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A nonlinear eigenvalue problem arising in a nanostructured quantum dot

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ABSTRACT

In this paper we investigate a minimization problem related to the principal eigenvalue of the *s*-wave Schrödinger operator. The operator depends nonlinearly on the eigenparameter. We prove the existence of a solution for the optimization problem and the uniqueness will be addressed when the domain is a ball. The optimized solution can be applied to design new electronic and photonic devices based on the quantum dots.

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1. Introduction

Quantum dot nanostructures have attracted broad interest in the past few years because of their unique physical properties and potential applications in micro- and nanoelectronic devices. In such nanostructures, the free carriers are confined to a small region of space by potential barriers. If the size of this region is less than the electron wavelength, the electronic states become quantized at discrete energy levels. Due to the possibility of precise control over the conductivity by adjusting the energy levels via the configuration, quantum dot structures have received tremendous attention from many physicists and scientists [1]. The problem of finding the energy states in these structures is regarded as an essential step to study the optical and electrical properties.

Motivated by the above explanation, in this paper we consider a nanostructure quantum dot and the Schrödinger equation governing it. We discus an efficient method that is capable to predict the configuration which has a minimum ground state energy.

Let us introduce the mathematical equations modeling the structure and an associated optimization problem. Let Ω be a bounded connected set in $\mathbb{R}^n$ with smooth boundary. Suppose that p_0 and q_0 are two Lebesgue measurable functions satisfying $0 \leqslant p_0,\ q_0 \leqslant h$ in Ω, where h is a positive constant. To avoid trivial situations, we assume that p_0 and q_0 are not constant functions. Define $\mathcal{P}$ and $\mathcal{Q}$ as the family of all measurable functions which are rearrangements of p_0 and q_0 respectively. For $p \in \mathcal{P}$ and $q \in \mathcal{Q}$, the governing Hamiltonian equation is the following *s*-wave Schrödinger equation [2],

$$-\frac{\hbar^2}{2m}\Delta u + q(x)u + 2\lambda p(x)u = \lambda^2 u, \quad \text{in} \quad \Omega, \quad u = 0, \quad \text{on} \quad \partial\Omega, \tag{1.1}$$

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where $\hbar$ stands for Planck 's constant, m is the mass of particle, λ is the first eigenvalue (ground state energy) and u is the corresponding eigenfunction (wave function).

In Schrödinger (1.1), the potential function is of the form

$$V(\lambda, x) = q(x) + 2\lambda p(x),$$

where it depends on the ground state energy. Let us mention that λ can be described as a function of p and q. Hence, we use notation $\lambda_{p,q}$ to emphasize its dependence on p and q.

We seek potentials that minimize the first eigenvalue corresponding to Eq. (1.1) relative to $\mathcal{P}$ and $\mathcal{Q}$. To determine the potential which gives the minimum ground state energy, we should study the following minimization problem

$$\inf_{p\in\mathcal{P}, q\in\mathcal{Q}} \lambda_{p,q}. \tag{1.2}$$

These type of optimization problems for eigenvalues of linear or nonlinear elliptic partial differential equations have been intensively attractive to mathematicians in the past decades. They have several applications as for instance the stability of vibrating bodies, the propagation of waves in composite media and the thermic insulation of conductors; see [3] for an overview of the topic. However, it should be mentioned that the majority of the investigated nonlinear models are nonlinear in their differential operator part [4–6].

Eq. (1.1) can be regarded as a nonlinear elliptic eigenvalue problem such that the nonlinearity is originated from the nonlinear dependence on the eigenvalue. We note that such systems have been under less attention in this field of study [7]. In the linear problems, the analysis of the eigenvalues is based essentially on the Rayleigh quotient associated with the eigenvalues. For nonlinear eigenvalue problem (1.1), we should apply the Rayleigh functional corresponding to the eigenvalue. In this paper we extend rearrangements techniques to find an optimal eigenvalue of a nonlinear problem. This eigenvalue minimization problem is more difficult than that of the linear problems due to the more complicated form of the Rayleigh functional. We hope this paper would be a motivation to further study in this direction.

One can find some quantum dot models where the Schrödinger equations governing them are nonlinear with respect to the energy [8–10].

Our paper is organized as follows. In the next section we review rearrangement theory with an eye on the optimization problem (1.2). In the third section we derive a formula for the first eigenvalue of the problem (1.1). Then we prove the existence of a solution to the problem (1.2). In the fourth section, we examine the uniqueness problem and we shall investigate the configuration of the unique solution. In the last section, we will give an overview of our results with a numerical example which shows the physical significance of the findings.

2. Preliminaries

In this section we state some results from the rearrangement theory related to our optimization problem (1.2). The reader can refer to [11,12] for further information about the rearrangement theory. In this paper, we denote with $|\mathcal{A}|$ the Lebesgue measure of the measurable set $\mathcal{A} \subset \mathbb{R}^n$.

Two Lebesgue measurable functions $p : \Omega \to \mathbb{R},\ p_0 : \Omega \to \mathbb{R}$ are said to be rearrangements of each other if

$$|\{x \in \Omega : p(x) \geqslant \alpha\}| = |\{x \in \Omega : p_0(x) \geqslant \alpha\}| \quad \forall \alpha \in \mathbb{R}. \tag{2.1}$$

The notation $p \sim p_0$ means that p and p_0 are rearrangements of each other. Consider $p_0 : \Omega \to \mathbb{R}$. The class of rearrangements generated by p_0, denoted $\mathcal{P}$, is defined as follows

$$\mathcal{P} = \{p : p \sim p_0\}.$$

Consider a function $q \in L^r(\Omega),\ r \geqslant 1$. A level set of this function is

$$\{x \in \Omega : \quad q(x) = \alpha\}, \quad \alpha \in \mathbb{R}.$$

Throughout this paper we shall write increasing instead of non-decreasing, and decreasing instead of non-increasing. The following two lemmas were proved in [11].

Lemma 2.1. *Let $p \in L^r(\Omega), r > 1$, and let $q \in L^s(\Omega),\ s = r/(r-1)$. Suppose that every level set of q has measure zero. Then, there exists an increasing function $\xi : \mathbb{R} \to \mathbb{R}$ such that $\xi(q)$ is a rearrangement of p. Furthermore, there exists a decreasing function $\eta : \mathbb{R} \to \mathbb{R}$ such that $\eta(q)$ is a rearrangement of p.*

We denote with $\overline{\mathcal{P}}$ the weak closure of $\mathcal{P}$ in $L^r(\Omega)$.

Lemma 2.2. *Let $\mathcal{P}$ be the set of rearrangements of a fixed function $p_0 \in L^r(\Omega),\ r > 1,\ p_0 \neq 0$, and let $q \in L^s(\Omega),\ s = r/(r-1),\ q \neq 0$. If there is an increasing function ξ such that $\xi(q) \in \mathcal{P}$, then*

$$\int_\Omega pq dx \leqslant \int_\Omega \xi(q) q dx \quad \forall p \in \overline{\mathcal{P}}$$

and the function $\xi(q)$ is the unique maximizer relative to $\overline{\mathcal{P}}$. Furthermore, if there is a decreasing function η such that $\eta(q) \in \mathcal{P}$, then

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