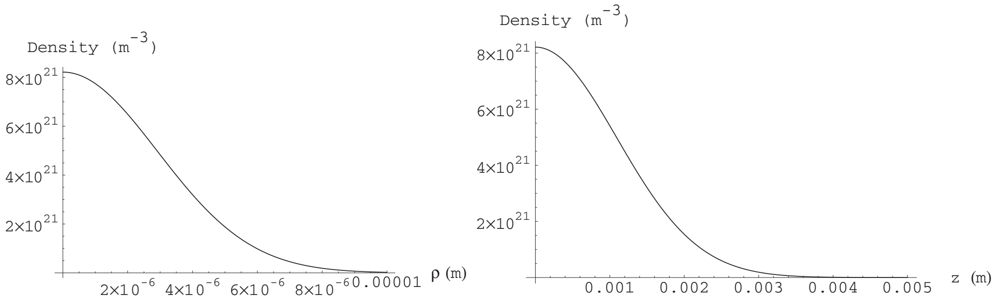

Figure 3. The density distribution plotted in radius and z dimension, respectively.

equation (29) so we obtain

$$\begin{aligned} &\frac{\omega_z}{2} + \frac{\gamma}{m\omega_z} - (N-1)a\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z} = \omega_z \\ &\frac{\omega_\rho}{2} + \frac{\alpha^2\omega_z}{\omega_\rho(\gamma\hbar + 2m\omega_z\theta)} - (N-1)a\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z} = \omega_\rho. \end{aligned} \tag{30}$$

Therefore, we can conclude that the wavefunction of the system can be written as

$$\phi_0(\mathbf{r}) = N^{1/2}\left(\frac{m\omega_\rho}{\pi\hbar}\right)^{1/2}\left(\frac{m\omega_z}{\pi\hbar}\right)^{1/4}\exp\left[-\left(\frac{m\omega_\rho}{2\hbar}\rho^2 + \frac{m\omega_z}{2\hbar}z^2\right)\right]. \tag{31}$$

We plot $\phi_0(\mathbf{r})$ as a function of ρ and z in three dimensions as shown in figure 2. This wavefunction is very narrow in the ρ direction and very wide in the z direction so we can calculate the size and the density distribution of the condensate cloud in the trap from the Gaussian curve in figures 2 and 3.

The length of the condensate in the ρ direction and the length in the z direction are $\left(2\hbar/m\omega_\rho\right)^{1/2} = 5.8251 \times 10^{-6}$ m $(2\hbar/m\omega_z)^{1/2} = 2.1872 \times 10^{-3}$ m. The width of the

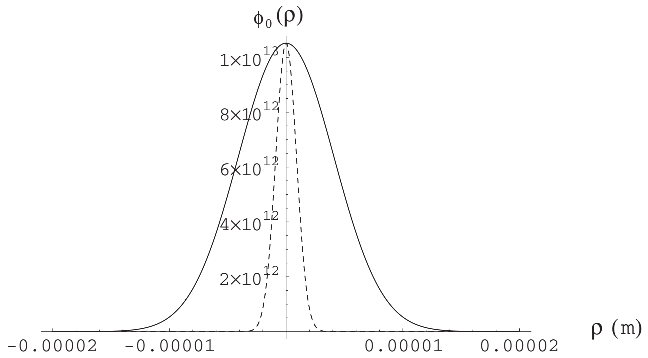

Figure 4. Wavefunctions plotted for various ρ. The solid line is the $\phi_0(\rho)$ wavefunction. The dashed line is the non-interaction wavefunction.

Table 1. Summary of parameters describing the two trap shapes used for achieving BEC and comparing the results from the experiments [1] to theory.

Parameter	Trap A		Trap B	
α/k_B (mK cm^{-1})	15.9		9.5	
γ/k_B (μK cm^{-2})	25		25	
θ/k_B (μK)	35 ± 2		34 ± 2	
	$\chi_c = \chi_m$	$\chi_c = \chi_m/2$	$\chi_c = \chi_m$	$\chi_c = \chi_m/2$
μ/k_B (μK)	1.9	3.8	1.3	2.6
$N_c(\times 10^9)$	1.2 ± 0.2	6.6 ± 1.3	1.2 ± 0.1	6.7 ± 0.5
Minimized parameter $\omega_\rho(2\pi$ Hz)	607.078	310.777	335.110	169.742
Minimized parameter $\omega_z(\times 10^{-5} 2\pi$ Hz)	434.248	212.992	640.245	317.724
$n_p(\times 10^{15}$ cm^{-3}) (experiment)	$4.8 \pm 0.4 \pm 1$	$9.7 \pm 0.7 \pm 2$	$3.3 \pm 0.1 \pm 0.7$	$6.5 \pm 0.2 \pm 1.3$
$n_p(\times 10^{15}$ cm^{-3}) (theory)	8.21	16.4	5.5	11.0
Length $2\rho_{max}$ (μm) (experiment)	15	21	20	28
Length $2\rho_{max}$ (μm) (theory)	11. 7	16.3	15.7	22.1
Length $2z_{max}$ (mm) (experiment)	5.5	7.8	4.5	6.4
Length $2z_{max}$ (mm) (theory)	4. 3	6.2	3.6	5.1
Total energy (J) (experiment)	2.25×10^{-20}	2.47×10^{-19}	1.54×10^{-20}	1.67×10^{-19}
Total energy (J) (theory)	2.47×10^{-20}	2.65×10^{-19}	1.65×10^{-20}	1.82×10^{-19}

condensate in the ρ direction is small compared with the length in the z direction which makes the condensate a thread shape. And then we can calculate the peak condensate density, the maximum density at the centre of the trap $|\phi(0,0)|^2 = N(m\omega_\rho/\pi\hbar)\,(m\omega_z/\pi\hbar)^{1/2} = 8.2130 \times 10^{15}$ cm^{-3}. We find that the ground state energy is in good agreement with the experimental result [1]. We can continue calculating energy in other trap shapes by path integral theory and compare them to calculations from the Thomas-Fermi approximation [1]. The results are shown in table 1.

Recall the ground state wavefunction from equation (29) and consider in ρ dimension.

$$\phi_0(\rho) = \sqrt{N}\left(\frac{m}{\pi\hbar}\left(\frac{\omega_z}{2} + \frac{\gamma}{m\omega_z} - (N-1)a\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z}\right)\right)^{1/4} \times \left(\frac{m}{\pi\hbar}\left(\frac{\omega_\rho}{2} + \frac{\alpha^2\omega_z}{\omega_\rho\,(\gamma\hbar + 2m\omega_z\theta)} - (N-1)a\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z}\right)\right)^{1/2} \times \exp\left[-\frac{m}{2\hbar}\left(\frac{\omega_\rho}{2} + \frac{\alpha^2\omega_z}{\omega_\rho\,(\gamma\hbar + 2m\omega_z\theta)} - (N-1)a\sqrt{\frac{m}{2\pi\hbar}}\omega_\rho\sqrt{\omega_z}\right)\rho^2\right]. \quad (32)$$

We now study the effect of the atom–atom interactions in the wavefunction in figure 4. The dashed line represents only the first two terms in equation (32) and the solid line is $\phi_0(\boldsymbol{\rho})$ which is broadened by repulsive atom–atom interaction and similarly for the z direction. Therefore, this is the reason why repulsive atom–atom interactions lead to an expansion of the condensate length in the z and ρ directions.

5. Conclusion

We have calculated the ground state energy and the wavefunction of Bose–Einstein condensation of atomic hydrogen by the many-body Feynman path integral theory. We predicted and studied the behaviour and properties of the hydrogen condensate such as the size of the condensate cloud, peak condensate density and the value of the ground state energy.

When Bose–Einstein condensation occurs, the macroscopic fraction of the hydrogen atoms occupies the lowest energy of about 10^{-20} J and all atoms have the same wavefunction. This wavefunction gives information about the size of the condensate and the density distribution. We found that many atoms occupy a very small volume under the influence of a magnetic trap and interaction among the atoms, the diameter is $\sim 12\ \mu$m and the length is $\sim$5 mm. The peak density is $\sim 8 \times 10^{15}$ cm^{-3}, which is maximum at the centre of the trap. However, hydrogen condensates are huge when compared with the other alkali metal atoms. These results have been obtained by the simple way used in [6]. Also, the results from path integral theory are in good agreement with the Thomas–Fermi approximation which is used for calculation in the experiment [1].

The calculation in Feynman path integral theory, however, is very complicated which very much differs from the simple Thomas–Fermi approximation. Nevertheless, Feynman's path integral has advantages over the Thomas–Fermi approximation in that it is more realistic since we do not neglect the kinetic energy term, although it is very small. The results are therefore more reliable. It is interesting to see if this method can be applied to study the properties of the excited states and other states of atomic hydrogen; it is our hope that this will be accomplished in the future.

Acknowledgments

The authors acknowledge the financial support from Thailand Research Fund (TRF).

References

[1] Fried D G 1999 Bose–Einstein condensation of atomic hydrogen *PhD Thesis* Massachusetts Institute of Technology

[2] Fried D G, Killian T C, Willmann L, Landhuis D, Moss S C, Greytak T J and Kleppner D 1998 Bose–Einstein condensation of atomic hydrogen *Phys. Rev. Lett.* **81** 3811

[3] Cesar C L, Fried D G, Killian T C, Polcyn A D, Sandberg J C, Yu I A, Greytak T J, Kleppner D and Doyle J M 1996 Two-photon spectroscopy of trapped hydrogen *Phys. Rev. Lett* **77** 255

[4] Feynman R P and Hibbs A R 1995 *Quantum Mechanics and Path Integrals* (Singapore: McGraw-Hill)

[5] Baym G and Pethick C J 1996 Ground-state properties of magnetically trapped Bose-condensed rubidium gas *Phys. Rev. Lett.* **76** 6

[6] Dalfovo F, Giorgini S, Pitaevskii L and Stringari S 1999 *Rev. Mod. Phys* **71** 463