# QBeC, a Python Library to simulate Bose-Einstein Condensation using Quantum Circuits

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## 1 Introduction

Bose–Einstein condensate (BEC) is a state of matter that is typically formed when a gas of bosons at low densities is cooled to temperatures very close to absolute zero. Under such conditions, a large fraction of bosons occupy the lowest quantum state, at which point microscopic quantum mechanical phenomena, particularly wavefunction interference, become apparent macroscopically. The idea of BEC originated in 1924-1925, when A. Einstein generalized a work of S. N. Bose on the quantum statistics for photons to a gas of non-interacting bosons. Based on the quantum statistics, Einstein predicted that, below a critical temperature, part of the bosons would occupy the same quantum state to form a condensate. The dynamics of BEC is described by Gross-Pitaevskii equation:

$$i\hbar\delta_t\psi(x,t) = \left[-\frac{\hbar^2}{2m}\nabla^2+\frac{m}{2}(\omega_\perp^2x^2+\omega_\perp^2y^2+\omega_z^2z^2)+\frac{4\pi\hbar^2a}{m}|\psi(x,t)|^2\right]\psi(x,t) \quad (1)$$

where m,a is the mass and scattering length of the atom and $\omega$ is the Harmonic trap frequency. The wave function is normalised to the number of atoms in condensate:

$$\int dx|\psi(x)|^2 = N \quad (2)$$

QBeC is built with the aim to simulate the dynamics of BEC on a quantum computer.

## 2 Reconstructing the problem for Quantum Computer

For this project, I have taken only the case of finding the ground state wavefunction of BEC. This gives us the non-linear Schrodinger Equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2+\frac{m}{2}(\omega_\perp^2x^2+\omega_\perp^2y^2+\omega_z^2z^2)+\frac{4\pi\hbar^2a}{m}|\psi(r)|^2\right]\psi(r) = \mu\psi(r) \quad (3)$$

where $\mu$ is the chemical potential. Thus taking the approach from Variational Quantum Eigensolver (VQE), the following energy functional is minimised:

$$E[\psi(r)] = \int dr \left[ -\frac{\hbar^2}{2m}|\nabla\psi(r)|^2 + \frac{m}{2}(\omega_\perp^2 x^2 + \omega_\perp^2 y^2 + \omega_z^2 z^2)|\psi(r)|^2 + \frac{4\pi\hbar^2 a}{m}|\psi(r)|^4 \right] \tag{4}$$

This energy functional can't be used yet, as the wave-function is not normalised to unity, which is essential to get correct results on quantum computer. This is done by taking the length co-ordinates in units of harmonic oscillator. To simplify, just the case of 1-D is taken:

$$a_\perp = \left( \frac{\hbar}{m\omega_\perp} \right)^{0.5} \tag{5}$$

rescaling the co-ordinates and energy:

$$r = a_\perp r_1 \tag{6}$$

$$E = \hbar\omega_\perp E_1 \tag{7}$$

For the non-linear interaction, the coefficient is defined now as:

$$u_1 = \frac{8\pi a N}{a_\perp} \tag{8}$$

Thus the energy functional now to be minimised is:

$$\frac{E_1}{N} = \int dr \left[ |\nabla_1\psi_1(r_1)|^2 + r_1^2|\psi_1(r_1)|^2 + u_1|\psi_1(r_1)|^4 \right] \tag{9}$$

and the non-linear Schrodinger equation:

$$\left[ -\nabla_1^2 + r_1^2 + u_1|\psi_1(r_1)|^2 \right]\psi_1(r_1) = 2\mu_1\psi_1(r_1) \tag{10}$$

So now we have a non-linear PDE to be solved. We break up the equation in the momentum and position space such as:

$$[D(-i\nabla) + V(r)]f(r) = Ef(r) \tag{11}$$

Using VQE we find try to approximate the wavefunction at minimum energy:

$$H = D(-i\nabla) + V(r) \geq E_{min} \tag{12}$$

The Hamiltonian is not included in the circuit as is done in typical VQE runs. Only the the wave-function, f(r), is constructed using an ansatz and the energy is calculated classically.

# 3 Results using QBeC

QBeC is a meant to be released as a python package to simulate the dynamics of BEC. For now, the focus is just on searching for ground state of BEC in 1-D. During the testing only optimiser that worked well was the Simultaneous Perturbation Stochastic Approximation (SPSA). Other optimizers such as ADAM and COBYLA seem to give incorrect results, with ADAM taking up quite large execution time. Below are the results from some of the runs.

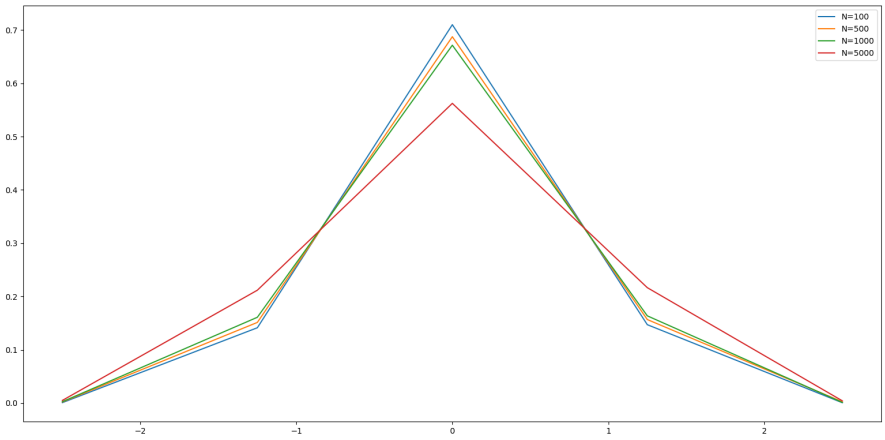


Figure 1: Ground state wave-function after BEC of Rubidium atoms. [qubits=3, SPSA=5000 iterations, ansatz=RealAmplitudes]

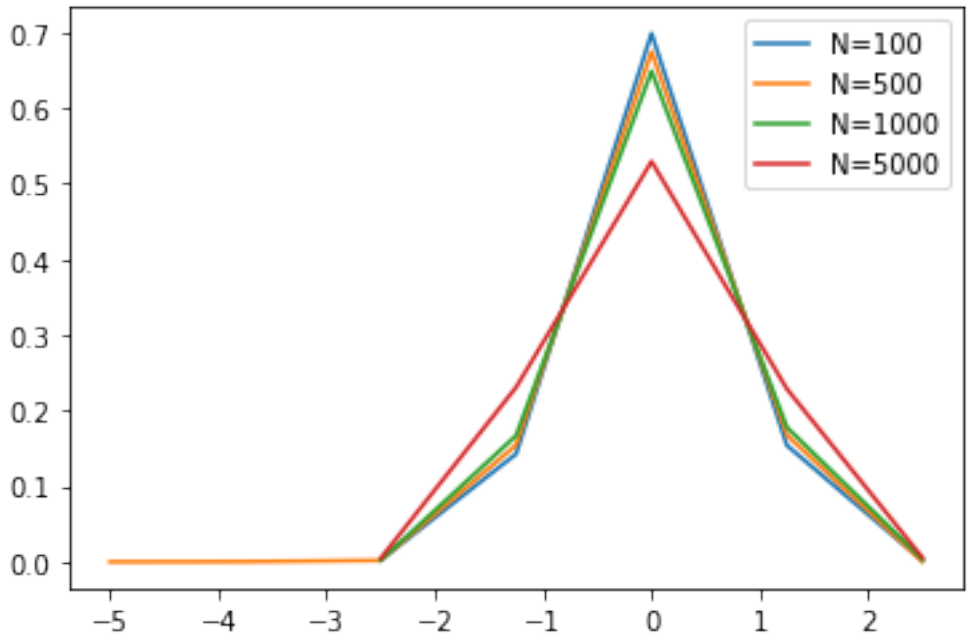


Figure 2: Ground state wave-function after BEC of Rubidium atoms. [qubits=3, SPSA=8000 iterations, ansatz=RealAmplitudes]

This is quite amazing to see. The probability peak is decreasing as the density of atoms increases. Although we can't the gaussian profile quite yet as the discretisation points are just $2^3 = 8$ for the Harmonic oscillator length 10. As the number of qubits are increased we get a more fine mesh and the gaussian profile is expected to be seen. Currently the computational time for $qubits > 4$ is quite large and a construction for problem specific ansatz is needed.

# 4 Next Steps for QBeC

In the current library, I have only have the provision to calculate the ground state wave-function of BEC. For next steps there is a need to provide for ansatz that are better suited for this problem. Some other functionalities such as vortex solutions, excited state solutions will also be included.