Electron-wave-function calculation in the continuous part of the spectrum: The case of slowly varying potential asymptotics

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In this paper we address the problem of calculating the free-state wave functions with predefined asymptotic behavior. It is shown that, in a number of cases, usable results may be obtained by the WBK (Wentzel-Brillouin-Kramers) approximation, but not by plain numerical integration of the Schrödinger equation if it is performed with accuracy normally provided by computers. For reference purposes, the calculation based on algebra implemented in MATHEMATICA® is done, enabling an arbitrary large number of significant digits to be used. The WBK-based calculation is found to offer reasonably low errors. [S1063-651X(96)03705-6]

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I. INTRODUCTION

The general method of finding the continuum (free)-state wave functions in time-independent quantum systems is to construct the scattering states by iterated use of the Lipmann-Schwinger equation [1]. A simpler procedure for practical use is to find the scattering states as linear combinations of waves in the asymptotic regions of the scattering potential. The method is generally applicable, regardless of the system symmetry, although it has been discussed mostly for spherically symmetric cases [1,2] due to their importance in atomic physics. The development of advanced technologies of semiconductor growth in the last two decades enabled fabrication of ultrathin quantum-confining structures, usually with plane symmetry. Finding the free-state wave functions in such structures is important in studying various physical phenomena [3–5]. This may be done by finding the scattering matrix, from which the wave functions are directly calculated.

An alternative procedure for calculating the wave functions in the continuum is by quasidiscretization, i.e., introduction of box boundary conditions (with distant walls), well known from elementary textbooks in quantum mechanics [6]. This method is straightforwardly applicable only for symmetric systems with asymptotically bounded potentials. There are two types of wave functions here—even and odd—which may exist in the quantization box of length L. As L increases towards infinity, pairs of distinct subsequent states merge into doubly degenerate states. Handling such wave functions is usually easier than with propagating waves, while both choices lead to identical final results. In the regions with flat potential (set equal to zero for convenience), the solutions of the Schrödinger equation are oscillatory in character, their initial phase being unknown at the beginning. This phase may be found by solving the equation for the modulation function (the position-dependent wave-function amplitude), equivalent to the Schrödinger equation. The method has been used, for instance, in calculating the self-consistent potential in inversion layers [7], and quantum-confined microstructures [8]. It turns out, however, that in realistic examples the calculation converges only for small charges accumulated in the well region. Although this suffices for some systems, such as those having a flat built-in potential and a modulated effective mass [8], the majority of real structures with finite binding potential accumulate a considerable charge in the well region, causing the calculation to diverge. This is due to a very slowly decaying electrostatic potential that appears, causing large numerical errors in conventional calculation when integrating the free-state wave functions, such that their values in the well region are meaningless.

In this paper we first point to the source of such errors (Sec. II), and illustrate, on realistic examples, that they can make the conventional calculation completely useless (Sec. III). Furthermore, we discuss how to alleviate the problem by using the WBK (Liouville-Green) approximation (Sec. IV). Thus, instead of solving the Schrödinger differential equation with ''constant tail'' boundary conditions, it is solved by using the asymptotic boundary conditions, in the way described previously in the Orr-Somerfeld problem [9]. Errors introduced by the WBK approximation itself are estimated by an arbitrary large precision algorithm in MATHEMATICA. It also allows one to estimate the minimum accuracy (the number of significant digits) that would be necessary to use in the conventional calculation to guarantee some required accuracy of the wave function. Comparison with high-accuracy reference results obtained by MATHEMATICA indicate that the double-precision arithmetic on a 32-bit digital computer (16 significant digits) will usually fail to give reliable results in the conventional implementation, while the WBK method, although itself approximate, happens to be quite accurate and reliable for practical purposes. Specific examples are also provided.

II. AN ANALYTICALLY SOLVABLE EXAMPLE

The wave function $\Psi(z)$ is to be found by solving the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dz^2}+V(z)\Psi(z)=E\Psi(z). \tag{1}$$

Here m denotes the electron mass, $V(z)$ the potential, $E(>0)$ the electron energy, and z the direction along which the potential varies (in case of semiconductor quantum wells, perpendicular to the well layer plane). The origin is taken in

the middle of the well. Here we imagine the infinite symmetric structure under consideration to be embedded in a quantizing box, its half length denoted as L. We should note that L appears in both the wave-function normalizing factor and in the density of states, and cancels out in any result for physical quantities. The wave function in regions with flat potential, i.e., far from the well, takes the form

$$\Psi(z)=\begin{cases} L^{-1/2}\cos(k_z z+\eta_e) & \text{(even state)} \\ L^{-1/2}\sin(k_z z+\eta_o) & \text{(odd state)}, \end{cases} \tag{2}$$

where $\eta_{(e,o)}$ is the initial phase of the even (odd) state, and k_z is the wave number, related to the energy as $E=\hbar^2 k_z^2/2m$. One may proceed to use the unity amplitude (unnormalized) wave function instead of (2), but the phases are still to be determined. Instead of solving the full Schrödinger equation, an efficient way to do this is to consider the *modulation function* $F(z)$, related to the full wave function as

$$\Psi(z)=F(z)\exp[i(k_z z+\eta)]. \tag{3}$$

Thus, $F(z)$ describes the deviation of the wave function from a simple plane wave. The remaining exponential factor in Eq. (3) actually enables one to derive the differential equation in $F(z)$ with no unknown parameters (the initial phases). If a form other than exponential was chosen, this advantage would be lost. The initial phase η is chosen so as to provide the required behavior of the wave function at the origin. Substituting Eq. (3) into (1), we find

$$\frac{d^2F}{dz^2}=-2ik_z\frac{dF}{dz}+U(z)F, \tag{4}$$

where $U(z)=2mV(z)/\hbar^2$. Here we consider the class of potentials that become flat beyond some $z=w$, i.e., $U(z>w)\equiv 0$, and the wave functions there have simple periodic form. The boundary conditions for the modulation function therefore read

$$F(w)=1, \quad \left.\frac{dF}{dz}\right|_{z=w}=0. \tag{5}$$

The modulation function $F(z)$ is constant in the region $z>w$, as directly follows from Eq. (4) with $V(z)\equiv 0$. The initial phase η can be found from [8]

$$\tan(\eta_e)=\frac{\mathrm{Im}(W)}{\mathrm{Re}(W)}, \quad W=\frac{i}{ik_z F(0)+F'(z)|_{z=0}} \tag{6}$$

for even states and from

$$\tan(\eta_o)=-\frac{\mathrm{Im}[F(0)]}{\mathrm{Re}[F(0)]} \tag{7}$$

for odd states.

To highlight the source of numerical difficulties described in Sec. I it is very instructive to consider the case of rectangular potential barrier, its height being V_0 and width $2w$ (Fig. 1). Equations (1) and (4) can then both be solved analytically. Here we compare the values of the two functions at

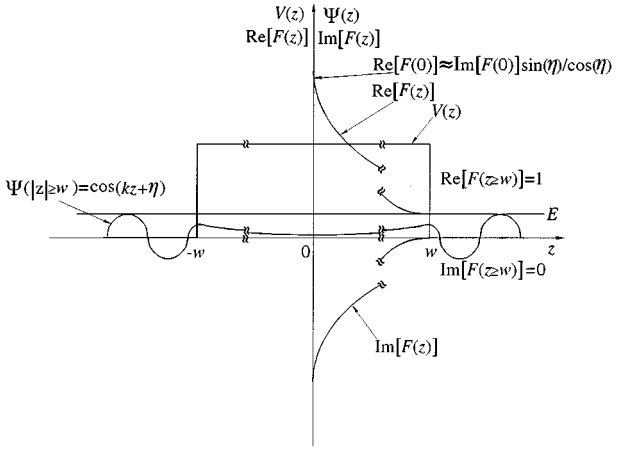

FIG. 1. Qualitative plot of the wave function and the modulation function in case of a wide rectangular barrier. While real and imaginary parts of the modulation function take values very much exceeding unity (in absolute value), their signs are opposite and the wave function is very small, and difficult for accurate evaluation.

the origin in the limit of very wide barrier layer. If $wk_n \gg 1$, the modulation function corresponding to an energy $E<V_0$ at $z=0$ is given by

$$F(0)\approx\frac{1}{2}\left(1-i\frac{k_z}{k_n}\right)\exp[(k_n+ik_z)w], \tag{8}$$

where $k_n=\sqrt{2mV_0/\hbar^2-k_z^2}$. Its amplitude increases with increasing barrier width.

The solution of the Schrödinger equation having, for instance, even parity, has the form $\Psi=C\cosh(k_n z)$ inside the barrier, with

$$C=\left[\cosh^2(k_n w)+\frac{k_n^2}{k_z^2}\sinh^2(k_n w)\right]^{-1/2}. \tag{9}$$

For very large w, the wave function at $z=0$ acquires values much smaller than 1. The even-state wave function may also be written as

$$\begin{aligned}\Psi_e(z)&=\mathrm{Re}\{F(z)\exp[i(k_z z+\eta_e)]\}\\ &=\mathrm{Re}[F(z)]\cos(k_z z+\eta_e)\\ &\quad-\mathrm{Im}[F(z)]\sin(k_z z+\eta_e).\end{aligned} \tag{10}$$

With both the real and imaginary parts of the wave function being on their own very large numbers, even a double precision arithmetic with 16 significant digits may not allow one to actually evaluate the wave function inside the barrier within this approach, its small amplitude being a result of almost complete cancellation of two very large terms.

The relationship between the modulation function and the wave function is illustrated in Fig. 1. In regions of constant potential the real part of the modulation function exponentially decays as z increases, tending towards unity, and the imaginary part also decays exponentially, but tends to zero. In the case of a very wide barrier the values of the real and imaginary parts are related according to the expression given in Fig. 1, and have opposite signs. In contrast to the very

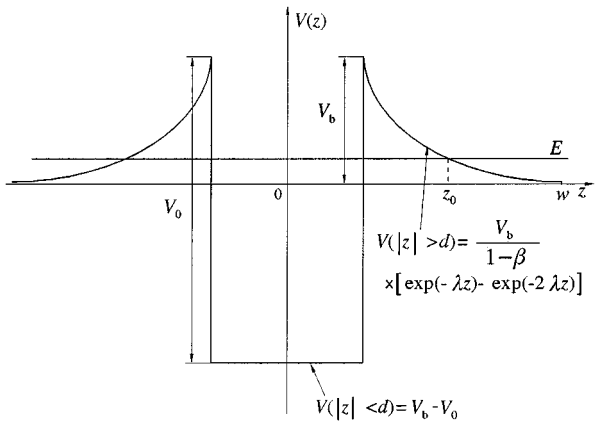

FIG. 2. An example of the potential used to check the validity of the conventional and the ''exact'' MATHEMATICA calculation of free-state wave functions, and also for finding the accuracy of the WBK approximation in this problem (Sec. IV). The potential is flat inside the well ($|z|<d$), and of Morse form outside ($|z|>d$). The right turning point z_0 is also indicated. Due to symmetry, the Schrödinger equation or the equivalent equation for the modulation function should really be solved only on the interval $z\in[0,\infty)$.

large values that they acquire, the wave function becomes diminishingly small, and a large number of significant digits in the value of F is really necessary to evaluate the wave function.

III. THE CONVENTIONAL AND THE ''EXACT'' CALCULATION

We now consider a realistic case of a symmetric rectangular semiconductor quantum well based on the $GaAs/Al_xGa_{1-x}As$ heterojunction, with the potential in the barrier, due to self-consistency effects, taken to be of Morse type (Fig. 2):

$$V(z)=\frac{V_b}{1-\beta}\left[\exp(-\lambda z)-\beta\,\exp(-2\lambda z)\right], \tag{11}$$

where V_b denotes the potential energy at the well-barrier boundary, while, roughly speaking, λ determines the decay rate, and β the point of the potential extremum. In this case the solution of Eq. (4) may be found in the form of a series [7]:

$$F(z)=\sum_{j=0}^{\infty} b_j e^{-j\lambda z}. \tag{12}$$

From Eq. (5) it follows that $b_0=1$. The coefficient b_1 is given by

$$b_1=\frac{V_b}{1-\beta}\,\frac{1}{\lambda^2-2i\lambda k_z}, \tag{13}$$

and higher-order ones by a recurrence relation

$$b_j=\frac{V_b}{1-\beta}\,\frac{b_{j-1}-\beta b_{j-2}}{\lambda j(\lambda j-2ik_z)}, \quad j\geq 2. \tag{14}$$

The potential inside the well is constant, and the wave function is of sine or cosine type.

This scheme is an alternative to direct numerical integration of Eq. (4). The accuracy of the results is, however, easier to control in this procedure than in numerical integration, which is the main reason it was employed in this work (also, it is somewhat faster, but otherwise there are no essential differences between the two). Yet, in a broad range of λ and β values, such that the Morse potential varies slowly, it delivers meaningless results for the wave function inside the well when calculated in the conventional (FORTRAN REAL*8, i.e., 8 bytes) implementation. The reason behind this is just the same as in the case of a rectangular barrier, discussed in Sec. II: the modulation function acquires such large values that a part or all of the significant digits necessary for the initial phase calculation get lost due to truncation errors.

The same procedure can also be built in the MATHEMATICA algorithm to take advantage of the arbitrary precision facility it offers [10] (at the expense of low speed, however). Results obtained that way may therefore be called ''exact.'' They may give a straight answer to whether any trust should be put into the outcome of the conventional (REAL*8) calculation. Additionally, they may serve for testing the accuracy of methods that are approximate *per se*, such as the WBK method considered in Sec. IV.

While various methods for estimating the effects of truncation errors exist, e.g., the interval or Karlsruhe arithmetic [11,12], in the problem we consider these errors seriously affect just one expression, and a simple error propagation analysis will suffice to estimate the necessary precision. The condition number for the even-state wave-function value at the origin is given by

$$\epsilon_{\Psi_e(0)}=\frac{\mathrm{Re}[F(0)]\cos(\eta_e)\,\epsilon_{\mathrm{Re}[F(0)]}}{\Psi_e(0)} - \frac{\mathrm{Im}[F(0)]\sin(\eta_e)\,\epsilon_{\mathrm{Im}[F(0)]}}{\Psi_e(0)}, \tag{15}$$

where ϵ on the right-hand side denotes the relative error of the quantity its subscript refers to. For the odd wave function the same quantity is to be determined from

$$\epsilon_{\Psi'_o|_{z=0}}=\frac{\mathrm{Im}[F'(z)|_{z=0}]\cos(\eta_o)\,\epsilon_{\mathrm{Im}[F(0)]}}{\Psi'_o(z)|_{z=0}} + \frac{\mathrm{Re}[F'(0)|_{z=0}]\sin(\eta_o)\,\epsilon_{\mathrm{Re}[F(0)]}}{\Psi'_o(z)|_{z=0}} + k_z\,\frac{\mathrm{Re}[F(0)]\cos(\eta_o)\,\epsilon_{\mathrm{Re}[F(0)]}}{\Psi'_o(z)|_{z=0}} - k_z\,\frac{\mathrm{Im}[F(0)]\sin(\eta_o)\,\epsilon_{\mathrm{Im}[F(0)]}}{\Psi'_o(z)|_{z=0}}. \tag{16}$$

It is assumed in Eqs. (15) and (16) that both $\sin(\eta)$ and $\cos(\eta)$ are determined accurately. If any of the terms in (15) or (16) exceeds unity in magnitude, errors tend to amplify in the course of calculation, making it ill conditioned [11]. It turns out, practically, that ill conditioning appears in the case of slowly varying potentials. Assuming the relative errors of

the input quantities are all equal, approximating the denominator of the right-hand side of the resulting expression by its geometric mean value, and replacing $\cos^2\eta$ and $\sin^2\eta$ with their average, we find from Eqs. (15) and (16) a rough estimate of the precision (number of significant digits in computation required to give one significant digit correct) for the wave function, or slope of the wave function, at the origin:

$$R_1=\begin{cases}\log_{10}|F(0)/\Psi_e(0)| & \text{for even states}\\ \frac{1}{2}\log_{10}\{[|F_o'(z)|_{z=0}|^2+k_z^2|F(0)|^2]/|\Psi_o'(z)|_{z=0}|^2\} & \text{for odd states.}\end{cases} \tag{17}$$

Two constant terms, $\log_{10}5$ for even states and $-\frac{1}{2}\log_{10}8$ for odd states, were neglected in comparison to the displayed terms in Eq. (17), which proved justified in all realistic situations.

IV. WBK CALCULATION

The difficulties that arise in finding the free-state wave functions, described in Secs. II and III may be alleviated by resorting to an approximate solution of the Schrödinger equation, given by the WBK method, instead of attempting to solve the exact Schrödinger equation (in whatever form). Consider the potential as given in Fig. 2. Denoting the right turning point coordinate as z_0, the wave function in the region $z>z_0$ may be generally written as [13]

$$\Psi(z>z_0)=\frac{A}{\sqrt{k(z)}}\cos\left(\int_{z_0}^{z}k(z')dz'-\frac{\pi}{4}\right)+\frac{B}{\sqrt{k(z)}}\sin\left(\int_{z_0}^{z}k(z')dz'-\frac{\pi}{4}\right) \tag{18}$$

or, in case of even states, as

$$\Psi(z>z_0)=\frac{G}{\sqrt{k(z)}}\cos\left(\int_{z_0}^{z}k(z')dz'+\eta_e\right). \tag{19}$$

Here $k(z)$ is the electron wave vector calculated at z, and it follows directly from (5) and the required pure oscillatory behavior of the wave function at infinite distances from the well center that

$$G=\sqrt{k_z}. \tag{20}$$

The boundary conditions at the well-barrier interface at $z=d$ require both the growing and decaying components of the wave function to be taken into account, although the wave function is growing in the region $d<z<z_0$. At $z=d$ the wave function is given by

$$\Psi(d)=-\frac{A}{\sqrt{|k(d)|}}\exp(I_d)+\frac{B}{2\sqrt{|k(d)|}}\exp(-I_d) \tag{21}$$

and its first derivative is

$$\left.\frac{d\Psi}{dz}\right|_{z=d}=\left(\frac{1}{2\sqrt{|k(d)|}}\left.\frac{d|k(z)|}{dz}\right|_{z=d}+\sqrt{|k(d)|}\right)\exp(I_d)A+\frac{1}{2}\left(-\frac{1}{2\sqrt{|k(d)|}}\left.\frac{d|k(z)|}{dz}\right|_{z=d}+\sqrt{|k(d)|}\right)\exp(-I_d)B, \tag{22}$$

where

$$I_d=\int_{d}^{z_0}|k(z')|dz'. \tag{23}$$

In the interior region $-d<z<d$ first one has to find the wave function $\Psi_{(i)}(z)$ (either numerically, or, if possible, analytically), with some preset value of the even-state wave-function amplitude at $z=0$. Values of A and B are then calculated by matching this solution to the WBK one at $z=d$, i.e.,

$$c_{11}A+c_{12}B=\Psi_{(i)}(d), \tag{24}$$

$$c_{21}A+c_{22}B=\left.\frac{d\Psi_{(i)}}{dz}\right|_{z=d}, \tag{25}$$

where the coefficients c_{ij} are given by Eqs. (21) and (22). This procedure is iterated until one gets, within an acceptable accuracy, that

$$A^2+B^2-G^2=0 \tag{26}$$

by an appropriate choice of the wave-function amplitude at $z=0$. The wave-function initial phase is then calculated from

$$\eta_e=I_f(w)-k_zw-2\pi\left[\mathrm{Int}\left(\frac{I_{z0}-k_zw}{2\pi}\right)-1\right], \tag{27}$$

where

$$I_{z0}=\int_{z0}^{w}k(z)dz \tag{28}$$

and

$$I_f(z)=\int_{z0}^{z}k(z)dz-\frac{\pi}{4}+\arctan\left(\frac{-A}{B}\right). \tag{29}$$

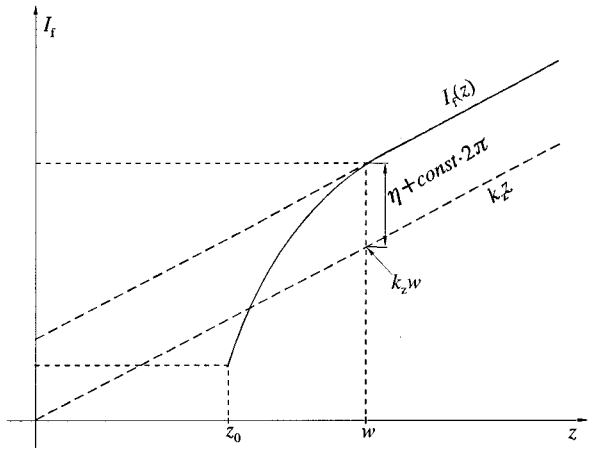

FIG. 3. Qualitative plot of the function $I_f(z)$, as defined in the text.

Here w denotes a suitably chosen value of z, such that the potential there becomes negligible, and the wave function acquires a simple harmonic behavior (Fig. 2). The function $I_f(z)$ is represented schematically in Fig. 3. In the region $z>w$ the wave number is constant, and I_f increases linearly with z. The initial phase, up to an integer multiple of π, is actually the distance between $I_f(z)$ and $k_z z$ lines, measured in the direction of I_f. The phase, strictly speaking, may be viewed as a continuous function of energy, or of the free electron wave vector k_z, and then the additional multiple of π to be added may be found from Levinson's theorem, according to the number of bound states in the well for $k_z=0$ [14,15]. However, since we aim at estimating the accuracy of the initial phase, it is convenient to allow its values in the range $[-\pi,+\pi]$ only, since a phase shift by $n\pi$, $n\in\mathbb{Z}$, does not affect the wave functions or the electron density.

For odd states the procedure is quite similar, except that it is the wave-function derivative, not the amplitude, that is preset at $z=0$. The initial phase is evaluated from Eq. (27), but with the I_f function defined differently, now reading

$$I_f(z)=\int_{z0}^{z} k(z)dz-\frac{\pi}{4}+\arctan\left(\frac{B}{A}\right). \tag{30}$$

Algorithmic steps in calculating the initial phase are displayed in Fig. 4.

In this formulation there are no cancellations of numbers very close to each other, which would bring about numerical difficulties as described in Secs. II and III. The only problem with the WBK method is that it is intrinsically approximate, and its accuracy should be tested against the ''exact'' results in a range of interesting cases.

V. NUMERICAL RESULTS AND DISCUSSION

For the purpose of numerical testing of the conventional and the WBK approach, we have performed a calculation for a realistic quantum-well structure, as given in Fig. 2. The values of the structure parameters used in numerical calculations are the particle mass $m=0.067m_0$, where m_0 is the free electron mass, corresponding to the electron effective mass in GaAs, the built-in potential $V_0=0.162$ eV, corresponding

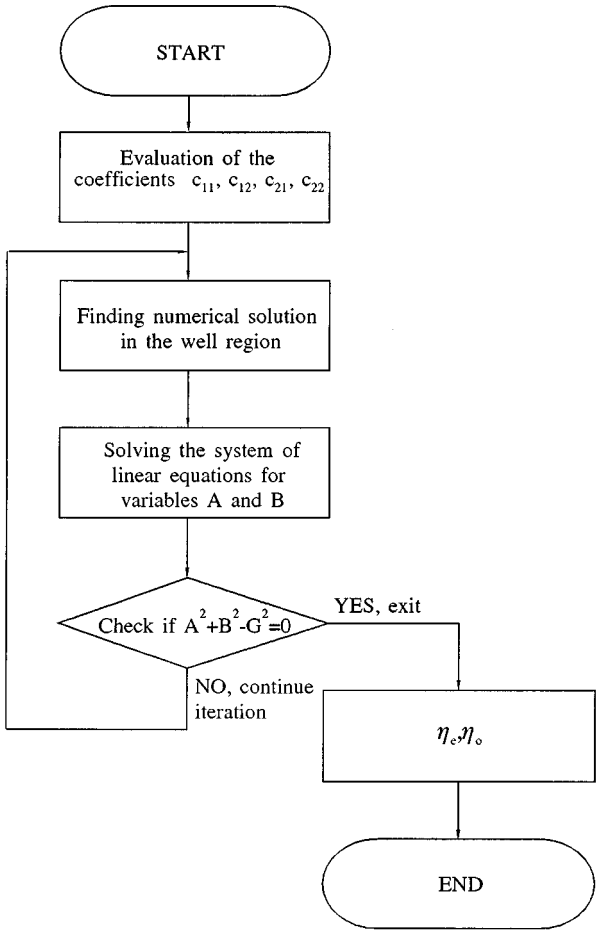

FIG. 4. The block diagram of the algorithm for calculation of wave functions with required asymptotic behavior, and of the initial phases of even and odd states, using the WBK approximation.

to the $GaAs/Al_{0.2}Ga_{0.8}As$ interface at $T=300$ K, the well width $2d=5$ nm, and the Morse potential parameters $V_b=0.1$ eV and $\beta=0.4$ (the potential outside the well is then decaying for any $\lambda>0$). The electron wave vector in the bulk is taken as $k_z=0.1$ nm^{-1}. Results obtained via the ''exact'' calculation, for various values of λ, are compared against those obtained within the approximate WBK calculation. The numerical value of $\hbar^2/2m_0$ is approximately taken as 0.0381 eV nm^2, convenient for MATHEMATICA computation with rational numbers. With this set of values taken, it turns out that other quantities entering the calculation, if expressed in nanometers, should be inserted as pure numbers (dimensionless).

To illustrate the complete failure of the conventional approach (with REAL*8 arithmetic) to this problem, in Fig. 5 we present the amplitudes of the even-state wave function and the modulation function (or their derivatives for odd states), as calculated in the well center, using the conventional and the MATHEMATICA algorithm. The modulation function found by the conventional calculation is quite accurate, but it is still useless for evaluating the wave function, due to truncation errors. Not only is the wave function inside the well grossly incorrect (compare with the ''exact'' MATHEMATICA values in Fig. 5), but also its behavior, as the parameter λ varies, is unphysical. With decreasing λ, i.e., widening the

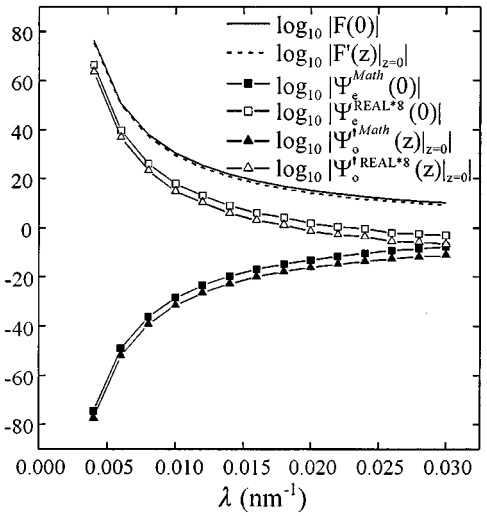

FIG. 5. Amplitudes of the wave function and the modulation function (for even state) and the derivatives of these quantities (for odd states) in the well center, calculated by the conventional (REAL*8) and the ''exact'' MATHEMATICA (MATH) approach for a range of values of λ in the Morse potential.

barrier, the wave function inside the well, as calculated in the conventional way, increases, while in fact it should decrease, as confirmed by the ''exact'' calculation in MATHEMATICA.

The relative errors occurring in the WBK calculation of the wave-function amplitude (derivative) at $z=0$ for even (odd) states are given in Fig. 6. The range of λ values ($0.004<\lambda<0.03$) was chosen so that ''exact'' results truncated to 200 significant digits could be obtained from the MATHEMATICA program. Lower values of λ (<0.004) would lead to excessive memory requirements due to both a very large number (over 650) of b_j coefficients, Eq. (14), and a large number of digits (>200) to be used. For $\lambda>0.03$ the WBK errors are larger, but good results may be obtained by plain numerical integration of the Schrödinger equation (with REAL*8 arithmetic), so this case needs no further considerations. The upper limit for the λ parameter where the WBK approximation may still be used decreases as the electron wave vector (energy) increases. This is accompanied by an increase of the wave-function modulus in the central region, and the conventional numerical integration of the Schrödinger equation may then be used.

As depicted in Fig. 6(a), the error in the even-state wave function has a fast (almost exponential) rise as λ increases. This error is negligible for small values of λ, i.e., the slowly decaying wave function, as is indeed expected for the WBK method. In the range of λ values stated above, the even- (odd-) state wave-function amplitudes (derivatives) in the well center are always low, meaning essentially complete depletion of the central region. This is because only low-lying free states contribute significantly to the charge density, and the corresponding wave functions have very small values in the vicinity of the well, due to a slowly decaying repulsive self-consistent potential. To give a numerical example, for $\lambda=0.004$ (which is the typical value of λ found in the first few iterations of the previously developed self-consistent procedure [8]) the wave-function amplitude varies from 10^{-75} at $z=0$ to the order of unit at $z=841$ (the right

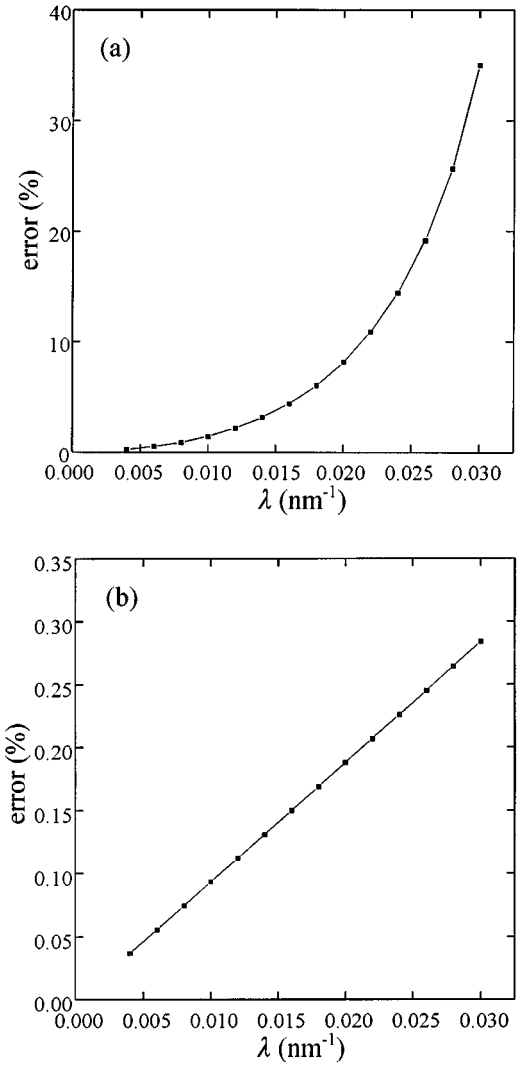

FIG. 6. The relative errors of the even-state wave-function amplitude (a), and the odd-state wave-function derivative (b), both taken at the quantum-well center, as they depend on the λ parameter in the Morse potential.

turning point). It is interesting to note that errors of even-state wave functions grossly exceed those of odd states. As displayed in Fig. 6(b), these latter increase approximately linearly with λ. The different behavior of the two is related to differences in their nature and conditions for using the WBK approximation.

As for the modulation function, it acquires very large values in the above range of λ. For example, with $\lambda=0.004$ the modulation function amplitude is as large as 10^{77}, and using 16 significant digits in calculation hardly makes any sense because the full wave-function amplitude is of the order of 10^{-75}. In Fig. 7 we give R_1, Eqs. (15) and (16), as it varies with the λ parameter. This number decreases with increasing λ (and also depends somewhat on energy), but generally is quite large, and indicates the necessity of using WBK-based calculation in order to get valid results.

The even- and odd-state initial phases as calculated by the ''exact'' (MATHEMATICA) and WBK method, denoted by superscripts MATH and WBK, respectively, are given in Table I. Since the phase is determined to within a factor $n\pi$, $n\in\mathbb{Z}$,

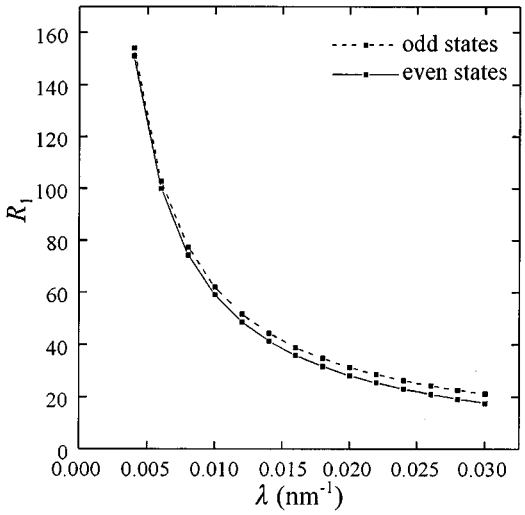

FIG. 7. Dependence of quantity R_1 (which is approximately equal the number of digits to be taken in computation, which guarantees one significant digit of the even-state wave function value and slope of the odd-state wave function in the well center), on the λ parameter in the Morse potential.

the accuracy of this calculation may be judged only from the absolute error. One can see from Table I that there is good agreement between the two approaches for all values of λ considered, more so if λ is smaller, and hence the potential variation slower, which is the usual situation where the WBK approximation works best.

VI. CONCLUSION

The usefulness and accuracy of the WBK approximation for calculating the continuous spectrum wave functions is explored. By comparison with high-precision calculations performed in MATHEMATICA we have shown that in a class of Morse potentials where plain integration of the Schrödinger equation fails, the WBK method delivers reasonably accurate results for the wave functions. Furthermore, the precision of the conventional calculation required to get (at least) one significant digit in the final result correct is estimated.

TABLE I. The even-(e) and odd-(o) state phases (in radians), as calculated by an ''exact'' MATHEMATICA (MATH) and an approximate WBK approach.

λ (nm^{-1})	η_e^{MATH}	η_e^{WBK}	η_o^{MATH}	η_o^{WBK}
0.004	−0.06458	−0.06301	1.50621	1.50778
0.006	1.70490	1.70725	−3.00749	−3.00514
0.008	−0.55235	−0.54921	1.01845	1.02159
0.010	3.11954	3.12347	−1.59285	−1.58892
0.012	−2.81038	−2.80566	−1.23958	−1.23487
0.014	1.92972	1.93522	−2.78267	−2.77717
0.016	−0.79858	−0.79230	0.77221	0.77849
0.018	1.96615	1.97321	−2.74624	−2.73917
0.020	−2.10541	−2.09756	−0.53462	−0.52676
0.022	−0.29604	−0.28740	1.27475	1.28339
0.024	1.21163	1.22106	2.78243	2.79186
0.026	2.48724	2.49745	−2.22515	−2.21494
0.028	−2.70268	−2.69168	−1.13189	−1.12089
0.030	−1.75529	−1.74350	−0.18450	−0.17271

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