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Generation of isospectral combinations of the potential and the effective-mass variations by supersymmetric quantum mechanics

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Abstract. The procedure is described for supersymmetric generation of combined potential and effective-mass variations, fully isospectral with an original potential. It relies on the standard supersymmetric technique, accompanied by the coordinate transform method. It enables one to generate families of isospectral potentials and isospectral effective-mass variations, both generally different from their original forms, with the number of free parameters larger than in the case of varying potential only, which may be of interest, e.g., in the design of semiconductor quantum wells.

1. Introduction

The problem of generating isospectral potentials in quantum mechanics has been considered for more than 50 years, but recently the research efforts on this topic have been considerably intensified. A new field, supersymmetric quantum mechanics (SUSYQM), devoted to this class of problems has emerged. The fundamental problem that SUSYQM deals with is in finding the family of potentials having the same spectrum of energies as some initial (original) potential (see, e.g., [1] for a review).

The standard SUSYQM handles the conventional Schrödinger equation with constant mass and variable potential. In some instances, however, the less conventional Schrödinger equation with both the position-dependent (effective) mass and the position-dependent potential is employed. The most extensive use of such an equation is in the physics of semiconductor nanostructures. This field has arisen due to the impressive development of sophisticated technologies of semiconductor growth, like molecular beam epitaxy, which made it possible to grow ultrathin semiconductor structures, with very prominent quantum effects (see e.g., [2] for a review). The motion of electrons in them may often be described by the envelope function effective-mass Schrödinger equation, where the material composition (i.e. the position) dependent effective mass of electrons replaces the constant particle mass in the conventional Schrödinger equation. The most popular of these structures is the semiconductor quantum well, and the Schrödinger equation here is effectively one-dimensional. Another instance where such an equation is employed, this time three-dimensional and with spherical symmetry, is in the pseudopotential-theory-based density functional calculations in solids: to reduce the computational load, model pseudopotentials with position-dependent electron mass which replace nonlocal pseudopotentials have been considered [3].

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It should be interesting, therefore, to extend the SUSYQM to handle cases with position-dependent mass. In this paper we first show how the standard SUSYQM procedure should be modified to become applicable to systems with position-dependent mass, generating families of isospectral potentials while leaving the original effective-mass variation unchanged. We then go to the main topic of this paper: to devise the procedure of generating families of isospectral Hamiltonians that involve the combination of both the potential *and* the effective-mass variation. All considerations are made for the one-dimensional Schrödinger equation.

2. Theoretical considerations

Within the envelope function effective-mass approximation the eigenenergies E and the envelope eigenfunctions ψ of the quantum well structure should be determined from the Schrödinger equation which takes the form [2]

$$-\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{m(z)}\frac{\mathrm{d}\psi}{\mathrm{d}z}\right)+qU_0(z)\psi = qE\psi \equiv \hat{H}_0\psi \tag{1}$$

where $q = 0.2627$ if energy, length and effective mass are expressed in eV, Å and free electron mass units, respectively. The effective mass is taken to be strictly positive, i.e., $m(z) > 0$ for all z.

Using the standard SUSYQM procedure [1] the initial Hamiltonian is first factorized as

$$\hat{H}_0 = \hat{A}^+\hat{A} + qE_0. \tag{2}$$

In equation (2) E_0 is one of the bound state eigenenergies of the Hamiltonian $\hat{H}_0$, and the operators $\hat{A}^+$ and $\hat{A}$ have the form

$$\hat{A}^+ = -\frac{\mathrm{d}}{\mathrm{d}z}\frac{1}{\sqrt{m(z)}} + W(z) \qquad \hat{A} = \frac{1}{\sqrt{m(z)}}\frac{\mathrm{d}}{\mathrm{d}z} + W(z) \tag{3}$$

where $W(z)$ is the superpotential, which is the solution of the nonlinear differential equation

$$W^2 - \frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{W}{\sqrt{m(z)}}\right)+q(E_0-U_0) = 0. \tag{4}$$

The solution of equation (4) may be written as

$$W(z) = -\frac{1}{\sqrt{m(z)}}\frac{\mathrm{d}}{\mathrm{d}z}[\ln\tilde{\psi}_0(z)] \tag{5}$$

where $\tilde{\psi}_0(z)$ is the general solution of the Schrödinger equation (1) for $E = E_0$. If $\psi_0(z)$ denotes the bound state wavefunction (and hence is a square-integrable function), then

$$\tilde{\psi}_0(z) = \psi_0(z)\left[C + \int_{z_0}^{z}\frac{m(z')}{\psi_0^2(z')}\,\mathrm{d}z'\right] \tag{6}$$

where C is an arbitrary constant. Using (6) the expression for the superpotential may be written as

$$W(z) = -\frac{1}{\sqrt{m(z)}}\frac{\mathrm{d}}{\mathrm{d}z}[\ln\psi_0(z)] - \frac{1}{\sqrt{m(z)}}\frac{\mathrm{d}}{\mathrm{d}z}\left\{\ln\left[C + \int_{z_0}^{z}\frac{m}{\psi_0^2}\,\mathrm{d}z'\right]\right\} \equiv W_1(z) + W_2(z). \tag{7}$$

The next step is to make the new Hamiltonian

$$\hat{H}_1 = \hat{A}\hat{A}^+ + qE_0 \tag{8}$$

its eigenspectrum being identical to that of $\hat{H}_0$, except that the state at $E = E_0$ is missing. The Hamiltonian $\hat{H}_1$ acting upon ψ_1 then gives

$$\hat{H}_1\psi_1 = -\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{m(z)}\frac{\mathrm{d}\psi_1}{\mathrm{d}z}\right)+qU_1(z)\psi_1 = qE\psi_1 \tag{9}$$

where the new potential $U_1(z)$ is given by

$$U_1(z) = U_0(z) - \frac{2}{q\sqrt{m}}\frac{\mathrm{d}W}{\mathrm{d}z} - \frac{1}{q\sqrt{m}}\frac{\mathrm{d}^2}{\mathrm{d}z^2}\frac{1}{\sqrt{m}}. \tag{10}$$

We should also note that the superpotential $W(z)$ and the potential $U_1(z)$ are related by

$$W^2 + \frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{W}{\sqrt{m}}\right) + q(E_0 - U_1) = 0. \tag{11}$$

By inserting the expression for the superpotential $W(z)$ into equation (11) we find that the term $W_2(z)$ causes a singularity in $U_1(z)$ for any value of the constant C. Furthermore, $W_2(z)$ causes a singularity in the expression for wavefunctions $\psi_{SSi}(z)$, and such wavefunctions would not be square integrable. Therefore, one has to set $W(z) = W_1(z)$, and the general solution of the Schrödinger equation $\hat{H}_1\psi_{10} = qE_0\psi_{10}$ takes the form

$$\psi_{10}(z) = \frac{\lambda + I(z)}{\psi_0(z)} \qquad I(z) = \int_{-\infty}^{z} \psi_0^2(z')\,\mathrm{d}z' \tag{12}$$

where λ is a constant. With E_0 not being an eigenvalue of $\hat{H}_1$, this solution is not square integrable (i.e. normalizable) for any value of λ. Then, another Hamiltonian is constructed as

$$\hat{H}_2 = \hat{A}_1^+\hat{A}_1 + qE_0. \tag{13}$$

The operators $\hat{A}_1^+$ and $\hat{A}_1$ in equation (13) have the same form as $\hat{A}^+$ and $\hat{A}$, except that ψ_0 is replaced by ψ_{10}. The Hamiltonian $\hat{H}_2$ is fully isospectral with $\hat{H}_0$, and the potential in it, $U_2(z) = U_{SS}(z)$, has the form

$$U_{SS}(z) = U_0(z) - \frac{2}{q\sqrt{m(z)}}\frac{\mathrm{d}}{\mathrm{d}z}\left\{\frac{1}{\sqrt{m(z)}}\frac{\mathrm{d}}{\mathrm{d}z}\ln[\lambda + I(z)]\right\} \tag{14}$$

where the constant λ may take any value outside the range $[-1, 0]$, otherwise the potential and the eigenfunctions would have singularities. The eigenfunctions $\psi_{SSi}(z)$, corresponding to this supersymmetric Hamiltonian, are related to the eigenfunctions $\psi_i(z)$ of $\hat{H}_0$ via

$$\psi_{SSi}(z) = -\psi_i(z) + \frac{\psi_0(z)\mu_i(z)}{\lambda + I(z)} \qquad \mu_i(z) = \int_{-\infty}^{z} \psi_0\psi_i\,\mathrm{d}z' \qquad i \neq 0 \tag{15}$$

$$\psi_{SS0}(z) = \frac{\sqrt{\lambda(\lambda+1)}\psi_0(z)}{\lambda + I(z)} \qquad i = 0. \tag{16}$$

It should be noted that ψ_0 in the above equations may denote any bound state of the Hamiltonian $\hat{H}_0$, not necessarily the lowest state.

A more general method of generating isospectral potentials has been described in [4]. Here one starts with the potential $U_0^*(z)$ and the corresponding Hamiltonian is factorized according to (see [5])

$$\hat{H}_0^* = \hat{A}^*\hat{A}^{*+} + q\epsilon = -\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{m(z)}\frac{\mathrm{d}}{\mathrm{d}z}\right) + qU_0^*(z) \tag{17}$$

where the operators $\hat{A}^*$ and $\hat{A}^{*+}$ have the same form as $\hat{A}$ and $\hat{A}^+$ except that $W(z)$ is replaced by $W^*(z)$. The factorization energy ϵ here is an energy below the ground state, and the corresponding solution is denoted as $\psi_{\epsilon 0}^*(z)$, i.e., $H_0^*\psi_{\epsilon 0}^* = q\epsilon\psi_{\epsilon 0}^*$. It follows that $\hat{A}^*\hat{A}^{*+}\psi_{\epsilon 0}^* = 0$, whereby $\hat{A}^{*+}\psi_{\epsilon 0}^* = 0$, and expression for the superpotential $W^*(z)$ directly follows:

$$W^*(z) = \frac{1}{\sqrt{m(z)}}\frac{\mathrm{d}}{\mathrm{d}z}\left[\ln\frac{\psi_{\epsilon 0}^*(z)}{\sqrt{m(z)}}\right]. \tag{18}$$

Now we define the new Hamiltonian $\hat{H}_1^* = \hat{A}^{*+}\hat{A}^* + q\epsilon$, with a new potential $U_1^*(z)$. Having in mind that $q(U_1^* - U_0^*) = \hat{A}^{*+}\hat{A}^* - \hat{A}^*\hat{A}^{*+}$ we find the expression for $U_1^*(z)$:

$$U_1^*(z) = U_0^*(z) - \frac{2}{q\sqrt{m}}\frac{\mathrm{d}W^*}{\mathrm{d}z} + \frac{1}{q\sqrt{m}}\frac{\mathrm{d}^2}{\mathrm{d}z^2}\frac{1}{\sqrt{m}}. \tag{19}$$

The energy ϵ is implicitly contained in the potential $U_1^*(z)$ via the solution of the Schrödinger equation $\psi_{1\epsilon}^*(z)$. Having in mind that $H_1^*\psi_{\epsilon 1}^* = q\epsilon\psi_{\epsilon 1}^*$, i.e. $\hat{A}^*\psi_{\epsilon 1}^* = 0$, we find

$$\psi_{\epsilon 1}^*(z) = \frac{\sqrt{m(z)}}{\psi_{\epsilon 0}^*(z)}. \tag{20}$$

Eigenenergies of the Hamiltonian $\hat{H}_0^*$ are $E_1, E_2, \ldots, E_n, \ldots$, and the corresponding eigenfunctions are $\psi_{10}^*, \psi_{20}^*, \ldots, \psi_{n0}^*, \ldots$. With the potential $U_1^*(z)$, the eigenfunctions corresponding to these energies are ψ_{n1}^*:

$$\psi_{n1}^*(z) = \frac{\hat{A}^{*+}\psi_{n0}^*}{\sqrt{q(E_n - \epsilon)}} = \frac{1}{\sqrt{q(E_n - \epsilon)}}\left(-\frac{\mathrm{d}\psi_{n0}^*}{\mathrm{d}z} + \frac{\psi_{n0}^*}{\psi_{\epsilon 0}^*}\frac{\mathrm{d}\psi_{\epsilon 0}^*}{\mathrm{d}z}\right). \tag{21}$$

The Hamiltonians with potentials $U_1^*(z)$ and $U_0^*(z)$ therefore have identical spectra, except that the one with $U_1^*(z)$ also has a state at energy ϵ, its eigenfunction being given by (20). *If the functions ψ_{n1}^*, as well as $\psi_{\epsilon 1}$, are to be free of singularities it is necessary that $\psi_{\epsilon 0}^*(z)$ is nodeless, if the new potential $U_1^*(z)$ is to have no new singularities other than those which $U_0^*(z)$ possibly had, it is again necessary that $\psi_{\epsilon 0}^*(z)$ is nodeless*. The condition necessary for $\psi_{\epsilon 0}^*(z)$ to be nodeless is given in [4, 6]. Assuming we have one nodeless solution $\psi_{\epsilon p}^*(z)$ of the Schrödinger equation with the potential $U_1^*(z)$ at energy ϵ, the general solution has the form

$$\psi_{\epsilon 0}^*(z) = \psi_{\epsilon p}^*(z)\left[\lambda + \int_{-\infty}^{z}\frac{m(z')}{\psi_{\epsilon p}^{*2}(z')}\,\mathrm{d}z'\right] \tag{22}$$

where λ is a constant. If $\psi_{\epsilon p}^*$ is nodeless then the value of the integral in (22) will be between zero and

$$I_{max} = \int_{-\infty}^{\infty}\frac{m(z')}{\psi_{\epsilon p}^{*2}(z')}\mathrm{d}z' > 0. \tag{23}$$

It follows that $\psi_{\epsilon 0}^*(z)$ will be nodeless provided λ is outside the region $(-I_{max}, 0)$. Clearly, if one sets some finite lower limit z_0 in the integral (22) then its values range between I_{min} and I_{max}, implying that $\psi_{\epsilon 0}^*(z)$ will be nodeless provided λ is outside the region $(-I_{max}, -I_{min})$. It may be interesting to explain the method of generating $\psi_{\epsilon,p}^*(z)$ for energies below that of the ground state. One first generates the solution $\psi_{\epsilon p-}^*(z)$ with the boundary condition $\psi_{\epsilon p-}^*(-\infty) = 0$. This solution has no zeros, and may be taken to be a positive, monotonously increasing function. Then one generates the solution $\psi_{\epsilon p+}^*(z)$ such that $\psi_{\epsilon p+}^*(\infty) = 0$. It also has no zeros, and may be taken to be a positive, monotonously decreasing function. A particular solution which also has no zeros may be written as a linear combination $\alpha\psi_{\epsilon,p-}^*(z) + \beta\psi_{\epsilon p+}^*(z)$, where α and β have the same sign. For simplicity one may take $\alpha = \beta = 1$, i.e. $\psi_{\epsilon p}^*(z) = \psi_{\epsilon p+}^*(z) + \psi_{\epsilon p-}^*(z)$.

We have presented in the above paragraph the method given in [4] generalized to the case of position-dependent effective mass. If the initial potential is that of the linear harmonic oscillator, and if the energy ϵ is downshifted by exactly Δ from the ground state (where Δ denotes the spacing between subsequent states), then the potential $U_1^*(z)$ depends on the parameter λ, and the energy spectrum is identical to that of the linear harmonic oscillator. This case was discussed in [7]. The case of an electron in Coulomb potential was analysed in [8, 9]. The potential corresponding to azimuthal quantum number $l = 1$ was taken as initial, and

the energy ϵ was the ground state energy for $l = 0$. The resulting potential $U_1^*(z)$ had the eigenspectrum identical to that of the Coulomb potential.

Both methods discussed here are known in the literature for the constant-mass case, and are here extended to handle the position-dependent effective-mass case. Also, both methods enable the generation of isospectral (or almost isospectral) potentials depending on a free parameter λ. Later, we will concentrate only on the SUSYQM case covered by equations (14)–(16), though the considerations may be rather straightforwardly applied to the case described by equations (19)–(21).

The modified SUSYQM procedure, as described above, enables one to generate the family of potentials $U_{SS}(z, \lambda)$ fully isospectral with the initial potential $U_0(z)$, while the effective-mass variation $m(z)$ remains unchanged. A question now arises: is it possible to generate the family of isospectral combinations of potential and effective-mass variations, both generally different from their original forms? The problem may be solved by using the coordinate transform method together with the SUSYQM transform, as will be described in further text.

We introduce a new coordinate y, related to the old coordinate z via $z = g(y)$, where the function $g(y)$ will be specified later. Also, we introduce the notation: $m(z) = m[g(y)] = \underline{m}(y)$, $\psi(z) = \psi[g(y)] = \underline{\psi}(y)$, etc. The Schrödinger equation (1) then takes the form (with $' \equiv \mathrm{d}/\mathrm{d}y$)

$$u'' + \{A(y) + q\underline{m}(y)[g'(y)]^2[E - \underline{U}_0(y)]\}u = 0 \tag{24}$$

where the new function $u(y)$ is related to $\underline{\psi}(y)$ via

$$u(y) = \text{const} \cdot [\underline{m}(y)g'(y)]^{-1/2}\underline{\psi}(y) \tag{25}$$

and

$$A(y) \equiv \frac{\underline{m}''(y)}{4\underline{m}(y)} - \frac{5}{16}\left(\frac{\underline{m}'(y)}{\underline{m}(y)}\right)^2. \tag{26}$$

It is important to note that equations (1) and (24) have identical spectra. With the wavefunctions $\psi(z)$ being square integrable, i.e., $\langle\psi(z)|\psi(z)\rangle = 1$, setting const $= 1$ in equation (25) and having in mind that $m(z) > 0$ we find that $\langle u(y)|u(y)\rangle = 1$ as well, i.e., the functions $u(y)$ also are square integrable. Now, choosing the function $g(y)$ so to satisfy

$$\underline{m}(y)g'(y)^2 = 1 \tag{27}$$

recasts equation (24) into

$$u'' + q\left[E - \left\{\underline{U}_0(y) - \frac{A(y)}{q}\right\}\right]u = 0 \tag{28}$$

which is the Schrödinger equation with the new potential $\underline{U}_0(y) - A(y)/q$ and the constant effective mass ($m = 1$ in free electron mass units). This form is simpler than equation (1), since it does not involve the position-dependent mass, and it has been extensively studied within the SUSYQM. Applying the SUSYQM to equation (28) we arrive at

$$u_{SS}'' + q\left[E - \left\{\underline{U}_{SS}^*(y) - \frac{A(y)}{q}\right\}\right]u_{SS} = 0 \tag{29}$$

where

$$\underline{U}_{SS}^*(y) = \underline{U}_0(y) - \frac{2}{q}[\ln\{\lambda + I(y)\}]'' \equiv \underline{U}_0(y) + \Delta U_{SS}(y, \lambda) \tag{30}$$

which follows directly from equation (14) by setting $m(z) = 1$. The corresponding wavefunctions $u_{SS}(y)$ are obtained from equations (15) and (16). The supersymmetric potential

$\underline{U}^*_{SS}(y)$ and the quantity $A(y)$ are fully determined once $U_0(z)$ and $m(z)$ are specified. In fact, equation (27) may be written as

$$\int_0^z \sqrt{m(z)}\,\mathrm{d}z = y = g^{-1}(z) \tag{31}$$

which defines (though in implicit form) the function $g(y)$, which thus enables finding $\underline{m}(y)$ and $\underline{U}_0(y)$, and hence also $\underline{U}^*_{SS}(y)$.

The Schrödinger equation (29) corresponds to some Schrödinger equation of the form (1) in the real space coordinate frame z_{SS}, but with modified effective-mass and potential variations $m_{SS}(z_{SS})$ and $U_{SS}(z_{SS})$, where the coordinate z_{SS} is related to y via $z_{SS} = g_{SS}(y)$, and

$$\underline{m}_{SS}(y)[g'_{SS}(y)]^2 = 1. \tag{32}$$

In order to go from equation (29) to

$$-\frac{\mathrm{d}}{\mathrm{d}z_{SS}}\left(\frac{1}{m_{SS}}\frac{\mathrm{d}\psi_{SS}}{\mathrm{d}z_{SS}}\right) + qU_{SS}(z_{SS})\psi_{SS} = qE\psi_{SS} \tag{33}$$

it is necessary to satisfy

$$\underline{U}_{SS}(y) - \frac{A_{SS}(y)}{q} = \underline{U}^*_{SS}(y) - \frac{A(y)}{q} \tag{34}$$

where $\underline{U}_{SS}(y) = U_{SS}[g_{SS}(y)] = U_{SS}(z_{SS})$, and $A_{SS}(y)$ has the same form as $A(y)$ except that $\underline{m}_{SS}(y)$ replaces $\underline{m}(y)$. The wavefunctions $\underline{\psi}_{SSi}(y)$ and $u_{SSi}(y)$ are related by

$$\underline{\psi}_{SSi}(y) = \sqrt[4]{\underline{m}_{SS}(y)}\,u_{SSi}(y). \tag{35}$$

With $\underline{m}_{SS}(y)$ determined, as will be explained further on, $g_{SS}(y) = z_{SS}$ may be found from (32), and then $\psi_{SSi}(z)$ also follows from (35). The wavefunctions obtained this way satisfy $\langle\psi_{SSi}(z_{SS})|\psi_{SSi}(z_{SS})\rangle = 1$.

The right-hand side of equation (34) is fully determined, and on the left-hand side there are two unknown functions, $\underline{m}_{SS}(y)$ and $\underline{U}_{SS}(y)$. One possibility of solving equation (34) is to write it as two equations:

$$\underline{U}_{SS}(y) = \underline{U}_0(y) + \zeta\,\Delta U_{SS}(y,\lambda) \tag{36}$$

$$-\frac{A_{SS}(y)}{q} = -\frac{A(y)}{q} + (1-\zeta)\Delta U_{SS}(y,\lambda) \tag{37}$$

where ζ is a dimensionless weighting parameter. Two characteristic values of this parameter are $\zeta = 0$ and $\zeta = 1$. These two cases will now be analysed in more detail.

(i) The case $\zeta = 1$. In this case equation (37) becomes $A_{SS}(y) = A(y)$, or, more explicitly:

$$\frac{\underline{m}''_{SS}(y)}{4\underline{m}_{SS}(y)} - \frac{5}{16}\left[\frac{\underline{m}'_{SS}(y)}{\underline{m}_{SS}(y)}\right]^2 = \frac{\underline{m}''(y)}{4\underline{m}(y)} - \frac{5}{16}\left[\frac{\underline{m}'(y)}{\underline{m}(y)}\right]^2. \tag{38}$$

This is a nonlinear differential equation in $\underline{m}_{SS}(y)$, since $\underline{m}(y)$ is known, as noted before. Now, introducing $\underline{m}_{SS}(y) = R^{-2}_{SS}(y)$ and $\underline{m}(y) = R^{-2}(y)$ we arrive at a more convenient form:

$$2R_{SS}(y)R''_{SS}(y) - (R'_{SS})^2 + 4R^2_{SS}\left[-\frac{R''(y)}{2R(y)} + \frac{(R')^2}{4R^2(y)}\right] = 0. \tag{39}$$

This type of nonlinear equation has been studied many years ago, and is well documented in [10]. Following the theory presented therein, the solution $R_{SS}(y)$ of the nonlinear equation (39) equals $s^2(y)$, where $s(y)$ is the general solution of the linear differential equation

$$s'' + \left[-\frac{R''}{2R} + \frac{(R')^2}{4R^2}\right]s = 0. \tag{40}$$

Since $\underline{m}_{SS}(y) = \underline{m}(y)$ certainly is a particular solution of equation (38), then $s_1(y) = \sqrt{R(y)}$ is a particular solution of the linear equation (40). From the theory of second-order linear differential equations, another particular solution of equation (40) is

$$s_2(y) = \sqrt{R(y)} \int_0^y \frac{\mathrm{d}y'}{R(y')} \tag{41}$$

and the required dependence $\underline{m}_{SS}(y)$ may be written as

$$\underline{m}_{SS}(y) = \frac{\underline{m}(y)}{[C_1 + C_2 \int_0^y \sqrt{\underline{m}(y')}\,\mathrm{d}y']^4} \tag{42}$$

where C_1 and C_2 are arbitrary real constants. Taking account of equation (32) the dependence of the 'new' coordinate z_{SS} on y may be written as

$$g_{SS}(y) = z_{SS} = \int_0^y \frac{\mathrm{d}y'}{\sqrt{\underline{m}_{SS}(y')}} = \int_0^y \frac{(C_1 + C_2 \int_0^{y'} \sqrt{\underline{m}(y'')}\,\mathrm{d}y'')^2}{\sqrt{\underline{m}(y')}}\,\mathrm{d}y'. \tag{43}$$

The dependence $m_{SS}(z_{SS})$ may then be found from equations (42) and (43). A special case occurs when $C_1 = 1$ and $C_2 = 0$. Then $\underline{m}_{SS}(y) = \underline{m}(y)$, wherefrom $g_{SS}(y) = g(y) = z$, i.e. $m_{SS}(z)$ coincides with the initial effective-mass dependence $m(z)$. In all other cases $m_{SS}(z) \neq m(z)$.

Introducing the notation $\eta(z_{SS}) \equiv g(g_{SS}^{-1}(z_{SS}))$ and $y(z_{SS}) = g_{SS}^{-1}(z_{SS})$, as well as $\underline{J}(y) \equiv (\underline{m}_{SS}(y)/\underline{m}(y))^{1/2}$, the new supersymmetric potential may be written as

$$U_{SS}(z_{SS}) = U_0[\eta(z_{SS})] - \frac{2}{q\sqrt{\underline{m}_{SS}(y)}} \frac{\mathrm{d}}{\mathrm{d}z_{SS}} \times \left\{ \frac{1}{\sqrt{\underline{m}_{SS}(y)}} \frac{\mathrm{d}}{\mathrm{d}z_{SS}} \ln \left[\lambda + \int_{-\infty}^{z_{SS}} \underline{J}(y)\psi_0^2[\eta(z_{SS})]\,\mathrm{d}z_{SS} \right] \right\}. \tag{44}$$

The function $U_{SS}(z_{SS})$ obtained in this way depends on three free parameters: λ, C_1, and C_2 (while $m_{SS}(z_{SS})$ depends only on C_1 and C_2). In the special case $C_1 = 1$ and $C_2 = 0$ equation (44) reduces to equation (14), as is indeed expected (note that equation (14) has been derived in a different way).

The normalized wavefunctions for the new system are given by

$$\psi_{SS}^i(z_{SS}) = \sqrt{\underline{J}(y)} \left[-\psi_i(\eta) + \frac{\psi_0(\eta) \int_{-\infty}^{z_{SS}} \psi_i(\eta)\psi_0(\eta)\underline{J}(y)\,\mathrm{d}z_{SS}}{\lambda + \int_{-\infty}^{z_{SS}} \underline{J}(y)\psi_0^2(\eta)\,\mathrm{d}z_{SS}} \right] \tag{45}$$

and

$$\psi_{SS}^0(z_{SS}) = \sqrt{\underline{J}(y)\lambda(\lambda+1)} \frac{\psi_0(\eta)}{\lambda + \int_{-\infty}^{z_{SS}} \underline{J}(y)\psi_0^2(\eta)\,\mathrm{d}z_{SS}}. \tag{46}$$

If $C_1 = 1$ and $C_2 = 0$ equations (45) and (46) turn into equations (15) and (16).

(ii) The case $\zeta = 0$. In this case $\underline{U}_{SS}(y) = \underline{U}_0(y)$ and $A_{SS}(y) = A(y) - q\Delta U_{SS}(y, \lambda) \equiv h(y, \lambda)$, and the nonlinear differential equation in $\underline{m}_{SS}(y)$ now takes the form

$$2R_{SS}R''_{SS} - (R'_{SS})^2 + 4R_{SS}^2 h(y, \lambda) = 0 \tag{47}$$

and its general solution may be written as

$$\underline{m}_{SS}(y) = \frac{1}{[C_1 s_1(y) + C_2 s_2(y)]^2} \tag{48}$$

where $s_{1,2}(y)$ are particular solutions of

$$s'' + h(y, \lambda)s = 0. \tag{49}$$

The functions $s_1(y)$ and $s_2(y)$ now cannot be written explicitly in analytic form (in terms of $\underline{m}(y)$), as was possible in case (i). With $\underline{m}_{SS}(y)$ determined according to (48), the procedure of finding $m_{SS}(z_{SS})$, $U_{SS}(z_{SS})$ and $\psi^i_{SS}(z_{SS})$ is fully analogous to that used in case (i), e.g.,

$$U_{SS}(z) = U_0[\eta(z_{SS})]. \tag{50}$$

For all other values of the 'weighting' parameter ζ (i.e. $\zeta \neq 0$ and $\zeta \neq 1$) the procedure is fully analogous to that in case (ii).

3. Numerical examples and discussion

For the purpose of numerical illustration of the theory given above, we use the textbook models of a rectangular quantum well with infinitely high barriers, and of a rectangular well with finite barriers and different masses in the well and barrier regions. In the first example the well width is $2d$ and the electron effective-mass m^* is constant. This simple model allows most of the procedure to be done analytically. For the same reason we consider case (i) only.

The initial potential $U_0(z)$ and mass $m(z)$ are thus

$$U_0(z) = 0 \qquad \text{and} \qquad m(z) = m^* \qquad \text{for} \quad -d < z < d. \tag{51}$$

The transition to the corresponding dependences on y is simple ($y = z\sqrt{m^*}$):

$$\underline{U}_0(y) = 0 \qquad \text{and} \qquad \underline{m}(y) = m^* \qquad \text{for} \quad -d\sqrt{m^*} < y < d\sqrt{m^*} \tag{52}$$

while equation (28) in this case becomes

$$u'' + qEu = 0 \tag{53}$$

with the boundary conditions $u(\pm d\sqrt{m^*}) = 0$ and $\langle u|u\rangle = 1$. From textbook quantum mechanics it is known that the normalized solutions of equation (53) are

$$u_i(y) = \frac{1}{\sqrt{d}\sqrt[4]{m^*}} \left\{ \begin{matrix} \sin \\ \cos \end{matrix} \right\} (\mathrm{i}Y) \qquad Y = \frac{\pi}{2\sqrt{m^* d}} y \tag{54}$$

where $\cos(\cdot)$ corresponds to $i = 1, 3, 5, \ldots$ and $\sin(\cdot)$ to $i = 2, 4, 6, \ldots$. Eigenenergies are given by

$$E_i = \frac{\pi^2}{4qm^*d^2} i^2. \tag{55}$$

The family of potentials isospectral to the original (51) is described by

$$U_{SS}(y, \lambda) = \underline{U}_0(y) + \Delta U_{SS}(y, \lambda) = \Delta U_{SS}(y, \lambda) = -\frac{2}{q}\{\ln[\lambda + I(y)]\}''. \tag{56}$$

Choosing the supersymmetric transform to be done in respect to the ground state, we have

$$I(y) = \frac{Y}{\pi} + \frac{1}{2} + \frac{\sin(Y)}{2\pi} \tag{57}$$

and

$$U_{SS}(y, \lambda) = \frac{1}{qd^2m^*[\lambda + I(y)]} \left\{ \pi \sin(Y) + \frac{[1 + \cos(2Y)]^2}{2[\lambda + I(y)]} \right\}. \tag{58}$$

Using equation (42) the $\underline{m}_{SS}(y)$ dependence may be written as

$$\underline{m}_{SS}(y) = \frac{m^*}{[C_1 + C_2\sqrt{m^*}y]^4}. \tag{59}$$

Instead of constants C_1 and C_2 it is more convenient to use new constants α and β defined as

$$\alpha \equiv 3C_2m^*d \qquad \text{and} \qquad \beta \equiv C_1^3 \tag{60}$$

so that equation (59) becomes

$$\underline{m}_{SS}(y) = \frac{m^*}{(\beta^{1/3} + \frac{\alpha}{3d\sqrt{m^*}}y)^4}. \tag{61}$$

The coordinates z_{SS} and y, from equation (43), are related by

$$z_{SS} = \frac{d}{\alpha}\left[\left(\beta^{1/3} + \frac{\alpha}{3d\sqrt{m^*}}y\right)^3 - \beta\right] \tag{62}$$

and the final expression for the effective mass reads

$$m_{SS}(z_{SS}) = \frac{m^*}{(\alpha z_{SS}/d + \beta)^{4/3}} \tag{63}$$

while $U_{SS}(z_{SS})$ may be obtained by substituting (62) into (58). However, this expression is too cumbersome to be reproduced here.

All physically different $m_{SS}(z_{SS})$ and $U_{SS}(z_{SS})$ will be obtained by giving only positive values to α and β. It follows from equation (63) that $m_{SS}(z_{SS})$ is a monotonously decreasing function if $3\beta^{1/3} > \alpha$, otherwise there exists a point z_{SS0} where the effective mass becomes infinite. This second case will be discussed in more detail below.

The SUSYQM transformed wavefunctions, as they depend on y, read

$$\underline{\psi}_{SSi}(y) = \sqrt[4]{\underline{m}_{SS}(y)}u_{SSi}(y,\lambda) = \frac{u_{SSi}(y,\lambda)\sqrt[4]{m^*}}{|\beta^{1/3} + \frac{\alpha}{3d\sqrt{m^*}}y|}. \tag{64}$$

The wavefunctions $u_{SSi}(y,\lambda)$ may be written analytically, by using equations (15) and (16), as well as (54) for the rectangular well. The functions $\psi_{SSi}(z_{SS})$ are then simply found by combining equations (64) and (62). These are inversely proportional to $r = \alpha z_{SS}/d + \beta$. If $3\beta^{1/3} > \alpha$, r is positive for all relevant values of z_{SS}. On the other hand, if $3\beta^{1/3} < \alpha$ then a point z_{SS0} exists where r changes its sign, which brings about the wavefunction singularity. In the vicinity of this point the singularity is of the form $\text{const}/(z_{SS} - z_{SS0})^{1/3}$, i.e. $\psi^2_{SSi} \sim (z_{SS} - z_{SS0})^{-2/3}$, which means that the wavefunctions are still square integrable, regardless of the singularity, and are physically acceptable.

Numerical results are presented for a 100 Å wide quantum well ($d = 50$ Å) with a constant effective mass ($m^* = 0.08$ in free electron mass units). Such quantum wells are realizable by using ternary semiconductor alloys, like $Al_xGa_{1-x}As$, although the assumption of infinitely high barriers is clearly an approximation. In figures 1 and 2 the calculated effective-mass and potential variations are given in cases $\alpha = 1.4$ and $\beta = 1.5$ (i.e. $3\beta^{1/3} > \alpha$), or $\alpha = 8$ and $\beta = 1.5$ (i.e. $3\beta^{1/3} < \alpha$). The value of the parameter $\lambda = 0.5$ was taken, as both small enough to produce the output quite different from the input (coincidence of the two occurs in the limit $\lambda \to +\infty$), and also large enough that the output functions are not 'unphysically' deformed (which occurs in the limit $\lambda \to 0$). It is also interesting to note that, by changing the values of α and β within the $\lambda \to +\infty$ limit, it is possible to construct the supersymmetric potentials which are rectangular, but have different widths from the original, and have nonconstant effective mass (full reproduction of the original potential and the constant mass occurs for $\alpha = 0$ and $\beta = 1$; the corresponding dependences $U_{SS}(z_{SS})$ and $m_{SS}(z_{SS})$ are displayed in figure 3). Finally, in figure 4 are displayed the wavefunctions of the lowest three states of the Hamiltonian obtained with $\alpha = 8$ and $\beta = 1.5$ (the case of $3\beta^{1/3} < \alpha$), when the wavefunctions have singularities but are normalizable.

In the second example we take the rectangular potential $U_0(z)$ and the effective-mass $m(z)$ variations, i.e., $U_0(z) = 0$ for $|z| < d$ and $U_0(z) = V_0$ otherwise, while $m(z) = m_w$ for $|z| < d$ and $m(z) = m_b$ otherwise. This model corresponds to the conventional semiconductor

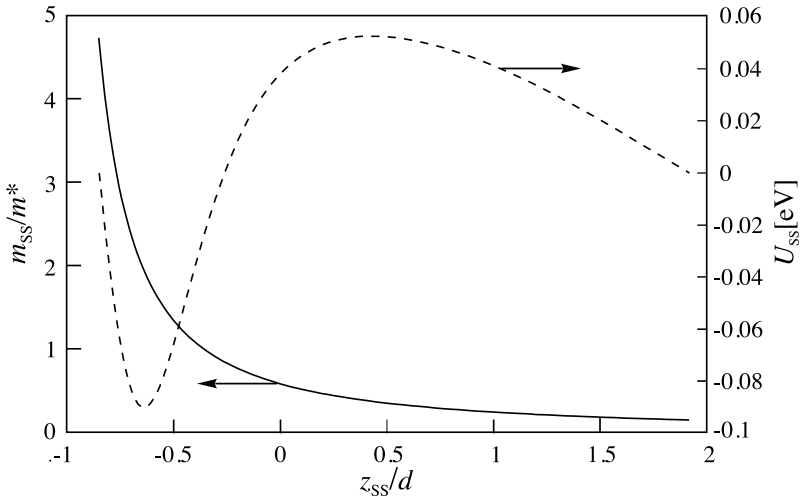

Figure 1. The $m_{SS}(z)$ and $U_{SS}(z)$ calculated when starting with a rectangular infinitely deep quantum well, $2d = 100$ Å wide. Other parameters: $m^* = 0.08$ (in free electron units), $\alpha = 1.4$, $\beta = 1.5$, and $\lambda = 0.5$. Arrows indicate from which vertical axis to read the values on the curves.

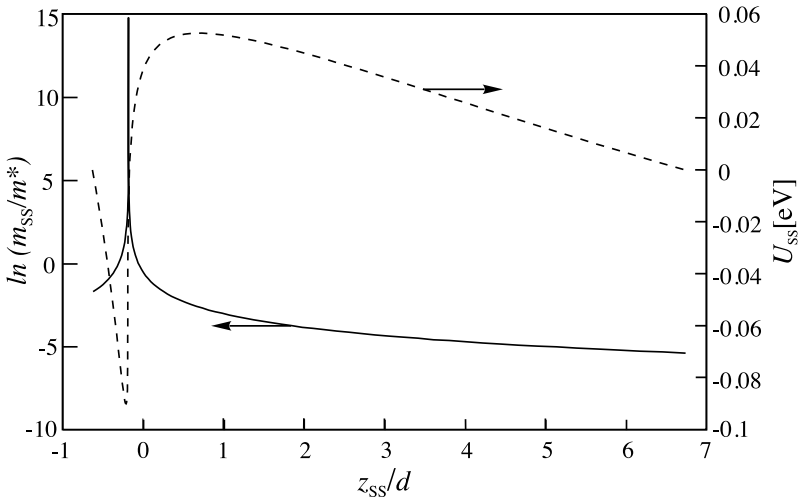

Figure 2. Same as in figure 1, but for $\alpha = 8$ and $\beta = 1.5$.

quantum wells, which have been extensively studied, both theoretically and experimentally [2]. The $y(z)$ dependence is here somewhat more complicated than in the previous example. By solving the differential equation (27) with the initial condition $y(z = 0) = 0$ we find

$$y = \begin{cases} y_d + \sqrt{m_b}(z - d) & z > d \\ \sqrt{m_w}z & |z| \leqslant d \\ -y_d + \sqrt{m_b}(z + d) & z < -d \end{cases} \tag{65}$$

where $y_d = \sqrt{m_w}d$. The well region thus maps into $|y| < y_d$, and the barrier region into $|y| > y_d$. The $\underline{m}(y)$ and $\underline{U}_0(y)$ dependences are very simple, being respectively m_w and zero in the well, and m_b and V_0 in the barriers. Using equations (42) and (43) we may thus

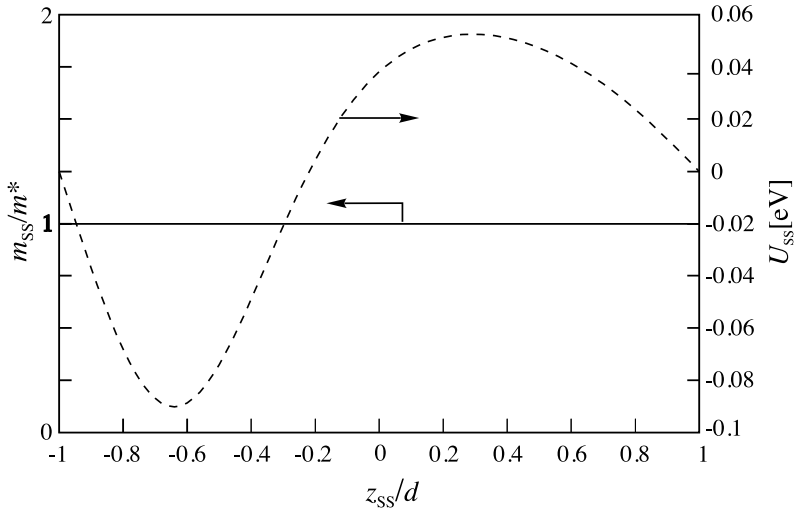

Figure 3. Same as in figure 1, but for $\alpha = 0$ and $\beta = 1$, which is equivalent to the standard SUSYQM case. Comparison of these results against those in figure 1 indicates substantial differences on the qualitative scale.

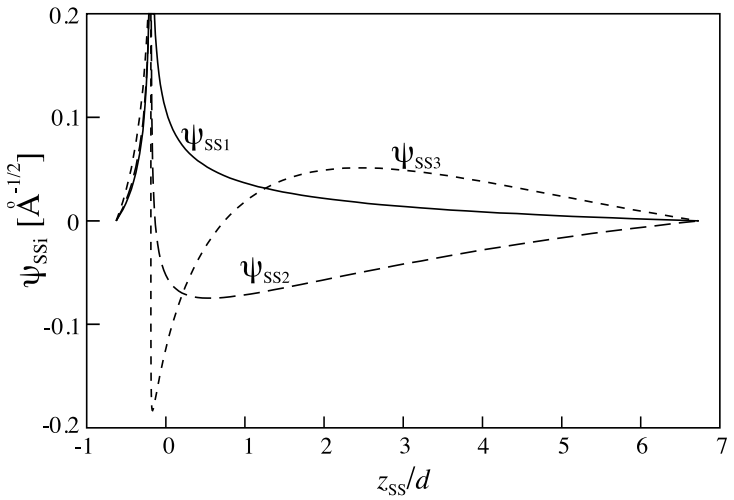

Figure 4. The normalized wavefunctions of the lowest three states, obtained with $\alpha = 8$ and $\beta = 1.5$, for the quantum well with parameters given in figure 1.

find analytic expression for the effective-mass variation $m_{SS}(z_{SS})$. In analogy to the previous example we introduce the new constants $\alpha \equiv 3C_2 m_w d$ and $\beta \equiv C_1^3$, and find that inside the well $m_{SS}(z_{SS})$ is given by equation (63) in which m^* should be substituted by m_w, where the well region $(-d \leqslant z \leqslant d)$ maps into $z_{SSmin} \leqslant z \leqslant z_{SS\,max}$ on the z_{SS} axis, where

$$(z_{SS})_{min}^{max} = d\left(\alpha\beta^{1/3} \pm \beta^{2/3} \pm \frac{\alpha^2}{27}\right) \tag{66}$$

with the constants α and β having only positive values. Inside the barriers the $m_{SS}(z_{SS})$

dependence reads

$$m_{SS}(z_{SS}) = \frac{m_b}{[\frac{\alpha}{d} r_m (z_{SS} - z_{1,2})]^{4/3}} \tag{67}$$

where z_1 is used in (67) for $z_{SS} \langle z_{SSmin}$ and z_2 for $z_{SS} \rangle z_{SSmax}$, with $z_{1,2}$ given by

$$z_{1,2} = \frac{(\beta^{1/3} \pm \frac{\alpha}{3})^3 d}{\alpha} \left[1 - \frac{1}{r_m}\right] - \frac{\beta d}{\alpha}. \tag{68}$$

In equations (67), (68) r_m is the ratio of effective masses in the the barrier and the well, $r_m = m_b/m_w$. Along with the above expressions the $z_{SS}(y)$ dependence should be given. Inside the well it is already given by equation (62), with m^* substituted by m_w, while in the barrier region we find

$$z_{SS}(y) = z_{1,2} + \frac{d}{\alpha r_m} \left[\beta \pm \frac{\alpha}{3} \mp \frac{\alpha}{3}\sqrt{r_m} + \frac{\alpha\sqrt{m_b}}{3 d m_w} y\right]^3 \tag{69}$$

where z_1 and lower signs are used for $z_{SS} \leqslant z_{SSmin}$, while z_2 and upper signs apply for $z_{SS} > z_{SSmax}$.

Due to the discontinuity of the effective mass at the well/barrier interfaces, the $u(y)$ functions are found as follows. Assuming all the solutions of equation (28) are normalized to unity, the constant in equation (25) equals one, so (25) may be written as

$$u(y) = \frac{\psi(z(y))}{\sqrt[4]{m(z(y))}} \tag{70}$$

i.e., in this case

$$u(y) = \frac{\psi(z(y))}{\sqrt[4]{m_{w,b}}} \tag{71}$$

in the well (barrier) regions. The functions $u(y)$ have discontinuities at $y = \pm y_d$ because $m_w \neq m_b$. Finally we note that the wavefunctions $\psi(z)$ are determined in the textbook manner, and the corresponding expressions will not be reproduced here.

Choosing the supersymmetric transform to be done in respect to the ground state, we have

$$\underline{U}_{SS}(y, \lambda) = \underline{U}_0(y) - \frac{2}{q}\left[\frac{2u_0 u_0'}{\lambda + I(y)} - \frac{u_0^4}{[\lambda + I(y)]^2}\right] \tag{72}$$

where $u_0(y) = \psi_0(z(y))/\sqrt[4]{m(z(y))}$ and $I(y) = \int_{-\infty}^{y} u_0^2 \, \mathrm{d}y'$. It is here interesting to note that, because of the discontinuities of $u(y)$ at $y = \pm y_d$, the function $\underline{U}_{SS}(y, \lambda)$ acquires the δ-functions at these points, i.e.,

$$\underline{U}_{SS}(y = \pm y_d, \lambda) = \mp \frac{4}{q} \frac{u_0(\pm y_d)}{\lambda + I(\pm y_d)} \left(\frac{1}{\sqrt[4]{m_b}} - \frac{1}{\sqrt[4]{m_w}}\right) \psi_0(z(\pm y_d)) \delta(y \mp y_d). \tag{73}$$

The expression for $I(y)$ is found analytically, but is too cumbersome to be reproduced here. Now, combining the expressions for $\underline{U}_{SS}(y, \lambda)$ and $z_{SS}(y, \alpha, \beta)$ we find the final expression for $U_{SS}(z_{SS}, \lambda, \alpha, \beta)$, which can also be written in a fully analytic, though quite cumbersome form. The expressions for the wavefunctions $\underline{\psi}_{SSi}(y)$ are obtained from equation (64). These are continous everywhere, including at $y = \pm y_d$. Then, using the $z_{SS}(y)$ dependence given above, we finally find the $\psi_{SSi}(z_{SS})$ wavefunctions. It is interesting to note a peculiarity occuring in these wavefunctions in the present example. Having in mind that $-\infty < y < +\infty$ and $\underline{m}(y) > 0$, it follows from equation (42) that for whatever values of the constants C_1 and C_2 (i.e., α and β) there exists a point y_0 where the denominator of (42) becomes zero. In the vicinity of the (corresponding to the z_{SS} axis) point z_{SS0} the wavefunction $\psi_{SSi}(z_{SS})$ diverges

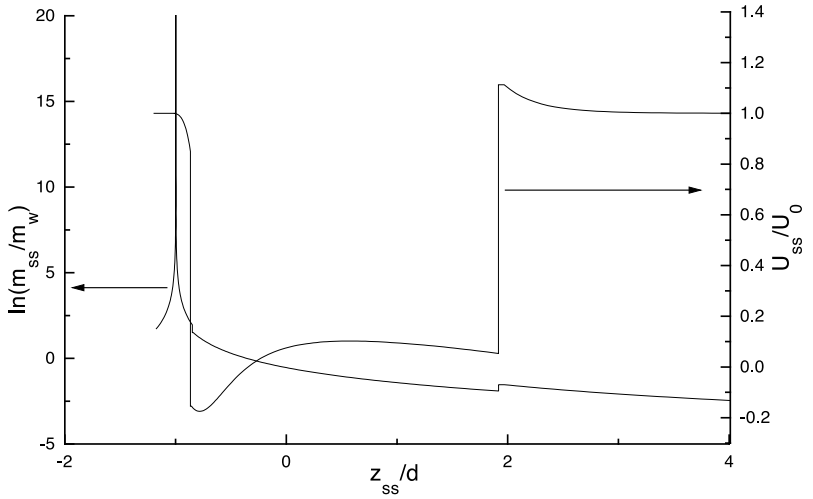

Figure 5. The $m_{SS}(z_{SS})$ and $U_{SS}(z_{SS})$ calculated when starting with a $2d = 100$ Å wide rectangular quantum well, with the barrier height $V_0 = 300$ meV. The effective masses in the well and the barrier amount to $m_w = 0.08$ and $m_b = 0.12$ (in free electron mass units), respectively, and the transform parameters are $\alpha = 1.4$, $\beta = 1.5$, and $\lambda = 0.5$.

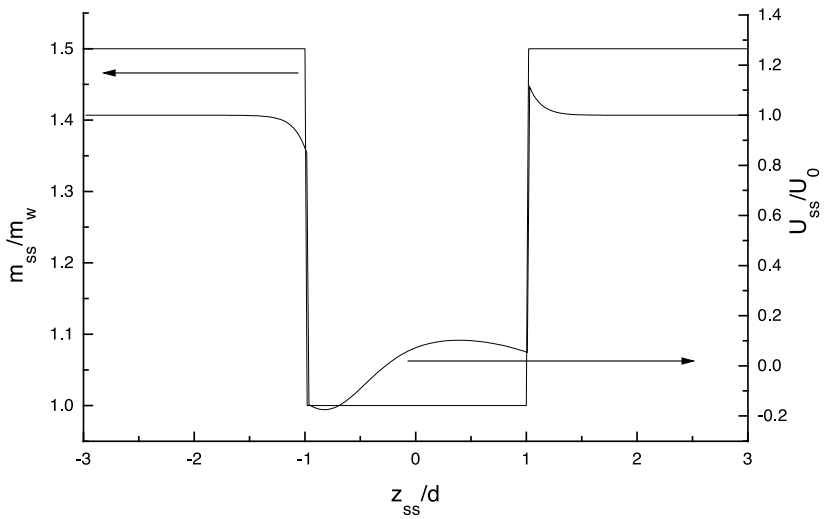

Figure 6. Same as in figure 5, but for $\alpha = 0$ and $\beta = 1$, equivalent to the standard SUSYQM case. Qualitative differences from the results in figure 5 should be noted.

as $\sim$const$/(z_{SS} - z_{SS0})^{1/3}$, thus remaining normalizable, just as was the case in the previous example.

To give a specific example, we made numerical calculations starting with a 100 Å wide quantum well with the effective mass in the well $m_w = 0.08$ and in the barriers $m_b = 0.12$, and the barriers height $V_0 = 300$ meV. These parameters correspond to a realistic semiconductor quantum well based on $Al_xGa_{1-x}As$ alloy [2]. In figure 5 we give the calculated $m_{SS}(z_{SS})$ and $U_{SS}(z_{SS})$ functions for the same set of parameters as in the previous example, i.e., $\alpha = 1.4$, $\beta = 1.5$, and $\lambda = 0.5$. We note that inside the barrier $U_{SS}(z_{SS})$ is very close to V_0 but

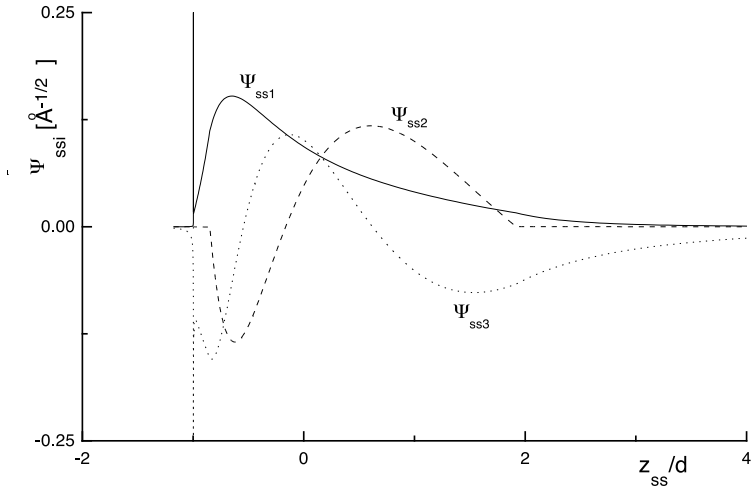

Figure 7. The normalized wavefunctions of the lowest three states of the quantum well with the parameters as in figure 5. Note that the wavefunctions in the vicinity of z_{SS0} are not δ-like, but are very sharp and the detailed shape cannot be displayed (see the text for more discussion).

changes considerably inside the well, while the effective mass $m_{SS}(z_{SS})$ varies considerably throughout the structure, and has a singularity at $z_{SS0} \approx 49$ Å. The corresponding results for $\alpha = 1$ and $\beta = 0$, which is the case of classical supersymmetry, are given in figure 6. Here only $U_{SS}(z_{SS})$ differs from $U_0(z)$, while $m_{SS}(z_{SS}) = m(z)$. It should be noted that the δ-function contributions to the potential $U_{SS}(z_{SS})$ at z_{SSmin} and z_{SSmax}, equation (73), are not displayed in figure 5 and 6. Finally, in figure 7 we display the wavefunctions $\psi_{SSi}(z_{SS})$ for the case $\alpha = 1.4$ and $\beta = 1.5$. With the point z_{SS0} being rather distant from the extrema of $u_{SSi}(y)$, the wavefunctions $\psi_{SSi}(z_{SS})$ each acquire an additional extremum due to the singularity at z_{SS0}. This is in contrast, e.g., to the wavefunctions $\psi_{SS1}(z_{SS})$ and $\psi_{SS2}(z_{SS})$ in the first case considered in this work, because there the point z_{SS0} was close to the extrema of $u_{SSi}(y)$.

4. Conclusion

Using the coordinate transform method the procedure of the supersymmetric transform was generalized to generate isospectral Hamiltonians with both the potential and the (variable) effective mass different, with adjustable degrees, from the original ones. In this respect the procedure differs from the standard SUSYQM which affects only the potential and leaves the effective mass, even if position-dependent, unchanged. Families of isospectral potentials depend on three, and families of effective masses on two free parameters, while the standard SUSYQM introduces one free parameter. The increased number of free parameters may be advantageous, e.g., in using this technique for the design and optimization of semiconductor quantum wells for some applications [11].

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