On the Transfer Matrix Method and the WKB Approximation for the Schrödinger Equation with Position-Dependent Effective Mass

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We have obtained a set of coupled differential equations from the continuous limit of the transfer matrix method. Decoupling such a set of equations yields an extension to the Wentzel-Kramers-Brillouin (WKB) approximation for the Schrödinger equation with a position-dependent effective mass (PDEM). In the classically allowed region, the decoupling is to ignore the reflection resulting from the variations of both the potential and effective mass. By considering an infinite-well example with a PDEM, it is shown that the extended WKB approximation can provide not only an estimation of the eigenenergies, but also an analytic form for the approximate wavefunctions.

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I. INTRODUCTION

The one-dimensional Schrödinger equation with a position-dependent effective mass (PDEM) has been introduced for many microstructures of current interest [1–4]. To understand such an equation analytically, exactly solvable examples have been discussed in the literature [5–7]. On the other hand the transfer matrix method [8–12] is a powerful numerical way to calculate the eigenvalues and eigenfunctions of the Schrödinger equation with a PDEM. To perform this numerical method, the space is divided into a series of slabs so that the effective mass and potential can be approximated as constants in a slab. By considering the conservation of the flux, it has been suggested that we should use the BenDaniel condition to match an eigenfunction at each boundary between two adjacent slabs [8–10, 13]. In Ref. [1], Ou, Cao, and Shen derived a dispersion relation for the one-dimensional Schrödinger equation with a PDEM by considering the analytic transfer matrix method. Such a dispersion relation contains an integral term of the Wentzel-Kramers-Brillouin (WKB) type. It is well-known that the WKB approximation [1, 14–17] provides important classical interpretations in the development of quantum mechanics. Hence it is

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interesting to probe the validity of the WKB approximation after incorporating the variation of the effective mass.

In this paper, a set of coupled differential equations is obtained by considering the continuous limit of the transfer matrix method. Decoupling such a set of equations, the approximate wavefunction of the analytic form

$$\psi(x) = \sqrt{\frac{m^*(x)}{k(x)}} \exp[\pm iS(x)/\hbar]$$
(1)

with

$$S(x) \equiv \int^{x} k(x')dx' \tag{2}$$

is derived in Section II when the effective mass $m^*(x)$ depends on the position x. Here V(x) is the potential, \hbar is the Planck constant divided by 2π , $k(x) \equiv \sqrt{2m^*(x)(E - V(x))}/\hbar$, and E is the eigenenergy. The phase S(x) is of the same form as that in the well-known WKB approximation except that $m^*(x)$ is position-dependent. Therefore, we can extend such an approximation for the one-dimensional Schrödinger equation with a PDEM from the transfer matrix method. When the effective mass becomes constant in space, the approximate solution given by Eq. (1) reduces to the conventional WKB-type function. As discussed in Section III, decoupling in the classically allowed region is to ignore the reflection due to the variations on the effective mass and/or potential. From our study, it becomes clear how to relate the numerical solution obtained from the transfer matrix method to the analytic WKB approximation. By considering an infinite-well example, it is shown that the extended WKB approximation can provide not only an estimation of the eigenenergies, but also an analytic way to understand the eigenfunctions when the effective mass is position-dependent. The conclusion is made in Section IV.

II. TRANSFER MATRIX METHOD AND THE APPROXIMATE WAVEFUNC-TION OF THE WKB-TYPE

When the effective mass m^* depends on the position x, it has been shown that the one-dimensional Schrödinger equation should be modified as [1–4]

$$-\frac{d}{dx}\frac{\hbar^2}{2m^*(x)}\frac{d}{dx}\psi(x) + V(x)\psi(x) = E\psi(x).$$
(3)

In this paper we assume that $m^*(x) > 0$. In addition, let $m^*(x)$ and V(x) be analytic functions. For convenience, in this section we only consider the classically allowed region where

$$E - V(x) > 0 \tag{4}$$

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at any point x. To extend the WKB approximation, the equation

$$\frac{d}{dx} \begin{bmatrix} t(x) \\ r(x) \end{bmatrix} = \mathbf{\Gamma}(x) \begin{bmatrix} t(x) \\ r(x) \end{bmatrix}$$
(5)

will be derived in this section by considering the continuous limit of the transfer matrix method. Here the position-dependent matrix is

$$\mathbf{\Gamma}(x) \equiv \begin{bmatrix} -ixk'(x) - \frac{m^*(x)}{2k(x)} \left(\frac{k(x)}{m^*(x)}\right)' & \frac{m^*(x)}{2k(x)} \left(\frac{k(x)}{m^*(x)}\right)' e^{-2ixk(x)} \\ \frac{m^*(x)}{2k(x)} \left(\frac{k(x)}{m^*(x)}\right)' e^{2ixk(x)} & ixk'(x) - \frac{m^*(x)}{2k(x)} \left(\frac{k(x)}{m^*(x)}\right)' \end{bmatrix},$$
(6)

where t(x) and r(x) are two complex functions. In this paper the notation f'(x) represents the derivative of any function f(x). With some calculation, we can see that Eq. (5) is equivalent to Eq. (3) if we set

$$\psi(x) = t(x)e^{ik(x)x} + r(x)e^{-ik(x)x}.$$
(7)

Then approximate solutions of the WKB type are obtained by decoupling Eq. (5). Therefore, we can relate the WKB-type solution to the transfer matrix method.

The transfer matrix method is a powerful numerical approach for solving Eq. (3) [8–10]. To perform such a method, as shown in Fig. 1, we can divide the space into a series of thin slabs, so that both the effective mass and potential can be approximated as constants in each slab. For convenience, each slab is labeled by an integer j sequentially from left to right. In the classically allowed region, the wavefunction $\psi(x)$ in a slab can be approximated as the linear superposition of two plane waves. Let x_j be the center point of the j-th slab and approximate the effective mass, potential, and wave number as $m_j^* = m^*(x_j)$, $V_j = V(x_j)$, and $k_j = k(x_j)$ in such a lab, respectively. Then the wave function is taken as

$$\psi(x) = t_j e^{ik_j x} + r_j e^{-ik_j x} \tag{8}$$

in the *j*-th slab. The coefficients t_j and r_j are the traveling components for two different directions. We shall consider the BenDaniel condition [13] to relate the coefficients of adjacent slabs [18, 19]. Based on such a condition, as shown in the Appendix, the coefficients t_{j+1} and r_{j+1} are related to t_j and r_j by

$$\begin{bmatrix} t_{j+1} \\ r_{j+1} \end{bmatrix} = \mathcal{T}_j \begin{bmatrix} t_j \\ r_j \end{bmatrix}$$
(9)

with the transfer matrix

$$\mathcal{T}_{j} = \begin{bmatrix} \frac{1}{2} \left(1 + \frac{k_{j}}{m_{j}^{*}} \frac{m_{j+1}^{*}}{k_{j+1}}\right) e^{i(k_{j} - k_{j+1})y_{j}} & \frac{1}{2} \left(1 - \frac{k_{j}}{m_{j}^{*}} \frac{m_{j+1}^{*}}{k_{j+1}}\right) e^{-i(k_{j} + k_{j+1})y_{j}} \\ \frac{1}{2} \left(1 - \frac{k_{j}}{m_{j}^{*}} \frac{m_{j+1}^{*}}{k_{j+1}}\right) e^{i(k_{j} + k_{j+1})y_{j}} & \frac{1}{2} \left(1 + \frac{k_{j}}{m_{j}^{*}} \frac{m_{j+1}^{*}}{k_{j+1}}\right) e^{-i(k_{j} - k_{j+1})y_{j}} \end{bmatrix} .$$
(10)

Here y_j is the point separating the *j*-th and (j + 1)-th slabs, so $x_{j+1} = (y_j + y_{j+1})/2$. It is shown in the Appendix that we can relate the transfer matrix \mathcal{T}_j to $\Gamma(\mathbf{x})$ by

$$\mathcal{T}_j = \mathbf{I} + \mathbf{\Gamma}(y_j) \Delta x_j + o(\Delta x_j^2), \qquad (11)$$

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FIG. 1: To perform the transfer matrix method, the space is divided into a series of slabs, in each of which both the potential and effective mass are approximated as constants. The points x_j and x_{j+1} represent the centers of the *j*-th and (j + 1)-th slabs, and y_j is the point separating these two slabs.

with
$$\Delta x_j \equiv x_{j+1} - x_j$$
 and

$$\mathbf{I} \equiv \begin{bmatrix} 1 & 0\\ 0 & 1 \end{bmatrix}.$$
(12)

Let $\Delta t_j \equiv t_{j+1} - t_j$ and $\Delta r_j \equiv r_{j+1} - r_j$. From Eqs. (9) and (11), we have the following set of equations:

$$\frac{1}{\Delta x_j} \begin{bmatrix} \Delta t_j \\ \Delta r_j \end{bmatrix} = \mathbf{\Gamma}(y_j) \begin{bmatrix} t_{x_j} \\ r_{x_j} \end{bmatrix} + o(\Delta x_j) \,. \tag{13}$$

By shrinking the widths of the slabs so that Δx_j approaches zero, the above equation can be reduced to Eq. (5) with the following correspondence:

$$\begin{bmatrix} t_j \\ r_j \end{bmatrix} \leftrightarrow \begin{bmatrix} t(x_j) \\ r(x_j) \end{bmatrix}.$$
(14)

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Thus we can obtain Eq. (5) by considering the continuous limit of the transfer matrix method. From Eqs. (8) and (14), we can see why the wave function is determined by Eq. (7) after obtaining r(x) and t(x).

In Eq. (5), the coefficients t(x) and r(x) are coupled to each other by the off-diagonal terms of $\Gamma(x)$. With some calculation, we can see from Eq. (11) that these terms come from the off-diagonal terms of \mathcal{T}_j , which correspond to the reflection due to the variations of the potential and/or effective mass [8–10]. If we ignore the reflection by neglecting the coupling between t(x) and r(x), we have the following decoupled equations:

$$\frac{d}{dx}t(x) \sim \left[-ixk'(x) - \frac{m^*(x)}{2k(x)}\left(\frac{k(x)}{m^*(x)}\right)'\right]t(x), \qquad (15)$$

$$\frac{d}{dx}r(x) \sim \left[ixk'(x) - \frac{m^*(x)}{2k(x)}\left(\frac{k(x)}{m^*(x)}\right)'\right]r(x).$$
(16)

Solving the above two first-order differential equations, we have

$$t(x)e^{ik(x)x} \sim c_1 \sqrt{\frac{m^*(x)}{k(x)}} \exp(iS(x)/\hbar),$$
 (17)

$$r(x)e^{-ik(x)x} \sim c_2 \sqrt{\frac{m^*(x)}{k(x)}} \exp(-iS(x)/\hbar).$$
 (18)

Here c_1 and c_2 are two constants. From Eq. (7), the approximate solution is of the form

$$\psi(x) \sim c_1 \sqrt{\frac{m^*(x)}{k(x)}} \exp(iS(x)/\hbar) + c_2 \sqrt{\frac{m^*(x)}{k(x)}} \exp(-iS(x)/\hbar).$$
 (19)

We shall set $c_1=0$ ($c_2=0$) such that t(x)=0 (r(x)=0) for the traveling wave moving to the right (left), and obtain the WKB-type function given by Eq. (1). Therefore, analytic functions of the WKB-type can be related to the numerical transfer matrix method by ignoring the reflection in the continuous limit.

III. DISCUSSION

In the last section, the approximate solution of the WKB-type is derived for the classically allowed region by ignoring the off-diagonal terms of $\Gamma(x)$ to thereby decouple Eq. (5). With increasing eigenenergy E, this is reasonable for k(x) >> 1, because the off-diagonal terms contain the factor $e^{\pm 2ik(x)x}$, which oscillates quickly under large k(x). On the other hand, the diagonal terms of $\Gamma(x)$ do not contain such an oscillating factor. Hence Eq. (1) provides a good approximation for the states with high energies, as in the conventional WKB approximation. Because the transfer matrix \mathcal{T}_i can be related to $\Gamma(x)$

by Eq. (11), we can expect that the numerical solution obtained by the transfer matrix method can be reduced to the WKB-type function as k(x) >> 1.

It has been shown that a dispersion relation of the WKB-type can be used to estimate the eigenenergies of the Schrödinger equation with a PDEM [1]. To further probe the extension of the WKB approximation to systems with a PDEM we consider the infinite quantum well, where

$$m^*(x) = \frac{m_1 - m_2}{2a}x + \frac{m_1 + m_2}{2} \tag{20}$$

and V(x) = 0 if |x| < a, while $V(x) = \infty$ if $|x| \ge a$. We do not need to consider how the phase changes at the turning points in this case [1, 14], and just need to set the eigenfunctions to be zero at $x = \pm a$. Hence we shall take $c_1 = -c_2 \equiv c$ in Eq. (19) to obtain the approximate eigenfunctions of WKB type:

$$\psi(x) \sim c_{\sqrt{\frac{m^*(x)}{k(x)}}} \sin(iS(x)/\hbar), \qquad (21)$$

if we set $S(x) = \int_{-a}^{x} \sqrt{2m^*(x')(E - V(x'))} dx'$ and require $S(a) = n\pi$. Here *n* is a nonnegative integer. Then we can obtain the WKB dispersion relation

$$E_n = \frac{9n^2(m_1 - m_2)^2 h^2}{128(m_1^{3/2} - m_2^{3/2})^2 a^2} \quad \text{with } n = 1, 2, 3, \dots .$$
(22)

On the other hand, we can reduce Eq. (3) as

$$\frac{d^2}{dy^2}u(y) = yu(y) \tag{23}$$

in such an example, if we set

$$y = -\left(\frac{(m_1 - m_2)E}{\hbar^2 a}\right)^{1/3} \left(x + \frac{m_1 + m_2}{m_1 - m_2}a\right)$$

and $u(y) = \psi'(x)/m^*(x)$. The solution of the above equation is a linear combination of Airy functions [17, 20], and thus it is easy to obtain the exact eigenvalues and wavefunctions. In Table 1, we compare the exact and approximate eigenenergies when $m_1 = 0.1 m_0$, $m_2 = 0.2 m_0$, and a = 5 nm. Here m_0 is the rest mass of the electron. We can see from Table 1 that the errors of the WKB approximation are reduced with increasing n. The error for the n=4 excited eigenlevel is only about 0.14%, and we can see from Fig. 2(a) that the corresponding WKB wavefunction is very close to the exact one. (In Fig. 2, both the approximate and exact wavefunctions are normalized such that $\int_{-a}^{a} |\psi(x)|^2 dx = 1$.) Therefore, the extended WKB approximation provides not only a good estimation for the eigenenergies, but also a good way to understand the wavefunctions. Figure 2(b) shows the square of the n = 4 wavefunction. The oscillating amplitudes, in fact, are proportional to the factor $\sqrt{m^*(x)/k(x)}$, as expected from Eq. (21).





FIG. 2: (a) The red dashed line and the black dotted line correspond to the exact wavefunction and the WKB approximate one. (b) The solid line is the square of the wavefunction and the dotted line is the envelope function proportional to $m^*(x)^{1/2}$.

n	WKB (eV)	Exact (eV)	Error (%)
1	0.0253	0.0258	1.93
2	0.1012	0.1018	0.55
3	0.2278	0.2283	0.25
4	0.4049	0.4055	0.14
5	0.6327	0.6333	0.09
6	0.9111	0.9117	0.06
7	1.2401	1.2407	0.05
8	1.6197	1.6203	0.04
9	2.0499	2.0505	0.03
10	2.5308	2.5313	0.02

TABLE I: The comparison of the WKB and exact eigenvalues for the solvable example discussed in the text.

For the tunneling through a classically forbidden region where E - V(x) < 0, it is known that we can obtain an estimation for the tunneling probability from the WKB approximation if the (effective) mass is constant. With some calculation, we can obtain Eq. (5) with the same $\Gamma(x)$ for the classically forbidden region from the continuous limit of the transfer matrix method. (It should be noted that k(x) becomes imaginary.) In addition, the WKB-type approximate solution given by Eq. (1) can still be obtained by decoupling Eq. (5). In fact, it is shown in Ref. [6] that Eq. (3) can be transformed to the conventional Schrödinger equation,

$$\left[\frac{d^2}{dy^2} - \frac{2}{\hbar^2}(\mathcal{V}(y) - E)\right]\phi(y) = 0, \qquad (24)$$

if we set $y = \int \sqrt{m^*(x)} dx$, $\phi(y) = \psi(x)/m^{*1/4}(x)$, and $\mathcal{V}(y) = V(x) + F(x)$. Here $\frac{\hbar^2}{dx^2} \left[\frac{d^2}{dx^2} m^*(x) - \frac{7}{2} (\frac{d}{dx} m^*(x))^2 \right]$

$$F(x) = -\frac{\hbar^2}{8m^*(x)} \left[\frac{\frac{d^2}{dx^2}m^*(x)}{m^*(x)} - \frac{7}{4} \left(\frac{\frac{d}{dx}m^*(x)}{m^*(x)}\right)^2 \right]$$

With some calculation, in fact, we can see that Eq. (1) can also be obtained from the conventional WKB-type function by considering such a transform after ignoring F(x). This



FIG. 3: A finite-well problem where both the effective mass and he potential have sharp jumps at the interfaces A_1 and A_2 . The regions denoted by (I), (II), and (III) are divided by these two interfaces.

approximation is reasonable when $m^*(x)$ varies so slowly that its derivatives are small. Because the WKB approximation may provide a suitable approximation to the above equation in the classically forbidden region, Eq. (1) also provides an extension of the WKB approximation when E - V(x) < 0.

Just as in the conventional WKB approximation, reflection is neglected if we use Eq. (1) to approximate the wavefunction. If the effective mass or potential has sharp jumps at some interfaces, we cannot ignore the reflection, and Eq. (1) does not give us a good approximate solution in the whole space. But we may apply Eq. (19) piecewisely to approximate the wavefunction. For example, consider a finite-well problem where the potential and effective mass have sharp jumps at two interfaces A_1 and A_2 , as shown in Fig. 3. We can divide the space into three regions denoted by (I), (II), and (III), respectively, and approximate the wavefunction by Eq. (19) in each region. Then we just need to consider the BenDaniel condition at A_1 and A_2 to obtain the approximate solution in the whole space.

IV. CONCLUSION

In this paper, we derived a set of first-order differential equations corresponding to the continuous limit of the transfer matrix method. Decoupling such a set of equations, an approximate wavefunction of the WKB-type is obtained for the one-dimensional Schrödinger equation with a position-dependent effective mass. In a classically allowed region, the decoupling is to ignore the reflections induced by the variations of the effective mass and potential. This is reasonable in the high-energy limit. From our derivation, it is clear how to relate the WKB approximation to the numerical solution obtained by the transfer matrix method when the effective mass is position-dependent. By considering an infinite-well example, it is shown that such an approximation can provide not only a simple estimation to eigenenergies, but also an analytic form which approximates the eigenfunctions.

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Appendix

In the transfer matrix method, the BenDaniel condition is taken into account to match ψ and ψ'/m^* , the wavefunction and its derivative divided by the effective mass, at the boundary of each slab. At the boundary y_j separating the *j*-th and (j + 1)-th slabs, we have

$$t_{j+1}e^{ik_{j+1}y_j} + r_{j+1}e^{-ik_{j+1}y_j} = t_je^{ik_jy_j} + r_je^{ik_jy_j}$$
(25)

by matching ψ , and

$$i\frac{k_{j+1}}{m_{j+1}^*}t_{j+1}e^{ik_{j+1}y_j} - i\frac{k_{j+1}}{m_{j+1}^*}r_{j+1}e^{-ik_{j+1}y_j} = i\frac{k_j}{m_j^*}t_je^{ik_jy_j} - i\frac{k_j}{m_j^*}r_je^{ik_jy_j}$$
(26)

by matching ψ'/m^* , if ψ is approximated by Eq. (8). We can obtain Eqs. (9) and (10) by relating t_{j+1} and r_{j+1} to t_j and r_j from the above two equations.

By introducing the function $h(x) \equiv k(x)/m^*(x)$, the factor

$$\frac{k_j}{m_j^*} \frac{m_{j+1}^*}{k_{j+1}} = \frac{h(x_j)}{h(x_{j+1})} = 1 - \frac{h'(y_j)}{h(y_j)} \Delta x + o(\Delta x^2).$$
(27)

Based on the above equation, we can obtain Eq. (11) as the first-order approximation with respect to Δx since $e^{\pm i(k_{j+1}-k_j)y_j} \sim 1 \pm iy_i k'(y_j) \Delta x$ and $e^{\pm i(k_{j+1}+k_j)y_j} \sim e^{\pm 2ik(y_j)y_j}$.

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