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RKFD Scheme for Quantum Reflection Model of Bose-Einstein Condensates (BEC) from Silicon Surface

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ABSTRACT

We applied the numerical combination of Runge-Kutta and Finite Difference (RKFD) scheme for a quantum reflection model of Bose-Einstein condensate (BEC) from a silicon surface. It is by the time-dependent Gross-Pitaevskii equation (GPE), a non-linear Schrödinger equation (NLSE) in the context of quantum mechanics. The role of cut-off potential δ and negative imaginary potential V_{im} is essential to estimating non-interacting BEC reflection models. Relying on these features, we performed a numerical simulation of the BEC quantum reflection model and calculated the effect of reflection probability R versus incident speed v_x. The model is based on the three rapid potential variations: positive-step potential $+V_{step}$, negative-step potential $-V_{step}$, and Casimir-Polder potential V_{CP}. As a result, the RKFD numerical scheme was successfully set up and applied to the quantum reflection model of BEC from the silicon surface. The numerical simulation results show that the reflection probability R decays exponentially to the incident speed v_x.

Keywords: Bose-Einstein Condensate, Gross-Pitaevskii Equation, Quantum Reflection, Casimir-Polder, Quantum Mechanics.

1. INTRODUCTION

The first experiment of a Bose-Einstein condensate (BEC), which experienced quantum reflection from a surface (e.g., semiconductor), was carried out by Pasquini et al. [1], [2], while the theoretical model developed by Scott et al. [3]. The study succeeds in revealing anomalous behavior of BEC at low incident speed. However, the saturation effect of reflectivity and its relationship to the dynamics of the collective complex is still far from clear, especially in describing the characteristics of BEC in kinetic energy and mean-field. The dimensional effect of BEC and the geometrical of semiconductors, i.e., nonplanar and micro-engineered surfaces for quantum reflections of BEC from a curved cylinder surface, may be seen as practical tools for further investigation of these unsolved anomalous behaviors. Then, the mean-field theory of the Gross-Piteavskii equation (GPE) became the primary framework to model the quantum reflection with the single atom Casimir-Polder theory [2]–[5].

GPE is a class of nonlinear Schrodinger equations (NLSE) with a macroscopic wave function ψ as a tool to characterize BEC at temperatures T far below the critical condensation temperature Tc (~ nano Kelvin). One set of GPE includes the potential trap and the mean-field of atom-atom interaction in gas that manifests as nonlinear terms. Attractive and repulsive interactions of atom-atom are accounted for in the GPE using the focusing constant a, which may be positive (focusing: $a>0$) or negative (defocusing: $a<0$) [6]. Meanwhile, the method to solve GPE is based

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on a numerical scheme rather than an analytical one. It is due to its mathematical complexity. In 1995, Ruprecht et al. [7] proposed the Crank-Nicolson method to solve GPE in describing inhomogeneous, weakly interacting BEC in small harmonic trap potentials at zero temperature. In addition, Bao et al. [8] in 2003 and Bao and Shen [9] in 2005 also achieved the spectral and pseudo-spectral methods. For the quantum reflection of BEC, Scott et al. [3] have relied on the Crank-Nicolson method in solving GPE. However, for algorithm efficiency, we propose a Runge-Kutta Finite Difference (RKFD) scheme for the case of BEC that undergoes quantum reflection. It was carried out to investigate the characteristics of quantum reflection of BEC from a surface.

2. MATHEMATICAL AND NUMERICAL FORMULATION

2.1 Mathematical Description

Let us consider the quantum reflection of BEC from a surface. We observe them for silicone surfaces based on one set of GPE models, which read as:

$$i\hbar\frac{\partial}{\partial t}\psi_j = -\frac{\hbar^2}{2m}\nabla_j^2\psi_j + V_j\psi_j + g_j\left|\psi_j\right|^2\psi_j\,. \tag{1}$$

where m is the atomic mass, $\hbar$ is the Planck constant, and the indexes j refers to 1D, 2D, or 3D systems. The first term on the right-hand side (RHS) of Eq (1) is the kinetic energy, where ∇_j^2 is the Laplace operator. The second term shows the external effect caused by harmonic potential trap V_j. At the same time, the third term represents the atom-atom interaction, where g_j is the interaction constant. For all dimensions systems, they are defined respectively as:

$$\nabla_j^2 = \begin{cases} \frac{\partial^2}{\partial x^2} \\ \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2} \\ \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2} \end{cases} ;\; V_j = \begin{cases} \frac{1}{2}\,m\omega_x^2x^2 \\ \frac{1}{2}m(\omega_x^2x^2+\omega_y^2y^2) \\ \frac{1}{2}m(\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2) \end{cases} ;\; g_j = \begin{cases} \frac{2\hbar^2a}{m}\left(\frac{m\omega_\perp}{\hbar}\right) = 2a\hbar\omega_\perp & j=1D, \\ \frac{\sqrt{8\pi}\,\hbar^2a}{m}\sqrt{\frac{m\omega_z}{\hbar}} & j=2D, \\ \frac{4\pi\hbar^2a}{m} & j=3D. \end{cases}$$

W.l.o.g, we reduce (1) into the dimensionless form. It aims to simplify calculations by setting normalization conditions $\int |\psi|^2\; dr = 1$ and some scaling parameters in (2).

$$t = \frac{\tau}{\omega_x};\;\; a_x = \sqrt{\frac{\hbar}{m\omega_x}};\;\; \tilde{x} = \frac{x}{a_x};\;\; \tilde{y} = \frac{y}{a_x};\;\; \tilde{z} = \frac{z}{a_x} \tag{2}$$

Substitute (2) into (1), and we will go to some steps of mathematical reduction. The dimensionless form of GPE can be written as

$$i\frac{\partial}{\partial t}\tilde{\psi}_j = \left[-\frac{1}{2}\tilde{\nabla}_j^2 + \tilde{V}_j + \kappa_j N\left|\tilde{\psi}_j\right|^2\right]\tilde{\psi}_j\,. \tag{3}$$

$\tilde{V}_j$ and κ_j are the dimensionless forms of the harmonic trap potential and the interaction constant of atom-atom, respectively; both values are:

$$\kappa_j = \begin{cases} 2a\frac{\omega_\perp}{\omega_x}\sqrt{\frac{m\omega_x}{\hbar}} \\ \sqrt{8\pi}a\sqrt{\frac{m\omega_z}{\hbar}} \\ 4\pi a\sqrt{\frac{m\omega_x}{\hbar}} \end{cases} ;\; \tilde{V}_j = \begin{cases} \frac{1}{2}\tilde{x}^2 & j=1D, \\ \frac{1}{2}\left(\tilde{x}^2+\gamma_y^2\tilde{y}^2\right) & j=2D, \\ \frac{1}{2}\left(\tilde{x}^2+\gamma_y^2\tilde{y}^2+\gamma_z^2\tilde{z}^2\right) & j=3D, \end{cases}$$

where $\gamma_y = \omega_y/\omega_x$; $\gamma_z = \omega_z/\omega_x$, and N is the total number of atoms.

2.2 Potential models

In this paper, we present the RKFD scheme for GPE (3) in a one-dimensional space, $j = 1D$ for $\kappa_j = 0$ (non-interacting case). The whole discussion deals with the quantum reflection of BEC in the context of equations. We set the displacement of the harmonic trap or the ground state BEC scene to accelerate it towards the surface. That is by setting a minimum harmonic trap on the surface. Since time t = 0 ms, we replace the harmonic trap along the x-axis at the point after Δx. It resulted in a scenario where BEC leads to a region of rapid potential energy variation $x \geq \Delta x$.

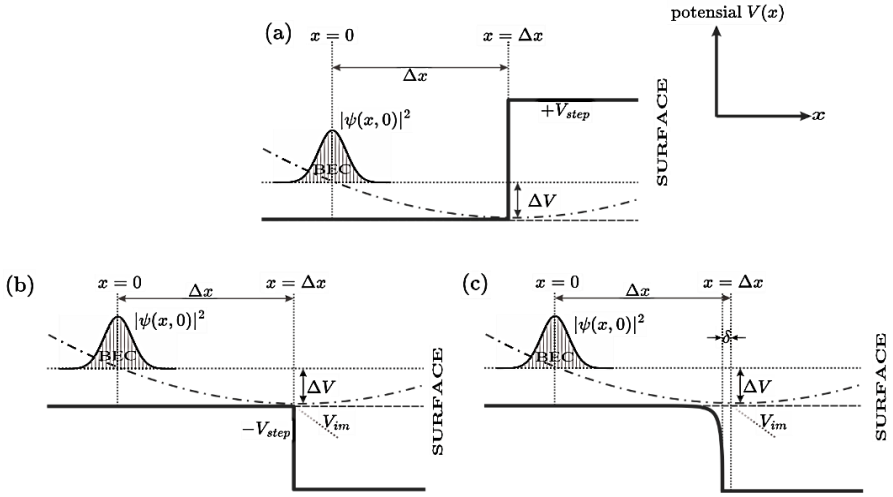

Figure 1. The potential scenario of the 1D quantum reflection model of BEC, at minimum of harmonic trap is $V_j + V_s$, where V_s is the types of surface potential ($+V_{step}$, $-V_{step}$ and V_{CP}).

As seen in Figure 1, the BEC move by the rapid potential variation, where the harmonic trap couples with three different potentials (at $x \geq \Delta x$), i.e.,

a. positive-step potential ($+V_{step}$), it represents the hardwall surface and indicates the classical reflection, no scattered or absorption atoms,
b. negative-step potential ($-V_{step}$), it represents the weak attractive potential, and
c. Casimir-Polder (CP) potential, $V_{CP} = -C_4/(x^3(x + \lambda'))$ where for C_4 = 1.6 x 10^{-55} Jm^{-4} and λ' is 100 nm for ^{87}Rb-Si [10]. The atom-atom scattered or absorption model at the surface (during a collision) is modeled by the imaginary potential V_{im} and the small offset δ (cut-off) to prevent the attractive CP potential varying rapidly near the surfaces.

2.3 RKFD Scheme

To observe the BEC quantum reflection, we solve the complex GPE problem by first discretizing the space x domain using the understanding of the finite difference method, $\tilde{\psi}(\tilde{x}, \tau) \rightarrow \tilde{\psi}_n(\tau)$. Hence, we can transform the Laplace operator $\tilde{\nabla}^2$ into a matrix operator **D2**:

$$\frac{\partial^2}{\partial \tilde{x}^2}\tilde{\psi}(\tilde{x}, \tau) = \frac{1}{dx}\left[\frac{\tilde{\psi}_{n+1}(\tau) - \tilde{\psi}_n(\tau)}{dx} - \frac{\tilde{\psi}_n(\tau) - \tilde{\psi}_{n-1}(\tau)}{dx}\right],$$

$$\frac{\partial^2}{\partial \tilde{x}^2}\tilde{\psi}(\tilde{x}, \tau) = \frac{\tilde{\psi}_{n+1}(\tau) - 2\tilde{\psi}_n(\tau) + \tilde{\psi}_{n-1}(\tau)}{(dx)^2},$$

$$\frac{\partial^2}{\partial \tilde{x}^2}\tilde{\psi}(\tilde{x},\tau) = \frac{1}{(\partial x)^2}\begin{pmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{pmatrix} \cdot \begin{pmatrix} \tilde{\psi}_1(\tau) \\ \tilde{\psi}_2(\tau) \\ \tilde{\psi}_3(\tau) \\ \tilde{\psi}_4(\tau) \\ \tilde{\psi}_5(\tau) \end{pmatrix},$$

$$\frac{\partial^2}{\partial \tilde{x}^2}\tilde{\psi}(\tilde{x},\tau) = \boldsymbol{D2}.\ \tilde{\psi}_n(\tau)\,, \tag{4}$$

where dx is the change of spatial grid points.

Using the definition of matrix operator **D2** in Eq (4), we can quickly write the RHS of GPE (3) into,

$$\frac{\partial}{\partial \tau}\tilde{\psi}_n(\tau) = f\left(\tilde{\psi}_n,\tau\right) = -i\left[\frac{1}{2}\mathbf{D2}.\tilde{\psi}_n(\tau) - \tilde{V}(\tilde{x})\tilde{\psi}_n(\tau) - \kappa N\left|\tilde{\psi}_n(\tau)\right|^2\tilde{\psi}_n(\tau)\right]. \tag{5}$$

Subsequently, we compromise the $f\left(\tilde{\psi}_n,\tau\right)$ function in (5) with the fourth order Runge-Kutta method. We write their solution as follows:

$$\tilde{\psi}_n(\tau+\Delta\tau) = \tilde{\psi}_n(\tau) + \frac{1}{6}\,\Delta\tau\,(K_1 + 2K_2 + 2K_3 + K_4) \tag{6}$$

τ is the time, $\Delta\tau$ is the step size, and K is a function of the average slope over the interval, which reads as,

$$K_1 = f\left(\tilde{\psi}_n,\tau\right)$$
$$K_2 = f\left(\tilde{\psi}_n + \frac{\Delta\tau}{2}K_1\right)$$
$$K_3 = f\left(\tilde{\psi}_n + \frac{\Delta\tau}{2}K_2\right)$$
$$K_4 = f\left(\tilde{\psi}_n + \Delta\tau\,K_3\right)$$

We refer to this as one set of RKFD schemes, in which the GPE (3) solution for BEC quantum reflection from a silicon surface is present at the end of this manuscript.

3. FLOWCHART AND ALGORITHM

Now, we can observe the quantum reflection model of BEC from solution (6) by some stages shown in flowcharts (see figure 2) or use the following simulation algorithm.

a. Initialize parameters, such as the atomic mass m, the Planck constant $\hbar$, the longitudinal trap frequency ω_x, the center of potential trap Δx, normalize constant A, and wave number k. At the same time, set the initial condition of the envelope ψ as Gaussian wave function: $\psi(x,0) \approx \exp\left(-\frac{m\omega_x}{2\hbar}x^2\right)$, as well as the potential trap V.
b. Provide the change of spatial grid points x (step size $h = dx$), the scaling unit a_x, and the center of the initial gaussian wave function x_0.
c. Transform the dimensionless Laplace operator $\tilde{\nabla}^2$ using the finite difference algorithm. We record the results as a matrix operator **D2**. If we are in python, it can be clear by *scipy.sparse.diags()* toolbox.
d. Rewrite the RHS of GPE (3) with the matrix operator **D2** features. Subsequently, provide the time interval for snapshot dt, the initial (t_0) and the final time (t_f).
e. Integrate GPE (5) from initial (t_0) to final time (t_f) using Runge-Kutta method to produce the numerical solution of $\psi(x,t)$. Again, if we are in python, we can solve it by using *integrate.solve_ivp* toolbox.

f. Plot the numerical solution $\psi(x,t)$ in x-coordinate. On the other hand, we can record the simulation along time t.

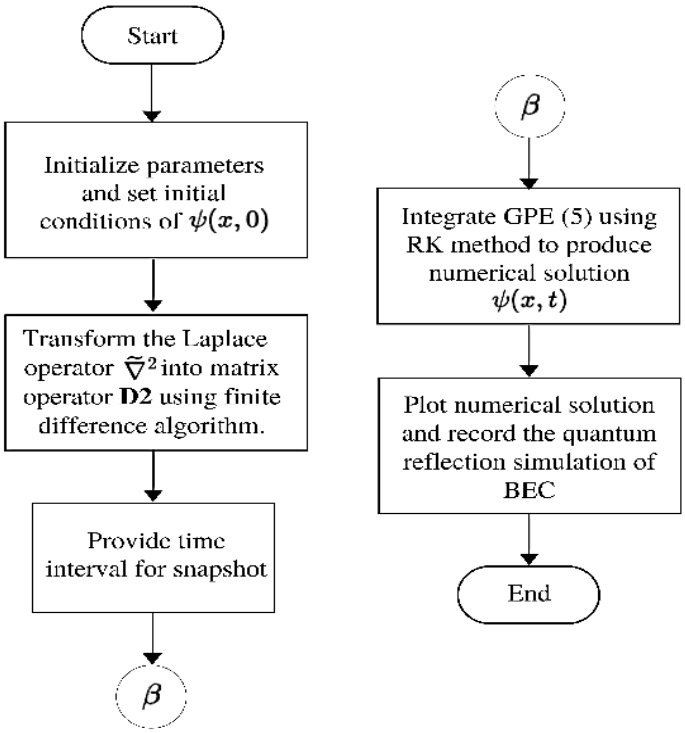

Figure 2. The flowchart of the algorithm for the numerical simulations

4. SUMMARY AND DISCUSSION

This section presents the quantum reflection simulations of BEC single atom ^{87}Rb from the silicon surface through the GPE solutions of (6) (see Figures 3). We create the benchmark by the compare our RKFD scheme simulation results with the Crank-Nicolson method used by Scott et al. [3] and the fourth-order Runge-Kutta method by Halif [10] in solving the GPE (3). Therefore, we selected the same parameters in references [3] and [10]. It is related to offset δ dan imaginary potential V_{im} as an essential feature to observe the correspondence of reflection probability R to incident speed v_x of a single atom ^{87}Rb moving toward to Si surface using the Gaussian wave function,

$$\psi(x,0) = (\frac{m\omega_x}{\hbar})^{1/4}\exp\,(-\frac{m\omega_x}{2\hbar}x^2) \tag{7}$$

(Note: the quantum reflection from Si surface).

The role of offset δ is to avoid the region where the CP potential model varies rapidly near the surface ($x \to 0$, $V_{CP} \to -\infty$). Regarding that, the imaginary potential V_{im} is the absorption model of atom-atom scattered on the surface. We found that recognizing the imaginary potential V_{im} reduces or removes the transmission process. In other words, it avoids interference when the value reaches the end of the box (or surface). Without the imaginary potential V_{im} , it would create an artificial reflection. For more knowledge about the role of offset δ dan V_{im} imaginary potential, we suggest reading ref [10].

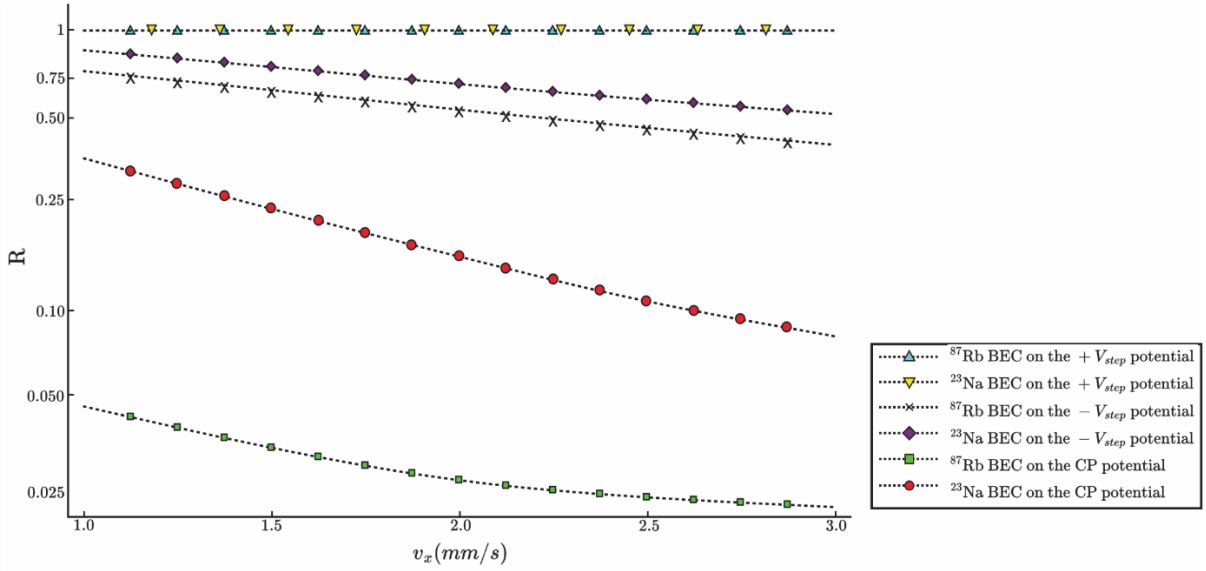

Figure 3. Reflection probability R versus incident speed v (mm/s) of non-interacting 87Rb and 23Na BEC in three different cases: Positive step potential, Negative step potential, and Casimir-Polder potential.

After observing the δ offset role and the V_{im} imaginary potential effect, we calculate the related reflection probability R to incident speed v_x for a single atom ^{87}Rb moving toward the Si surface. In classical reflection context, i.e., the positive-step potensial $+V_{step}$, the BEC is totally reflected by hard wall. Meanwhile, for negative-step $-V_{step}$ and V_{CP} Casimir-Polder potential, we found that only a few atom-atom is reflected, where the atom-atom transmitted by the imaginary potential V_{im} are absorbed in the surface. However, it is slightly different compared to the theoretical model of Scott et al. [3] that uses ^{23}Na atoms. The relation of reflection probability R versus incident speed v_x for a single atom ^{87}Rb moving toward Si is lower than for ^{23}Na by a factor of ~10 on $v_x = 1$ mm/s. It is due to the mass of ^{87}Rb atom much greater than ^{23}Na atom. Hence, we assess that the RKFD scheme is good enough to be used in BEC quantum reflection studies from a surface.

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