Eigenvalue problems of a two-dimensional Schrödinger operator with nonparabolic effective mass

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In this paper, we study the eigenvalue problem for the Schrödinger operator on a two dimensional disk with nonparabolic effective mass approximation. Here the effective mass depends on the energy states. Our results mainly concern with the number of energy states lying in a wire and the monotonicity of energy states with respect to the depth of the wire. © 2004 American Institute of Physics.

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\section{I. INTRODUCTION}

Semiconductor quantum wires (or dots) are nanoscale structures in which the carriers are confined in two (or three) dimensions. The carriers exhibit wavelike properties in quantum wires and dots, and discrete energy states exist for the structures. These structures have recently attracted intensive research, on their physical phenomena and the corresponding practical applications (see, e.g., Ref. 1). Methods like photoluminescence\textsuperscript{2} and capacitance-voltage spectroscopy\textsuperscript{3} have been used to study the electronic and optical properties of quantum dots. For practical applications, quantum wires and dots play an important role in optoelectronic devices such as infrared photodetectors,\textsuperscript{4} quantum dots laser,\textsuperscript{5} memory device,\textsuperscript{6} and quantum computing systems.\textsuperscript{7}

In this paper, we study the eigenvalue problem for the Schrödinger operator on a disk $D = \{(r, \theta)| \, r \in (0,R_1) \cup (R_1,R_2), \, \theta \in [0,2\pi]\}$:

\begin{equation}
-\hbar^2 \frac{\partial^2 \psi}{\partial m(r,\lambda)^2} + \frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} + V(r) \psi(r,\theta) = \lambda \psi(r,\theta), \tag{1.1}
\end{equation}

where the potential function $V$ is defined by

\begin{equation}
V(r) = \begin{cases} 
0, & r < R_1 \\
0, & R_1 < r \leq R_2. 
\end{cases} \tag{1.2}
\end{equation}

and the nonparabolic effective mass $m(r,\lambda)$ is defined by

\begin{equation}
m(r,\lambda) = \begin{cases} 
m_1(\lambda), & r < R_1 \\
m_2(\lambda), & R_1 < r \leq R_2. 
\end{cases} \tag{1.3}
\end{equation}

Equation (1.1) is equipped with the Dirichlet boundary condition:

\begin{equation}
\psi(R_2,\theta) = 0, \quad \theta \in [0,2\pi]. \tag{1.4}
\end{equation}

We also impose the interface conditions at $r = R_1$ and $\theta \in [0,2\pi]$:

\begin{equation}
\psi(R_1^-,\theta) = \psi(R_1^+,\theta) \tag{1.5}
\end{equation}
and
\[
\frac{1}{m_1(\lambda)} \frac{\partial \psi}{\partial r}(R_1^-, \theta) = \frac{1}{m_2(\lambda)} \frac{\partial \psi}{\partial r}(R_1^+, \theta).
\] (1.6)

Throughout this paper, we further assume that

(i) The effective mass \( m_1(\lambda) \), \( m_2(\lambda) \geq 0 \) are \( C^1 \) and increasing for \( \lambda \in [0, c] \).

(ii) The product \( m_2(\lambda)(c - \lambda) \) is decreasing for \( \lambda \in [0, c] \).

Remark 1.1: In Refs. 8–10, for a quantum wire of small size, the nonparabolic effective mass \( m(\lambda) \) in (1.3) is approximated by
\[
\frac{1}{m_j(\lambda)} \approx \frac{P_j^2}{h^2} \left( \frac{2}{\lambda + a_j - c_j} + \frac{1}{\lambda + a_j - c_j + \delta_j} \right), \quad j = 1, 2,
\] (1.7)
where \( P_j \), \( a_j \), and \( \delta_j \) stand for the momentum, main energy gap and spin–orbit splitting in the \( j \)th region, respectively. The semiconductor band structure parameters are
\[
c_1 = 0, \quad a_1 = 0.235, \quad \delta_1 = 0.81, \quad P_1 = 0.2875;
\]
\[
c_2 = c = \text{the depth of the potential wire}, \quad a_2 = 1.59, \quad \delta_2 = 0.8, \quad P_2 = 0.1993.
\]

By taking the derivatives of \( m_1(\lambda) \) and \( m_2(\lambda)(c - \lambda) \) with respect to \( \lambda \), one can easily verify, for
\[
0 < c \leq \frac{a_2}{2},
\]
that the nonparabolic effective mass approximations \( m_j(\lambda) \) (\( j = 1, 2 \)) satisfy (H1) and (H2).

Such problem and its generalization have been studied by many authors (see, e.g., Refs. 11–16 and the work cited therein). Their results mainly focus on the ratios of and the gaps between eigenvalues. We are led to investigate, in this paper, the eigenstates lying in the wire by the following work. In Refs. 17 and 18, the spatial tunneling (from one hole to another) occurs in coupled quantum wells [one-dimensional (1D)] when the energy states in both wells are aligned. In the case of the hole tunneling in the coupled quantum dots, the tunneling mechanisms are significantly more complicated, due to the band mixing effect. When the energy states are approximately aligned between heavy hole and light hole, mixing tunneling occurs. Moreover, it was reported in Ref. 19 that a chaotic tunneling effect was generated when tunneling occurs. Our effort here aims towards understanding these phenomena. Note also that the discretization of the one-dimensional Schrödinger operator with constant effective mass has recently been reported in Ref. 20.

This paper is organized as follows. In Sec. II, we apply separation of variables and derive the secular equations for (1.1):
\[
f_k(\lambda) = g_k(\lambda) \quad (k = 0, 1, 2, \ldots; \quad \lambda \in [0, c]),
\]
from which \( \lambda \) can be solved. In Sec. III, we show for all \( k \) that \( f_k(\lambda) \) is decreasing and \( g_k(\lambda) \) is increasing. Furthermore, we shall show that \( g_k(\lambda) \) is continuous in \( [0, c] \). In Sec. IV, we utilize the results in Secs. II and III to find the exact number of energy states lying in the wire, i.e., those eigenvalues in \( [0, c] \). We shall give a sufficient and necessary condition which guarantees the existence of at least one energy state in the wire. The monotonicity of the energy state with respect to \( c \), the depth of the wire, is also obtained. Section V contains some brief concluding remarks.

II. SECULAR EQUATIONS

In this section we shall derive the secular equations for the eigenvalue problem (1.1). To this end, we apply the technique of separation of variables, assuming that the wave function \( \psi \) satisfies
\[ \psi(r, \theta) = u(r) \omega(\theta). \]  
\[ \text{(2.1)} \]

Substituting (2.1) into (1.1) we get
\[ \frac{r^2}{u(r)} \left\{ -\frac{\hbar^2}{2} \left( \frac{d^2 u}{dr'^2} + \frac{1}{r} \frac{du}{dr'} \right) + m(r, \lambda) \left[ V(r) - \lambda \right] u(r) \right\} = \frac{\hbar^2}{2} \frac{1}{\omega(\theta)} \frac{d^2 \omega}{d \theta^2}. \]  
\[ \text{(2.2)} \]

Furthermore, the boundary condition (1.4) becomes
\[ u(R_2) = 0, \]  
\[ \text{(2.3)} \]
and the interface conditions (1.5) and (1.6), respectively, become
\[ u(R_1^-) = u(R_1^+) \]  
\[ \text{(2.4)} \]
and
\[ \frac{1}{m_1(\lambda)} \frac{du}{dr}(R_1^-) = \frac{1}{m_2(\lambda)} \frac{du}{dr}(R_1^+). \]  
\[ \text{(2.5)} \]

As (2.2) holds for all values of \( r \in [0, R_1] \cup (R_1, R_2] \) and \( \theta \in [0, 2\pi] \), both sides of the equation equal to a constant. Consequently, the right hand side of (2.2) implies that the function \( \omega(\theta) \) satisfies the following boundary value problems:
\[ \frac{\omega''(\theta)}{\omega(\theta)} = -k^2, \quad \omega(0) = \omega(2\pi), \quad \omega'(0) = \omega'(2\pi), \]
where \( k = 0, 1, 2, \ldots \). For convenience, we shall denote
\[ \alpha = \sqrt{2m_1(\lambda)}\lambda/\hbar^2, \quad \beta = \sqrt{2m_2(\lambda)}(c - \lambda)/\hbar^2. \]  
\[ \text{(2.6)} \]

Similarly, the left hand side of (2.2) implies, for \( k = 0, 1, 2, \ldots, \)
\[ r^2u'' + ru' + (r^2\alpha^2 - k^2)u = 0, \quad \text{for } 0 < r < R_1 \]  
\[ \text{(2.7)} \]
and
\[ r^2u'' + ru' - (r^2\beta^2 + k^2)u = 0, \quad \text{for } R_1 < r < R_2. \]  
\[ \text{(2.8)} \]

Let \( J_k \) be Bessel functions of the first kind of order \( k \), which satisfies the Bessel’s equation \( r^2u'' + ru' + (r^2 - k^2)u = 0 \). Let \( I_k \) and \( K_k \), respectively, be the modified Bessel functions of the first and second kind of order \( k \), which are linearly independent solutions of the modified Bessel’s equation \( r^2u'' + ru' - (r^2 + k^2)u = 0 \).

For a given \( k \), (2.7) and (2.8) imply that the solution of (2.2) is given by
\[ u(r) = AJ_k(\alpha r), \quad \text{for } 0 < r < R_1 \]  
\[ \text{(2.9)} \]
and
\[ u(r) = BJ_k(\beta r) + CK_k(\beta r), \quad \text{for } R_1 < r \leq R_2, \]  
\[ \text{(2.10)} \]
where \( A, B, \) and \( C \) are constant coefficients to be determined. Note that Bessel functions of the second kind are absent in (2.9) because of the boundedness of the eigenfunction \( \psi(r, \theta) = u(r) \omega(\theta) \).

Now, applying the boundary condition (2.3) to (2.10), we obtain
Applying the interface conditions (2.4) and (2.5) to (2.9) and (2.10), we have
\[ AJ_\ell(\alpha R_1) = B[I_k(\beta R_1) - D_k K_k(\beta R_1)] \] (2.12)
and
\[ \frac{A}{m_1(\lambda)} \alpha J'_\ell(\alpha R_1) = \frac{B}{m_2(\lambda)} \beta[I'_k(\beta R_1) - D_k K'_k(\beta R_1)]. \] (2.13)

Dividing (2.13) by (2.12), we can show that an eigenvalue of (1.1) is a root of the secular equations
\[ f_k(\lambda) = g_k(\lambda) \quad (k=0,1,2,...), \] (2.14)
where
\[ f_k(\lambda) = \frac{1}{m_1(\lambda)} \frac{\alpha J'_\ell(\alpha R_1)}{J_\ell(\alpha R_1)} \] (2.15)
and
\[ g_k(\lambda) = \frac{1}{m_2(\lambda)} \frac{\alpha J'_\ell(\alpha R_1)}{J_\ell(\alpha R_1)}, \quad \tilde{g}_k(\lambda) = \frac{\beta[I'_k(\beta R_1) - D_k K'_k(\beta R_1)]}{I_k(\beta R_1) - D_k K_k(\beta R_1)}. \] (2.16)

Remark 2.1. Assumptions \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) are not involved in the derivation of the secular equations (2.14). Thus, (2.14) holds for any effective mass \( m(r, \lambda) \) and can be used in numerical computations involving the eigenvalues of (1.1).

III. MONOTONICITY OF \( f_k \) AND \( g_k \)

In this section, we shall study the monotonicity of \( f_k \) and \( g_k \) with respect to \( \lambda \) and \( c \). To this end, we first quote some well-known and useful properties of \( J_k \), \( I_k \), and \( K_k \), as well as the Comparison Theorem [Ref. 21, p. 24] for differential equations.

Proposition 3.1 (Ref. 22, p. 79): Let \( k \) be a nonnegative integer. Then the following properties hold.

(i) \[ J_k(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n! \Gamma(n+k+1)} \left( \frac{x}{2} \right)^{2n+k}, \text{ where } \Gamma(\cdot) \text{ is the gamma function.} \]

(ii) \[ I_k(x) = \sum_{n=0}^{\infty} \frac{\left( \frac{x}{2} \right)^{2n+k}}{n! \Gamma(n+k+1)}. \]

(iii) \[ K_k(x) = -J_k(x) \ln \frac{x}{2} + \frac{1}{2} \sum_{n=0}^{k-1} (-1)^n \frac{(k-n-1)!}{n!} \left( \frac{x}{2} \right)^{k-2n} \]
\[ + (-1)^{k+1} \sum_{n=0}^{\infty} \frac{\left( \frac{x}{2} \right)^{k+2n}}{n!(n+k)!} \left( \frac{\Gamma'(n+1)}{\Gamma(n+1)} + \frac{\Gamma'(n+k+1)}{\Gamma(n+k+1)} \right), \text{ for } k \geq 1. \]
\[ K_0(x) = -I_0(x) \ln \frac{x}{2} + \frac{1}{2} \sum_{n=0}^{\infty} \left( \frac{x}{2} \right)^{2n} \frac{\Gamma'(n+1)}{n!\Gamma(n+1)}. \]

(iv) \( I_k(x), K_k(x) > 0, \) for \( x > 0. \)

(v) \( I_{k+1} + I_{k-1} = 2I_k', \quad I_0' = I_1. \)

(vi) \( K_{k+1} + K_{k-1} = -2K_k', \quad K_0' = -K_1. \)

(vi) \( W[I_k(x), K_k(x)] = -\frac{1}{x} \) where \( W\{\cdot, \cdot\} \) denotes the Wronskian of two functions.

**Theorem 3.1 (Comparison Theorem):** Let \( u \) and \( v \) be, respectively, the solutions of the differential equations

\[ y' = F(y, x), \quad z' = G(z, x) \]

where \( F(\eta, x) \leq G(\eta, x) \) in the strip \( a \leq x \leq b, \) and \( F \) and \( G \) satisfy the Lipschitz condition. If \( u(a) \leq v(a) \) then \( u(x) \leq v(x), \) for all \( x \in [a, b]. \)

Now, we are ready to prove the monotonicity properties of \( f_k \) and \( g_k, \) with a modified Prüfer transform\(^1\) for linear second-order boundary value problems.

**Proposition 3.2:** Assume that (H1) and (H2) in Sec. I hold.

(i) For each \( k, \) \( f_k(\lambda) \) is decreasing.

(ii) \( f_k|_{\lambda=0}=k/m_1(0)R_1. \)

**Proof:** For a given \( k, \) denote \( u(r) = J_k(\alpha r). \) Then \( u \) satisfies the differential equation (2.7). Note that \( f_k(\lambda) = u'(R_1)/[m_1(\lambda)u(R_1)], \) and define the modified Prüfer transform

\[ \tan \phi(r, \lambda) = \frac{u'(r)}{m_1(\lambda)u(r)}. \quad (3.1) \]

Differentiating (3.1) and with the help of (2.7), we can show that \( \phi \) satisfies the first-order differential equation

\[ \phi' = F(\phi, r, \lambda) := \frac{uu'' - (u')^2}{m_1(\lambda)} \left[ \frac{1}{m_1(\lambda)} \left( \frac{u'}{u} \right)^2 + \frac{u''}{u} \right] = \left[ -\frac{2\lambda}{h^2} + \frac{k^2}{m_1(\lambda)r^2} \right] \cos^2 \phi - \frac{1}{r} \sin \phi \cos \phi - m_1(\lambda) \sin^2 \phi. \quad (3.2) \]

Routine calculations, with the help of Proposition 3.1 (i), then yield

\[ \frac{u'}{m_1(\lambda)u} = \sqrt{\frac{2\lambda}{m_1(\lambda)h^2} \frac{J_k'(\sqrt{2m_1(\lambda)\lambda/h^2} r)}{J_k(\sqrt{2m_1(\lambda)\lambda/h^2} r)} = \frac{k}{m_1(\lambda)r} = \frac{\lambda r}{(k+1)h^2} + O(m_1(\lambda)\lambda^2 r^3).} \quad (3.3) \]

Consequently, for \( \lambda_1 > \lambda_2 \) and a sufficiently small \( r_0 > 0, \) we arrive at

\[ \frac{u'(r)}{m_1(\lambda)u(r)} \bigg|_{r = r_0, \lambda = \lambda_1} \leq \frac{u'(r)}{m_1(\lambda)u(r)} \bigg|_{r = r_0, \lambda = \lambda_2}, \]

hence
On the other hand, it follows from (3.2) that $F$ is Lipschitz continuous for $r \in [r_0, R_1]$ and is decreasing with respect to $\lambda$. Thus, from (3.4) and Theorem 3.1, we have $\phi(R_1, \lambda_1) \leq \phi(R_1, \lambda_2)$. From (2.15), (3.1) and the definition of $u(r)$, assertion (i) follows. Assertion (ii) is a direct consequence of (3.3).

\begin{proof}
Since $K_k(x)$ never vanishes, we define $h(x) := I_k(x)/K_k(x)$. Using Proposition 3.1 (vii), it follows that $h'(x) = [xK_k(x)^2]^{-1} > 0$, and the assertion follows.
\end{proof}

Proposition 3.4: Assume $m_2(\lambda) > 0$, for $\lambda \in [0, c]$. For any nonnegative integer $k$, we have

\begin{enumerate}
  \item $\overline{g}_k(\lambda)$ on (2.16) is continuous and nonpositive on $[0, c)$, and so is $g_k(\lambda)$.
  \item $\lim_{c \to c^-} g_k(\lambda) = \begin{cases} m_2(\lambda)R_1 \ln R_1/R_2 \; & k=0, \\
                        m_2(\lambda)R_1(R_1^2-R_2^2)^{-1} \; & k>1. \end{cases}$
\end{enumerate}

\begin{proof}
Applying Proposition 3.3 to (2.16), together with (2.11), we can show that the denominator of $\overline{g}_k$ is negative, implying that $\overline{g}_k$ is continuous. From Proposition 3.1 (v) and (vi), it follows that the numerator of $\overline{g}_k$ is positive. Thus, $\overline{g}_k(\lambda) < 0$ for $0 < \lambda < c$. As $\overline{g}_k = \overline{g}_k/m_2(\lambda)$ and $m_2(\lambda) > 0$, assertion (i) holds.

To prove assertion (ii), a straightforward application of \textsc{Mathematica} on Proposition 3.1 (ii) and (iii) produces

$$
\frac{K_k(\beta R_2) I'_k(\beta R_1) - I_k(\beta R_2) K'_k(\beta R_1)}{K_k(\beta R_2) I_k(\beta R_2) - I'_k(\beta R_1) K_k(\beta R_1)}
= \begin{cases} 
\beta R_1 \ln \frac{R_1}{R_2}^{-1} + O(\beta), & k=0 \\
\left( \beta R_1 \ln \frac{R_1}{R_2} \right)^{-1} + O(\beta), & k>1. 
\end{cases}
$$

when $\beta$ is sufficiently small. The fact that $\beta \to 0$ as $\lambda \to c$ leads to assertion (ii).
\end{proof}

Proposition 3.5: Assume that $(\mathcal{H}1)$ and $(\mathcal{H}2)$ hold. Then for any nonnegative integer $k$,

\begin{enumerate}
  \item $g_k$ is increasing with respect to $\lambda$ for $0 \leq \lambda < c$, and
  \item $\overline{g}_k$ is decreasing with respect to $c$.
\end{enumerate}

\begin{proof}
We first show that $\overline{g}_k$ in (2.16) is decreasing with respect to $\beta$. Let

$$
u(r) = I_k(\beta r) - D_k K_k(\beta r).$$

Define the Prüfer transform $\tan \phi = v = u'/u$. With (2.8) and a similar argument as in the proof of Proposition 3.2, we can show that $\overline{g}_k(\lambda) = v \big|_{r=R_1}$ and $\phi$ satisfies

$$
\phi' = \frac{1}{r^2} \left( \cos^2 \phi \right) (\beta^2 r^2 + k^2) - \frac{1}{r} \sin \phi \cos \phi - \sin^2 \phi.
$$

From Proposition 3.3, it follows for each $\beta$ that $u(r, \beta) = 0$ only when $r = R_2$. Together with the definitions of the Bessel functions $I_k$ and $K_k$, we prove that $\nu$ is continuous for $0 < r < R_2$ and
IV. MAIN RESULTS

In this section, we shall prove the main result of this paper. Denote the eigenvalue of (1.1) by 
\[ \lambda_{k,j} \quad (k=0,1,2,\ldots, j=1,2,\ldots), \]
Corresponding to the jth root of the kth secular equation (2.14). We also define 
\[ s_{k,j} \quad (k=0,1,2,\ldots, j=1,2,3,\ldots) \]
to be the real number such that \[ \sqrt{2m_1(s_{k,j})s_{k,j}-R_1/h} \]
is the jth root of the kth Bessel function \( J_k \), with \( s_{k,0}=0 \). It is easy to see that \( s_{k,j} \quad (j=1,2,\ldots) \)
are the singularities of \( f_k \). Note that \( \{s_{k,j}\} \) are well-defined, since \( (H1) \) implies that the function 
\[ \lambda \mapsto m_1(\lambda) \lambda \]
is increasing from zero to infinity in \( [0,\infty) \). Using the properties of \( f_k \) and \( g_k \) in Propositions 3.2, 3.4, and 3.5, we sketch \( f_k(\lambda) \) and \( g_k(\lambda) \) in Fig. 2.

We now prove the first main result that exactly counts the number of eigenvalues of (1.1) which lie in the wire.

Theorem 4.1. Assume that \( (\mathcal{H}1) \) and \( (\mathcal{H}2) \) hold. Suppose \( s_{k,n}<c<s_{k,n+1} \) for some \( n \geq 0 \). If 
\[ f_k(c)<g_k(c), \] then \( \lambda_{k,1}, \ldots, \lambda_{k,n+1} \) lie in the wire; otherwise, \( \lambda_{k,1}, \ldots, \lambda_{k,n} \) lie in the wire and
\( \lambda_{k,n+1} \) is out of the wire. Moreover, for any given size and depth of the wire in (1.1), there exists \( \tilde{R}_2 \) such that there is at least one energy state lying in the wire for \( R_2 > \tilde{R}_2 \).

**Proof:** For a fixed \( k \), define \( d(l) = f_k(l) - g_k(l) \). It follows from Propositions 3.2 and 3.5 that \( d \) is decreasing in \( l \). Since \( g_k \) is continuous on \( [0,c] \), \( d \) has only singularities \( s_{k,1}, s_{k,2}, \ldots, s_{k,n} \) in \( (0,c) \). But \( f_k(0) > 0 \) and \( g_k(0) < 0 \) imply that \( \lambda_{k,j} \in (s_{k,j}, s_{k,j+1}) \), \( j = 1, 2, \ldots, n \). The existence of \( \lambda_{k,n+1} \) in \( (s_{k,n}, \gamma) \) comes from the inequality \( f_k(c) < g_k(c) \).

To complete the proof, it suffices to consider the case when \( s_{k,1} = c \) we see that \( f_0 \) is continuous on \( [0,c] \), with \( f_0(0) = 0 \), \( f_0(c) = 0 \). Using Proposition 3.4, we have \( g_0(c) = [m_2(c) R_1 \ln(R_1/R_1)]^{-1} \to 0 \) as \( R_2 \to \infty \). The assertion follows. \( \square \)

**Remark 4.1.** (i) A direct consequence of the last assertion of Theorem 4.1 is that when the domain of (1.1) is degenerated to the entire plane, i.e., \( R_2 = \infty \), there is at least one energy state lying in the wire.

(ii) From a computational point of view, all discrete energy states of (1.1) lying in the wire \( [0, c] \) can easily be computed by applying Newton’s iteration or the bisection method to the secular equations (2.14), with \( s_{k,j} \) as initial guesses.

The second main result shows that the increasing monotonicity of the energy state holds with respect to the depth \( c \) of the wire.

**Theorem 4.2.** Each energy state lying in the wire increases as \( c \) increases.

**Proof:** Let \( d(\lambda) = f_k(\lambda) - g_k(\lambda) \). As in the proof of Theorem 4.1, the result follows from Proposition 3.5 (ii). \( \square \)

**V. CONCLUDING REMARKS**

We conclude this paper with some brief remarks and speculation on future works.

The non-parabolic effective mass approximations in (1.7) proposed in Refs. 9 and 10 satisfy satisfy \((\Omega(1)) \) and \((\Omega(2)) \) for specified \( c \). These approximations are thus applicable, for some specific \( c \), in our main Theorems. With assumptions \((\Omega(1)) \) and \((\Omega(2)) \), the monotonicity properties of \( f_k \) and \( g_k \) are ensured. Hence, the roots of (2.14) can be computed by classical iterative methods (e.g., Newton’s method or bisection method). Without assumptions \((\Omega(1)) \) and \((\Omega(2)) \), the monotonicity properties of \( f_k \) and \( g_k \) does not always hold, so it cannot guarantee that there is a unique root of (2.14) between two consecutive singularities. Hence, the number of energy states lying in the wire from Theorem 4.1 becomes a lower bound.

Analogously, the main results of (1.1) in this paper with Neumann boundary conditions can be proved. It may be of interest to study the eigenvalue problem for the Schrödinger operator (or discretized Schrödinger operator) on a 3D the cylindrical domain with Dirichlet or Neumann boundary condition.
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