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# Exact bound-state wavefunctions for potentials varying from the double well to the single well 

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#### Abstract

We reduce the Schrödinger equation on the full line, the potential of which varies from the double well to the single well depending on the value of some parameter $a$, to a Heun's type equation, the solution of which recalls the hypergeometric series. The eigenvalue equation, which determines the energy of bound states, follows from the usual requirement that the wavefunction be zero at infinity. Transforming this equation into the infinite continued-fraction expansion we easily obtain the approximate eigenvalue. We compare it with that evaluated exactly and see that the difference is less than $0.5 \%$ for any value of the parameter $a$.


## 1. Introduction

The theoretical treatments of tunnelling phenomena are usually based on some kind of approximation. Assuming that the probability of tunnelling is small, we express the particle state as the even or odd combination of wavefunctions which describes the quantum motion in only one of the potential wells separated by the central barrier. In this way, for example, the energy splitting of the lowest even and odd bound states is calculated. In the wKB approach it is proportional to the amplitude of the tunnelling probability corresponding to the barrier (Landau-Lifshitz 1958). This is also why the probability of localising a particle in one well oscillates with the frequency, which is proportional to this energy difference. Some recent references on this coherence problem at non-zero temperatures and in real systems with dissipation of the energy of motion are den Boer and de Bruyn Onboter (1980), Caldeira and Leggett (1981), Widom and Clarke (1982), Voss and Webb (1982) and Bray and Moore (1982).

From this point of view the double-well potentials, for which the Schrödinger equation on the full line can be exactly solved, represent an interesting problem as they allow comparison with the approximative formula. The investigated potential used here

$$
\begin{align*}
& V(a, y)=\left[4 a /\left(a-t^{2}\right)^{2}\right]\left[\left(3 a-\frac{5}{2}\right) t^{4}+\left(a^{2}-5 a+3\right) t^{2}-\frac{1}{2} a^{2}+a\right] \\
& t \equiv \tanh \left[(2 a)^{1 / 2} y\right] \tag{1}
\end{align*}
$$

is more interesting as it corresponds to a real physical problem and its double-well form passes to the one-well form by varying only the value of parameter $a$ from
$a=1+\varepsilon(\varepsilon>0)$ to $a=\infty$. It can also be easily generalised to the four-well potential and the Schrödinger equation retains the analytic solvability.

In $\S 2$ properties of the potential (1) are investigated, especially in the double-well region. We solve the Schrödinger equation on the full line for this potential in § 3 . As we are concentrating on the bound-state solutions, we initially review the properties of the ground-state solution and then we give the solution for the only excited state. The general approach consists in reducing the primary Schrödinger equation to Heun's equation in the interval $[0,1]$. Its solution, expressed in terms of power series, becomes less divergent at $z=1$, when we impose the usual boundary condition, which determines the eigenvalues. The eigenvalue equation is also written in the form of the infinite continued-fraction expansion. There is an alternative solution, which leads to Heun's equation again but with different defining parametres. At the end of the section we sketch the scattering solutions.

We derive two approximate analytic formulae for the binding energy of the only excited state as a function of parameter $a$ from the infinite continued-fraction expansion and compare them with the exact numerical values in § 4. Both derived formulae can be related to variational solutions of the problem, which apply simple forms of wavefunction. The concluding remarks form the content of $\S 5$.

## 2. The Schrödinger equation

The Schrödinger equation, with which we are concerned in this paper, was first derived by one of the authors (Hudák 1981) in connection with the stability analysis of some solutions for the double sine-Gordon equation with respect to small perturbations. This equation reads

$$
\begin{equation*}
\mathrm{d}^{2} F\left(\omega^{2}, y\right) / \mathrm{d} y^{2}+\left[\omega^{2}-V(a, y)\right] F\left(\omega^{2}, y\right)=0, \quad y \in(-\infty,+\infty) \tag{2}
\end{equation*}
$$

where the potential $V(a, y)$ is given by (1). Compared with the quoted paper we use a new parameter $a=1+\lambda / 2$ instead of $\lambda \in(0, \infty)$ and put $y_{0}=0$, thus fixing the symmetry centre of the potential $V(a, y)$ at the origin.

If $a>5$ the potential $V(a, y)$ assumes the maximum value $V=2 a$ at $y= \pm \infty$ and the minimum value $V=2(2-a)$ at $y=0$. This minimum turns into the local maximum for $a<5$ and new minima $V=-2-\left[(a-1)^{2} / 4\right]$ appear at $y_{m}=$ $\pm(2 a)^{-1 / 2} \tanh ^{-1}\left\{[a(5-a) /(7 a-3)]^{1 / 2}\right\}$ at the same time. The potential $V(a, y)$ is characterised by two wells below the critical value $a_{\mathrm{c}}=5$ and by a single well above this value as demonstrated in figure 1. Continuously varying the value of $a$ we completely change the form of the potential.

We can also characterise the potential $V(a, y)$ by the distance $l=2\left|y_{m}\right|$ between the centres of two wells in the double-well region. We have $l \approx$ $(10)^{1 / 2}(5-a) / 32+\mathrm{O}\left[(5-a)^{2}\right]$ as $a \rightarrow 5^{-}$and $l \approx-2^{-1 / 2} \ln \left[\frac{1}{2}(a-1)\right]+\mathrm{O}[(a-1) \ln (a-1)]$ as $a \rightarrow 1^{+}$. The energy excess of the barrier is $\delta E_{\mathrm{B}} \approx(a-5)^{2} / 4 \approx 25,6 l^{2}$ as $l \rightarrow 0^{+}$and $\delta E_{\mathrm{B}} \approx 4-4 \exp \left(-2^{1 / 2} l\right)$ as $l \rightarrow \infty$. The difference $\delta E_{\mathrm{M}}=4+2(a-1)+(a-1)^{2} / 4$ between the absolute maximum and minimum of the potential energy displays similar behaviour: $\delta E_{\mathrm{M}} \approx 4+4 \exp \left(-2^{1 / 2} l\right)$ as $l \rightarrow \infty$, but $\delta E_{\mathrm{M}} \approx 16-64(2 / 5)^{1 / 2} l$ as $l \rightarrow 0^{+}$.

Introducing the new energy parameter $b$ and the new variable $x$

$$
\begin{equation*}
b^{2}=1-\omega^{2} / 2 a, \quad l=(2 a)^{1 / 2} y \tag{3}
\end{equation*}
$$



Figure 1. The potential $V(a, x)$ is characterised by two wells below the critical value $a_{c}=5$ and by a single well above this value: curve a, $a=1,25$; curve $\mathrm{b}, a=3,25$; curve c, $a=6,25$.


Figure 2. The density $w_{i}(x)$ of the probability of observing a quantum particle at the point $x$ for three typical values of the potential parameter $a$ : curve $a$, $a=1,25$; curve b; $a=3,25$; curve c, $a=6,25$. Note that for $2<a<5$ there are two minima of the potential $V(a, x)$ but only a single minimum in the probability $w_{1}(x)$.
we obtain the more familiar form of the Schrödinger equation

$$
\begin{equation*}
\frac{\mathrm{d}^{2}}{\mathrm{~d} x^{2}} F(b, x)=\left(b^{2}-2 \frac{(a-1)\left[a+3(\tanh x)^{2}\right]}{\left[a-(\tanh x)^{2}\right]}\left[1-(\tanh x)^{2}\right]\right) F(b, x), \tag{4}
\end{equation*}
$$

in which the potential tends to zero as $|x| \rightarrow \infty$. Since the potential in (4) is always attractive, there is at least one bound state for any $a \in(1, \infty)$ (cf Landau and Lifshitz 1958, for example).

## 3. Bound states

The zero oscillation mode $\omega=0$ found by Hudák (1981) is the ground state of (4), for which we obtain $b=1$. The corresponding normalised eigenfunction is

$$
\begin{equation*}
F(1, x)=\left[4+\frac{2(a-1)}{\sqrt{a}} \ln \left(\frac{\sqrt{a}+1}{\sqrt{a}-1}\right)\right]^{-1 / 2}\left\{[\cosh (x+\Delta)]^{-1}+[\cosh (x-\Delta)]^{-1}\right\} \tag{5}
\end{equation*}
$$

where

$$
\begin{equation*}
\tanh \Delta=1 / \sqrt{a} \tag{6}
\end{equation*}
$$

Figure 2 shows the density $w_{1}(x)=|F(1, x)|^{2}$ of the probability of observing a quantum particle at the point $x$ for three typical values of the potential parameter $a(a=1,25$, $a=3,25, a=6,25)$. Its value at the symmetry centre $x=0$

$$
\begin{equation*}
w_{1}(0)=\frac{2(a-1)}{2 a+\sqrt{a}(a-1) \ln [(\sqrt{a}+1) /(\sqrt{a}-1)]} \tag{7}
\end{equation*}
$$

can be expressed in terms of the distance $l$ in the double-well region ( $1<a<5$ ). This probability vanishes exponentially, $w_{1}(0) \approx 2 \exp \left(-2^{1 / 2} l\right)$, as $l \rightarrow \infty$ and assumes the finite value $w_{1}(0)=4 /\left[5+4 \sqrt{5} \ln \left(\frac{1}{2}(1+\sqrt{5})\right]\right.$ as $l \rightarrow 0^{+}$.

There is a well known procedure (Kamke 1943) by means of which we reduce the number of bound states. This procedure consists in introducing a new eigenfunction

$$
\begin{equation*}
U(b, x)=F(1, x)(\mathrm{d} / \mathrm{d} x)[F(b, x) / F(1, x)], \tag{8}
\end{equation*}
$$

instead of $F(b, x)$, which now solves the Schrödinger equation (4) with the transformed potential

$$
\begin{align*}
W(a, x)= & 2\left(\frac{\mathrm{~d}}{\mathrm{~d} x} \ln F(1, x)\right)^{2}-2+2 \frac{(a-1)\left[a+3(\tanh x)^{2}\right]}{\left[a-(\tanh x)^{2}\right]}\left[1-(\tanh x)^{2}\right] \\
& =-\frac{2}{(\cosh x)^{2}}\left(1-\frac{a-1}{a-(\tanh x)^{2}}\right), \tag{9}
\end{align*}
$$

and with the same eigenenergy $-b^{2}$. As (9) represents an attractive potential, but less attractive than $-2 /(\cosh x)^{2}$, there then exists just one bound state of the transformed equation (4). This means finally that there are two bound states $b=1$ and $0<b<1$ in the primary equation (4) for $1<a<\infty$.

We find them by inserting

$$
\begin{equation*}
t=\tanh (x) \quad \text { and } \quad F(b, x)=\left[\left(1-t^{2}\right)^{b / 2} /\left(a-t^{2}\right)\right] f\left(b, t^{2}\right) \tag{10}
\end{equation*}
$$

into (4). The eigenfunction $f(b, z),\left(z=t^{2}\right)$ then solves Heun's equation (Kamke 1943, formula 2.328):

$$
\begin{align*}
& H(a, q ; \alpha, \beta, \gamma, \delta ; z) \equiv z(1-z)(a-z) h^{\prime \prime} \\
&+\left\{(\alpha+\beta+1) z^{2}-[\alpha+\beta+1+a(\gamma+\delta)-\delta] z+\gamma a\right\} h^{\prime}+(\alpha \beta z-q) h=0 \tag{11}
\end{align*}
$$

where
$a=a, \quad q=\frac{1}{4} a(b-1)(b+2), \quad \alpha=\frac{1}{2}(b-1), \quad \beta=\frac{1}{2}(b-2), \quad \gamma=\frac{1}{2}, \quad \delta=b+1$,
i.e. the parameters $q, \alpha, \beta$ and $\delta$ depend on the eigenvalue $b$.

Solutions of (11) can be expanded into the series

$$
\begin{equation*}
\sum_{n=0}^{\infty} c_{n, r}(a, q ; \alpha, \beta, \gamma, \delta) z^{n+r} \tag{13}
\end{equation*}
$$

in the interval $0 \leqslant z \leqslant 1$ in which we are interested. The coefficients $c_{n, r}$ fulfil the recurrence relations

$$
\begin{gather*}
c_{n+1, r}=\left(\frac{(n+r+\gamma+\delta-1)(n+r)+q / a}{(n+r+\gamma)(n+r+1)}+\frac{(n+r)(n+r+\alpha+\beta-\delta)}{a(n+r+\gamma)(n+r+1)}\right) c_{n, r} \\
-\frac{(n+r+\alpha-1)(n+r+\beta-1)}{a(n+r+\gamma)(n+r+1)} c_{n-1, k} \quad(n=-1,0, \ldots, \infty), \\
c_{-2, r}=c_{-1, r}=0, \quad c_{0, r}=1 . \tag{14}
\end{gather*}
$$

Putting $n=-1$ we see that $r=0$ or $r=1-\gamma$. The value $r=0$ labels an even function of $t$ and we denote the corresponding series (12) by $F\left(a, q_{i} \alpha, \beta, \gamma, \delta ; z\right)$ in accordance
with Kamke (1943). If $\gamma$ is not an integer, which is the case when $\gamma=\frac{1}{2}, r=1-\gamma=\frac{1}{2}$ labels the second independent solution of (10). It is an odd function of $t$ and reads $z^{1-\gamma} F\left(a, q_{1} ; \alpha-\gamma+1, \beta-\gamma+1,2-\gamma, \delta ; z\right)$ in the notation introduced, where $q_{1}=$ $q+(1-\gamma)[\alpha+\beta+1-\gamma+(a-1) \delta]$. The function $F(a, q ; \alpha, \beta, \gamma, \delta ; z)$ exhibits similar properties to the more familiar hypergeometric function $F(\mu, \nu ; \rho ; z)$. It diverges at $z=1$, in general, like the geometric series, as the solution of the recurrence relations (14) is

$$
\begin{equation*}
c_{n, r}(a, q ; \alpha, \beta, \gamma, \delta) \sim A_{r}(a, q ; \alpha, \beta, \gamma, \delta)+B_{r}(a, q ; \alpha, \beta, \gamma, \delta) a^{-n} \tag{15}
\end{equation*}
$$

in the asymptotic region $n \gg 1$. This means according to (10) and (12), that the eigenvalue equation, which determines the eigenvalue $b$, reads

$$
\begin{equation*}
\lim _{n \rightarrow \infty} c_{n, r}(a, q ; \alpha, \beta, \gamma, \delta)=0 \tag{16}
\end{equation*}
$$

Although even then the logarithmically divergent part $(b-1)(1-1 / a) z \ln (1-z)$ remains in the series (13), according to (14), it is harmless in the bound-state wavefunction (10) as the total product function tends to zero as $|t| \rightarrow 1$.

Since the eigenvalue equation (16) is somewhat impractical, we replace it by another one, which is more amenable to an approximate solution. Denoting factors multiplying $c_{n, r}$ and $-c_{n-1, r}$ respectively in (14) by $\mu_{n+r}$ and $\nu_{n+r}$ respectively, we transform (14) into the reverse recurrence relation

$$
\begin{equation*}
\rho_{n, r}=\frac{c_{n+1, r}}{c_{n, r}}=\frac{\nu_{n+r+1}}{\mu_{n+r+1}-\rho_{n+1, r}} \quad(n=0, \ldots, \infty) \tag{17}
\end{equation*}
$$

which turns into the infinite continued-fraction expansion

$$
\begin{equation*}
\rho_{0, r}=\mu_{r}=\frac{\nu_{1+r}}{\mu_{1+r}} \frac{\nu_{2+r}}{-\mu_{2+r}} \frac{\nu_{3+r}}{-\mu_{3+r}}-\ldots \tag{18}
\end{equation*}
$$

by successive iterations into the new eigenvalue equation.
If we insert $b=1$ into the set of parameters (12), their values are $a=a, q=0, \alpha=0$, $\beta=-\frac{1}{2}, \gamma=\frac{1}{2}, \delta=2$, so that $\mu_{0}=\nu_{1}=0$ (for $r=0$ ), which corroborates Hudák's eigenvalue $b^{2}=1$ and eigenfunction $\left(1-t^{2}\right)^{1 / 2} /\left(a-t^{2}\right)$. The eigenvalue of the only excited state $0<b<1$ is determined by the $r=\frac{1}{2}$ alternative of equation (18) and the corresponding eigenfunction is an odd function of $x$ with nodes at $x=0$ and $x= \pm \infty$ respectively.

This excited state is a ground state for the transformed potential (9). The product form of the corresponding transformed eigenfunction $U(b, x)$,

$$
\begin{equation*}
U(b, x)=\left(1-t^{2}\right)^{b / 2} u\left(b, t^{2}\right), \quad t=\tanh (x) \tag{19}
\end{equation*}
$$

which is analogous to ( 10 ), ensures the desirable asymptotic behaviour of the boundstate wavefunction. Inserting this expression into the Schrödinger equation with potential (9) we get Heun's equation (11) for $u(b, z)$ again, but now the set of parameters (12) is

$$
\begin{equation*}
a=a, \quad q=\frac{1}{4} a(b+1) b-\frac{1}{2}, \quad \alpha=\frac{1}{2}(b-1), \quad \beta=\frac{1}{2}(b+2), \quad \gamma=\frac{1}{2}, \quad \delta=b+1 . \tag{20}
\end{equation*}
$$

The ground-state wavefunction $U(b, x)$ is given by the $r=0$ alternative of formulae (13)-(18), so that we have two formally different expressions for the wavefunction of
the excited state of (4)

$$
\begin{align*}
F(b, x)= & \frac{\left(1-t^{2}\right)^{b / 2}}{a-t^{2}} t F\left(a, \frac{a}{4} b(b+3)-1 ; \frac{b}{2}, \frac{b-1}{2}, \frac{3}{2}, b+1 ; t^{2}\right) \\
= & \frac{\left(1-t^{2}\right)^{1 / 2}}{a-t^{2}} \int_{0}^{t} \mathrm{~d} s\left(1-s^{2}\right)^{b / 2-3 / 2}\left(a-s^{2}\right) \\
& \quad \times F\left(a, \frac{a}{4} b(b+1)-\frac{1}{2} ; \frac{b+2}{2}, \frac{b-1}{2}, \frac{1}{2}, b+1 ;-s^{2}\right), \quad t=\tanh (x) \tag{21}
\end{align*}
$$

both expressed by Heun's solution $F\left(\ldots ; \ldots ; t^{2}\right)$.
Not only solutions for bound states but also solutions for the scattering states can be expressed by means of functions $F(\ldots ; \ldots ; z)$. The parameters $q, \alpha, \beta$ and $\delta$ are now complex numbers as $b=-i k$ and $k^{2}>0$ is the energy of the scattered particle. As the potential in (4) is symmetric we now find solutions of the Schrödinger equation for either half-line $x \geqslant 0$ and $x \leqslant 0$ separately and then match them at $x=0$. Because the scattering wavefunctions are neither even nor odd functions of $x$, they are linear combinations of two independent solutions that are given by the $r=0$ and $r=\frac{1}{2}$ alternative of formulae (10) and (13)-(15). This combination must be taken such that the wavefunction (10) remains finite as $x \rightarrow \pm \infty$ and that it respects the prescribed boundary conditions of the particular scattering problem as $x \rightarrow \pm \infty$ at the same time. Realisation of the sketched procedures also leads automatically to the determination of the other physically important quantities like the transmission and reflection amplitudes.

## 4. Approximate solutions

We begin with the eigenvalue problem for the excited state $b$. If we choose values (12) for the parameters of Heun's equation, its eigenvalue $b$ is determined by equation (18), in which we put $r=\frac{1}{2}$. As $\rho_{n, 1 / 2} \sim a^{-1}$, according to (15) for the eigenvalue $b$ in the asymptotic region of $n$, we cut off the infinite expansion at some large enough value of $n$ and substitute $\nu_{n} /\left(\mu_{n}-a^{-1}\right)$ for $\rho_{n-1,1 / 2}$. We get an approximate equation polynomial expression in $b$, the positive root of which, $b<1$, is an approximate value of $b$.

This procedure is much simplified provided that $\nu_{3 / 2}$ is very small for some reason. If we neglect it completely, the approximate eigenvalue equation reads $\mu_{1 / 2}=$ $\left(b^{2}+3 b-4 / a\right) / 6$ according to (14) and (12), i.e. the eigenvalue

$$
\begin{equation*}
b=\frac{1}{2}(9+16 / a)^{1 / 2}-\frac{3}{2}=8 / a\left[(9+16 / a)^{1 / 2}+3\right] \tag{22}
\end{equation*}
$$

It is roughly equal, i.e. $b \approx a^{-1}$, especially as $a \rightarrow 1^{+}$. But then the absolute value of $\nu_{3 / 2}=(b-1) b / 20 a$ is very small indeed $\left|\nu_{3 / 2}\right| \approx(a-1) / 20 a^{3} \leqslant 1 / 135$. When we insert $b=1 / a$ into the infinite continued-fraction, which divides $\nu_{3 / 2}$ according to (18), we see that its value moves round the value $\frac{1}{2}$. Thus the eigenvalue equation is

$$
b^{2}+3 b-(4 / a)+\frac{3}{5} c\left[(a-1) / a^{3}\right]=0
$$

i.e.

$$
\begin{equation*}
b=\frac{1}{2}\left[9+(16 / a)-\frac{3}{5} c\left[(a-1) / a^{3}\right]\right\}^{1 / 2}-\frac{3}{2}, \tag{23}
\end{equation*}
$$

where the unknown constant $c \approx 1$ according to the theoretical estimate obtained.

We have calculated numerically the binding energies $b^{2}$ using the computer program, which issues from the very effective method of determining the eigenvalues of the one-dimensional Schrödinger equation (cf Úlehla et al 1981). The numerical results are given in the second column of table 1. As the relative deviation of these values and those according to formula (22) assumes its maximum value $7.04 \%$ at $a=2.1$ (see the third column of table 1), we have chosen constant $c$ in (23) such that the numerical value and the value given by (23) to be equal at this point. We obtain $c=1.025$ and the values of the corresponding binding energy as a function of parameter $a$ differ from those calculated numerically by less than $0.5 \%$.

Table 1. The binding energy $b^{2}$ as a function of parameter $a$. Listed are exact values $E$ and the approximate values according to formulae (22) and (24).

| $a$ | $E$ | $(22)$ | $(24)$ |
| :--- | :--- | :--- | :--- |
| 1.1 | 0.8362 | 0.8578 | 0.8801 |
| 1.2 | 0.7156 | 0.7446 | 0.7822 |
| 1.3 | 0.6217 | 0.6529 | 0.7011 |
| 1.4 | 0.5465 | 0.5775 | 0.6330 |
| 1.5 | 0.4849 | 0.5146 | 0.5750 |
| 1.6 | 0.4336 | 0.4617 | 0.5253 |
| 1.7 | 0.3905 | 0.4166 | 0.4821 |
| 1.8 | 0.3537 | 0.3779 | 0.4444 |
| 1.9 | 0.3221 | 0.3445 | 0.4113 |
| 2.0 | 0.2947 | 0.3153 | 0.3820 |
| 2.1 | 0.2707 | 0.2898 | 0.3559 |
| 3.1 | 0.1366 | 0.1456 | 0.1990 |
| 4.1 | 0.0828 | 0.0876 | 0.1289 |
| 5.1 | 0.0557 | 0.0585 | 0.0908 |
| 6.1 | 0.0400 | 0.0419 | 0.0677 |
| 7.1 | 0.0302 | 0.0314 | 0.0525 |
| 8.1 | 0.0236 | 0.0245 | 0.0420 |
| 11.1 | 0.0130 | 0.0134 | 0.0243 |
| 21.1 | 0.0038 | 0.0038 | 0.0076 |
| 31.1 | 0.0018 | 0.0018 | 0.0037 |

As there is an alternative solution for the excited state given by (19), (11) and (20-21), we applied the described procedure to the set of parameters (20) also. Unlike the preceding case we cannot now estimate the RHS of (18) (with $r=0$ ) to a good accuracy. If we neglect it completely, we get $\mu_{0}=0=b(b+1) / 2-1 / a$, i.e.

$$
\begin{equation*}
b=\frac{1}{2}(1+8 / a)^{1 / 2}-\frac{1}{2} . \tag{24}
\end{equation*}
$$

This root assumes the exact value for $a \rightarrow 1$ as well as for $a \rightarrow \infty$, but within the interval $a \in(1, \infty)$ the agreement with the numerical value is much worse than that of formula (22) (see the fourth column of table 1). The only way of recovering formula (24) is to replace $8 / a$ by $8[1-(a-1) / 3 a] / a$ as it has asymptotic behaviour for $a \rightarrow \infty$, differing only slightly from that given by the numerical evaluation and it is identical with formula (22) to an order $1 / a$. The resulting formula:

$$
\begin{equation*}
b=\frac{1}{2}\left[1+16 / 3 a+8 / 3 a^{2}\right]^{1 / 2}-\frac{1}{2} \tag{25}
\end{equation*}
$$

gives the numerical values, which agree with the second column to a minimum accuracy of $1 \%$. This is why we prefer formula (23).

At the same time, formulae (22) and (24) reflect two possibilities of finding the approximate wavefunction using the variational calculation. We evaluate the average value of the total energy for the potential of equations (4) and (9) respectively for this purpose. In the first case we substitute the function

$$
\begin{equation*}
F(p, x)=\left[1-(\tanh x)^{2}\right]^{p / 2}\left[a-(\tanh x)^{2}\right]^{-1} \tag{26}
\end{equation*}
$$

for the wavefunction (10), while in the second case we insert

$$
U(p, x)=\left[1-(\tanh x)^{2}\right]^{p / 2}
$$

i.e.
$F(p, x)=\frac{\left[1-(\tanh x)^{2}\right]^{1 / 2}}{a-(\tanh x)^{2}} \int_{0}^{x} \mathrm{~d} y\left[1-(\tanh y)^{2}\right]^{(p-1) / 2}\left[a-(\tanh y)^{2}\right]$
instead of (19). The average values $E_{v}$ and $E_{w}$ are, correspondingly,

$$
\begin{gather*}
E_{v}=\frac{3}{2} p-\frac{4}{a}+\frac{3}{4}+\frac{3}{8\left(p-\frac{1}{2}\right)}+\left(-p-\frac{1}{2}+\frac{2}{a}-\frac{1}{4} \frac{1}{p-\frac{1}{2}}\right)\left(1-\frac{1}{a}\right) \\
\times\left(\frac{\mathrm{d}}{\mathrm{~d} t} \ln F\left(2, \frac{3}{2} ; p+\frac{3}{2} ; z\right)\right)_{z=1 / a}  \tag{28}\\
E_{w}=\frac{p}{2}-\frac{9}{4}+\frac{9}{8\left(p+\frac{1}{2}\right)}+2\left(1-\frac{1}{a}\right) F\left(\frac{1}{2}, 1 ; 1-p ; 1-\frac{1}{a}\right) . \tag{29}
\end{gather*}
$$

The integrals appearing in the average values just define the different types of hypergeometric function $F(\mu, \nu ; \rho ; z)$ that we have successively reduced to those written in (28) and (29) using the relations of Bateman and Erdélyi (1953). The minima of expressions (28) and (29) are, in fact, given by formulae (22) and (24) respectively in the limits $a \rightarrow 1^{+}$and $a \rightarrow \infty$.

## 5. Concluding remarks

The fact that the Schrödinger equation on the full line with the double-well potential (1) or even the more general potential is analytically solvable, can be attributed to the final Heun form of the transformed equation, the solution of which does not differ very much from the hypergeometric series. The alternative solution (19), which again results in the equation of Heun's type and which is based on the transformation (9) is useful only when the form of the ground-state wavefunction is simple. The phenomenological formula (25), though practically useful, is in fact misleading as it is derived from formula (23), which only has a theoretical justification.

Note. After completion of this article, a paper by W M Zheng on 'The Darboux transformation and solvable double-well potential models for Schrödinger equations' appeared (Zheng 1984). In the paper Zheng derives a potential from the Weber equation, which varies its form from the double well to the single well depending on
the value of a parameter, using the Darboux transformation. The Darboux transformation and allied transformations are often used now in studying various aspects of solutions of the Schrödinger equation. The first paper of this kind was probably the paper by Grum (1955) on 'Associated Sturm-Liouville Systems'. We express our sincere thanks to the referee, who attracted our attention to a certain similarity between some investigations in our paper and in that of Zheng.

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