# Wave function for smooth potential and mass step

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The one-dimensional Schrödinger equation, derived from the general form of the effective-mass Hamiltonian $(m^{\eta}\mathbf{p}m^{\epsilon}\mathbf{p}m^{\rho}+m^{\rho}\mathbf{p}m^{\epsilon}\mathbf{p}m^{\eta})/4+V$ with $\eta+\epsilon+\rho=-1$, is solved exactly for a system with smooth potential and *mass* step. The wave function depends on the Heun function, which is a generalization of the hypergeometric function. The effective-mass Hamiltonian and the connection rules for a system with abrupt heterojunction are deduced from the study of the limiting case when the smooth step potential and mass tend to an abrupt potential and mass step. [S1050-2947(99)05101-X]

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## I. INTRODUCTION

The study of physical systems with position-dependent mass have known a new development over the last years. This interest is due to the recent progress of crystal-growth techniques (molecular-beam-epitaxy technique, for example) for the production of a nonuniform semiconductor specimen. An important and widely used theory for the determination of electronic properties of semiconductors is the effective-mass approximation [1]. This theory, originally developed to treat homogeneous crystals, has been extended to nonuniform materials in which the carrier effective mass depends on the position.

Since the momentum and the mass operators do not commute, a question concerning the correct form of the kinetic-energy operator of the generalized Hamiltonian has arisen. This question is directly related to the connection rules for the wave function across an abrupt heterojunction. Von Roos [2] was the first to suggest the following form of the kinetic-energy operator:

$$\hat{T}=\tfrac{1}{4}(m^{\eta}\mathbf{p}m^{\varepsilon}\mathbf{p}m^{\rho}+m^{\rho}\mathbf{p}m^{\varepsilon}\mathbf{p}m^{\eta}), \tag{1}$$

where $\eta+\varepsilon+\rho=-1$. This two-parameter class operator is, by construction, a Hermitian quantum-mechanical operator corresponding to the classical kinetic energy. Various special cases of Eq. (1) have appeared in the literature, viz [3–7],

$$\hat{T}=\frac{1}{4}\left[\frac{1}{m}\,p^2+p^2\,\frac{1}{m}\right], \tag{2}$$

$$\hat{T}=\frac{1}{2}\left[\mathbf{p}\,\frac{1}{m}\,\mathbf{p}\right], \tag{3}$$

$$\hat{T}=\frac{1}{2}\left[\frac{1}{\sqrt{m}}\,p^2\,\frac{1}{\sqrt{m}}\right]. \tag{4}$$

To try to limit the choice of the $\eta$ and $\varepsilon$ parameters of Eq. (1), two strategies have been adopted. The first one consists in calculating, via the effective-mass approximation, some observables of a particular model. Then, these results are compared either with experimental data, or with exact results of simple models. Thus, Morrow and Brownstein [8] have shown that $\eta=\rho$; otherwise, the wave function is forced to vanish at the heterojunction boundary, which is clearly an unphysical result. Thomsen, Einevoll, and Hemmer [9] reach the same result $\eta=\rho$; otherwise, the ground-state energy diverges in the abrupt limit. Let us point out here that the $\eta=\rho$ restriction excludes the form (2). Using the restricted Hamiltonian resulting from the $\eta=\rho$ constraint,

$$H=\tfrac{1}{2}(m^{\eta}\mathbf{p}m^{\varepsilon}\mathbf{p}m^{\eta})+V, \tag{5}$$

contradictory choices of the $\varepsilon$ parameter have been proposed. Reformulating the connection rule problem by first extrapolating the effective-mass wave function on the two sides of the heterojunction across the interface, as if the semiconductor were homogeneous, Zhu and Kroemer [7] arrive at the conclusion that $\varepsilon=0$. Comparing the results of Kroning-Penney's calculation of electron transmission from a set of $\delta$-function scatterers and the transmission coefficient obtained via the effective-mass theory, Morrow [10] arrives at the same conclusion that $\varepsilon\approx 0$. In return, other workers have proposed $\varepsilon=-1$: Von Roos and Mavromatis [6], by using the Kohn-Luttinger representation and canonical transformation, or Galbraith and Duggan [11], by comparing the calculated optical transition energies with experimental values. The study of the matching conditions of the wave function, across an abrupt heterojunction in three dimensions, has led Morrow [12] to change his first conclusion $\varepsilon\approx 0$ [10] to $\varepsilon=-1$.

The second strategy tries to tackle the problem with a fundamental point of view, i.e., without using a particular form of potential and mass. Within this frame, and using the path-integral formalism, Yung and Yee [13] arrive at the following effective-mass Hamiltonian:

$$H=\frac{1}{2}\left(\mathbf{p}\,\frac{1}{m}\,\mathbf{p}\right)+\frac{\hbar^2}{6}\,\frac{m''}{m^2}-\frac{\hbar^2}{4}\,\frac{m'^2}{m^3}+V, \tag{6}$$

where $m'(x)\equiv dm(x)/dx$ and $m''(x)\equiv d^2m(x)/dx^2$. In a recent work Lévy-Leblond [14], using the notion of instantaneous Galilean invariance, reaches form (3). Moreover, he shows that not only the use of position-dependent mass gives correct approximation, but it is also a conceptually consistent approach.

Thus, opinions were divided on the choice of the $\varepsilon$ parameter, although the majority of these works incline to form (3). Besides, in a preceding paper [15], we have used this form (3) to calculate the Green's function, via the path integral formalism, for step and rectangular-barrier potentials and masses. It is to be noticed that, practically, in all the above-mentioned works, applications are made for piecewise flat potential and mass. Nevertheless, models with continuous smoothly variable potential and mass are also interesting to study. In a recent work [16], we have proposed a solution of the one-dimensional Schrödinger equation resulting from the kinetic-energy operator (3) for a system with smooth potential and mass step. We have also shown that the behavior of the transmission coefficient, as a function of the energy, is similar to that of the case of an abrupt potential and mass step.

The approach of the present paper is quite different from the two above-mentioned strategies. The one-dimensional Schrödinger equation, derived from the generalized kinetic-energy operator (1), is considered without any restriction in the values of the $\eta$ and $\varepsilon$ parameters. This generalized Schrödinger equation is solved for a system with continuous and smoothly variable potential and mass, namely, for potential and mass with smooth step shape. Assuming the values of $\eta$, $\rho$, and $\varepsilon$ to be universal, and by studying the limiting case, when the smooth potential and mass step tend to an abrupt potential and mass step, we will arrive at the conclusion that the correct kinetic Hamiltonian for an abrupt heterojunction is form (3). This form (3) implies that the connection rules of the wave function across abrupt interface are the continuity of $\Psi(x)$ and $[1/m(x)][d\Psi(x)/dx]$.

In Sec. II we solve the generalized Schrödinger equation. In Sec. III we study two limiting cases, namely, when the smooth potential and mass tend to an abrupt potential and mass step, and when the width of the mass step is vanishing. The conclusion is given in Sec. IV

## II. GENERALIZED SCHRÖDINGER EQUATION

The one-dimensional time-independent Schrödinger equation, derived from the generalized kinetic-energy operator (1), can be written

$$-\frac{\hbar^2}{4}\,m^{\eta}(x)\,\frac{d}{dx}\left\{m^{\varepsilon}(x)\,\frac{d}{dx}\,[m^{\rho}(x)\Psi(x)]\right\}-\frac{\hbar^2}{4}\,m^{\rho}(x)\,\frac{d}{dx}\times\left\{m^{\varepsilon}(x)\,\frac{d}{dx}\,[m^{\eta}(x)\Psi(x)]\right\}+[V(x)-E]\Psi(x)=0, \tag{7}$$

or

$$\frac{d^2\Psi(x)}{dx^2}-\frac{m'(x)}{m(x)}\,\frac{d\Psi(x)}{dx}+\left\{\tfrac{1}{2}[\rho(\rho+\varepsilon-1)+\eta(\eta+\varepsilon-1)]\,\frac{m'^2(x)}{m^2(x)}+\frac{(\rho+\eta)}{2}\,\frac{m''(x)}{m(x)}+\frac{2m(x)}{\hbar^2}\,[E-V(x)]\right\}\Psi(x)=0. \tag{8}$$

The smooth potential and mass step are chosen equal to

$$V(x)=\frac{V_0}{2}\left(1+th\,\frac{x}{2r}\right), \tag{9}$$

$$m(x)=\overline{m}+\frac{\Delta m}{2}\,th\,\frac{x}{2r}, \tag{10}$$

where $\overline{m}=(m_1+m_2)/2$, $\Delta m=m_2-m_1$, $V_0$ and $r$ are positive constants. The potential increases from the value $V=0$ for $x=-\infty$ to the value $V=V_0$ for $x=+\infty$. The mass increases (decreases) if $m_1<m_2$ (if $m_1>m_2$), from the value $m=m_1$ for $x=-\infty$ to the value $m=m_2$ for $x=+\infty$. The significant variations are occurring in the range $x\in\,]-2r,2r[$:

$$V(-2r)\cong 0.119V_0,\quad m(-2r)\cong 0.119\Delta m,$$

$$V(2r)\cong 0.889V_0,\quad m(2r)\cong 0.889\Delta m.$$

The change of the independent variable

$$z=\tfrac{1}{2}\left(1-th\,\frac{x}{2r}\right) \tag{11}$$

transforms the coefficients of Eq. (8) into rational functions of the new $z$ variable, and maps the original interval $x\in\,]-\infty,+\infty[$ to $z\in\,]0,1[$. Potential (9) and mass (10) then take the forms $V(z)=-V_0(z-1)$ and $m(z)=-\Delta m(z-a)$, where

$$a=\frac{m_2}{m_2-m_1}. \tag{12}$$

With the abbreviations

$$\nu^2=\frac{2m_2r^2}{\hbar^2}\,(V_0-E),\quad \mu^2=-\frac{2m_1r^2E}{\hbar^2},\quad \omega^2=\frac{2\Delta m r^2V_0}{\hbar^2}, \tag{13}$$

the generalized Schrödinger equation becomes

$$\frac{d^2\Psi(z)}{dz^2}+\left[\frac{1}{z}+\frac{1}{(z-1)}-\frac{1}{(z-a)}\right]\frac{d\Psi(z)}{dz}+\left\{(a-1)\theta-\varphi+\nu^2-\mu^2+a\omega^2+(\theta+2\varphi-\omega^2)z-\frac{a\nu^2}{z}+\frac{(a-1)\mu^2}{(z-1)}+\frac{a(a-1)\theta}{(z-a)}\right\}\frac{\Psi(z)}{z(z-1)(z-a)}=0, \tag{14}$$

where

$$\theta=-(\rho+\eta+\rho\eta),\quad \varphi=\frac{\rho+\eta}{2}=-\frac{(1+\varepsilon)}{2}. \tag{15}$$

Equation (14) is a Heun-type equation in its general form [17–19], i.e., a second-order linear homogeneous differential equation with four singularities $z=0$, 1, $a$, $\infty$, all regular. Since all the singularities are regular, Eq. (14) belongs to the class of Fuchsian equations. The change of the dependent variable

$$\Psi(z)=z^{\nu}(z-1)^{\mu}(z-a)^{1-\sqrt{1-\theta}}f(z) \tag{16}$$

transforms Eq. (14) into the normal form of a Heun equation

$$\begin{aligned}&\frac{d^2f(z)}{dz^2}+\left[\frac{(2\nu+1)}{z}+\frac{(2\mu+1)}{(z-1)}+\frac{(1-2\sqrt{1-\theta})}{(z-a)}\right]\frac{df(z)}{dz}\\&\quad+\{a[\omega^2-(\nu+\mu)(\nu+\mu+1)]+\nu(2\sqrt{1-\theta}-1)-\varphi-1\\&\quad+\sqrt{1-\theta}+[(\nu+\mu+1-\sqrt{1-\theta})^2\\&\quad-\omega^2+2\varphi+\theta]z\}\frac{f(z)}{z(z-1)(z-a)}=0.\end{aligned} \tag{17}$$

With the following abbreviations,

$$\begin{gathered}\alpha=\sqrt{\omega^2-2\varphi-\theta}+\nu+\mu+1-\sqrt{1-\theta},\\ \beta=-\sqrt{\omega^2-2\varphi-\theta}+\nu+\mu+1-\sqrt{1-\theta},\\ \gamma=2\nu+1,\quad \delta=1-2\sqrt{1-\theta},\\ b=a[\omega^2-(\nu+\mu)(\nu+\mu+1)]+\nu(2\sqrt{1-\theta}-1)-\varphi-1\\ +\sqrt{1-\theta},\end{gathered} \tag{18}$$

the solution of Eq. (17), which is regular in the vicinity of $z=0$ and belongs to the exponent *zero*, is the Heun function defined by the series [20]

$$f_1(z)=CF(a,b;\alpha,\beta,\gamma,\delta;z)\equiv C\left\{1-\frac{b}{\gamma a}+\sum_{s=2}^{\infty}c_s z^s\right\}, \tag{19}$$

where the $c_s$ coefficients of the series are determined by the difference equation

$$\begin{aligned}(s+2)(s+1+\gamma)ac_{s+2}={}&\{(s+1)^2(a+1)+(s+1)\\&\times[\gamma+\delta-1+(\alpha+\beta-\gamma)a]-b\}\\&\times c_{s+1}-(s+\alpha)(s+\beta)c_s,\end{aligned} \tag{20}$$

with the initial conditions $c_0=1$, $c_1=-b/\gamma a$, and $c_s=0$ if $s<0$. Constant $C$ will be fixed by the boundary conditions. Series (19) converges inside a circle centered at the origin $z=0$ and whose radius is the distance from the origin to the nearer of the two singular points $z=1$ and $z=a$. Thus, series (19) converges for $|z|<1$ if $|a|>1$, i.e., if $m_1<2m_2$ and $m_1\neq m_2$. In the case where $|a|<1$, i.e., if $m_1>2m_2$, series (19) converges for $|z|<|a|$. In the latter case an analytic continuation to ensure convergence for $|z|<1$ may be obtained by introducing, into the differential equation (17), the change of the independent variable $z'=1-z$.

The wave function (16) becomes

$$\Psi(z)=Cz^{\nu}(z-1)^{\mu}(z-a)^{1-\sqrt{1-\theta}}F(a,b;\alpha,\beta,\gamma,\delta;z). \tag{21}$$

We study now the asymptotic behavior, when $x\to\pm\infty$, of the wave function (21). First, when $x\to+\infty$, or $z\approx\exp(-x/r)\to0$, the Heun function is equal to 1 when $z=0$; then we have

$$\begin{aligned}\Psi(z)\underset{z\to0}{\to}&\,Ce^{i\pi(\mu+1-\sqrt{1-\theta})}a^{1-\sqrt{1-\theta}}\exp\left(-\frac{\nu x}{r}\right)\\&=C'\exp\left(-\frac{\nu x}{r}\right).\end{aligned} \tag{22}$$

Two cases have to be considered. (a) $E<V_0$, $\nu>0$ is real. The wave function vanishes exponentially as would be expected when $E<V_0$. We obtain $\Psi\to C'\exp(-Kx)$, where

$$K^2=\frac{\nu^2}{r^2}=\frac{2m_2}{\hbar^2}(V_0-E). \tag{23}$$

(b) $E>V_0$, $\nu=-ik_2r$ is imaginary, then $\Psi\to C'\exp(ik_2x)$, where

$$k_2^2=\frac{2m_2}{\hbar^2}(E-V_0). \tag{24}$$

For the limit when $x\to-\infty$, or $z\to1$, we have $1-z\approx\exp(x/r)\to0$; we use the following formula, which links the $z$ and $1-z$ argument functions,

$$\begin{aligned}F(a,b;\alpha,\beta,\gamma,\delta;z)={}&F(a,b;\alpha,\beta,\gamma,\delta;1)\\&\times F(1-a,-b-\alpha\beta;\alpha,\beta,1+\alpha+\beta-\gamma-\delta,\delta;1-z)\\&+(1-z)^{\gamma+\delta-\alpha-\beta}F(a,b-\alpha\gamma[\gamma+\delta-\alpha-\beta];\gamma+\delta-\alpha,\gamma+\delta-\beta,\gamma,\delta;1)\\&\times F(1-a,-b-\alpha\beta-[\gamma+\delta-\alpha-\beta][\gamma+\delta-a\gamma];\gamma+\delta-\alpha,\gamma+\delta-\beta,1+\gamma+\delta-\alpha-\beta,\delta;1-z).\end{aligned} \tag{25}$$

We have established this formula in Appendix A of [16]. The wave function (21) is then transformed into

$$\begin{aligned}\Psi(z)={}&Cz^{\nu}(z-1)^{\mu}(z-a)^{1-\sqrt{1-\theta}}\{F(a,b;\alpha,\beta,\gamma,\delta;1)F(1-a,-b-\alpha\beta;\alpha,\beta,1+\alpha+\beta-\gamma-\delta,\delta;1-z)\\&+(1-z)^{\gamma+\delta-\alpha-\beta}F(a,b-a\gamma[\gamma+\delta-\alpha-\beta];\gamma+\delta-\alpha,\gamma+\delta-\beta,\gamma,\delta;1)\\&\times F(1-a,-b-\alpha\beta-[\gamma+\delta-\alpha-\beta][\gamma+\delta-a\gamma];\gamma+\delta-\alpha,\gamma+\delta-\beta,1+\gamma+\delta-\alpha-\beta,\delta;1-z)\}.\end{aligned} \tag{26}$$

Thus, when $x \to -\infty$, or $z \to 1$, the wave function has the following behavior:

$$\Psi \xrightarrow[x \to +\infty]{} C''\{e^{\mu/xr} + Re^{-\mu/xr}\}, \tag{27}$$

where the quantity $|R|^2$ is the reflection coefficient given by

$$|R|^2 = \left| \frac{F(a, b - a\gamma[\gamma+\delta-\alpha-\beta]; \gamma+\delta-\alpha, \gamma+\delta-\beta, \gamma, \delta; 1)}{F(a,b;\alpha,\beta,\gamma,\delta;1)} \right|^2. \tag{28}$$

The wave function (21) can finally be written

$$\Psi(x) = \left[\frac{1}{2}\left(1 - th\,\frac{x}{2r}\right)\right]^{\nu}\left[\frac{1}{2}\left(1 + th\,\frac{x}{2r}\right)\right]^{\mu} \times \left[\frac{1}{2}\left(1 - 2a - th\,\frac{x}{2r}\right)\right]^{1-\sqrt{1-\theta}} \times \frac{F\left(a,b;\alpha,\beta,\gamma,\delta;\, \frac{1}{2}\left(1 - th\,\frac{x}{2r}\right)\right)}{F(a,b;\alpha,\beta,\gamma,\delta;1)}. \tag{29}$$

Setting $\mu = ik_1 r$, where

$$k_1^2 = \frac{2m_1}{\hbar^2} E, \tag{30}$$

we can summarize the limits of the wave function

$$\Psi(x) = \begin{cases} e^{ik_1x} + Re^{-ik_1x} & \text{for } x \to -\infty \\ Ce^{-Kx} \quad \text{if } E > V_0 & \text{for } x \to +\infty \\ Ce^{ik_2x} \quad \text{if } E < V_0 & \text{for } x \to +\infty. \end{cases} \tag{31}$$

Thus, we recover the asymptotic behavior of a plane wave coming from the left side. Moreover, if $E < V_0$, $\mu = ik_1 r$ is imaginary and $\nu > 0$ is real, the numerator and denominator of the reflection coefficient (28) are complex conjugates, and then we have $|R|^2 = 1$. We also recover this case of total reflection when $E = V_0$, $\nu = 0$.

## III. LIMITING CASES

### A. Abrupt potential and mass step

We consider the limiting case when the smooth potential and mass step tend to an abrupt potential and mass step, i.e., when the $r$ parameter of Eqs. (9)–(11) tends to 0. For this purpose, and using the fact that Heun's function is invariant by interchange of $\alpha$ and $\beta$ argument, we can rewrite the reflection coefficient (28) in the following equivalent form:

$$|R|^2 = \left| \frac{F(a,\tilde{b};\tilde{\alpha},\tilde{\beta},\gamma,\delta;1)F(a,\tilde{b};\tilde{\beta},\tilde{\alpha},\gamma,\delta;1)}{F(a,b;\alpha,\beta,\gamma,\delta;1)F(a,b;\beta,\alpha,\gamma,\delta;1)} \right|, \tag{32}$$

where

$$\tilde{\alpha} = \gamma+\delta-\alpha, \quad \tilde{\beta} = \gamma+\delta-\beta, \quad \tilde{b} = b - a\gamma[\gamma+\delta-\alpha-\beta]. \tag{33}$$

We use, now, the following relation between two contiguous Heun functions:

$$(\beta-\gamma-\delta)F(a, b+1-a+(a-1)\beta + a\alpha - a\delta; \alpha, \beta-1, \gamma, \delta+1; z) = (\alpha z + \beta - \gamma - \delta)F(a,b;\alpha,\beta,\gamma,\delta;z) + z(z-1) \times \frac{dF(a,b;\alpha,\beta,\gamma,\delta;z)}{dz}. \tag{34}$$

The establishment of this relation needs lengthy calculations. We do not give here the details of these calculations. However, the method for obtaining this relation is equivalent to that of Appendix B of Ref. [16]. Particularly, for $z = 1$ relation (34) becomes

$$F(a,b;\alpha,\beta,\gamma,\delta;1) = \frac{(\beta-\gamma-\delta)}{(\alpha+\beta-\gamma-\delta)} F(a, b+1-a + (a-1)\beta + a\alpha - a\delta; \alpha, \beta-1, \gamma, \delta+1; 1). \tag{35}$$

We now transform each Heun's function of expression (32) by the intermediary of Eq. (35),

$$|R|^2 = \left| \frac{(\tilde{\beta}-\gamma-\delta)(\tilde{\alpha}-\gamma-\delta)}{(\beta-\gamma-\delta)(\alpha-\gamma-\delta)} \right| \left| \frac{(\alpha+\beta-\gamma-\delta)^2}{(\tilde{\alpha}+\tilde{\beta}-\gamma-\delta)^2} \right| \left| \frac{F(a, \tilde{b}+1-a+(a-1)\tilde{\beta}+a\tilde{\alpha}-a\delta; \tilde{\alpha}, \tilde{\beta}-1, \gamma, \delta+1; 1)}{F(a, b+1-a+(a-1)\beta+a\alpha-a\delta; \alpha, \beta-1, \gamma, \delta+1; 1)} \right| \times \left| \frac{F(a, \tilde{b}+1-a+(a-1)\tilde{\alpha}+a\tilde{\beta}-a\delta; \tilde{\beta}, \tilde{\alpha}-1, \gamma, \delta+1; 1)}{F(a, b+1-a+(a-1)\alpha+a\beta-a\delta; \beta, \alpha-1, \gamma, \delta+1; 1)} \right|. \tag{36}$$

The assumption that the values of $\eta$, $\rho$, and $\varepsilon$ are universal, implies that, in our case, these values are independent of the $r$ parameter. Substituting in this last expression the $\alpha$, $\beta$, $\gamma$, $\delta$, and $b$ parameters by their values in Eq. (18), and the $\tilde{\alpha}$, $\tilde{\beta}$, and $\tilde{b}$ parameters by Eq. (33), we find that the second term of Eq. (36) is equal to 1, and the last two terms tend to 1 when $r \to 0$. Finally, we arrive at

$$\lim_{r\to 0}|R|^2=\lim_{r\to 0}\left|\frac{[(a-1)\nu+a\mu]^2+2a(a-1)(\nu+\mu)(1-\sqrt{1-\theta})+2a(a-1)(1+\varphi-\sqrt{1-\theta})}{[(a-1)\nu-a\mu]^2+2a(a-1)(\nu-\mu)(1-\sqrt{1-\theta})+2a(a-1)(1+\varphi-\sqrt{1-\theta})}\right|. \tag{37}$$

We see that if $1+\varphi-\sqrt{1-\theta}\neq 0$, we have $\lim_{r\to 0}|R|^2=1$, which corresponds to a completely reflective barrier. Furthermore, to avoid this unphysical result we must have $1+\varphi-\sqrt{1-\theta}=0$, or with help of Eq. (15),

$$1-\sqrt{1+\rho+\eta+\rho\eta}+\frac{\rho+\eta}{2}=0. \tag{38}$$

Under this last condition, Eq. (37) reduces to

$$\lim_{r\to 0}|R|^2=\lim_{r\to 0}\left|\frac{[(a-1)\nu+a\mu]^2+2a(a-1)(\nu+\mu)(1-\sqrt{1-\theta})}{[(a-1)\nu-a\mu]^2+2a(a-1)(\nu-\mu)(1-\sqrt{1-\theta})}\right|. \tag{39}$$

We remark that if $\theta\neq 0$, Eq. (39) tends to

$$\lim_{r\to}|R|^2=\frac{\nu+\mu}{\nu-\mu}\equiv\frac{k_1-k_2}{k_1+k_2}, \tag{40}$$

and furthermore, if $a\to\infty$, i.e., when the width of the mass step is vanishing $(m_1=m_2=m)$, we will have

$$\lim_{\substack{r\to 0\\ a\to\infty}}|R|^2=\frac{\tilde{k}_1-\tilde{k}_2}{\tilde{k}_1+\tilde{k}_2}\neq\left(\frac{\tilde{k}_1-\tilde{k}_2}{\tilde{k}_1+\tilde{k}_2}\right)^2\equiv|R|_0^2, \tag{41}$$

where $\tilde{k}_1=\sqrt{2mE/\hbar^2}$, $\tilde{k}_2=\sqrt{2m(E-V_0)/\hbar^2}$, and $|R|_0^2$ is the reflection coefficient of an abrupt potential step with constant mass. Thus, in order that

$$\lim_{\substack{r\to 0\\ a\to\infty}}|R|^2=|R|_0^2,$$

we must have $\theta=0$, or with the help of Eq. (15),

$$-(\rho+\eta+\rho\eta)=0. \tag{42}$$

In short, in order that

$$\lim_{r\to 0}|R|^2\neq 1$$

and

$$\lim_{\substack{r\to 0\\ a\to\infty}}|R|^2=|R|_0^2,$$

the two conditions (38) and (42) must be verified simultaneously,

$$\rho+\eta+\rho\eta=0$$

and

$$2-2\sqrt{1+\rho+\eta+\rho\eta}+\rho+\eta=0. \tag{43}$$

This system has the unique solution

$$\rho=\eta=0, \tag{44}$$

which, with help of the condition $\eta+\varepsilon+\rho=-1$, gives

$$\varepsilon=-1. \tag{45}$$

We then arrive at the conclusion that form (3) is the correct form of the effective-mass Hamiltonian for an abrupt potential and mass step. Other works have presented, through an exact model calculation, arguments in favor of form (3). We can quote the work of Thomsen, Einevoll, and Hemmer [9], where a $\delta$-function potential, situated at the interface between two materials, has been used as a test case for the Hamiltonian (5). In [21], Einevoll and Hemmer have used a heterostructure consisting of two homogeneous materials, both described by one-dimensional Kroning-Penney lattice, and the local potential has been taken to be a square well. Finally, the work of Einevoll, Hemmer, and Thomsen [22] with superlattices, quantum wells, and localized potentials, has been taken as a test model.

Form (3) implies [8,14] that the connection rules of the wave function across abrupt interface are the continuity of $\Psi(x)$ and $[1/m(x)][d\Psi(x)/dx]$. Lévy-Leblond [23], applying these connection rules to a one-dimensional system with an abrupt potential and mass step, has found the following reflection coefficient:

$$|R|^2=\left(\frac{\dfrac{k_1}{m_1}-\dfrac{k_2}{m_2}}{\dfrac{k_1}{m_1}+\dfrac{k_2}{m_2}}\right)^2. \tag{46}$$

We can observe that, under conditions (38) and (42), the reflection coefficient (37) reduces to

$$\lim_{r\to 0}|R|^2=\lim_{r\to 0}\left|\frac{[(a-1)\nu+a\mu]^2}{[(a-1)\nu-a\mu]^2}\right|, \tag{47}$$

which, after substituting $a$ by Eq. (12), $\nu$ and $\mu$ by their definitions in Eq. (13), is exactly equal to Eq. (46).

### B. Smooth potential step with constant mass

The second limiting case considered is when the width of the mass step is vanishing $(m_1=m_2=m)$, i.e., when the parameter $a$ defined by Eq. (12) tends to infinity. For this purpose, we appeal to the following limit [24]

$$\lim_{a\to\infty}F(a,ac;\alpha,\beta,\gamma,\delta;z)={}_2F_1(\eta+\sqrt{\eta^2+c},\eta-\sqrt{\eta^2+c};\gamma;z) \tag{48}$$

where

$$\eta=\frac{\alpha+\beta-\delta}{2}, \quad \gamma\neq -n(n=0,1,2,\ldots).$$

This limit (48) gives the case where the Heun function degenerates, by confluence of the singular points $a$ and $\infty$, into a hypergeometric function. Applying this limit (48) for the Heun functions contained in the expression of the reflection coefficient (28), we find

$$\lim_{a\to\infty}|R|^2=\left|\frac{{}_2F_1(\overline{\nu}-\overline{\mu},\overline{\nu}-\overline{\mu}+1;2\overline{\nu}+1;1)}{{}_2F_1(\overline{\nu}+\overline{\mu},\overline{\nu}+\overline{\mu}+1;2\overline{\nu}+1;1)}\right|^2$$
$$=\left|\frac{\Gamma(+2\overline{\mu})\Gamma(\overline{\nu}-\overline{\mu})\Gamma(\overline{\nu}-\overline{\mu}+1)}{\Gamma(-2\overline{\mu})\Gamma(\overline{\nu}+\overline{\mu})\Gamma(\overline{\nu}+\overline{\mu}+1)}\right|^2=|\overline{R}|^2, \tag{49}$$

where

$$\overline{\nu}^2=\frac{2mr^2}{\hbar^2}(V_0-E), \quad \overline{\mu}^2=-\frac{2mr^2E}{\hbar^2}, \tag{50}$$

and $|\overline{R}|^2$ is the reflection coefficient for a system with a constant mass and potential smooth step obtained in [25]. We have used the relation

$${}_2F_1(\alpha,\beta;\gamma;1)=\frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)} \tag{51}$$

to transform the hypergeometric functions contained in Eq. (49) into a gamma function.

## IV. CONCLUSION

In the present paper we have proposed a solution of the Schrödinger equation, derived from the generalized effective-mass Hamiltonian $H_{\mathrm{gen}}=(m^{\eta}\boldsymbol{p}m^{\varepsilon}\boldsymbol{p}m^{\rho}+m^{\rho}\boldsymbol{p}m^{\varepsilon}\boldsymbol{p}m^{\eta})/4+V$ with $\eta+\varepsilon+\rho=-1$, without any restriction in the $\eta$ and $\varepsilon$ parameters, for a one-dimensional system with smooth potential and mass step. Assuming the values of $\eta$, $\rho$, and $\varepsilon$ to be universal, and by studying the limiting case when the smooth potential and mass step tend to an abrupt potential and mass step, we have shown that the parameters must take the values $\eta=\rho=0$, $\varepsilon=-1$, which suggests that the appropriate form of the effective-mass Hamiltonian for an abrupt heterojunction is the form $H_{\mathrm{abrupt}}=[\boldsymbol{p}m^{-1}\boldsymbol{p}]/2+V$. This form implies that the connection rules of the wave function across abrupt interface are the continuity of $\Psi(x)$ and $[1/m(x)][d\Psi(x)/dx]$.


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