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A simple approximation for eigenvalues in quantum theory

H Mitter† and K Yamazaki‡

† Institut für Theoretische Physik der Universität, A-8010 Graz, Austria
‡ Physics Department, College of General Education, Kyoto University, Kyoto 606, Japan

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Abstract. An approximation method for the determination of energy levels in quantum theory is discussed which starts from a scaled set of eigenstates of a solvable model. It is shown that the lowest approximation fulfils certain relations which also hold exactly. The approximation is tested by comparison with numerically computed eigenvalues in several cases. The errors turn out to be moderate in most of these and depend very little on typical coupling constants.

1. Introduction

For many practical applications, numerical methods for the accurate calculation of energy eigenvalues in quantum mechanics are widely used. Sometimes one would prefer, however, a simple method by means of which one may obtain quick information on orders of magnitude, together with analytical expressions, which are simple enough to be used as an input for further studies. The method to be described below is of this type. The basic idea—the use of a scaled set of eigenstates of some solvable Hamiltonian—is not entirely new: it has been used in some special models as a starting point for numerical calculations. Here we shall consider this idea in a general context. We shall show that a certain choice of the scaling parameter may be preferable. Some exact relations are then valid even in the lowest approximation and the scaling parameter acts in fact as a (nonlinear) variational parameter. In order to obtain some information on the reliability we shall compare the results obtained in this approximation with results based on numerical integration of the Schrödinger equation for various models.

2. Description of the method

The method to be described can be used both for one-dimensional problems and problems with central symmetry. In order to deal with both cases we employ the usual Schrödinger scaling. We start from the Hamiltonian

$$H = (\hbar^2/2m\kappa^2)h, \qquad h = h_{\text{kin}} + V(q), \tag{1}$$

with some appropriate scaling factor κ. We use dimensionless dynamical variables p, q

$$[q, p] = \mathrm{i}. \tag{2}$$

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For one-dimensional problems we have

$$h_{\text{kin}} = p^2, \qquad x = \kappa q, \qquad p_x = \hbar p/\kappa. \tag{3a}$$

For problems with central symmetry we have

$$h_{\text{kin}} = p^2 - \frac{2\mathrm{i}}{q}p + \frac{l(l+1)}{q^2}, \qquad r = \kappa q, \qquad \frac{1}{r}(\boldsymbol{r}\cdot\boldsymbol{p}) = \hbar p/\kappa \tag{3b}$$

with the quantum number l of orbital angular momentum. The potential is assumed to depend only on q in both cases. In order to formulate the method we consider another Hamiltonian

$$\hat{h} = h_{\text{kin}} + W(q) \tag{4}$$

whose normalised eigenstates $|n\rangle$ and eigenvalues w_n

$$(\hat{h} - w_n)|n\rangle = 0, \qquad \langle n|n\rangle = 1,$$

are assumed to be known. In previous papers (Feranchuk and Komarov 1982, Yamazaki 1984) the harmonic oscillator potential has been used as a 'reference potential' W in a determination of eigenvalues for the quartic anharmonic oscillator in one dimension. The method is extended here to other reference potentials. It is this extension which allows for a discussion of problems with central symmetry (where operator techniques are inconvenient). For central symmetry the states $|n\rangle$ may also depend on l: this dependence is suppressed in the notation used here.

We consider the unitary operator

$$U(\theta) = \exp(\theta G) \tag{5}$$

with a real parameter θ and

$$G = -\tfrac{1}{2}\mathrm{i}(pq + qp). \tag{6}$$

It is observed that G generates a scale transformation

$$U^{-1}(\theta)F(p, q)U(\theta) = F(\mathrm{e}^{-\theta}p, \mathrm{e}^{\theta}q)$$

(for a proof cf the appendix).

Now we consider the states

$$|n, \theta\rangle = U(\theta)|n\rangle \tag{7}$$

where θ is allowed to depend on n (and l for central symmetry). It has to be kept in mind that the states (7) are normalised, but neither orthogonal nor complete for non-trivial dependence of θ on n. The lowest approximation to the eigenvalue ε_n of h is defined by

$$\varepsilon_n^{(0)} = \langle n, \theta_0|h|n, \theta_0\rangle \tag{8}$$

where θ_0 is a solution of the equation

$$(\partial/\partial\theta)\langle n, \theta|h|n, \theta\rangle = 0. \tag{9}$$

If this equation has several solutions, we have to select an appropriate one. Reality of θ_0 is clearly a necessary condition. In most applications we have found only one real solution. Higher approximations are found by perturbation theory with

$$h_n^{(1)} = h - |n, \theta_0\rangle\varepsilon_n^{(0)}\langle n, \theta_0|$$

as perturbation term. The calculation has to be done for each level separately with individual $\theta_0(n)$ determined from (9). Here we shall consider, however, only the lowest approximation.

3. Properties of the lowest approximation

The special choice of θ as parameter of a scale transformation (in contrast to other possible variational parameters) has favourable consequences and provides for simplifications which we shall now study.

By differentiation we obtain from (9)

$$(\partial/\partial\theta)\langle n,\theta|h|n,\theta\rangle = (\partial/\partial\theta)\langle n|U^{-1}(\theta)hU(\theta)|n\rangle = \langle n,\theta|[h,G]|n,\theta\rangle.$$

Thus we can use

$$\langle n,\theta_0|[h,G]|n,\theta_0\rangle = 0 \tag{10}$$

instead of (9) as an equation for θ_0. Evaluating the commutator using (6) and the commutation relations (2) we obtain

$$\langle n,\theta_0|-2h_{\mathrm{kin}} + q\,\partial V/\partial q|n,\theta_0\rangle = 0. \tag{11}$$

For exact eigenstates of h this is the virial theorem. Thus we see that our lowest approximation fulfils the virial theorem which allows for reliable estimates of eigenvalues in many cases.

Another useful property of the lowest approximation is found if we assume that h depends on some parameter λ

$$h = h(\lambda). \tag{12}$$

The parameter θ depends on λ in this case and the lowest eigenvalue contains λ both explicitly via h and implicitly via θ:

$$\varepsilon_n^{(0)}(\lambda) = \langle n,\theta(\lambda)|h(\lambda)|n,\theta(\lambda)\rangle.$$

Differentiation with respect to λ gives

$$\mathrm{d}\varepsilon_n^{(0)}/\mathrm{d}\lambda = \langle n,\theta(\lambda)|\mathrm{d}h/\mathrm{d}\lambda|n,\theta(\lambda)\rangle + (\mathrm{d}\theta/\mathrm{d}\lambda)(\partial/\partial\theta)\langle n,\theta|h|n,\theta\rangle.$$

The last term vanishes because of (9) so that we obtain

$$\mathrm{d}\varepsilon_n^{(0)}/\mathrm{d}\lambda = \langle n,\theta|\mathrm{d}h/\mathrm{d}\lambda|n,\theta\rangle. \tag{13}$$

For exact eigenstates and eigenvalues this is the Hellmann–Feynman theorem. It should be observed, however, that we have used only (9) and not (7) in this derivation: therefore (13) would hold for any other parametrisation as well.

The equations for the determination of θ_0 and the lowest eigenvalue can be rewritten using the formulae given above. Thus we may use

$$\begin{aligned} \mathrm{e}^{2\theta}(\partial/\partial\theta)\langle n|V(q\,\mathrm{e}^{\theta})|n\rangle &= \mathrm{e}^{2\theta}\langle n|q\,\mathrm{e}^{\theta}V'(q\,\mathrm{e}^{\theta})|n\rangle \\ &= 2(w_n - \langle n|W|n\rangle) \end{aligned} \tag{14}$$

for the determination of θ_0. With a solution of (14) we have

$$\begin{aligned} \varepsilon_n^{(0)} &= \langle n|V(q\,\mathrm{e}^{\theta_0})|n\rangle + \tfrac{1}{2}\mathrm{e}^{\theta_0}\langle n|qV'(\mathrm{e}^{\theta_0}q)|n\rangle \\ &= \langle n|V(q\,\mathrm{e}^{\theta_0})|n\rangle + (w_n - \langle n|W|n\rangle)\,\mathrm{e}^{-2\theta_0}. \end{aligned} \tag{15}$$

Therefore the lowest approximation amounts essentially to a computation of the diagonal element of V between eigenstates of $\hat{h}$. For simple reference potentials this computation can be done analytically for a large class of potentials V.

If W is chosen homogeneous,

$$W = Aq^{\beta}, \tag{16}$$

the virial theorem for $\hat{h}$ gives

$$w_n - \langle n|W|n\rangle = [\beta/(2+\beta)]w_n \tag{17}$$

which provides for a further simplification. The factor A in (16) can be taken as unity without loss of generality, since it can be absorbed in θ.

The close connection with a variational procedure is established by another equivalent way to formulate the lowest approximation. Let $\langle q|n\rangle$ be a normalised eigenfunction of the Hamiltonian (4). The function

$$\langle q|\psi_\alpha(n)\rangle = \alpha^{\mu}\langle \alpha q'|n\rangle \tag{18}$$

with a constant (positive) factor α and $\mu = \frac{1}{2}$ (resp $\frac{3}{2}$) in the one-dimensional (resp spherically symmetric) case is then also normalised. In terms of the scaled dynamical variables $q = \alpha q'$, $p = p'/\alpha$ we have $h_{\text{kin}}(p', q') = \alpha^2 h_{\text{kin}}(p, q)$ and obtain

$$\langle \psi_\alpha(n)|h|\psi_\alpha(n)\rangle = \alpha^2\langle n|h_{\text{kin}}(p, q)|n\rangle + \langle n|V(q/\alpha)|n\rangle.$$

Taking

$$\alpha = \mathrm{e}^{-\theta}$$

this agrees with (15). Therefore the lowest approximation can be considered as a variational approach with the trial function (18) and α as variational parameter. This implies that the energy of the exact ground state $n = 0$ is lower than the result obtained in first approximation by the present method.

Finally we consider problems in which V consists of a homogeneous potential (16) plus a perturbation

$$V = W + \lambda V_1(q). \tag{19}$$

We try a Taylor expansion around $\lambda = 0$

$$\varepsilon_n^{(0)}(\lambda) = \varepsilon_n^{(0)}(0) + \lambda\varepsilon_n^{(0)\prime}(0) + \tfrac{1}{2}\lambda^2\varepsilon_n^{(0)\prime\prime}(0) + \ldots.$$

In order to compute the first term we have to solve (14) with $V = W$. Using relation (17) we obtain after a few elementary steps

$$\theta(\lambda = 0) = 0, \qquad |n, \theta(0)\rangle = |n\rangle, \qquad \varepsilon_n^{(0)}(0) = w_n.$$

For the next term we use (13) and obtain

$$\varepsilon_n^{(0)\prime}(0) = \langle n|V_1(q)|n\rangle.$$

The third term is found by differentiation of (13). We have

$$(\mathrm{d}/\mathrm{d}\lambda)|n, \theta(\lambda)\rangle = U'(\theta)|n\rangle\theta'(\lambda) = G|n, \theta(\lambda)\rangle\theta'.$$

For $\langle n, \theta(\lambda)|$ we obtain the opposite sign, since $U^{+}(\theta) = U(-\theta)$. Therefore

$$\mathrm{d}^2\varepsilon_n^{(0)}(\lambda)/\mathrm{d}\lambda^2 = -\theta'(\lambda)\langle n, \theta(\lambda)|[G, V_1(q)]|n, \theta(\lambda)\rangle. \tag{20}$$

Thus

$$\varepsilon_n^{(0)}(\lambda) = w_n + \lambda\langle n|V_1(q)|n\rangle + \tfrac{1}{2}\lambda^2\theta'(0)\langle n|[G, V_1(q)]|n\rangle + \ldots . \tag{21}$$

For small λ our lowest approximation agrees therefore with the perturbation expansion at least up to first order in λ, whenever an expansion in powers of λ is meaningful.

4. Application to one-dimensional problems

For these problems it seems natural to use the harmonic oscillator

$$W = q^2, \qquad \beta = 2, \qquad w_n = 2n+1. \tag{22}$$

The eigenstates are

$$|n\rangle = (a^+)^n|0\rangle(1/\sqrt{n!}), \qquad a|0\rangle = 0,$$

with the usual creation and destruction operators

$$q = (1/\sqrt{2})(a+a^+), \qquad p = (1/\mathrm{i}\sqrt{2})(a-a^+), \qquad [a, a^+] = 1.$$

It is worth noting that the scale transformation generated by (6)

$$G = \tfrac{1}{2}(a^{+2} - a^2) \tag{23}$$

corresponds to a transformation familiar from solid state physics (Bogoliubow, Primakoff, Holstein) which gives new ladder operators

$$b = U(\theta)aU^{-1}(\theta) = a\cosh\theta - a^+\sinh\theta \tag{24}$$

so that the states (7) become

$$|n, \theta\rangle = (b^+)^n|0, \theta\rangle(1/\sqrt{n!}), \qquad b|0, \theta\rangle = 0, \qquad [b, b^+] = 1. \tag{25}$$

The matrix element in (14), (15) can be explicitly evaluated for several potentials. An example is

$$V(q) = \sum_{m=0}^{s} C_m q^{2m}, \tag{26}$$

$$\langle n|V(q\,\mathrm{e}^{\theta})|n\rangle = \sum_m C_m S_{n,m}\,\mathrm{e}^{2m\theta}, \tag{27}$$

with

$$S_{n,m} = \frac{(2m)!}{2^{2m}m!}\sum_{k=0}^{m} 2^k \binom{n}{k}\binom{m}{k}. \tag{28}$$

This result can be obtained using algebraic techniques for ladder operators. Equation (14) becomes an algebraic equation of degree $(s+1)$ for $\mathrm{e}^{2\theta}$. The anharmonic oscillator containing the terms with $m = 1, 2$ has been examined before (Yamazaki 1984). The cubic equation for $\mathrm{e}^{2\theta}$ has only one admissible root and the method has reproduced the exact eigenvalues (known from extensive numerical examination of the Schrödinger equation) with small errors (<2%) for arbitrary (positive) coefficients C_1, C_2. Higher approximations as indicated in § 2 reduce the error considerably.

The extension to higher anharmonic terms is straightforward with the formulae given above. As long as all coefficients C_m are non-negative, there is always only one admissible root $\mathrm{e}^{2\theta_0}$, since the matrix element (27) is positive.

Here we shall concentrate on the example

$$V = \pm \mu q^{2k} + \lambda q^{2l}, \qquad l > k > 0;\ \lambda > 0;\ \mu > 0. \tag{29}$$

The upper sign corresponds to some anharmonic oscillator, the lower one to a double well. For both signs we have only one admissible root. With

$$K(n, l) = (n+\tfrac{1}{2})/lS_{n.l}, \qquad C(n, k) = kS_{n.k}/(n+\tfrac{1}{2}), \qquad C(n, 1) = 1, \tag{30}$$

the equation for $\alpha = e^{2\theta}$ reads

$$\lambda \alpha^{l+1} = K(1 \mp \mu C \alpha^{k+1}). \tag{31}$$

The lowest approximation for the eigenvalues is

$$\begin{aligned} \varepsilon_n^{(0)}(\mu, \lambda) &= \lambda(l+1)S_{n.l}\alpha^l \pm \mu(k+1)S_{n.k}\alpha^k \\ &= \frac{(n+\frac{1}{2})(l+1)}{\alpha l}\left(1 \pm \mu \frac{(l-k)}{k(l+1)} C\alpha^{k+1}\right). \end{aligned} \tag{32}$$

Scaling μ and λ, we obtain by elementary methods

$$\varepsilon_n^{(0)}(1, \lambda) = \lambda^{1/(l+1)} \varepsilon_n^{(0)}(\lambda^{-(k+1)/(l+1)}, 1) \tag{33}$$

which is valid also for the exact eigenvalues (see e.g. Simon (1970) for $k = 1$; the extension is trivial). Thus our approximation reproduces also those analyticity properties with respect to the coupling constant which are a consequence of relation (33).

In order to arrive at expansions either for large or for small coupling we have to solve (31) iteratively. For large λ/small μ we obtain

$$\varepsilon_n^{(0)} = \frac{(n+\frac{1}{2})}{kl}\left(\frac{\lambda}{K}\right)^{1/(l+1)}\left[k(l+1) \pm l\mu C\left(\frac{K}{\lambda}\right)^{(k+1)/(l+1)} + \dots\right]. \tag{34}$$

For the opposite situation small λ/large μ the two signs of μ must be investigated separately. For the oscillator the bracket on the RHS of (31) assumes small values (α approaches a constant). We obtain

$$\varepsilon_n^{(0)} = \frac{(n+\frac{1}{2})}{kl}(\mu C)^{1/(k+1)}\left(l(k+1) + \frac{k\lambda}{K}(\mu C)^{-(l+1)/(k+1)} + \dots\right). \tag{35a}$$

For the double well the bracket does not vanish because of $\alpha > 0$. We have to iterate for large α and obtain

$$\varepsilon_n^{(0)} = (n+\tfrac{1}{2})\left[-\frac{(l-k)\mu C}{kl}\left(\frac{\mu KC}{\lambda}\right)^{k/(l-k)} + \left(\frac{\lambda}{\mu KC}\right)^{1/(l-k)} + \dots\right]. \tag{35b}$$

It is evident that the expansion (21) is not allowed for the double well.

Extensive and accurate numerical results are available for the sextic oscillator and double-well (Balsa and Pló 1983) and for the quartic double-well (Balsa *et al* 1983). We have compared the results of formula (32) with these. For the sextic oscillator ($k = 1$, $l = 3$, $\mu = +1$) the error amounts again to a few percent in a large region of λ and n. Even for the extreme value $\lambda = 10^4$ (where one would not trust naively any approximation based on the harmonic oscillator) the error is only 6.6% for $n = 0$ and 4.3% for $n = 1$. For $2 \leqslant n \leqslant 39$ the error is smaller than 2.6% for $10^{-3} \leqslant \lambda \leqslant 10^4$. This is probably due to the scaling properties (11) resp (33) of our approximation. For the quartic double-well ($k = 1$, $l = 2$, $\mu = -1$) and its sextic counterpart ($k = 1$, $l = 3$, $\mu = -1$) the relative errors amount to a few percent for $\lambda > 1$ and $n > 0$. For the

ground state with $\lambda = 1$ the error is 7% for the quartic and 14% for the sextic well. In general, the error becomes smaller with growing n and λ. The approximation becomes unreliable for smaller values of λ. In particular the negative eigenvalues (i.e. those which are situated below the central peak of the well which corresponds to $\varepsilon_n = 0$ here) are reproduced with large errors.

An improvement can be obtained using shifted ladder operators, whereby the shift acts as an independent variational parameter, and taking parity into account (see Feranchuk and Komarov (1982); their quantity ω corresponds to our $\exp(-2\theta)$). The calculation becomes, however, quite complicated.

Some information is still contained in our formula even on the negative levels. Since very little is known exactly on double-well potentials, this information may give some hints, even if it is not very accurate. We can look for which value $\lambda = \lambda_0(n)$ the nth eigenvalue (32) assumes the value zero. Setting the bracket in the last form of (32) equal to zero and inserting the corresponding value of α into (31) we obtain

$$\lambda_0(n) = \frac{(n+\frac{1}{2})(1+k)}{(l-k)S_{nl}} \left(\frac{\mu(l-k)C(n,k)}{k(l+1)} \right)^{(l+1)/(k+1)}. \tag{36}$$

Since the eigenvalues decrease with λ, we may state that for $\lambda < \lambda_0(0)$ one level ($n = 0$) is situated below the central peak (i.e. inside the double well), for $\lambda < \lambda_0(1)$ two levels ($n = 0, 1$) etc. Since the exact eigenvalue for the ground state is lower than the approximative one, $\lambda_0(0)$ is an *exact* upper bound on the value of the coupling constant for which the ground state lies inside the well. The other values $\lambda_0(n)$ are probably only useful for rough estimates.

5. Application to problems with central symmetry

For problems with central symmetry one may choose Coulomb eigenstates as a basis for the method. In this case we have

$$W = -2/q, \qquad \beta = -1, \qquad w_n = -1/n^2. \tag{37}$$

The eigenstates are represented by

$$\langle q|n, l\rangle = \frac{1}{nq} \left(\frac{(n-l-1)!}{(n+l)!} \right)^{1/2} \left(\frac{2q}{n} \right)^{l+1} L_{n-l-1}^{(2l+1)} \left(\frac{2q}{n} \right) e^{-q/n}. \tag{38}$$

Here L denotes the Laguerre polynomials and the integers n, l are restricted by $n \geqslant l+1$, $l = 0, 1, 2, \ldots$. The crucial matrix element is

$$\langle n, l|V(q\,e^{\theta})|nl\rangle = \frac{(n-l-1)!}{2n(n+l)!} \int_0^{\infty} dx\, x^{2l+2} e^{-x} (L_{n-l-1}^{(2l+1)}(x))^2 V\left(\frac{xn}{2} e^{\theta} \right) \tag{39}$$

which can again be evaluated explicitly for a class of potentials: results for exponential dependence (Yukawa type potential) can be found in e.g. Gradshteyn and Ryzhik (1965). For powers of q it is simpler to use recurrence relations of the Laguerre polynomials and their orthogonality properties.

Here we shall consider as a simple example the 'funnel' potential

$$V(q) = \lambda q - (1-\lambda) q^{-1} \tag{40}$$

which is used as a phenomenological potential for quark–anti-quark bound states. In

this case we obtain

$$n^2\langle n, l|V(q\,e^{\theta})|n, l\rangle = A\,e^{\theta} - (1-\lambda)\,e^{-\theta} \tag{41}$$

with

$$A = \tfrac{1}{2}\lambda n^2[3n^2 - l(l+1)]. \tag{42}$$

We obtain a cubic equation for $y = e^{\theta}$

$$Ay^3 + (1-\lambda)y - 2 = 0. \tag{43}$$

In terms of its (only) real solution the lowest approximation for the eigenvalues is

$$\varepsilon_{nl}^{(0)} = [3 - 2y(1-\lambda)]/(ny)^2. \tag{44}$$

For small λ this agrees with perturbation theory because of (21). For $\lambda \simeq 1$ we obtain the expansion

$$\varepsilon_{nl}^{(0)} = 3\left(\frac{\lambda}{4}\right)^{2/3} M^{2/3} - \frac{(1-\lambda)}{n}\left(\frac{\lambda}{4}\right)^{1/3} M^{1/3} + \ldots, \qquad M = \frac{3n^2 - l(l+1)}{n}. \tag{45}$$

We have compared the results of formula (44) for the lowest six levels $l+1 \leqslant n \leqslant l+6$ with $0 \leqslant l \leqslant 5$ in the range $0.1 \leqslant \lambda \leqslant 0.9$ with exact results on the level sequence (Grosse and Martin 1980) and with results of numerical calculations. Our formula reproduces the sequence

$$\varepsilon_{1S} < \varepsilon_{2P} < \varepsilon_{2S} < \varepsilon_{1D} < \varepsilon_{2P} < \varepsilon_{3S} < \varepsilon_{1F} < \varepsilon_{2D} < \ldots.$$

The inequality

$$3\varepsilon_{1P} \geqslant \varepsilon_{1D} + 2\varepsilon_{1S}$$

is fulfilled and the energy difference between the second and first eigenvalue $\varepsilon_2(l) - \varepsilon_1(l)$ decreases with growing l, always throughout the range in λ considered. In comparison with numerically calculated eigenvalues (H Grosse, private communication) the relative error depends very little on λ so that the dependence of individual eigenvalues on the coupling is reproduced rather accurately. The magnitude of the relative error depends, however, on the quantum numbers. The worst results were obtained for the S-states ($l = 0$), where we have found errors of 6–9% and in one case ($n = 1$, $l = 0$, $\lambda = 0.1$) even 13%. For the other states the error is smaller and decreases with growing l. The first term in (45) (i.e. the asymptotic formula for $\lambda = 1$) gives, however, wrong results: all eigenvalues turn out too large in comparison with the numerical results. The inequality given above remains valid, however, and the level sequence is obeyed with the exception of $\varepsilon_{3S} = \varepsilon_{1F}$. The difference between the second and the first level with given l increases slightly with l and thus shows a wrong tendency. Thus our approximation is not reliable for λ very close to 1. This is to be expected, since we have used Coulomb eigenfunctions which are certainly not appropriate for a potential differing so radically from $1/q$ as (40) does for $\lambda = 1$. It is remarkable enough that the approximation works for $\lambda = 0.9$.

6. Conclusion

In most of the cases studied the approximation discussed here has turned out reasonable in the sense that the eigenvalues are reproduced with moderate errors. The most

important aspect is in our opinion that the errors are to a considerable extent independent of typical coupling constants so that the approximation is neither of the weak nor of the strong coupling type. This property is plausible, since some exact relations are fulfilled already in the lowest approximation. This approximation can be used as a starting point for further studies, since explicit analytical expressions can be found in many cases. Some caution on the reliability is still appropriate, however, since we have only tested eigenvalues and not eigenfunctions. The problem of higher approximations in a systematic treatment has not been considered here. For the one-dimensional cases studied in § 4 such a scheme can be constructed algebraically: this has been done in Yamazaki (1984) for the quartic anharmonic oscillator and has improved the accuracy considerably; a generalisation is straightforward, but simplicity is of course lost. For spherically symmetric problems higher approximations are all but evident. Whether the basic idea of our method can be extended successfully to problems with continuous spectra and/or more degrees of freedom remains an open problem.

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Appendix

Here we indicate a proof of the relation

$$U^{-1}(\theta)F(p,q)U(\theta)=F(\mathrm{e}^{-\theta}p,\mathrm{e}^{\theta}q).$$

We shall consider the special example

$$f_{\alpha\beta}(\theta):=U^{-1}(\theta)p^{\alpha}q^{\beta}U(\theta)$$

with arbitrary (real) α,β. With the explicit form (5) we have

$$(\mathrm{d}/\mathrm{d}\theta)f_{\alpha\beta}(\theta)=-U^{-1}(\theta)[G,p^{\alpha}q^{\beta}]U(\theta).$$

The commutator can be evaluated using (6) and (2). The result is

$$[G,p^{\alpha}q^{\beta}]=(\alpha-\beta)p^{\alpha}q^{\beta}.$$

Thus we obtain the differential equation

$$(\mathrm{d}/\mathrm{d}\theta)f_{\alpha\beta}(\theta)=(\beta-\alpha)f_{\alpha\beta}(\theta).$$

Together with the initial condition

$$f_{\alpha\beta}(\theta=0)=p^{\alpha}q^{\beta}$$

we obtain by integration

$$f_{\alpha\beta}(\theta)=(\mathrm{e}^{-\theta}p)^{\alpha}(\mathrm{e}^{\theta}q)^{\beta}.$$

The proof is extended immediately to products $p^{\alpha}q^{\beta}p^{\gamma}q^{\delta}\ldots$ and formal series of such products and applies therefore to rather general functions F.

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