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LETTER TO THE EDITOR

Shape invariant potentials in SUSY quantum mechanics and periodic orbit theory

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Abstract
We examine shape invariant potentials (excluding those that are obtained by scaling) in supersymmetric quantum mechanics from the standpoint of periodic orbit theory. An exact trace formula for the quantum spectra of such potentials is derived. On the basis of this result, and Barclay's functional relationship for such potentials, we present a new derivation of the result that the lowest order SWKB quantisation rule is exact.

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In non-relativistic quantum mechanics certain potentials are amenable to exact analytic solution. For a subset of these soluble potentials, the energy spectrum may be expressed explicitly as an algebraic function of a single quantum number. Such potentials occur either in one space dimension, or are central potentials in higher dimensions. For the latter, an effective potential in the radial variable can be defined for each partial wave. Some examples of such potentials are Coulomb, harmonic oscillator, Morse, Rosen–Morse, etc [1]. These potentials also have the property that the lowest order WKB quantization rule, together with the appropriate Maslov index (that may change from potential to potential [2]), leads to exact results. For central potentials, the Langer prescription [3] for the centrifugal barrier, together with half-integer quantization, can also be employed [4].

In supersymmetric (SUSY) quantum mechanics, these exactly solvable potentials are found to be translationally shape invariant [5]. Combining SUSY and WKB, Comtet *et al* [6] found that the lowest order SWKB calculation needs neither the Maslov index nor the Langer correction to yield the exact result. The purpose of this paper is to understand this result from the point of view of the periodic orbit theory (POT) [7], rather than the higher order WKB corrections [8]. Regarding the latter, we should point out a largely overlooked paper by Barclay [4], in which he showed that the higher order WKB terms converge in these potentials to yield an energy-independent correction, which may be absorbed into the Maslov index. For SWKB, all the higher order terms vanish. Although we do not make the WKB expansion, we arrive at the same result in a novel application of POT.

We first set the notation by reviewing the relevant equations of SUSY QM. Consider a potential $V(x; a_1)$ of a single variable x, and a set of parameters denoted by a_1. One defines a 'super potential'

$$W(x; a_1) = -\frac{\hbar}{\sqrt{2m}} \frac{\phi_0'(x)}{\phi_0(x)},$$

where $\phi_0(x)$ is the ground state solution of the Schrödinger equation at energy E_0 for the potential $V(x, a_1)$, and a prime denotes the spatial derivative. Let us define

$$V_1(x; a_1) = (V(x; a_1) - E_0), \tag{1}$$

so that the ground state energy of the Hamiltonian

$$H_1 = -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_1(x; a_1)$$

lies at zero energy, i.e., $E_0^{(1)} = 0$. Then it is easy to show that

$$V_1(x; a_1) = W^2(x; a_1) - \frac{\hbar}{\sqrt{2m}} W'(x; a_1).$$

The SUSY partner Hamiltonian H_2 has the potential $V_2(x; a_1)$, and has an energy spectrum identical to that of H_1, except for the absence of the zero-energy state. The ground state of H_2, denoted by $E_0^{(2)}$ coincides with the first excited state $E_1^{(1)}$ of H_1, and so on. The partner potential $V_2(x; a_1)$ is

$$V_2(x; a_1) = W^2(x; a_1) + \frac{\hbar}{\sqrt{2m}} W'(x; a_1).$$

Shape invariance in the partner potentials is defined by the relation

$$V_2(x; a_1) = V_1(x; a_2) + R(a_1), \tag{2}$$

where the new parameters a_2 are some function of a_1, and the remainder $R(a_1)$ is independent of the variable x. We restrict our consideration of shape invariance to those cases where a_2 and a_1 are related by translation, $a_2 = a_1 + \alpha$. It is then straightforward to show, by constructing a hierarchy of Hamiltonians, that the complete eigenvalue spectrum of H_1 is given by [1]

$$E_n^{(1)} = \sum_{k=1}^{n} R(a_k), \qquad n \geqslant 1, \tag{3}$$

$$E_0^{(1)} = 0. \tag{4}$$

The rhs of the above may be expressed as a monotonic function $f_1(n)$ of the quantum number n, so that

$$E_n^{(1)} = f_1(n); \qquad f_1(0) = 0. \tag{5}$$

For the shape invariant potentials we consider here, $f_1(n)$ is an algebraic function. Using this property, we proceed to obtain an exact expression for the quantum density of states of H_1 in the spirit of periodic orbit theory. This entails a division of the density of states into a smooth and an oscillating part as a function of a continuous classical variable E. To this end, we may write

$$\delta\big(E - E_n^{(1)}\big) = \delta(E - f_1(n)) = \delta(n - F_1(E))F_1'(E), \tag{6}$$

where the algebraic relation $E_n = f_1(n)$ has been inverted to define

$$n = F_1(E). \tag{7}$$

Note that we have used the algebraic expression between integer n and E_n to provide the relationship for continuous variables in equation (7). The continuous function $F_1(E)$ that we obtain in this way will be shown to satisfy the requirements of POT and classical mechanics (see equations (14)–(18)). In this sense, our choice of $F_1(E)$ using equation (7) is not only natural, but also necessary.

For the spectrum under consideration, $f_1(0) = 0$ implies the condition

$$F_1(0) = 0. \tag{8}$$

The quantum density of states $g_1(E)$ for the discrete spectrum of H_1 is defined as

$$g_1(E) = \sum_{n=0}^{\infty} \mathrm{d}(n)\delta\big(E - E_n^{(1)}\big), \tag{9}$$

where $\mathrm{d}(n)$ is the degeneracy of states at $E = E_n$. Writing $\mathrm{d}(n) = \mathrm{d}(F_1(E)) \equiv D(E)$, and using equation (6), we obtain

$$g_1(E) = D(E)F_1'(E)\sum_{n=0}^{\infty}\delta(n - F_1(E)). \tag{10}$$

($D(E) = 1$ for one-dimensional potentials). We now use the identity

$$\sum_{n=0}^{\infty}\delta(n - x) = \sum_{k=-\infty}^{\infty} \mathrm{e}^{2\mathrm{i}\pi kx}, \qquad x \geqslant 0, \tag{11}$$

to obtain the desired expression [7, 11]

$$g_1(E) = D(E)F_1'(E)\left[1 + 2\sum_{k=1}^{\infty}\cos[2\pi k F_1(E)]\right]. \tag{12}$$

For a given $F_1(E)$, this is an *exact* expression for the quantum density of states $g_1(E)$. It is in the form of a trace formula in POT [7, 10] when $F_1(E)$ (to within a dimensionless additive constant η) is identified with the action $S_1(E)$ of the primitive classical periodic orbit of the potential $V_1(x)$:

$$\frac{S_1(E)}{h} = F_1(E) + \eta, \tag{13}$$

$$S_1(E) = 2\sqrt{2m}\int_{x_1}^{x_2}\sqrt{E - V_1}\,\mathrm{d}x. \tag{14}$$

In the above, x_1 and x_2 are the classical turning points at which $E = V_1(x)$ (for economy in notation, we write $V_1(x, a_1) = V_1(x)$). The (h-independent constant) η may be determined by using equation (13), and applying the condition given by equation (8) for $E = 0$. We then obtain

$$\eta = \frac{S_1(0)}{h}. \tag{15}$$

We may prove equation (13) by noting that the (smooth) Thomas–Fermi density of states, given by the first term on the rhs of equation (12), is the Laplace inverse of the classical canonical partition function [12] of the Hamiltonian $H_1^{cl}(x, p) = p^2/2m + V_1(x)$:

$$F_1'(E) = \mathcal{L}_E^{-1} Z_1^{cl}(\beta) = \frac{1}{2\pi\mathrm{i}}\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} Z_1^{cl}(\beta)\,\mathrm{e}^{\beta E}\,\mathrm{d}\beta. \tag{16}$$

Since

$$Z_1^{cl}(\beta) = \frac{1}{h}\int \exp[-\beta H_1^{cl}(x, p)]\,\mathrm{d}x\,\mathrm{d}p$$
$$= \frac{1}{2\pi\hbar}\sqrt{\frac{2m\pi}{\beta}}\int_{-\infty}^{\infty}\exp[-\beta V_1(x)]\,\mathrm{d}x, \tag{17}$$

it follows from (16) that

$$F_1'(E) = \frac{\sqrt{2m}}{2\pi\hbar}\int_{x_1}^{x_2}\frac{\mathrm{d}x}{\sqrt{[E - V_1(x)]}}. \tag{18}$$

From this, equation (13) follows on integration over energy. Note that $F_1'(E)/h$ is the period of the classical periodic orbit and is unique, whereas $F_1(E)$ involves a constant of integration, η. Using equation (7) together with (13), (14), we obtain the important result that the lowest order WKB quantization rule is *exact* for V_1 :

$$S_1(E) = \oint p(x)\,\mathrm{d}x = (n+\eta)h, \tag{19}$$

where $p(x) = \sqrt{2m[E - V_1(x)]}$. We also see that the constant η is the so-called Maslov index which may vary from one potential to another.

The Maslov index η may be eliminated from the quantisation rule by employing the superpotential formalism, and the result of Barclay and Maxwell [13]. They made the important observation that the shape invariant class of potentials under consideration obey one or other of the following equations:
Class 1

$$\frac{\hbar}{\sqrt{2m}}\frac{\mathrm{d}W}{\mathrm{d}x} = A + BW^2(x) + CW(x), \tag{20}$$

or Class 2

$$\frac{\hbar}{\sqrt{2m}}\frac{\mathrm{d}W}{\mathrm{d}x} = A + BW^2(x) + CW(x)\sqrt{(A + BW^2)}, \tag{21}$$

where A, B and C are constants. Using these equations, we now show that $S_1(E)$, as defined by equation (14), obeys the relation (x_{1s}, x_{2s} are the turning points in SWKB)

$$S_1(E) = 2\sqrt{2m}\int_{x_{1s}}^{x_{2s}}\sqrt{E - W^2}\,\mathrm{d}x + h\eta. \tag{22}$$

To this end, note that the action S_1 can be expressed as an inverse Laplace transform

$$S_1(E) = \sqrt{2m\pi}\,\mathcal{L}_E^{-1}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-\beta[W^2 - \hbar W'/\sqrt{2m}]}}{\beta^{3/2}}\,\mathrm{d}x. \tag{23}$$

At this point, for simplicity of notation, let us temporarily put $\hbar/\sqrt{2m} = \gamma$. Expanding the exponential in powers of W', we have

$$S_1(E) = \sqrt{2m\pi}\,\mathcal{L}_E^{-1}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-\beta W^2}}{\beta^{3/2}}\left(1 + \sum_{k=0}^{\infty}\frac{(\gamma\beta W')^{k+1}}{(k+1)!}\right)\mathrm{d}x. \tag{24}$$

$$= 2\sqrt{2m}\int_{x_{1s}}^{x_{2s}}\sqrt{E - W^2}\,\mathrm{d}x + \sum_{k=0}^{\infty}\frac{\hbar}{(k+1)!}\frac{\partial^k}{\partial E^k}\int_{-\sqrt{E}}^{\sqrt{E}}\frac{(\gamma W')^k}{\sqrt{E - W^2}}\,\mathrm{d}W. \tag{25}$$

Note that now the limits in x are replaced by the condition $W^2(x) = E$. The integral for $k = 0$ may be done immediately, yielding π. To evaluate the integrals for integer $k \geqslant 1$, we assume that $\gamma W'$ obeys Barclay's equation (20) (class 1) or (21) (class 2).

For class 1, we require integrals of the type

$$I_k = \int_{-\sqrt{E}}^{\sqrt{E}} \frac{(A + BW^2 + CW)^k}{\sqrt{E - W^2}}\, \mathrm{d}W. \tag{26}$$

On expanding the numerator, terms with odd powers of W vanish on integration. One now sees that only the piece of I_k involving the highest power of W^2 survives the differentiation in equation (25). Consider the integral with W^{2k}. With the substitution $W = \sqrt{E}\sin\theta$

$$\int_{-\sqrt{E}}^{\sqrt{E}} \frac{W^{2k}}{\sqrt{E - W^2}}\, \mathrm{d}W = E^k \int_{-\pi/2}^{\pi/2} \sin^{2k}\theta\, \mathrm{d}\theta \tag{27}$$

$$= E^k \frac{(2k-1)!!}{(2k)!!}\pi. \tag{28}$$

Accordingly, equation (25) reduces to

$$S_1(E) = 2\sqrt{2m} \int_{x_{1s}}^{x_{2s}} \sqrt{E - W^2}\, \mathrm{d}x + \hbar\pi \left(1 + \sum_{k=1}^{\infty} \frac{B^k (2k-1)!!}{(k+1)(2k)!!}\right). \tag{29}$$

By construction, $W^2(x)$ has coincident turning points at $E = 0$, so the first term on the RHS above vanishes at this energy. Comparing with equation (15), we deduce that

$$\begin{aligned}\eta &= \frac{1}{2}\left(1 + \sum_{k=1}^{\infty} \frac{B^k (2k-1)!!}{(k+1)(2k)!!}\right) \\ &= \frac{1}{B}[1 - \sqrt{1 - B}].\end{aligned} \tag{30}$$

Note, from equation (20), that B is independent of Planck's constant h. Comparing now with equation (13), we deduce our main result

$$2\pi\hbar F_1(E) = \sqrt{2m} \oint \sqrt{E - W^2}\, \mathrm{d}x. \tag{31}$$

Using equation (7) we get as the *exact* result the SWKB expression

$$\oint \sqrt{2m(E - W^2)}\, \mathrm{d}x = 2\pi\hbar n, \qquad n = 0, 1, 2, 3, \ldots \tag{32}$$

which yields the quantum spectrum of $V_1(x)$.

A similar derivation may be carried through for class 2 superpotentials obeying equation (21). The starting point, as before, is equation (25), and the integral to be considered is now of the form

$$J_k = \int_{-\sqrt{E}}^{\sqrt{E}} \frac{(A + BW^2)^k \left(1 + \frac{CW}{\sqrt{A+BW^2}}\right)^k}{\sqrt{E - W^2}}\, \mathrm{d}W. \tag{33}$$

The second bracketed term in the numerator on the RHS may be expanded binomially, and the terms in odd powers of W vanish on integration. We then have

$$J_k = \sum_{n=0}^{n_{\max}} \frac{k!}{(k-2n)!(2n)!} \int_{-\sqrt{E}}^{\sqrt{E}} \frac{(A + BW^2)^{k-n}(CW)^{2n}}{\sqrt{E - W^2}}\, \mathrm{d}W, \tag{34}$$

where $n_{\max} = k/2$ for k even, and $(k-1)/2$ for k odd. The highest power of W in the numerator is again W^{2k} and again only terms with this highest power (with coefficient $B^{k-n}C^{2n}$) will survive when J_k is differentiated k-times. Accordingly, equation (25) reduces to

$$S_1(E) = 2\sqrt{2m} \int_{x_{1s}}^{x_{2s}} \sqrt{E - W^2}\, \mathrm{d}x + \hbar\pi \left(1 + \sum_{k=1}^{\infty} \frac{(2k-1)!!}{(k+1)(2k)!!} \sum_{n=0}^{n_{\max}} \frac{k! B^{k-n} C^{2n}}{(k-2n)!(2n)!}\right). \tag{35}$$

The main results given earlier by equation (31), (32) remain valid.

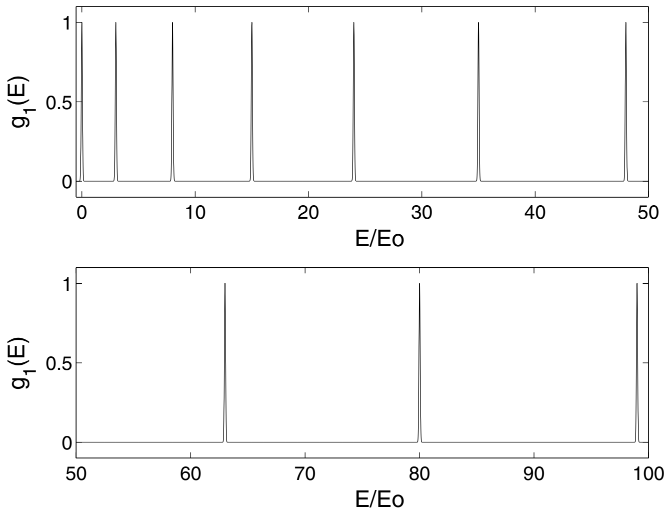

Figure 1. Numerical evaluation of the trace formula (12) for the infinite square well where $F_1(E) = (1 + E/E_0)^{1/2} - 1$. In the figure, E is plotted in units of E_0. To ensure uniform lineshapes, correct degeneracies, and strict numerical convergence, we have employed the usual prescription used in numerical semiclassics (see, for example, section 5.5 of [7]) which is to convolve the trace formula with a Gaussian of width σ. For this particular calculation, we have truncated the sum at $k_{\max} = 10^4$ while prescribing $\sigma = 0.05$.

The summation in equation (35) can be done similarly to that in equation (30). The inner summation provides the mean of $(B \pm C\sqrt{B})^k$. Then we find

$$\eta = \frac{1}{2z_+}[1 - \sqrt{1 - z_+}] + \frac{1}{2z_-}[1 - \sqrt{1 - z_-}]$$

where

$$z_\pm = B \pm C\sqrt{B}. \qquad (36)$$

These results (30), (36) are a simple demonstration of the relation between WKB and SWKB, which Barclay [4] approached in a different manner.

It may now be instructive to illustrate our results with a few examples:

(1) Infinite square well. In this example, $W(x) = -\hbar\pi/(\sqrt{2m}L)\cot(\pi x/L)$. It belongs to class 1 with $A = \hbar^2\pi^2/(2mL^2) = E_0$, $B = 1$ and $C = 0$. The quantum spectrum of V_1 is given by $f(n) = n(n+2)E_0$, with $n = 0, 1, 2, \ldots$. Then $F_1(E) = (1 + E/E_0)^{1/2} - 1$. A careful numerical evaluation of the trace formula (12) with this $F_1(E)$ reproduces the quantum spectrum (see figure 1). It is also easy to check equation (31) by evaluating the action integral of $W^2(x)$ analytically, and equation (22) using equation (30) ($\eta = 1$).

(2) Three-dimensional harmonic oscillator in the lth partial wave. In this example $W(r) = \sqrt{2m}\omega r/2 - \hbar/(\sqrt{2m})(l+1)/r$. It belongs to class 2 with $A = \hbar\omega$, $B = 1/(2l+2)$ and $C = -\sqrt{B}$. The quantum spectrum, measured from the lowest state in a fixed partial wave is $f(n) = 2n\hbar\omega$, so $F(E) = E/(2\hbar\omega)$. Again, equation (31) may be checked explicitly.

To verify equation (22), we find from equation (36) that

$$\eta = \tfrac{1}{2} + \tfrac{1}{2}\left[\ell + \tfrac{1}{2} - \sqrt{\ell(\ell+1)}\right] \qquad (37)$$

in this example. The first 1/2 represents the usual half-integer quantisation in LOWKB, while the terms in square brackets arise from the sum of order $\hbar^2$ and higher corrections. As discussed in detail by Seetharaman [14] and Barclay [4] they can be removed by adopting the Langer prescription. We have also checked other examples analytically.

In conclusion, we have given a new proof that lowest order SWKB quantisation is exact, starting from periodic orbit theory, rather than by examining the higher order WKB terms. The key ingredients have been an invertible algebraic expression for the energy spectrum, and Barclay and Maxwell's [4, 13] insight about shape invariant potentials.

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