

## On the numerical solution of the Gross-Pitaevskii equation for an isolated vortex in trapped gas

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### Abstract

*In this paper, the solution of the Gross-Pitaevskii equation is obtained numerically and the spread of the boson molecules in the vortex examined. In our study, we considered the attractive interaction for which the coupling constant is negative and the vortex is generated in harmonic potential. Our results show that, for attractive interaction, the boson molecules spread out from the centre of the vortex as the strength of the interaction increases.*

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**Keywords:** Bose-Einstein condensation; Vortex; Harmonic potential

### 1.0 Introduction

Bose-Einstein condensation (BEC) has commanded intense research efforts since its theoretical inception in 1925, and its experimental observation in 1995 [1-3]. BEC exhibits a topological defect (TD) which appears in cross-disciplinary subfields of physics. This is the consequence of the topology of the order parameter in the condensate [4]. Quantized vortex is a prime example of this. In 2004, Kasamatsu et al [5] obtained a new effective vortex-molecular field that features a pseudospin texture with meron pairs in Bose-Einstein condensates (BECs).

When a trapped gas is cooled to BEC, laser beams can be used to stir the condensate such that the phase of the condensate wave function is moderated to produce a desired velocity field. In this method of vortex formation, if the stirring or rotation frequency  $\Omega$  is below certain critical value  $\Omega_{c1}$ , no special motion is observed, for a rotational frequency above this critical value, lines of singularity appear in the velocity field of the trapped condensate. These singularities are called the vortex filaments and they correspond to a quantized circulation of the velocity along a closed contour around the vortex [6]. For  $\Omega = \Omega_{c1}$ , a single vortex is formed while  $\Omega > \Omega_{c1}$  produces more vortices. At different occasions, Abo-Shaeer et al [10] and Haljan et al [11] reported the creation of lattices with up to  $\sim 200$  vortices. However, the number of vortices that can be generated is different in harmonic and anharmonic traps. The radial trap frequency  $\omega$ , which sets the scale of  $\Omega_{c1}$ , limits the rotational rate in harmonic trap. In other words, as the angular frequency of rotation of the gas approaches the transverse trapping frequency, the centrifugal force approaches the restoring force exerted by the trap and the atoms become more and more weakly contained. This limitation is overcome in anharmonic trapping potential [12]. In this present paper, we limit ourselves to a vortex generated in harmonic trapping potential since our aim is to isolate a single vortex for analysis. Vortex has also been observed in a number of BECs trapped in magnetic potential [7, 8, 9]. Despite this work on single – component condensates, the spread of the molecules of the condensates within the vortex has not been reported to the best of our knowledge.

In this paper we investigate the particular characteristic of boson molecules within the vortex in the condensate using a numerical scheme developed Laoye et al [15]. The rest of the paper is organized as follows: in section 2. we present the derivation of the Gross-Pitaevskii (GP) equation, a mean-field model, used to describe the dynamical behaviour of the condensate molecules. In section 3, we seek the solution of the GP equation by a numerical scheme. We conclude the paper in section 4.

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## 2.0 The GP equation

A trapped gas of  $N$  interacting bosons that is under the influence of an external magnetic potential of  $V_{ext}(r)$  can be described by many-body Hamiltonian in second quantization as

$$H = \int dr \Psi^\dagger(r) \left[ -\frac{\eta^2}{2m} \nabla^2 + V_{ext}(r) \right] \Psi(r) + \frac{1}{2} \int dr dr' \Psi^\dagger(r) \Psi^\dagger(r') V(r-r') \Psi(r') \Psi(r) \quad (2.1)$$

where  $\Psi(r)$  and  $\Psi(r')$  are boson field operators that annihilate and create a particle at position  $r$  respectively and  $V(r-r')$  is the two-body interatomic potential. The field operator  $\Psi(r)$  can be considered in Heisenberg picture. This means that we can determine the time evolution of the operator  $\Psi(r,t)$  using the Heisenberg equation with the many-body Hamiltonian in equation (2.1)

$$i\eta \frac{\partial}{\partial t} \Psi(r,t) = \left[ -\frac{\eta^2}{2m} \nabla^2 + V_{ext}(r) + \int dr' \Psi^\dagger(r',t) \times V(r'-r) \Psi(r',t) \right] \Psi(r,t) \quad (2.2)$$

BEC is observed in an ultra-cold situation. In a dilute and cold gas, only binary collisions at low energy are relevant, which are characterized by only the s-wave scattering length [13]. In this condition, the particle interaction is independent of the details of the two-body potential. Consequently, the two-body interatomic potential  $V(r'-r)$  in equation (2.2) can be replaced as follows;

$$V(r'-r) = g \delta(r'-r) \quad (2.3)$$

In this presentation, the right hand side measures the effective interaction in the condensate, where  $g$  is the coupling constant, which measures the strength of the interaction. Equation (2.3) allows the replacement of field operator  $\Psi(r,t)$  with the condensate wave function  $\Phi(r,t)$ . Using equation (2.3), equation (2.2) becomes

$$i\eta \frac{\partial}{\partial t} \Phi(r,t) = \left[ -\frac{\eta^2}{2m} \nabla^2 + V_{ext}(r) + g |\Phi(r,t)|^2 \right] \Phi(r,t) \quad (2.4)$$

The equation is known as the GP equation. The condensate wave function can be written as

$$\Phi(r,t) = \phi(r) \exp\left(\frac{i\mathcal{E}t}{\eta}\right) \quad (2.5)$$

where  $\mu$  is the chemical potential.

The wave function  $\Phi$  is normalized to the total number of particles as  $\int dr |\Phi|^2 = N$

$$\left[ -\frac{\eta^2}{2m} \nabla^2 + V_{ext}(r) + g |\phi(r)|^2 \right] \phi(r) = \mathcal{E} \phi(r) \quad (2.6)$$

This equation is a form of the nonlinear Schrodinger equation, the nonlinearity arises from the mean-field term. The external magnetic potential which is the trapping potential is usually represented by the harmonic potential

$$V_{ext}(r) = \frac{1}{2} m \omega_{h0}^2 r^2 \quad (2.7)$$

where  $\omega_{h0} = \sqrt[3]{\omega_x \omega_y \omega_z}$  is the geometric average of the oscillator frequency  $\omega_{h0}$ , also defines the harmonic

oscillator length as  $\omega_{h0} = \sqrt{\eta/m\omega_{h0}}$ . If length is measured in terms of  $\omega_{h0}$ , equation (2.6) becomes

$$\left[ -\nabla^2 + r^2 + g |\phi(r)|^2 \right] \phi(r) = 2\mathcal{E} \phi(r) \quad (2.8)$$

All quantities in this equation are now dimensionless and the normalization condition now satisfies  $\int dr |\phi(r)|^2 = 1$ . To incorporate vortex structure,  $\phi$  equation (2.8) can be written as

$$\phi(r) = \phi(r) \exp(-i\mu\vartheta/\eta) \exp(-ik_z z) \quad (2.9)$$

Caroli et al [14] used equation (2.9) to describe a cylindrical vortex structure with  $\mu$  the orbital angular momentum quantum number which takes on integral values  $0, \pm 1, \pm 2, \pm 3, \dots$  and  $k_z$  the  $z$ -component of the momentum. Equation (2.8) becomes

$$\left[ -\frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \frac{\mu^2}{r^2} + k_z^2 + r^2 + g \phi^2(r) \right] \phi(r) = 2\mathcal{E} \phi(r) \quad (2.10)$$

In Ref. [15], equation (2.10) was solved for  $\mu = 0$  where no vortex structure is observed. We considered the case where  $\mu > 0$  for which vortex structure is incorporated. The solution of equation (2.10) is sought near the origin of the vortex core, which reduces equation (2.10) to

$$\left[ r^2 \frac{d^2}{dr^2} + r \frac{d}{dr} + (r^2 (2\mathcal{E} - k_z^2) - \mu^2) \right] \phi(r) = 0 \quad (2.11)$$

By making the substitution  $x = (2\mathcal{E} - k_z^2)^{1/2} r$ , we obtain a Bessel equation (2.12). For  $2\mathcal{E} - k_z^2 = 1$ , we obtain equation (2.13) whose solution is  $\phi(r) = J_\mu(r)$ . Equation (2.13) gives the initial conditions required for the solution of equation (2.10).

$$\left[ x^2 \frac{d^2}{dx^2} + x \frac{d}{dx} + (x^2 - \mu^2) \right] \phi_n(r) = 0 \quad (2.12)$$

$$\left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + \frac{(r^2 - \mu^2)}{r^2} \right] \phi(r) = 0 \quad (2.13)$$

### 3.0 Results

The variations of the wave function of the BECs are shown in fig. 1. In this result, we implemented the quartic Runge-Kutta algorithm for equation (2.10); equation (2.13), which is the Bessel equation of the first

order, gives the initial condition for the problem with  $J_\mu(r) = \sum_{n=0}^{\infty} \frac{(-1)^n (0.5r)^{(\mu+2n)}}{n!(n+\mu)!}$  estimated for  $\mu = 1$

and  $r = 0.01$ . The solution is sought for  $g = (-1, -45, -50)$ , which shows attractive interaction within the condensate molecules. We observe that as the strength of interaction increases the wave function peaks away from the centre of the vortex core and the particles tend to spread out. In other words, the radius of the vortex increases.

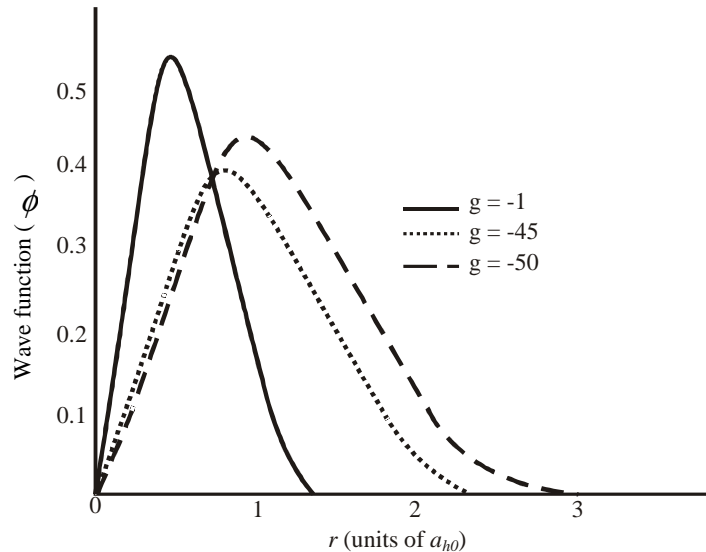


Figure 3.1: Condensate wave function for attractive interaction

### 4.0 Conclusion

This paper solved the GP equation numerically and examined the spread of the molecules in the vortex using the quartic Runge-Kutta method. The presented numerical results show that, for attractive interaction, the boson molecules spread out from the centre of the vortex as the strength of the interaction increases.

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