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QUANTUM CONTROL OF NANOPARTICLES AT LOW TEMPERATURE*

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Abstract

In this work, quantum control of nanoparticles will be considered at low temperature. It would be quite interesting for scientists and researchers to take the well known nanoparticles at the scale of 10^{-9}m(=1nm) as they are at proper low temperature. It is desired to create Bose-Einstein-Condensates (BEC) with the nanoparticles. In our former study (cf. [Wang, 2016]) of controlling nanoparticle, the density function theory (DFT) described by time-dependent Schrödinger equation had been utilized to apply control theory to nanoparticles at matter surface. In the framework of Thomas-Fermi (TF) model, nanoparticles governed quantum system had been considered in the complex Hilbert spaces. In this investigation, the factor of temperature will be taken account into time dependent Schrödinger equation. First, physically, a lot of questions will be arising in here for the control purpose of BEC phenomena of low temperature. Such as, whether BEC can be created using nanoparticles? what can the nanoparticles do at low temperature? which differences have for the nanoparticles BEC than other size particles? how control would be proceeded for nanoparticles at magnetic-electric field? Second, theoretically, how to apply of quantum control theory to nanoparticles BEC in the framework of variational theory? Then, how to get the first hand theoretic results to do nanoparticles control at low temperature.
Review current contributed work and literatures, the survey of control Bose-Einstein-Condenstates had been occurred at amount of areas and had obtained significant milestone results as atomic particles (e.g. ^{87}Rb, ^{7}Li, ^{23}Na,^{52}Cr, ^{39}K) cooling to temperature below of BEC thresholds. Indeed, the behavior of nanoparticles at the room temperature had also been considered, and had already been created to Carbon (C) nanotube, nanowire, nanomotor, nanorod as advanced materials. Particularly, the focus point is nanoparticles at low temperature, what is happened? the exciting and attractive conclusion will be hoped in this paper. As a kind of prediction, this theoretical research for control of nanoparticles would be fairly interesting, the control theory could be applied to these sort of nanoparticles perfectly. Without lost of generality, the nanoparticles composed BEC will be much more useful and can be quickly utilized to real society in the world. It is good to connect these researches to chemical and physical laboratory, and to do further interdisciplinary work concerning the control of quantum system.

Key words

Quantum control, Bose-Einstein-Condensates, Nanoparticles, Complex Hilbert spaces.

1 Introduction of Basic Idea

For a long time, people knew the nanoparticles and Bose-Einstein-Condensates separately in each subject or research field (cf. [Bose, 1924], [Einstein, 1924]). Two most interesting phenomenas had been frequently considered at amount of areas for various purposes. Such as one can make the nano-tube, nano-motor, nano-chip, nano-rod, and so forth. Based on those frontier results, the advance materials had been developed and even used in our usual life (nanocrystal ceramic are already in use by US Navy). Meanwhile, Bose-Einstein-Condensates (BEC) had been created at low temperature using molecules and atom since the middle and later of last century. The curious question is how to create a nanoparticles based BEC? That is, using 10^{-9}m (i.e $1\sim$ several nm) sized particles to create a condensate as they are under ultra-cold temperature condition. Definitely, there are many questions will be arising in here.

i). whether BEC can be created using nanoparticles?
ii). what can nanoparticles do at low temperature?

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iii). which differences have for nanoparticles BEC than other size particles?
iv). how control will be proceeded for nanoparticles at magnetic-electric field?
v). what is the connection between nanoparticles and BEC?
vi). what is usefulness of nanoparticles based BEC?

For such proposed problems, it is possible to consider in the following points:

Firstly, it needs to do theoretic prediction for nanoparticles based Bose-Einstein-Condensates. If such a BEC can be created using nano-particles at low temperature (i.e. near zero temperature -273K), then it can be called as nano-BEC or nano condensate. Although it is unknown for us whether such a nano-BEC will be certainly possess good properties, it is rather to believe that it must be a difference than a general condensate. The evidence at published paper "Bose-Einstein condensation in a plasmonic lattice" (Nature Physics 14, p. 739) to know that "the new condensate can produce light pulses that are extremely short and so may offer faster speed for information processing and imaging application". Quote that "Such device should be much faster and use less energy than their electronic counterparts".

Secondly, numerical approach can be proceed for the simulation of such a particular nano-BEC. It desired that a completely different results can be obtained in the direction of nano science research and condensed matter physics.

Thirdly, theoretical control can be considered, and can be applied optimal control theory to nonlinear cubic time-depended Schödinger equation, namely Gross-Pitaevskii (G-P) equation with the condition of low temperature for nanoparticles.

For the restrict of physical experiments, in the viewpoint of control field, mathematically, third problem will be taken account into our target in this paper.

2 Theoretical Control of Nano-BEC

Before the mathematical symbolic calculation, there are many kind of thoughts swarmed at the topic of BEC created by nanoparticles. A lot of predictions or guesses can be considered in this direction. Suppose nano-BEC had both chemical and physical properties of nano materials and condensates, in other word, it should be possess both of them. Then, not only at the materials science, but also at the condensates physics, such sorts of nano-BEC could attract a great deal attention that not limited to academic level, it would be a huge extension to realistic world. In practice, it just like the human can not reach to a very high temperature except self body temperature 35°C∼37°C, it is also difficult for live species to reach low temperature at all. If the material of nano-BEC can be created at ultra-cold external condition, it can be used to replace human for working at low temperature of hard environment. It means that, some day, people may have nano-tube, nano-motor, nano-rod and nano-chip at low temperature. If such a dramatic material could be created, it would bring revolutionary change in industrial, engineering, aerospace, medical therapy as well as outspaces (such as moon), and spread to other fields.

Now, let us introduce the physical model posed for the nanoparticles based Bose-Einstein-Condensates. Two difference points should be focused:

1). particles size: 10^{-9}m nanoparticle.

2). temperature: ultra-cooling technique created low temperature.

By reviewing current literatures and contributed papers as the reference and citation, there are a lot of cooling technique used in the lab: laser cooling technique; electronic-magnetic cooling technique; optical cooling technique (cf. [Rice and Zhao, 2000]). For create N number bosonic atoms based Bose-Einstein-Condensates in lab experiments, usually take atomic particles such as: ^{23}Na, ^{87}Rb, ^{133}Cs. For example,

- Temperature of creating Bose-Einstein Condensate: $T_b = \frac{h^2}{2\pi mk}(\frac{N}{2.612V})^{2/3}$.
- The number of atoms in a BEC: $N(T) = N\{1 - (T/T_b)^{3/2}\}$.
- Thermal de-Broglie wave length: $\lambda = \frac{h}{\sqrt{3mkT}}$.

Here h is Planck constant, T_b is the below threshold of temperature. m is the mass of same particles. If an ultra-cold vapor of bosonic atoms are trapped in magnetic well, pure condensates will be created as they are cooled to a temperature below the BEC threshold. After that creation, these BEC are located into a optical lattice potential.

More precisely in physics, Bose Einstein Condensates is an state of matter in which bosons collectively occupy the energetic ground state of a quantum system.

If changing the boson atoms into a 10^{-9}m sized nanoparticles, whether above phenomena could be appeared? That is, whether the Bose-Einstein-like condensates can be created at what kind of low temperature with cooling technology? In fact, in our nanoparticles condensate, the physical approach is used to make metallic and metal oxide ceramic nanoparticles. it involved evaporation of a solid metal followed by rapid condensation to form nanosized clusters that settle in the form of a powder. Currently, various vaporizing metal can be used and variation of the medium into which the vapor is released affects the nature and size of the particles.

Our idea is that, if create Bose-Einstein-Condensates itself using nanoparticle, it might not be worked. But if using nanoparticles to create condensates which like BEC should be existed!

Fortunately, after submission of the abstract of poster "Quantum control of nanoparticle at low temperature" to the American Chemical Society National Meeting 2018

(PHYS Poster Session, Control ID: 2953973) at January 24, 2018. The new condensate had been created with gold nanoparticles, see paper "Bose-Einstein condensation in a plasmonic lattice", April 16, 2018, Nature Physics 14. Thanks to the team of Aalto University.

Thus, overcome the physical possibility, it is realistic to directly create condensate BEC with nanoparticles (e.g. Au). In our physical model, two factors needed to be involved at the system. T and T_b represent the temperature and its below threshold. The size of nanoparticle could be 1nm or few nanometer.

Suppose N number of nanoparticles are used to create a condensate, and $n = 1, 2, 3, ...N$. Then, as the vacuum chamber cooling to untra low temperature, the velocity of nanoparticles are slow, just like atomic and molecule particles, nanoparticles is easily to be probed and measured (at the condensed moment, the slow motion of particles is described by Langevin equation for the calculation of their movement, it's exclusive at this paper).

At first, introduce quantum system of nanoparticles for $\mathbf{x} = (x_1, x_2, x_3) \in \mathbf{R}^3$, the Gross-Pisaevskii (G-P) equation (cf. [Pitaevskii and Stringari, 2003]) governed Bose-Einstein-Condensates take the form of

$$\mathbf{i}\hbar\frac{\partial\psi_n}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi_n + (V^1(\mathbf{x}) + V^2(\mathbf{x}) + V^3(\mathbf{x}))\psi_n + N\nu|\psi_n|^2\psi_n, \quad (1)$$

for $n = 1, 2, \cdots, N$. In here, $\hbar$ is Planck constant, m is a nanoparticle mass, $\psi_n(\mathbf{x}, t)$ is condensate wave function of n-th particle at BEC, N is the total number of condensed nanoparticles, and $\nu = 4\pi\hbar^2 a_s/m$ is interacting constant of ground state of nanoparticle, where $a_s \in \mathbf{R}$ is s wave characteristic scattering length. $\mathbf{i}$ is unit of imaginary part at complex space. Usually, given the initial function $\psi_n(\mathbf{x}, 0) = \psi_n^0(\mathbf{x})$ for $\mathbf{x} \in \mathbf{R}^3$.

Next, our task in the rest of this section is to discuss the expression of V^1, V^2, V^3 for the nanoparticle setting in quantum system (1).

In quantum system (1), it needs to set potential terms in the cooling temperature. For unified to set $\mathbf{V}(\mathbf{x}, t) = V^1(\mathbf{x}, t) + V^2(\mathbf{x}, t) + V^3(\mathbf{x}, t)$. To be difference, denote M as the total mass of N nanoparticles.

V^1: The external potential $V^1(\mathbf{x})$ is electro-magnetic field for creating BEC of N nanoparticle, without lost of generality, for instance, usually set $V^1(\mathbf{x}) = M\sigma_0^2\frac{|\mathbf{x}|^2}{2}$, trapped frequency $\sigma_0 = 2\pi|\mathbf{x}_0|^2 \in \mathbf{R}^3$. Harmonic oscillator is configured as example

$$V^1 = \frac{M}{2}(\omega_{x_1}^2 x_1^2 + \omega_{x_2}^2 x_2^2 + \omega_{x_3}^2 x_3^2)\,.$$

This setting is depending on the physics structure of experiments used of creation.

V^2: In real lab, optical potential for nanoparticle can be configured as

$$V^2(\mathbf{x}) = \mu\sum_{k=1}^{3}\frac{\hbar^2\mathbf{x}^2}{M}\sin^2(x_k x_k),\ x_k \in \mathbf{R}^3,$$

and $\mu > 0$ is a dimensionless parameter for representing the depth of optical lattice. The trapped field can adjust the optical frequencies along the directions of x_1, x_2, x_3 axis. Other kind of optical apparatus can be also confining, e.g. $V^2 = \hbar\frac{\Omega(t)}{2\Delta}(1 + \cos(2k_L\mathbf{x} - \delta_L t))$, where k_L wave vector; δ_L is difference of two beam; Ω is single photon Rabi frequency; Δ detuning. It rely on the structure of optical lattice.

V^3: The varying size of nanoparticles, or distance between each nanoparticles can be formed as $V^3 = \sum_{i=1}^{N} V_i\psi_i$, where V_i are constant coefficients of i-th nanoparticle. $i = 1, 2, ..., N$.

Additionally, a_s in scattering coefficients ν need have adjustment and confinement at the physical lab. In particular, V^3 represented all nanoparticles size potential, it can vary at the nano scale (unit 1nm=10^{-9}m). For quantum materials, V^3 can take qubits as calculation in recent papers.

3 Control Theory of Nano-BEC

For three dimension Gross-Pitaevskii equation (1), set $\boldsymbol{\psi} = (\psi_1, \psi_2, \cdots, \psi_N)$. Denote complex scalar function $\psi_n(\mathbf{x}, t)$ and operator $\hat{\psi}_n(\mathbf{x}, t)$, then $\psi_n(\mathbf{x}, t) = \langle\hat{\psi}_n(\mathbf{x}, t)\rangle$.

Hamiltonian:

$$\mathbf{H} = \int_\Omega \hat{\boldsymbol{\psi}}^*(\mathbf{x})[-\frac{\hbar^2}{2M}\Delta + \tilde{\mathbf{V}}(\mathbf{x})]\hat{\boldsymbol{\psi}}(\mathbf{x})d\mathbf{x} + N\frac{4\pi\hbar^2 a_s}{2M}\int_\Omega\int_\Omega \hat{\boldsymbol{\psi}}^*(\mathbf{x})\hat{\boldsymbol{\psi}}^*(\mathbf{y})\hat{\boldsymbol{\psi}}(\mathbf{x})\hat{\boldsymbol{\psi}}(\mathbf{y})d\mathbf{x}d\mathbf{y}.$$

$\hat{\boldsymbol{\psi}}^*$ is conjecture (field) operator of $\hat{\boldsymbol{\psi}}$, and in here $\hat{\boldsymbol{\psi}}$ or $\hat{\boldsymbol{\psi}}^*$ is annihilate or create operator of nanoparticle.

$[\hat{\boldsymbol{\psi}}(\mathbf{x}), \hat{\boldsymbol{\psi}}^*(\mathbf{y})] = \delta(\mathbf{x} - \mathbf{y}),\ \ [\hat{\boldsymbol{\psi}}^*(\mathbf{x}), \hat{\boldsymbol{\psi}}^*(\mathbf{y})] = 0.$

Lagrangian:

$$\mathcal{L} = \frac{1}{2}\mathbf{i}\hbar\Big[\frac{\partial\boldsymbol{\psi}^*(\mathbf{x}, t)}{\partial t}\boldsymbol{\psi}(\mathbf{x}, t) - \boldsymbol{\psi}^*(\mathbf{x}, t)\frac{\partial\boldsymbol{\psi}(\mathbf{x}, t)}{\partial t}\Big] + \frac{\hbar^2}{2M}|\nabla\boldsymbol{\psi}(\mathbf{x}, t)|^2 + \mathbf{V}(\mathbf{x}, t)|\boldsymbol{\psi}(\mathbf{x}, t)|^2 + \frac{1}{2}N\nu|\boldsymbol{\psi}(\mathbf{x}, t)|^4.$$

More precisely, for discrete nanoparticles size potential, denote matrix $\tilde{V}^3 = \text{diag}\{V^{31}, V^{32}, \cdots, V^{3N}\}$,

$$\tilde{\mathbf{V}}(\mathbf{x}) = M\sigma_0^2\frac{|\mathbf{x}|^2}{2} + \mu\sum_{k=1}^{3}\frac{\hbar^2\mathbf{x}^2}{M}\sin^2(x_k x_k) + \tilde{V}^3.$$

Therefore, $\tilde{\mathbf{V}}(\mathbf{x})$ is $N \times N$ matrix function.

Two focus comments:

(A). Nanoparticles Size Potential: $\tilde{V}_3$ is roughly in the

form of matrix. Theoretically, it is not in details and rigorously any more, owing no specified experiments and particles in this paper.

(a) Non-interacting particles: If involved nanoparticle is non-interacting single particles, clearly, the formulation in Hamiltonian and Lagrangian become: $V^{31} = V^{32} = \cdots = V^{3N} \equiv V^0$, then for $N \times N$ unit matrix $\mathbf{I}$

$$\hat{\boldsymbol{\psi}}^*(\mathbf{x})\tilde{V}^3\hat{\boldsymbol{\psi}}(\mathbf{x}) = \hat{\boldsymbol{\psi}}^*(\mathbf{x})V_0\mathbf{I}\hat{\boldsymbol{\psi}}(\mathbf{x}) = V_0\hat{\boldsymbol{\psi}}^*(\mathbf{x})\hat{\boldsymbol{\psi}}(\mathbf{x}),$$

where V_0 is a constant.

(b) Interacting particles: If particles in the creation of condensate is interacting with other type particles, then matrix $\tilde{V}^{ij} \neq \mathbf{I}$, i.e. each element of the diagonal matrix is a non-zero constant, which representing the coupling coefficients between different particles. At that time, the Gross-Pitaeskii equation coupled with bose condensed regime to compose a simultaneously system equations. Such as interacting condensate ^{87}Rb $\sim^{41}$K, or ^{87}Rb $\sim^{85}$Rb mixtures.

(B). Condensed Temperature:

a). The critical (below) temperature as T_b.

b). Temperature T at thermal de-Broglie wave length λ which formed in lot of expression. Such as $\lambda_T = \sqrt{2\pi\hbar^2/(mk_BT)} \simeq 10\mu m$ for gold nanoparticles (size 3$\sim$14 nm), where k_B is Bolztmann constant, $\hbar$ is reduced Planck constant, and m is involved nanoparticles mass. Usual it depended on lab experimental setting and particles type.

Most of the published papers considered zero temperature, and finite temperature condensate. The dependence of temperature for the creation of condensates had been well investigated at chemical physics field. The last one is easily to understand, there is a finite threshold $T_b \neq 0$ for temperature to create a condensate ($0 \leq T \leq T_b$, $T_b \approx 5K$ for Au nanoparticle $\sim$ 1.4 nm). The first one zero temperature, it means $T_b = 0$ (-273K) absolute zero degree temperature. It indicated, the creation of a type particles at certain temperature (neglected at calculation), it can be differed with creation at any temperature (room temperature T=300K or other finite temperature). Usually, scaled temperature T/T_b used in calculation (e.g. $0.1 \leq T/T_b \leq 1.4$)

To a nanoparticles based BEC or BEC composed nanoparticles, the influence of temperature yet become a central problem.

3.1 Mathematical Formulation

In this subsection, at the framework of variational method to do mathematical setting (cf. [Dautray and Lions, 1992], [Lions, 1971], [Pitaevskii and Stringari, 2003]). Let Ω be an open bounded set of $\mathbf{R}^3$ and $Q = (0,T) \times \Omega$ for $T > 0$, set $\mathbf{x} = (x_1, x_2, x_3)$, and $(t, \mathbf{x}) \in Q$. Assume that the external potential term $\mathbf{V}(\mathbf{x}, t)$ is total control input, which can be a variable for representing the forces acting at BEC system (1). For selected nano particles type, V^3 is depended only on the spatial variable $\mathbf{x}$. The electron-magnetic field $V^1(\mathbf{x}, t)$ and optical field $V^2(\mathbf{x}, t)$ depended both spatial $\mathbf{x}$ and time variable t, and take the same formulation for all nanoparticles (cf. [Rice and Zhao, 2000]).

For a clear picture to prove the existence theorem of weak solution. Set nonlinear term $f_1 = \mathbf{V}(\mathbf{x}, t)\psi_n$ and $f_2 = N\nu|\psi_n|^2\psi_n$ to get a free G-P system of (1) as

$$\mathbf{i}\hbar\frac{\partial\psi_n}{\partial t} = \frac{\hbar^2}{2m}\Delta\psi_n + f_1 + f_2, \tag{2}$$

where $\hbar$ is Planck constant, m is a nanoparticle mass, $\psi_n(\mathbf{x}, t)$ is condensate wave function of n-th particle at BEC, N is the total number of condensed nano-particles. Initial function $\psi_n(\mathbf{x}, 0) = \psi_n^0(\mathbf{x})$ for $\mathbf{x} \in \Omega \subset \mathbf{R}^3$. Set $f = f_1 + f_2$ if needed.

Introduce two Hilbert space $H = L^2(\Omega)$ and $V = H_0^1(\Omega)$, and define their norm and inner product as usual. For complex-valued function ψ_n, define the complex space $\mathbb{L}^2(\Omega)$ and $\mathbb{H}_0^1(\Omega)$ corresponding to $L^2(\Omega)$ and $H_0^1(\Omega)$, use the notations $\mathbb{H} = \mathbb{L}^2(\Omega), \mathbb{V} = \mathbb{H}_0^1(\Omega)$ for complex Hilbert spaces (cf. [Dautray and Lions, 1992], [Lions, 1971]). Furthermore, $\mathbb{V}'$ denote complex conjugate space of $\mathbb{V}$. Then, $(\mathbb{V}, \mathbb{H})$ is a complex Gelfand triple spaces $\mathbb{V} \hookrightarrow \mathbb{H} \hookrightarrow \mathbb{V}'$, in which the embeddings are continuous, dense and compact. To differ the function at complex space, denote $\boldsymbol{\psi}, \boldsymbol{\phi}$ as notation of wave functions. For $\boldsymbol{\psi}_n = \psi_n^1 + \mathbf{i}\psi_n^2 \in \mathbb{L}^2(\Omega)$, where $\psi_n^1, \psi_n^2 \in L^2(\Omega)$, to define the norm of $\boldsymbol{\psi}_n$ in complex space $\mathbb{L}^2(\Omega)$ as

$$\|\boldsymbol{\psi}_n\|_{\mathbb{L}^2(\Omega)} = (\|\psi_n^1\|_{L^2(\Omega)}^2 + \|\psi_n^2\|_{L^2(\Omega)}^2)^{\frac{1}{2}}.$$

If $\boldsymbol{\psi}_n = \psi_n^1 + \mathbf{i}\psi_n^2 \in \mathbb{L}^2(\Omega)$ and $\boldsymbol{\phi}_n = \phi_n^1 + \mathbf{i}\phi_n^2 \in \mathbb{L}^2(\Omega)$, then inner product of $\boldsymbol{\psi}_n$ and $\boldsymbol{\phi}_n$ in complex space $\mathbb{L}^2(\Omega)$ is defined by

$$\begin{aligned}(\boldsymbol{\psi}_n, \boldsymbol{\phi}_n)_{\mathbb{L}^2(\Omega)} &= ((\psi_n^1, \phi_n^1)_{L^2(\Omega)} + (\psi_n^2, \phi_n^2))_{L^2(\Omega)}) \\ &+\mathbf{i}((\psi_n^2, \phi_n^1)_{L^2(\Omega)} - (\psi_n^1, \phi_n^2)_{L^2(\Omega)}).\end{aligned}$$

For $\boldsymbol{\psi}_n \in \mathbb{H}_0^1(\Omega)$, the norm of $\boldsymbol{\psi}_n$ in complex space $\mathbb{H}_0^1(\Omega)$ is

$$\|\boldsymbol{\psi}_n\|_{\mathbb{H}_0^1(\Omega)} = (\|\psi_n^1\|_{H_0^1(\Omega)}^2 + \|\psi_n^2\|_{H_0^1(\Omega)}^2)^{\frac{1}{2}}.$$

If $\boldsymbol{\psi}_n, \boldsymbol{\phi}_n \in \mathbb{H}_0^1(\Omega)$, then inner product of $\boldsymbol{\psi}_n$ and $\boldsymbol{\phi}_n$ in complex space $\mathbb{H}_0^1(\Omega)$ is defined as

$$\langle\boldsymbol{\psi}_n, \boldsymbol{\phi}_n\rangle_{\mathbb{H}_0^1(\Omega)} = \langle\psi_n^1, \phi_n^1\rangle_{H_0^1(\Omega)} + \langle\psi_n^2, \phi_n^2\rangle_{H_0^1(\Omega)}.$$

Denote $\boldsymbol{\psi} = (\boldsymbol{\psi}_1, \boldsymbol{\psi}_2, \cdots, \boldsymbol{\psi}_N)$, and $\mathcal{V} = \mathbb{V}^N, \mathcal{H} = \mathbb{H}^N$ if needed. Using the vectors and matrics notation to rewrite the free G-P system (2) as

$$\begin{cases}\mathbf{i}\hbar\dfrac{\partial\boldsymbol{\psi}}{\partial t} = \dfrac{\hbar^2}{2m}\Delta\boldsymbol{\psi} + \boldsymbol{f}_1 + \boldsymbol{f}_2 \text{ in } Q, \\ \boldsymbol{\psi}(\mathbf{x}, 0) = \boldsymbol{\psi}^0(\mathbf{x}) \text{ on } \Omega,\end{cases} \tag{3}$$

where $\boldsymbol{f}_1 = \Big(\mathbf{V}(\mathbf{x},t)\psi_1, \mathbf{V}(\mathbf{x},t)\psi_2, \cdots, \mathbf{V}(\mathbf{x},t)\psi_N\Big)$, $\boldsymbol{f}_2 = \Big(N\nu|\psi_1|^2\psi_1, N\nu|\psi_2|^2\psi_2, \cdots, N\nu|\psi_N|^2\psi_N\Big)$. Denote $\boldsymbol{f} = \boldsymbol{f}_1 + \boldsymbol{f}_2$. Clearly, by the configuration in section 2, nonlinear term $\boldsymbol{f}$ can be taken easily as $\boldsymbol{f} \in L^2(0,T;\mathcal{V}')$ or $\boldsymbol{f} \in L^2(0,T;\mathcal{H})$. Assume that $\boldsymbol{f}(t) \in \mathcal{V}'$ in here.

DEFINITION 1 (Solution space) Complex space $W(0,T)$ is called a solution space of $\boldsymbol{\psi}$ for free G-P system (3), if defined by

$$W(0,T) = \{\boldsymbol{\psi} |\ \boldsymbol{\psi} \in L^2(0,T;\mathcal{V}), \boldsymbol{\psi}' \in L^2(0,T;\mathcal{V}')\}.$$

Its norm can be defined by

$$\|\boldsymbol{\psi}\|_{W(0,T)} = \Big(\|\boldsymbol{\psi}\|^2_{L^2(0,T;\mathcal{V})} + \|\boldsymbol{\psi}'\|^2_{L^2(0,T;\mathcal{V}')}\Big)^{\frac{1}{2}}.$$

For $\boldsymbol{\psi}, \boldsymbol{\phi} \in W(0,T)$, define inner product as

$$\langle \boldsymbol{\psi}, \boldsymbol{\phi}\rangle_{W(0,T)} = \langle \boldsymbol{\psi}, \boldsymbol{\phi}\rangle_{\mathcal{V}} + \langle \boldsymbol{\psi}', \boldsymbol{\phi}'\rangle_{\mathcal{V}'}.$$

Hence, $W(0,T)$ is a complex Hilbert space equipped by above norm and inner product.

DEFINITION 2 (Weak solution) *A function $\boldsymbol{\psi}$ is said as weak solution of BEC system described by free G-P equation* (3) *for N nanoparticles, if $\boldsymbol{\psi} \in W(0,T)$ and satisfy weak form*

$$\int_0^T\!\!\int_\Omega \mathbf{i}\hbar\frac{\partial \boldsymbol{\psi}}{\partial t}\boldsymbol{\eta} d\mathbf{x}dt = \frac{\hbar^2}{2M}\int_0^T\!\!\int_\Omega \nabla\boldsymbol{\psi}\nabla\boldsymbol{\eta} d\mathbf{x}dt + \int_0^T\!\!\int_\Omega \mathbf{V}\boldsymbol{\psi}\boldsymbol{\eta} d\mathbf{x}dt + N\nu\int_0^T\!\!\int_\Omega |\boldsymbol{\psi}|^2\boldsymbol{\psi}\boldsymbol{\eta} d\mathbf{x}dt, \quad (4)$$

where $\boldsymbol{\eta}$ is a arbitrary function by the means of distribution in space $\mathcal{D}'(0,T)^N$, $\boldsymbol{\eta} \in C^1(0,T;\mathcal{V})$ and take $\boldsymbol{\eta}(T) = 0$.

3.2 Existence of Weak Solution

Cite the results for BEC in papers (cf. [Wang and Belavkin, 2009], [Wang and Belavkin, 2012], [Wang, 2018]), it is easy to obtain the proof of existence theorem of weak solution for nanoparticles at system (2).

THEOREM 3 (Existence theorem of weak solution) *For $\boldsymbol{\psi}_0 \in \mathcal{V}$ of N nanoparticles, then there exists a unique weak solution $\boldsymbol{\psi} \in W(0,T)$ for G-P equation* (1).

proof: As in [Lions, 1971], using Faedo-Galerkin method to construct an approximate solution for free nano BEC system (2). From Gelfand triple spaces, the two embeddings in $\mathbb{V} \hookrightarrow \mathbb{H} \hookrightarrow \mathbb{V}'$ are dense, continuous and compact, therefore, their N product spaces $\mathcal{V} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{V}'$ is also a Gelfand triple spaces, their embeddings are also dense, continuous and compact. Then there exists an orthogonal basis of $\mathbb{H}$, $\{w^j\}_{j=1}^\infty$ consisting of eigenfunctions of $A = \Delta$, such that $Aw^j = \lambda^j w^j$ for all j, $0 < \lambda^1 \leq \lambda^2 \leq, \cdots, \lambda^j \to \infty$ as $j \to \infty$. G^i is the orthogonal projection of $\mathbb{H}$ (or $\mathbb{V}$) onto the space spanned by $\{w^1, \cdots, w^i\}$. Let's use index i to represent the approximate solution which differed with weak solution, it is also exactly the dimension of spanned approximate space. For each $n \in N$, an approximate solution is defined for G-P equation (1) by

$$\psi_n^i(t) = \sum_{j=1}^i a_n^{ij}(t)w^j, \quad i = 1, 2, \cdots, N,$$

where $a_n^{ij}(t)$ is real-valued coefficient function. Set $A_n^i = [a_n^{i1}, a_n^{i2}, \cdots, a_n^{ii}]$, $\boldsymbol{\omega} = [w^1, w^2, \cdots, w^i]^T$, then $\psi_n^i = A_n^i\boldsymbol{\omega}$. Thus, their vector approximate solution of $\boldsymbol{\psi}$ is given by

$$\boldsymbol{\psi}^i = \begin{pmatrix} \psi_1^i(t) \\ \psi_2^i(t) \\ \vdots \\ \psi_N^i(t) \end{pmatrix} = \begin{pmatrix} \sum_{j=1}^i a_1^{ij}(t)w^j \\ \sum_{j=1}^i a_2^{ij}(t)w^j \\ \vdots \\ \sum_{j=1}^i a_N^{ij}(t)w^j \end{pmatrix}. \quad (5)$$

Notice that, by the embeddings of Gelfand triple spaces, at weak form for ψ_n^i, the conjugate paring of dual space V, V' at nonlinear term can be calculated by inner product of space H as $\langle\cdot,\cdot\rangle_{V,V'} = (\cdot,\cdot)_H$. Multiply w^k to both sides at detailed weak form (4) for ψ_n^i, use inner product instead of integration, substitute functional ψ_n with approximate solution ψ_n^i, then $\psi_n^i(t)$ satisfy ordinary differential equation ($1 \leq i \leq N$) as

$$\begin{cases} \mathbf{i}\hbar\sum_{j=1}^i \frac{\partial a_n^{ij}(t)}{\partial t}(w^j, w^k) \\ = \frac{\hbar^2}{2m}\sum_{j=1}^i a_n^{ij}(t)(\nabla w^j, \nabla w^k) + f(\sum_{j=1}^i a_n^{ij}(t)(w^j), w^k). \\ \sum_{j=1}^i a_n^{ij}(t)(w^j, w^k)(0) = (\psi_{n0}^i, w^k). \end{cases} \quad (6)$$

Then convert system (6) to an ordinary differential equation of coefficients $\{a_n^{ij}(t)\}$ for $n = 1, 2, \cdots, N$ and $j = 1, 2, \cdots, i$.

For simplification, similarly, here is to use the vectors and matrix formulation, through the notation of inner product, taking test function $\boldsymbol{\eta} = \boldsymbol{\omega}$. That is, multiply $\boldsymbol{\omega}$ to both sides of (4), substitute vector functional $\boldsymbol{\psi}^i$ defined in (5), for free system (2), then to get

$$\begin{cases} \mathbf{i}\hbar\frac{\partial \boldsymbol{\psi}^i}{\partial t}(\boldsymbol{\omega}, \boldsymbol{\omega}) = \frac{\hbar^2}{2M}(\nabla\boldsymbol{\psi}^i, \nabla\boldsymbol{\omega}) + (f(\boldsymbol{\psi}^i), \boldsymbol{\omega}), \\ (\boldsymbol{\psi}^i(0), \boldsymbol{\omega}) = (\boldsymbol{\psi}_0^i, \boldsymbol{\omega}). \end{cases} \quad (7)$$

By the orthogonal properties $(w^j, w^k) = \begin{cases} 0 & j \neq k \\ 1 & j = k. \end{cases}$, for more detail, denote

$$\mathbf{a} = \Big(a_n^{ij} \Big)_{N\times 1}, \ \mathcal{A} = \Big((\nabla w^j, \nabla w^k) \Big)_{N\times N},$$
$$\mathcal{F} = \Big(f(\sum_{j=1}^{i} a_n^{ij}(t)(w^j), w^k) \Big)_{N\times 1},$$
$$\mathbf{a}(0) = \Big(a_n^{ij}(0) \Big)_{N\times 1}, \ \mathbf{a}_0 = \Big((\psi_0^i, w^k) \Big)_{N\times 1}.$$

Then, convert the equations (6), (7) to vectors and matrix representation as

$$\begin{cases} \dfrac{d\mathbf{a}}{dt} - \mathcal{A}\mathbf{a} = \mathcal{F} \ \text{ in } [0,T], \\ \mathbf{a}(0) = \mathbf{a}_0. \end{cases} \tag{8}$$

By Carathéodory theory of ordinary differential equation (ODE), ensure a unique local solution of $\{a_n^{ij}\}$ for ODE (8). Hence, using the solved coefficients to compose approximate solution $\{\psi_n^i\}$, $i = 1, 2, \cdots, N$ for free system (2) as well as G-P system (1). Consequencely, that prove the existence of weak solution.

Let's consider the uniqueness of weak solution. Without lost of generality, to controlled system (1), for ψ_{n0}^i, there exists a $\psi_{n0} \in \mathbb{V}$ such that

$$\psi_{n0}^i \to \psi_{n0} \ \text{ strongly in } \ \mathbb{H}_0^1(\Omega).$$

It means that

$$\boldsymbol{\psi}_0^i \to \boldsymbol{\psi}_0 \ \text{ strongly in } \ \mathcal{H}.$$

Take the analogous argument for $\{\psi_n^i\}$, there is a function $\psi_n \in \mathbb{V}$, such that $\|\psi_n^i - \psi_n\|_{\mathbb{V}} \to 0$ as $i \to \infty$. That is, the approximate solution ψ_n^i is bounded in $L^\infty(0,T;\mathbb{V})$.

Suppose that $\{\psi_n^i\}$ and $\{\psi_n^k\}$ are two solutions of G-P equation (1) for ψ_{n0}^i and ψ_{n0}^k. From weak form (4) to get

$$\begin{aligned} &\frac{\mathbf{i}\hbar}{2}\frac{d}{dt}\|\psi_n^i - \psi_n^k\|_{\mathbb{H}}^2 + \frac{\hbar^2}{2m}\|\psi_n^i - \psi_n^k\|_{\mathbb{V}}^2 \\ &\le \|\mathbf{V}^i(\mathbf{x})(\psi_n^i - \psi_n^k)\|_{\mathbb{H}}^2 + N\nu\Big\||\psi_n^i|^2\psi_n^i - |\psi_n^k|^2\psi_n^k\Big\|_{\mathbb{H}}^2, \end{aligned}$$

where $\mathbf{V}^i$ denote the i-th column element of $N \times N$ matrix $\mathbf{V}(\mathbf{x})$. More precisely, for real-valued function $\mathbf{V}^i(\mathbf{x})$, it is easily to estimate the norm of nonlinear term as

$$\|\mathbf{V}^i(\mathbf{x})(\psi_n^i - \psi_n^k)\|_{\mathbb{H}}^2 \le \|\mathbf{V}^i\|_{L^2(\Omega)^N}^2 \|\psi_n^i - \psi_n^k\|_{\mathbb{H}}^2.$$

Further, to estimate the norm of last term as

$$\begin{aligned} \Big\||\psi_n^i|^2\psi_n^i - |\psi_n^k|^2\psi_n^k\Big\|_{\mathbb{H}}^2 &\le \|\psi_n^i\|_{\mathbb{H}}^2 \Big\|\psi_n^i - \psi_n^k\Big\|_{\mathbb{H}}^2 \\ &+ \Big\||\psi_n^i| - |\psi_n^k|\Big\|_{\mathbb{H}}^2 \Big\|(|\psi_n^i| + |\psi_n^k|)\psi_n^k\Big\|_{\mathbb{H}}^2. \end{aligned}$$

In here, if set $C(t) = \max\Big\{\|\mathbf{V}^i\|_{L^2(\Omega)^N}^2, \|\psi_n^i\|_{\mathbb{H}}^2 + \Big\|(|\psi_n^i| + |\psi_n^k|)\psi_n^k\Big\|_{\mathbb{H}}^2\Big\}$ and $I^{ik}(t) = \|\psi_n^i(t) - \psi_n^k(t)\|_{\mathbb{H}}^2 + \|\psi_n^i(t) - \psi_n^k(t)\|_{\mathbb{V}}^2$, set $\lambda = \max\Big\{\dfrac{\mathbf{i}\hbar}{2}, \dfrac{\hbar^2}{2M}\Big\}$ and $C'(t) = C(t)/\lambda$, then to get that

$$\frac{d}{dt}I^{ik}(t) \le C'(t)I^{ik}(t).$$

Set $I^{ik}(0) = \|\psi_{n0}^i - \psi_{n0}^k\|_{\mathbb{H}}^2 + \|\psi_{n0}^i - \psi_{n0}^k\|_{\mathbb{V}}^2$, from Gronwall inequality that

$$I^{ik}(t) \le \exp\Big(\int_0^T C'(t)dt\Big)I^{ik}(0).$$

It implied $\psi_n^i - \psi_n^k \to 0$ as $i, k \to \infty$. Moreover, above argument is also valid for N particles of system (7), that is $\boldsymbol{\psi}^i - \boldsymbol{\psi}^k \to 0$ as $i, k \to \infty$. It is the uniqueness of weak solution $\boldsymbol{\psi}$ respect to initial function $\boldsymbol{\psi}_0 \in \mathcal{V}$. Thus, by the boundedness of norm of $\boldsymbol{\psi}^i$ at spaces $L^2(0,T;\mathbb{H}), L^2(0,T;\mathbb{V})$ to know that there exist $\boldsymbol{\psi}(t)$ such that $\boldsymbol{\psi}^i(t) \to \boldsymbol{\psi}(t)$ at $\mathbb{H}$ and $\mathbb{V}$. Furthermore, the inclusive of spaces $C^N(0,T;\mathbb{H}) \subset W(0,T)$ to sure Theorem 3.

At the weak form (4), $\boldsymbol{f} \in L^2(0,T;\mathcal{V}')$ and $\boldsymbol{\eta} \in C^1(0,T;\mathcal{V})$. Certainly, for nonlinear term $\boldsymbol{f} \in L^2(0,T,\mathcal{H})$ in the free system (2), much more simplified proof can be straightforwardly attained.

□

4 Quantum Control of Nano-BEC

Suppose $Q = \Omega \times [0,T]$ and set $\mathbf{V} = V^1 + V^2 + V^3$, $\mathcal{U} = L^2(Q)^{N\times N}$ is the space of controls $\mathbf{V}$, and $\mathcal{U}_{ad}$ is a admissible set of $\mathcal{U}$. By the virtual of Existence theorem of weak solution to free system (3), there is a mapping from control space to solution space $\mathbf{V} \to \boldsymbol{\psi}(\mathbf{V})$: $\mathcal{U} \to \mathcal{V}$, which is continuous.

As is well known that the nanoparticle cooled at an vacuum chamber, its motion become slow, and can be measured and probed to do terminal observation by photograph, scanning electron micrograph, computer monitor at real time duration $[0,T]$ and final time t_f. The cost function of N nanoparticles for controlled G-P system (1) can be given in the form of

$$J(\mathbf{V}) = \epsilon^1\|\boldsymbol{\psi}^f(\mathbf{V}) - \boldsymbol{\psi}^{\text{target}}(\mathbf{V})\|_{\mathcal{H}}^2 + \epsilon^2\|\mathbf{V}\|_{\mathcal{U}}^2. \tag{9}$$

In criteria function (9), control $\mathbf{V} \in \mathcal{U}_{ad}$, $\boldsymbol{\psi}^{\text{target}}(\mathbf{V}) = (\psi_1^{\text{target}}(\mathbf{V}), \cdots, \psi_N^{\text{target}}(\mathbf{V}))$ is vector target state, and $\boldsymbol{\psi}^f(\mathbf{V}) = (\psi_1^f(\mathbf{V}), \cdots, \psi_N^f(\mathbf{V}))$ is observed final vector state of N nanoparticles at final time t_f. In here $\epsilon^i, i = 1, 2$ are weighted coefficients for balancing the calculated values of inherent cost and running cost.

Quantum optimal control is to solve two fundamental problems for nanoparticles system based Bose-Einstein-Condensate (cf. [Wang, 2021]):

i). Find an element $\mathbf{V}^*$ in $\mathcal{U}_{ad}$ satisfying G-P system (1) for nanoparticles such that
$$J(\mathbf{V}^*) = \inf_{\mathbf{V}\in\,\mathcal{U}_{ad}} J(\mathbf{V}).$$
ii). Characterize such a $\mathbf{V}^*$.

For N nanoparticles, $\mathbf{V}^*$ is called as quantum optimal control for G-P system (1) subject to cost function (9).

THEOREM 4 (Existence of quantum optimal control) *For $\boldsymbol{\psi}_0 \in \mathcal{V}$ of N nanoparticles, if $\mathcal{U}_{ad}$ is closed convex (bounded) admissible subset of $\mathcal{U}$, then there exists at least one quantum optimal control $\mathbf{V}^*$ of Bose-Einstein-Condensates system* (1) *subject to cost function* (9).

Proof. Set $J = \inf_{\mathbf{V}\in\mathcal{U}_{ad}} J(\mathbf{V})$, since $\mathcal{U}_{ad}$ is non-empty, there is a sequence $\{\mathbf{V}^k\}$ in $\mathcal{U}_{ad}$ such that $\inf_{\mathbf{V}\in\,\mathcal{U}_{ad}} J(\mathbf{V}) = \lim_{k\to\infty} J(\mathbf{V}^k) = J$. Since $\{J(\mathbf{V})\}$ is bounded in $\mathbf{R}^+$, and $\mathcal{U}_{ad}$ is closed and convex (bounded) subset of $\mathcal{U}$, there exist a subsequence (denoted as same symbol) of $\{\mathbf{V}^k\}$ can be chosen, and there exist a $\mathbf{V}^* \in \mathcal{U}_{ad}$, such that

$$\mathbf{V}^k \to \mathbf{V}^* \text{ weakly in } \mathcal{U} \text{ as } k \to \infty. \tag{10}$$

By the Existence Theorem 3 of weak solution to get estimate $\|\boldsymbol{\psi}\|^2_{\mathcal{H}} + \|\boldsymbol{\psi}\|^2_{\mathcal{V}}$ is bounded for $\boldsymbol{\psi}$ of N nanoparticles. For control $\mathbf{V}^k$, by the boundedness of $\mathcal{U}_{ad}$ to know that

$$\boldsymbol{\psi}(\mathbf{V}^k) \text{ is bounded in } L^2(0,T;\mathcal{H}) \cap L^2(0,T;\mathcal{V}).$$

Set $\boldsymbol{\psi}^* = \boldsymbol{\psi}(\mathbf{V}^*)$, there exist a subsequence (denoted as same notation) of $\{\boldsymbol{\psi}(\mathbf{V}^k)\}$ and a $\boldsymbol{\psi}^* \in W(0,T)$ such that

$$\boldsymbol{\psi}(\mathbf{V}^k) \to \boldsymbol{\psi}^* \text{ weakly in } L^2(0,T;\mathcal{H}) \cap L^2(0,T;\mathcal{V}).$$

as $k \to \infty$. Since the embedding $\mathcal{V} \hookrightarrow \mathcal{H}$ is compact, from Aubin-Lions-Temam theorem (cf. [Temam, 1997]), then there is a $\bar{\boldsymbol{\psi}} \in \mathcal{H}$ that

$$\boldsymbol{\psi}(\mathbf{V}^k) \to \bar{\boldsymbol{\psi}} \text{ strongly in } L^2(0,T;\mathcal{H})$$

as $k \to \infty$, and the analogical argument for derivatives of $\boldsymbol{\psi}$ as

$$\frac{\partial \boldsymbol{\psi}(\mathbf{V}^k)}{\partial t} \to \frac{\partial \bar{\boldsymbol{\psi}}}{\partial t} \text{ weakly in } L^2(0,T;\mathcal{V}'), \tag{11}$$
$$\nabla\boldsymbol{\psi}(\mathbf{V}^k) \to \nabla\bar{\boldsymbol{\psi}} \text{ weakly in } L^2(0,T;\mathcal{H}), \tag{12}$$

as $k \to \infty$. Denote $\boldsymbol{\psi}^k = \boldsymbol{\psi}(\mathbf{V}^k)$, therefore, for N nanoparticles, by the definition of weak form (4) to get

$$\int_0^T\!\!\int_\Omega -\mathbf{i}\hbar\boldsymbol{\psi}^k\frac{\partial\boldsymbol{\eta}}{\partial t}d\mathbf{x}dt = \int_0^T\!\!\int_\Omega\Big[-\frac{\hbar^2}{2M}\frac{\partial\boldsymbol{\psi}^k}{\partial\mathbf{x}}\frac{\partial\boldsymbol{\eta}}{\partial\mathbf{x}} + \mathbf{V}^k\boldsymbol{\psi}^k\boldsymbol{\eta} + N\nu|\boldsymbol{\psi}^k|^2\boldsymbol{\psi}^k\boldsymbol{\eta}\Big]d\mathbf{x}dt. \tag{13}$$

Using convergence results (10), (11), (12), and taking $k \to \infty$ in (13) to yield that

$$\int_0^T\!\!\int_\Omega -\mathbf{i}\hbar\bar{\boldsymbol{\psi}}\frac{\partial\boldsymbol{\eta}}{\partial t}d\mathbf{x}dt = \int_0^T\!\!\int_\Omega\Big[-\frac{\hbar^2}{2M}\frac{\partial\bar{\boldsymbol{\psi}}}{\partial\mathbf{x}}\frac{\partial\boldsymbol{\eta}}{\partial\mathbf{x}} + \mathbf{V}^*\bar{\boldsymbol{\psi}}\boldsymbol{\eta} + N\nu|\bar{\boldsymbol{\psi}}|^2\bar{\boldsymbol{\psi}}\boldsymbol{\eta}\Big]d\mathbf{x}dt$$

for all $\boldsymbol{\eta} \in C^1(0,T;\mathcal{V})$. It implies that $\bar{\boldsymbol{\psi}}$ is a weak solution of (1) in the sense of distribution $\mathcal{D}'(0,T)^N$ on $(0,T)$. By the uniqueness of weak solution for BEC system (1) for nanoparticles to find that $\bar{\boldsymbol{\psi}} = \boldsymbol{\psi}(\mathbf{V}^*)$. Then, by Gelfand triple spaces $\mathcal{V} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{V}'$, for $\boldsymbol{\psi}$ to get

$$\boldsymbol{\psi}(\mathbf{V}^k) \to \boldsymbol{\psi}(\mathbf{V}^*) \quad \text{strongly in } L^2(0,T;\mathcal{H}),$$
$$\boldsymbol{\psi}^f(\mathbf{V}^k) \to \boldsymbol{\psi}^f(\mathbf{V}^*) \quad \text{strongly in } \mathcal{H}$$

as $k \to \infty$. Since the norm $\|\cdot\|_{\mathbb{L}^2(\Omega)^N}$ are lower semi-continuous in weak topology of $\mathcal{H}$ for N nanoparticles

$$\liminf_{k\to\infty} \|\boldsymbol{\psi}^f(\mathbf{V}^k) - \boldsymbol{\psi}^{\text{target}}\|^2_{\mathcal{H}} \geq \|\boldsymbol{\psi}^f(\mathbf{V}^*) - \boldsymbol{\psi}^{\text{target}}\|^2_{\mathcal{H}}.$$

Vice versa, by the weak convergence (10) to know that $\liminf_{k\to\infty}(\mathbf{V}^k,\mathbf{V}^k)_{\mathcal{U}} \geq (\mathbf{V}^*,\mathbf{V}^*)_{\mathcal{U}}$ at the real space $L^2(Q)^{N\times N}$. Therefore, for cost function (9), $J = \liminf_{k\to\infty} J(\mathbf{V}^k) \geq J(\mathbf{V}^*)$, and $J(\mathbf{V}^*) = \inf_{\mathbf{V}\in\mathcal{U}_{ad}} J(\mathbf{V})$. It means that $\mathbf{V}^*(\mathbf{x},t)$ is quantum optimal control of nanoparticles BEC system (1) respect to the criteria function (9). □

REMARK 5 Not all of the N nanoparticles to be used in the creation of a condensate, usual there is a loss for a creation with cooling technique. For instance, if the condensed rate for example 87%, then the loss rate is 13%.

REMARK 6 At very high temperature, whether particles have the phenomena such as condensates or other extremely physical status?

Remarkable, although use the cubic Schrödinger equation, G-P system (1), to describe the wave package of nano BEC, physically, the motion of nanoparticle BEC is real-valued function. Therefore, necessary optimality condition of cost function (9) can be given by

$$\begin{aligned} &J'(\mathbf{V}^*)(\mathbf{V}-\mathbf{V}^*)\\ &= \epsilon^1\Big(\boldsymbol{\psi}^f(\mathbf{V}^*) - \boldsymbol{\psi}^{\text{target}}, \boldsymbol{\psi}^f(\mathbf{V}) - \boldsymbol{\psi}^f(\mathbf{V}^*)\Big)_{\mathcal{H}}\\ &\quad +\epsilon^2(\mathbf{V}^*,\mathbf{V}-\mathbf{V}^*)_{\mathcal{U}} \geq 0, \quad \forall\mathbf{V}\in\mathcal{U}_{ad}. \end{aligned} \tag{14}$$

In here, $J'(\mathbf{V}^*)(\mathbf{V}-\mathbf{V}^*)$ is the Gâteaux derivative of cost function $J(\mathbf{V})$ at $\mathbf{V}^*$ in the direction of $\mathbf{V}-\mathbf{V}^*$.

The proof of following Theorem can be found at [Wang and Belavkin, 2009], [Wang and Belavkin, 2012], [Wang, 2018] for nanoparticles immediately.

THEOREM 7 (Optimality system) For $\boldsymbol{\psi}_0 \in \mathcal{V}$, and control problem for G-P system (1) to cost function (9), if $\mathcal{U}_{ad}$ is closed convex (bounded) admissible subset of $\mathcal{U}$, then quantum optimal control $\mathbf{V}^*$ is characterized by optimal (Euler-Lagrange) system as

$$\begin{cases} \mathbf{i}\hbar\dfrac{\partial \boldsymbol{\psi}}{\partial t} = \dfrac{\hbar^2}{2M}\Delta\boldsymbol{\psi} + \mathbf{V}^*\boldsymbol{\psi} + N\nu|\boldsymbol{\psi}|^2\boldsymbol{\psi} \quad \text{in Q}, \\ \boldsymbol{\psi}(0) = \boldsymbol{\psi}_0 \ \text{ on } \Omega. \end{cases} \tag{15}$$

$$\begin{cases} \mathbf{i}\hbar\dfrac{\partial \mathbf{p}}{\partial t} \\ = \dfrac{\hbar^2}{2M}\Delta\mathbf{p} + \mathbf{V}^*\mathbf{p} + 2N\nu|\boldsymbol{\psi}|\boldsymbol{\psi}\mathbf{p} + N\nu|\boldsymbol{\psi}|^2\mathbf{p} \text{ in Q}, \\ \mathbf{i}\mathbf{p}(T) = \boldsymbol{\psi}^f(\mathbf{V}^*) - \boldsymbol{\psi}^{\text{target}} \quad \text{on } \Omega. \end{cases} \tag{16}$$

$$\epsilon^1\int_0^T\int_\Omega \boldsymbol{\psi}^*\mathbf{p}(\mathbf{V}^*)(\mathbf{V}-\mathbf{V}^*)d\mathbf{x}dt + \epsilon^2(\mathbf{V}^*, \mathbf{V}-\mathbf{V}^*)_{\mathcal{U}} \geq 0 \quad \forall \mathbf{V} \in \mathcal{U}_{ad}. \tag{17}$$

In here, $\mathbf{p} \in W(0,T)$ is weak solution of adjoint system (16) corresponding to weak solution $\boldsymbol{\psi}$ of optimal nanoparticles BEC system (15). The inequality (17) is necessary optimality condition for quantum optimal control $\mathbf{V}^*(\mathbf{x},t)$ of N nanoparticles. As to the control term $\mathbf{V}^*\boldsymbol{\psi}$, rewritten as $\boldsymbol{\psi}\mathbf{V}^*$, then $\boldsymbol{\psi}^*$ is the conjugate functional of $\boldsymbol{\psi}$, which is coefficient operator of the control function.

Proof. The variational calculation to deduce adjoint system (16) can be directly obtained by citing reference [Wang, 2021] for the nonlinear parabolic system given by partial differential equation. This is a distributed control problems for terminal observation with cost function (9). The conjugate operator for nonlinear term in the G-P equation (15) can be calculated easily as appeared at adjoint system. Cite [Wang, 2016] and [Wang, 2018], take the derivative of $f = f_1 + f_2$ respect to variable $\boldsymbol{\psi}$ in free system (2) to get that

$$\frac{\partial f}{\partial \boldsymbol{\psi}} = \frac{\partial(f_1+f_2)}{\partial \boldsymbol{\psi}} = \mathbf{V} + 2N\nu|\boldsymbol{\psi}|\boldsymbol{\psi} + N\nu|\boldsymbol{\psi}|^2.$$

Then, roughly get the right hand of adjoint system as

$$(\mathbf{V} + 2N\nu|\boldsymbol{\psi}|\boldsymbol{\psi} + N\nu|\boldsymbol{\psi}|^2)\mathbf{p}.$$

More precisely, consider the weak solution of state system (15), by taking the test function $\boldsymbol{\eta} = \mathbf{p}$ and $\boldsymbol{\eta}(T) = \mathbf{p}(0) = 0$ as

$$\int_0^T\int_\Omega \mathbf{i}\hbar\frac{\partial \boldsymbol{\psi}}{\partial t}\mathbf{p}d\mathbf{x}dt = -\frac{\hbar^2}{2M}\int_0^T\int_\Omega \nabla\boldsymbol{\psi}\nabla\mathbf{p}d\mathbf{x}dt + \int_0^T\int_\Omega \mathbf{V}^*\boldsymbol{\psi}\ \mathbf{p}d\mathbf{x}dt + N\nu\int_0^T\int_\Omega (|\boldsymbol{\psi}|^2\boldsymbol{\psi})\ \mathbf{p}d\mathbf{x}dt. \tag{18}$$

Denote $\boldsymbol{\psi}_t = \dfrac{\partial \boldsymbol{\psi}}{\partial t}$, in (18), use the notation of inner product of $L^2(\Omega)$ to find that

$$\mathbf{i}\hbar(\boldsymbol{\psi}_t, \mathbf{p}) = -\frac{\hbar^2}{2M}(\nabla\boldsymbol{\psi}, \nabla\mathbf{p}) + (\mathbf{V}^*\boldsymbol{\psi},\ \mathbf{p}) + N\nu(|\boldsymbol{\psi}|^2\boldsymbol{\psi}, \mathbf{p}).$$

That is

$$\mathbf{i}\hbar(\boldsymbol{\psi}_t, \mathbf{p}) = -\frac{\hbar^2}{2M}(\nabla\boldsymbol{\psi}, \nabla\mathbf{p}) + (f(\boldsymbol{\psi}), \mathbf{p}). \tag{19}$$

For first term in (19), calculate without considering the coefficients, then integration by part respect to variable t to know

$$\int_0^T\int_\Omega \frac{\partial \boldsymbol{\psi}}{\partial t}\mathbf{p}d\mathbf{x}dt = \int_\Omega (\boldsymbol{\psi}\mathbf{p})\big|_0^T d\mathbf{x} - \int_\Omega\int_0^T \boldsymbol{\psi}\frac{\partial \mathbf{p}}{\partial t}dtd\mathbf{x} = (\boldsymbol{\psi}^f(\mathbf{V}^*) - \boldsymbol{\psi}^{\text{target}}, \boldsymbol{\psi}(T))_{L^2(\Omega)} - \int_0^T\int_\Omega \boldsymbol{\psi}\frac{\partial \mathbf{p}}{\partial t}d\mathbf{x}dt. \tag{20}$$

Namely, use the inner product at space $L^2(\Omega)$ to get that

$$(\boldsymbol{\psi}_t, \mathbf{p}) = (\boldsymbol{\psi}^f(\mathbf{V}^*) - \boldsymbol{\psi}^{\text{target}}, \boldsymbol{\psi}(\mathbf{V}^*, T)) - (\boldsymbol{\psi}, \mathbf{p}_t). \tag{21}$$

For second term in (19), by the space $\mathbb{V} = \mathbb{H}_0^1(\Omega)$ to know that $\boldsymbol{\psi}$ and $\mathbf{p}$ are 0 at the boundary $\partial\Omega$, therefore, via system (18), it can be calculated as

$$-\frac{\hbar^2}{2M}\int_\Omega [\Delta\boldsymbol{\psi}]\ \mathbf{p}\ d\mathbf{x} = -\frac{\hbar^2}{2M}\int_\Omega \boldsymbol{\psi}\ [\Delta\mathbf{p}]\ d\mathbf{x}.$$

Namely, in the notation of inner product as

$$(-\Delta\boldsymbol{\psi}, \mathbf{p}) = (\boldsymbol{\psi}, -\Delta\mathbf{p}). \tag{22}$$

Now, substitute (21) and (22) into (19) to get that

$$\mathbf{i}\hbar(\boldsymbol{\psi}, \mathbf{p}_t) - \frac{\hbar^2}{2M}(\boldsymbol{\psi}, \Delta\mathbf{p}) = \mathbf{i}\hbar(\boldsymbol{\psi}^f(\mathbf{V}^*) - \boldsymbol{\psi}^{\text{target}}, \boldsymbol{\psi}(\mathbf{V}^*, T)) + (\boldsymbol{\psi}, f^*_{\boldsymbol{\psi}}(\boldsymbol{\psi})\mathbf{p}), \tag{23}$$

where $f_{\boldsymbol{\psi}} = \dfrac{\partial f(\boldsymbol{\psi})}{\partial \boldsymbol{\psi}}$, and $f^*_{\boldsymbol{\psi}}$ is conjugate operator of $f_{\boldsymbol{\psi}}$. Set $\mathbf{i}p(T) = \boldsymbol{\psi}^f(\mathbf{V}^*) - \boldsymbol{\psi}^{\text{target}}$, and consider test function $\mathbf{p}(0) = 0$, by (23), it means that

$$(\boldsymbol{\psi}, \mathbf{i}\hbar\mathbf{p}_t - \frac{\hbar^2}{2M}\Delta\mathbf{p} + f^*_{\boldsymbol{\psi}}\mathbf{p}) = (\boldsymbol{\psi}(T), \mathbf{i}\mathbf{p}(T)) - (\boldsymbol{\psi}(0), \mathbf{i}\mathbf{p}(0)).$$

Then by the arbitrary of $\boldsymbol{\psi}$ in the $L^2(\Omega)$ space to get that, responding to state solution $\boldsymbol{\psi} \in W(0,T)$, adjoint system for $\mathbf{p} \in W(0,T)$ can given as

$$\mathbf{i}\hbar\frac{\partial \mathbf{p}}{\partial t} - \frac{\hbar^2}{2M}\Delta\mathbf{p} = (\mathbf{V} + 2N\nu|\boldsymbol{\psi}|\boldsymbol{\psi} + N\nu|\boldsymbol{\psi}|^2)\mathbf{p}.$$

with value at T as $\mathbf{i}\mathbf{p}(T) = \boldsymbol{\psi}^f(\mathbf{V}^*) - \boldsymbol{\psi}^{\text{target}}$. Hence, it is verified adjoint system (16).

Next is to rewrite the necessary optimal condition (14) by using adjoint system (16). Denote $J(\mathbf{V}) = J_1(\mathbf{V}) + J_2(\mathbf{V})$, calculate the Gâteaux of $J_1(\mathbf{V})$ by definition as

$$\begin{aligned} & J_1'(\mathbf{V}^*)(\mathbf{V}-\mathbf{V}^*) \\ &= \lim_{\lambda\to 0}\frac{2}{\lambda}\Big(\boldsymbol{\psi}^f(\mathbf{V}^*)-\boldsymbol{\psi}^{\text{target}}, \\ & \qquad [\boldsymbol{\psi}^f(\mathbf{V}^*+\lambda(\mathbf{V}-\mathbf{V}^*))-\boldsymbol{\psi}^f(\mathbf{V}^*)]\Big). \end{aligned} \tag{24}$$

Above discussion to $\mathbf{V}^*$ in (18), (20) and (21) are also valid for control variable $\mathbf{V}$, that is

$$(\boldsymbol{\psi}_t, \mathbf{p}) = \Big(\boldsymbol{\psi}^f(\mathbf{V})-\boldsymbol{\psi}^{\text{target}}, \boldsymbol{\psi}(T)\Big) - (\boldsymbol{\psi}, \mathbf{p}_t). \tag{25}$$

By formulate (18) to get that

$$\begin{aligned} & \Big(\boldsymbol{\psi}^f(\mathbf{V}^*)-\boldsymbol{\psi}^{\text{target}}, \boldsymbol{\psi}(T)\Big)_{L^2(\Omega)} \\ & -\int_0^T\!\!\int_\Omega \boldsymbol{\psi}[\mathbf{i}\hbar\frac{\partial \mathbf{p}}{\partial t} - \frac{\hbar^2}{2M}\Delta\mathbf{p}]\, d\mathbf{x}dt \\ &= \int_0^T\!\!\int_\Omega \mathbf{V}^*\boldsymbol{\psi}\ \mathbf{p}d\mathbf{x}dt + N\nu\int_0^T\!\!\int_\Omega |\boldsymbol{\psi}|^2\boldsymbol{\psi}\ \mathbf{p}d\mathbf{x}dt. \end{aligned} \tag{26}$$

For the weak solution of adjoint system (16), taking test function $\boldsymbol{\eta} = \boldsymbol{\psi}$ to get the following formulation

$$\begin{aligned} & \int_0^T\!\!\int_\Omega [\mathbf{i}\hbar\frac{\partial \mathbf{p}}{\partial t} - \frac{\hbar^2}{2M}\Delta\mathbf{p}]\boldsymbol{\psi}d\mathbf{x}dt \\ &= \int_0^T\!\!\int_\Omega (\mathbf{V}^* + 2N\nu|\boldsymbol{\psi}|\boldsymbol{\psi}\mathbf{p} + N\nu|\boldsymbol{\psi}|^2\mathbf{p})\boldsymbol{\psi}\ d\mathbf{x}dt. \end{aligned} \tag{27}$$

Compare (26) and (27) to get that

$$\begin{aligned} & (\boldsymbol{\psi}^f(\mathbf{V}^*)-\boldsymbol{\psi}^{\text{target}}, \boldsymbol{\psi}(T))_{\mathcal{H}} \\ &= 2\int_0^T\!\!\int_\Omega \mathbf{V}^*\boldsymbol{\psi}\ \mathbf{p}d\mathbf{x}dt + 2N\nu\int_0^T\!\!\int_\Omega |\boldsymbol{\psi}|^2\boldsymbol{\psi}\ \mathbf{p}\ d\mathbf{x}dt. \\ &+ \int_0^T\!\!\int_\Omega 2N\nu|\boldsymbol{\psi}|\boldsymbol{\psi}\mathbf{p}\ d\mathbf{x}dt. \end{aligned} \tag{28}$$

By (25), set $\boldsymbol{\psi}(T) = \boldsymbol{\psi}^f(\mathbf{V}^*+\lambda(\mathbf{V}-\mathbf{V}^*)) - \boldsymbol{\psi}^f(\mathbf{V}^*)$ in (28) to find that

$$\begin{aligned} & \frac{1}{2}\Big(\boldsymbol{\psi}^f(\mathbf{V}^*)-\boldsymbol{\psi}^{\text{target}}, \boldsymbol{\psi}^f(\mathbf{V}^*+\lambda(\mathbf{V}-\mathbf{V}^*))-\boldsymbol{\psi}^f(\mathbf{V}^*)\Big)_{\mathcal{H}} \\ &= \int_0^T\!\!\int_\Omega \lambda(\mathbf{V}-\mathbf{V}^*)\boldsymbol{\psi}\ \mathbf{p}\ d\mathbf{x}dt. \end{aligned} \tag{29}$$

Indeed, in (24), $\lim\limits_{\lambda\to 0}\dfrac{1}{\lambda}[\boldsymbol{\psi}^f(\mathbf{V}^*+\lambda(\mathbf{V}-\mathbf{V}^*))-\boldsymbol{\psi}^f(\mathbf{V}^*)]$ is the Gâteaux derivative of $\boldsymbol{\psi}^f$ at $\mathbf{V}^*$ in the direction of $\mathbf{V}-\mathbf{V}^*$. Therefore, substitute (29) into (24), for $\forall\mathbf{V}\in\mathcal{U}_{ad}$, the necessary optimality condition (14) can be converted to

$$\int_0^T\!\!\int_\Omega \boldsymbol{\psi}^*\mathbf{p}(\mathbf{V}^*)(\mathbf{V}-\mathbf{V}^*)d\mathbf{x}dt + (\mathbf{V}^*, \mathbf{V}-\mathbf{V}^*)_{\mathcal{U}} \geq 0.$$

It is verified Theorem 7. □

The results obtained in Theorem 7 are agree with the conclusion in physics field [Hohenester, 2007].

In additional, at the physical viewpoint, if select the specified control space $\mathcal{U}_{ad}$, quantum optimal control $\mathbf{V}^*$ will have Bang-Bang principle for nano-BEC (cf. [Wang, 2016]).

5 Discussion

For posed nanoparticles created Bose-Einstein-Condensates problem, control of such a quantum system is quite interesting issue and there are many unknown mysteries need to solve not only at the control theory of applied mathematics, but also at the chemical physics field. Indeed, a lot of questions will be also questions if without collaborating with the area of chemistry and physics.

The essential task for such a cutting-edge problem extremely require interdisciplinary work together to explore.

(i) whether there is nano sized particles (gold nanoparticle, its stability both in size and temperature), we yet find that can be condensed?

(ii) whether some materials or matter, had already being a nano-sized condensates?

In the standpoint of mathematics, no answer to response at present.

Nanoparticles composed advance materials as well as quantum materials, would be continuously attract our attention for several decades or much long time. It would be exciting journey for exploring and discovering the research results crossing subjects.

6 Conclusion

In this paper, nanoparticles created condensates had been considered originally as control objective. It tried to find the quantum optimal control as the nanoparticle cooling to a low temperature, and condensed. In fact, currently, it is certainly to know that, to molecules and atoms, such kind of investigation had been taken, and a great deal excellent work had been reported in contributed papers, such as at IPACS (cf. [Romero-Meléndez and González-Santos, 2017]).

Nano condensates, is a big topic for future research at theoretical issues, numerical analysis, computational approach and experimental demonstration and simulation. It is also a promising research direction in further study and survey. Personally, thanks to the discovery of the nanoparticles created condensate with gold metal for making this work meaningful.

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