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Abstract
Based on the analytical transfer matrix method (ATMM), the universal dispersion equation determining the energy spectrum for an arbitrary potential function experienced by a particle with arbitrary position-dependent effective mass distribution is obtained. As an illustrative example, for a given mass distribution $m(x)$ and a potential function $V(x)$, our predicted results are in complete agreement with the exact ones. The energy spectrum of a harmonic oscillator with nonconstant mass is obtained. Since the exact solutions to Schrödinger equation with nonconstant effective mass are a valuable means for checking and improving models and numerical methods in the study of electronic properties, the ATMM will find wide applications in material science and condensed matter.

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1. Introduction

The motion of free carriers (electrons and holes) in semiconductors of nonuniform chemical composition is sometimes described by means of a Hamiltonian possessing a position-dependent effective mass, and the Schrödinger equation with position-dependent effective mass have also found wide applications in the study of electronic properties of quantum dots [1], quantum liquids [2], semiconductor superstructures [3] and so on. In fact, numerous examples can be found in the literature [4, 5] where the effective-mass approximation is claimed to produce good results, provided that suitable values are chosen.

Until recently, the solutions to this problem have been extensively developed. A general form of the generator of $su(1, 1)$ was employed to show that the solutions are free from the choice of parameters for position-dependent mass [6]. The universal formalism of supersymmetric quantum mechanics was extended by Plastino *et al* [7] to the Schrödinger equation with position-dependent effective mass. Coordinate transformation in supersymmetric quantum mechanics was used in [8] to generate isospectral potentials with

position-dependent mass. The ordering ambiguity of the mass and momentum operator and its effect on the exact solution were addressed in [9]. It is easily found that most of them solve Schrödinger equation according to the procedure: for a given mass distribution, their aims are to obtain the energy spectrum and potential function. However, the obtained potential function is dependent on the mass distribution and a known potential function for which the solutions to Schrödinger equation can be derived, which hampers their applications in actual physical systems. Furthermore, most of the methods mentioned above did not give the constraints imposed on the mass distribution or the potential function such that the problem becomes solvable.

In our work [10], an exact method for solving the Schrödinger equation with constant mass was developed by using the analytical transfer matrix method (ATMM). It was demonstrated that the ATMM can be applied to an arbitrary potential function, and the dispersion equation reads

$$\int_{x_{t1}}^{x_{t2}} \kappa(x)\,\mathrm{d}x + \phi(s) = (n+1)\pi \qquad (n = 0, 1, 2, \ldots) \tag{1}$$

where $\kappa(x)$ is defined by $\hbar\kappa(x) = \sqrt{2m[E - V(x)]}$, which is the local momentum of a particle with constant mass m whose total energy is E. The concept of phase contribution $\phi(s)$ due to the scattering of sub-waves is put forward and the phase shift at the classical turning point is proved to be exactly π, regardless of whether it is in the limit of short wave or long wave. These two substantial improvements play a crucial role in deriving the exact energy spectrum. In [11], we have successfully derived the energy splitting in symmetric double-well potentials with the ATMM. So it is clear that the ATMM is a powerful tool for energies of the bound states.

2. Exact dispersion equation

We discuss here that the ATMM can give exact energy spectrum when it is applied to an arbitrary potential well in which the effective mass of the particle is position dependent. Von Roos [12] was the first to suggest the following form of the kinetic energy operator $\mathbf{T} = \frac{1}{4}(m^\eta \mathbf{P}m^\varepsilon \mathbf{P}m^\rho + m^\rho \mathbf{P}m^\varepsilon \mathbf{P}m^\eta)$, where $\eta + \varepsilon + \rho = -1$. Apparently, different ordering renders different energy spectrum and wavefunction, however, the literature [13–15] shows that the single-particle wavefunction and eigenenergies comply with a Schrödinger equation of the form

$$\left[-\nabla \frac{\hbar^2}{2m(x)}\nabla + V(x)\right]\psi(x) = E\psi(x) \tag{2}$$

where $m(x)$ and $V(x)$ are arbitrary mass distribution and arbitrary potential well, respectively, and $\mathbf{P} = -\mathrm{i}\hbar\nabla$ with $\rho = 0, \varepsilon = -1$ and $\eta = 0$. The following analysis is based on equation (2).

When the term $E - V(x)$ vanishes, the two classical turning points x_{t1} and x_{t2} are always given. We simultaneously truncate the tail of the profile of $V(x)$ and of mass $m(x)$ at two appropriate points x_C and x_D, which are far away from the turning points, and divide the regions (x_C, x_{t1}), (x_{t1}, x_{t2}) and (x_{t2}, x_D) into l, f and g section layers with equal width d, respectively. Each layer is with piecewise constant potential energy and the effective mass. The truncation certainly affects the values of energy levels, as compared to the situation in an idealized system. The effects will clearly be negligible if the potential at the truncation points is very much larger than energies of relevant levels. The discretized Schrödinger equation for

the ith region with constant potential energy V_i and constant effective mass m_i can be written as

$$\frac{d^2}{dx^2}\psi_i(x) + \kappa_i^2\psi_i(x) = 0 \qquad (x_{i-1} \leqslant x \leqslant x_i) \tag{3}$$

with

$$\kappa_i(x) = \pm\sqrt{2m_i[E - V_i]}/\hbar \tag{4}$$

where the subscript i is an integer ranging from 1 to $l + f + g$, $\psi_i(x)$ representing the wavefunction in the ith section layer and κ_i stands for the wavevector in the same layer along the x direction. If $\kappa_i^2 \geqslant 0$, the energy E is above the barrier V_i, and physically it is an oscillatory wave solution. While for $\kappa_i^2 \leqslant 0$, it is an evanescent wave solution. Equation (4) is still valid if one substitutes $\kappa_i = i\alpha_i$ and uses the equalities, $\cos(i\alpha_i x) = \cosh(\alpha_i x)$ and $\sin(i\alpha_i x) = i\sinh(\alpha_i x)$.

The solution of equation (3) can be written as a superposition of left and right travelling plane wavefunctions

$$\psi_i(x) = A_i\exp[j\kappa_i(x - x_{i-1})] + B_i\exp[-j\kappa_i(x - x_{i-1})] \qquad (x_{i-1} \leqslant x \leqslant x_i) \tag{5}$$

and the wavefunction connection rules across an abrupt interface are (i) the continuity of the wavefunction

$$\psi_{i-1}(x_{i-1}) = \psi_i(x_{i-1}) \tag{6}$$

and (ii) the continuity of the flux

$$\frac{1}{m_{i-1}}\frac{d}{dx}\psi_{i-1}(x_{i-1}) = \frac{1}{m_i}\frac{d}{dx}\psi_i(x_i). \tag{7}$$

From the discussion above, the transfer matrices corresponding to the rth, uth and vth section layers can be written as

$$M_r = \begin{bmatrix} \cosh(\alpha_r d) & \frac{m_r}{\alpha_r}\sinh(\alpha_r d) \\ \frac{\alpha_r}{m_r}\sinh(\alpha_r d) & \cosh(\alpha_r d) \end{bmatrix} \qquad \alpha_r = \sqrt{2m_r[V_r - E]}/\hbar \tag{8}$$

$$M_u = \begin{bmatrix} \cos(\kappa_u d) & \frac{m_u}{\kappa_u}\sin(\kappa_u d) \\ -\frac{\kappa_u}{m_u}\sin(\kappa_u d) & \cos(\kappa_u d) \end{bmatrix} \qquad \kappa_u = \sqrt{2m_u[E - V_u]}/\hbar \tag{9}$$

and

$$M_v = \begin{bmatrix} \cosh(\alpha_v d) & \frac{m_v}{\alpha_v}\sinh(\alpha_v d) \\ \frac{\alpha_v}{m_v}\sinh(\alpha_v d) & \cosh(\alpha_v d) \end{bmatrix} \qquad \alpha_v = \sqrt{2m_v[V_v - E]}/\hbar \tag{10}$$

where the subscripts r, u and v are integers ranging from 1 to l, from $l + 1$ to $l + f$ and from $l + f + 1$ to $l + f + g$, respectively. We define

$$P_C = \sqrt{2m(x_C)[V(x_C) - E]}/\hbar \tag{11}$$

and

$$P_D = \sqrt{2m(x_D)[V(x_D) - E]}/\hbar \tag{12}$$

which are the equivalent attenuation coefficients at the points x_C and x_D, respectively.

By employing the transfer matrix method, the following matrix equation is given:

$$\begin{bmatrix} \psi(x_C) \\ \frac{1}{m(x_C)}\psi'(x_C) \end{bmatrix} = \left(\prod_{r=1}^{l} M_r\right)\left(\prod_{t=l+1}^{l+f} M_t\right)\left(\prod_{v=l+f+1}^{l+f+g} M_v\right)\begin{bmatrix} \psi(x_D) \\ \frac{1}{m(x_D)}\psi'(x_D) \end{bmatrix}. \tag{13}$$

and the prime $'$ in equation (13) denotes the derivative with respect to x.

After simple algebra manipulation, if l, f and $g \to \infty (d \to 0)$, we obtain the simple dispersion equation

$$\int_{x_{t1}}^{x_{t2}} \kappa(x) \, dx + \phi(s) = n\pi + \arctan\left(\frac{P_l}{\kappa_{l+1}} \frac{m_{l+1}}{m_l}\right)$$

$$+ \arctan\left(\frac{P_{l+f+1}}{\kappa_{l+f}} \frac{m_{l+f}}{m_{l+f+1}}\right) \qquad (n = 0, 1, 2, \ldots) \tag{14}$$

where the term $\phi(s)$ is determined from

$$\phi(s) = \sum_{u=l+1}^{l+f-1} \left[\phi_{u+1} - \arctan\left(\frac{\kappa_{u+1}}{\kappa_u} \frac{m_u}{m_{u+1}} \tan \phi_{u+1}\right)\right] \tag{15}$$

with

$$\phi_u = \arctan\left(\frac{P_u}{\kappa_u}\right) \tag{16}$$

and

$$P_u = \kappa_u \left[\arctan\left(\frac{P_{u+1}}{\kappa_u} \frac{m_u}{m_{u+1}}\right) - \kappa_u d\right] \tag{17}$$

$$P_r = \alpha_r \frac{(1/m_r)\sinh(\alpha_r d) + (P_{r-1}/\alpha_r)\cosh(\alpha_r d)}{\cosh(\alpha_r d) + (P_{r-1}/\alpha_r m_r)\sinh(\alpha_r d)} \tag{18}$$

$$P_v = \alpha_v \frac{(1/m_v)\sinh(\alpha_v d) + (P_{v+1}/\alpha_v)\cosh(\alpha_v d)}{\cosh(\alpha_v d) + (P_{v+1}/\alpha_v m_v)\sinh(\alpha_v d)} \tag{19}$$

$$P_0 = P_C, \quad P_{l+f+g+1} = P_D. \tag{20}$$

In equation (14), n is the quantum number and equation (14) is the universal dispersion equation determining the energy spectrum for an arbitrary potential function experienced by a particle with position-dependent effective mass.

If we equate $\kappa_{q+1}/m_{q+1} = \kappa_q/m_q$ in equation (15), which means we have neglected the potential profile difference of the neighbouring sections of layers, we obtain $\phi(s) = 0$, thus $\phi(s)$ can also be interpreted as the phase contribution due to the scattering of the sub-waves. If we do not take the variation of effective mass into account, i.e., the mass distribution $m(x) = $ constant, then equation (14) is reduced to equation (1) which is a natural consequence. Furthermore, the values of κ_{l+1} and κ_{l+f} at the classical turning points are both zero, so

$$\arctan\left(\frac{P_l}{\kappa_{l+f}} \frac{m_{l+1}}{m_l}\right) = \arctan\left(\frac{P_{l+f+1}}{\kappa_{l+f}} \frac{m_{l+f}}{m_{l+f+1}}\right) = \frac{\pi}{2} \tag{21}$$

which means that the phase shift at the classical turning points for the particle whose effective mass is position dependent is exactly equal to π.

3. Results

For the purpose of numerical illustration of the above theory, we consider the choice of the mass distribution $m(x)$ used in [7]

$$m(x) = \left(\frac{\alpha + x^2}{1 + x^2}\right)^2 \qquad m(0) = \alpha^2 \quad m(\pm\infty) = 1 \tag{22}$$

Table 1. Comparison of the energy spectrum for harmonic oscillator with nonconstant effective mass to that with constant mass using the ATMM ($\hbar = 1$).

n	0	1	2	3	4	5
E (constant)	0.500 00	1.500 00	2.500 00	3.500 00	4.500 00	5.500 00
E (nonconstant)	0.315 40	0.872 11	1.507 15	2.187 14	2.896 62	3.628 41

n	6	7	8	9	10	11
E (constant)	6.500 00	7.500 00	8.500 00	9.500 00	10.500 00	11.500 00
E (nonconstant)	4.377 91	5.141 92	5.918 14	6.704 83	7.500 64	8.304 48

n	12	13	14	15	16	17
E (constant)	12.500 00	13.500 00	14.500 00	15.500 00	16.500 00	17.500 00
E (nonconstant)	9.115 47	9.932 87	10.756 01	11.584 57	12.417 89	13.255 66

and the potential function $V(x)$ is determined from

$$V(x) = \frac{1}{2}[x + (\alpha - 1)\tan^{-1}(x)]^2 + \frac{(\alpha - 1)}{2(\alpha + x^2)^4}[3x^4 + (4 - 2\alpha)x^2 - \alpha] \quad (23)$$

which is a shape-invariant potential function characterized by one single parameter α. The reason that we choose the above example is that it possesses the following exact energy spectrum:

$$E_n = \left(n + \tfrac{1}{2}\right) \qquad (n = 0, 1, \ldots) \tag{24}$$

so that we can compare our result with it, though the chosen potential function (23) is very complex. On the other hand, the energy spectrum is the spectrum of a harmonic oscillator with constant mass. After the numerical calculations we obtained the energy spectrum for the potential function (23) with the formalism (14), i.e., $E_0 = 0.5$, $E_1 = 1.5$, $E_2 = 2.5$, $E_3 = 3.5, \ldots$. The agreement is seen to be excellent, which shows that our method is exact. For simplicity, we do not test other examples.

It is well known that the standard model of harmonic oscillator with constant mass plays an important role in theoretical physics. But in some particular situations, the constant mass is replaced by the effective mass which may be position dependent. Next we consider the harmonic oscillator in the potential well $V(x) = \frac{1}{2}x^2$ and it is with the position-dependent effective mass distribution (22) when $\alpha = 2$. The energy eigenvalues E (nonconstant) are listed in table 1, compared with the energy eigenvalues E (constant) for the constant mass $m = 1$.

It can be seen that the energy eigenvalues we obtained have a greater shift compared with the energy eigenvalues with constant mass, i.e., all of them decrease a lot. We look forward to the exact results showing a valuable means for checking and improving models and numerical methods in the study of electronic properties. At the same time, the results will challenge the standard model for which the mass of harmonic oscillator is constant. Because there are no results obtained by other methods, we can not compare our results with them. The concept of phase contribution is very important for deriving the exact energies, but we still cannot find the integral instead of sum form (15). Although some numerical methods such as Numerov or Runge–Kutta integration are straightforward, they can not supply the deep insight as the ATMM does, i.e., the ATMM gives the exact phase shift at the turning point and a better understanding of the phase contribution due to sub-waves scattering. Although the effective mass approximation is not exact in actual applications, the ATMM is exact for the Schrödinger equation with nonconstant effective mass through finer divisions, for example, we divide the whole potential profile ($x_C < x < x_D$) into 10^4 layers.

4. Conclusions

Dispersion equation (14) is presented in a simple and clear manner, whose terms are physically explicit and it can be applied to arbitrary potential wells in which the effective mass distribution of the particle can also be arbitrary, and the ATMM differs essentially from the methods mentioned in paragraph 2, i.e., it is not necessary to know in advance a potential function for which the solution of Schrödinger equation must be known. The method will find wide applications in calculating the exact values of lifetime for electrons in quantum wells with an applied electric field and it is able to determine the total lifetime of quasi-bound energy levels in the presence of inelastic scattering mechanisms, which are qualitatively modelled by an energy broadening imaginary potential. In addition, it can solve the transmission problems easily. In fact, we can derive the exact profiles of the mass distribution and potential function according to the energy spectrum of a real physical system through the inverse analytical transfer matrix method (IATMM). Since the Schrödinger equation for a spherically symmetric potential can be transformed into a one-dimensional equation, all such problems can also be solved using the same method. All of them mentioned above are in progress.

Acknowledgments

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