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1984 J. Phys. A: Math. Gen. 17 2177

(http://iopscience.iop.org/0305-4470/17/11/014)

J. Phys. A: Math. Gen. 17 (1984) 2177–2190. Printed in Great Britain

Evasive levels in quantisation through wavepacket coupling: a semi-classical investigation

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Received 27 July 1983, in final form 3 January 1984

Abstract. A new method is presented to introduce classical mechanics elements into the problem of obtaining the spectrum of an operator $\hat{H}(\hat{p}, \hat{q})$. A finite-rank functional space is created by centring complex wavepackets on a discrete number of points on an equi-energy of the classical $H(p, q)$ and by placing real wavepackets in the classically forbidden region. The latter span the active subspace, $\mathcal{P}$, and the former the inactive subspace, $\mathcal{Q}$, for an application of the method of Bloch–Horowitz. Depending on the rank retained for $\mathcal{Q}$, some levels can be calculated with an extreme accuracy in a simple model while others remain evasive. A semi-classical study of the Green function in the inactive subspace $\mathcal{Q}$, classically allowed, gives a clear explanation of this phenomenon and sheds new light on the significance of this semi-classical approximation for the propagator. An extension to the problem of barrier penetration is proposed.

1. Introduction

There have been a few attempts (Voros 1977, Knoll and Schaeffer 1976, Schaeffer 1978, Balian and Bloch 1974, Kleinert and Reinhardt 1979) to incorporate information from classical mechanics into the quantum mechanical problem which investigates the possibility that an energy E corresponds to an eigenvalue of an operator H. Both the real case (quantisation) and the complex case (barrier penetration and scattering) have been investigated. So far two lines of thought have retained most of the attention. The first originates from WKB with an essentially classical starting point with quantum corrections eventually added through matching conditions between classically allowed and forbidden regions. The second originates from the classical limit of the functional integral representation for the Green function $G(E)$—inverse of H. When this integral is limited or can be reduced to a sum of trajectories in the space of spatial coordinates (Feynman's integral), a link with WKB can be established (Orland 1980, Zinn-Justin 1983).

We submit that there is another approach which is yet capable of introducing classical mechanics elements into the solution of the quantum problem.

The simplification it brings comes from the use of the Bloch–Horowitz Hamiltonian, H', which reduces the problem to one of diagonalisation of a finite-rank Hamiltonian (Bloch and Horowitz 1958). The novelty comes from our using it backward and from defining the active/passive subspaces by using discrete phase-space wavepackets as state vectors (Giraud *et al* 1976). Backward means that the classically allowed region

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0305-4470/84/112177+14$02.25

will constitute the passive or $\mathcal{Q}$-subspace. The active or $\mathcal{P}$-subspace where diagonalisation of H' is carried out is the classically forbidden region. It follows that the asymptotic region is taken 'exactly' into account whereas the propagator which enters H' can be treated in the classical limit of a functional integral representation because it is defined in the $\mathcal{Q}$-subspace which is here classically allowed. Furthermore, we are not beset with problems of matching wavefunctions at the boundary between classically allowed and forbidden regions.

2. Theory

First we must recall that the Bloch–Horowitz method of diagonalising an auxiliary Hamiltonian H' in an active or $\mathcal{P}$-subspace, instead of diagonalising the exact Hamiltonian H in the full space, is exact in the sense that it is not in itself an approximation. With P and Q the projectors on $\mathcal{P}$ and $\mathcal{Q}$ respectively, H' is

$$H' = PHP + PHQ(E - QHQ)^{-1}QHP \equiv H'(E), \tag{1}$$

where the idempotent operators P and Q must satisfy

$$PQ = QP = 0, \tag{2}$$

$$P + Q = \mathbb{1}. \tag{3}$$

The diagonalisation of $H'(E)$ is subject to a self-consistent condition

$$E = \text{eigenvalue}\,(H'(E)). \tag{4}$$

For the sake of illustration let us consider the problem of quantisation in the well of figure 1(*a*). For a trial energy E, the classical motion is limited to the 'inside region' between q_- and q_+. Figure 1(*b*) shows the phase-space trajectory for

$$H = T(p) + V(q)$$

corresponding to that energy. We select the inside or classically allowed region as the passive or inactive subspace for the Bloch–Horowitz treatment. Consequently the projector Q will be built from wavepackets $|z_i\rangle = |q_i, p_i\rangle$,

$$Q = \sum_{i,j} |z_i\rangle W_{ij} \langle z_j|, \tag{5}$$

where the wavepacket $|z_i\rangle$ can be chosen most conveniently as a boosted Gaussian, see equation (23). The sum over i and j covers the dots (●) of figure 1(*b*) which must be chosen so as to constitute a sufficiently complete subset of states. This point will be made clearer in § 5 of this paper where the signature of insufficient completeness is found as the lack of connectedness of classical trajectories. The matrix W is simply the inverse of the overlap matrix N

$$N_{ij} = \langle z_i | z_j \rangle. \tag{6}$$

We define the $\mathcal{P}$-subspace as the classically forbidden region of phase-space and consequently the projector P is defined from the complex wavepackets $|\gamma_n\rangle = |q_n, p_n\rangle$,

$$P = \sum_{n,m} |\gamma_n\rangle W_{nm} \langle \gamma_m|, \tag{7}$$

where the sum is over the crosses (×) of figure 1(*b*). In practice it is sufficient to limit

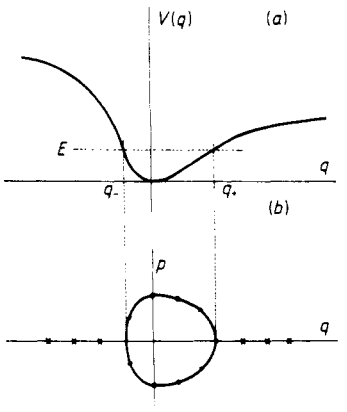

Figure 1. Schematic illustration of (*a*) a potential $V(q)$ and (*b*) the classical phase-space trajectory at an energy E.

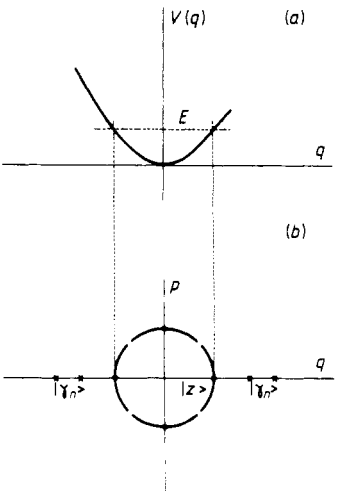

Figure 2. As figure 1 but for a one-dimensional harmonic oscillator specifying the P and Q subspaces. The dots (●) indicate the centres of the phase-space packets used to span Q. The crosses (×) play the same role for P.

oneself to real wavepackets i.e. centred on the q-axis with $p_n = 0$. Furthermore the finite range of H provides a way to limit the number of packets required to adequately generate P, as the correction term in H', equation (1), is proportional to $|P\hat{H}Q|^2$. This is a practical means of satisfying approximately condition (3). Condition (2) is easily satisfied by replacing the $|\gamma_n\rangle$ which span $\mathcal{P}$ by the $|\bar{\gamma}_n\rangle$:

$$|\bar{\gamma}_n\rangle = \mathcal{N}_n(1-Q)|\gamma_n\rangle, \tag{8}$$

with $\mathcal{N}_n$ a suitable normalisation factor. Hence (2) is exactly and easily satisfied.

It follows that both QHQ and H' become finite-rank operators. Thus the propagator

$$G(E) = (E - QHQ)^{-1} \tag{9}$$

is trivial to calculate and the diagonalisation of $H'(E)$ is easily carried out under the constraint (4). This diagonalisation of $H'(E)$ is carried out in the $\mathcal{P}$-subspace which corresponds to the classically forbidden region, which is thus automatically taken into account. This is in opposition to WKB-based methods where the role of the classically forbidden region must be brought in through boundary matching corrections (Fröman and Fröman 1965). The rescattering term of H' which plays a major role is weighted by the propagator of QHQ which is responsible for the dynamics in the classically allowed region. Thus a semi-classical estimate of this propagator is possible whereas it would have been impossible had we reversed the roles of $\mathcal{P}$ and $\mathcal{Q}$.

The self-consistent condition (4) may lead to a graphic search for the eigenvalue as can be seen in figure 3 (which will be discussed later) with the asymptote given by QHQ and the correct eigenvalue given by $E = E' = \text{eigen}(H'(E))$.

At this point classical mechanics has been used only to help define P and Q for the quantum problem. The link between classical and quantum models can be

developed further with the introduction of the phase-space functional integral representation for the propagator $G(E)$ of equation (9). As is well known, the stationary phase approximation of this integral will take us into a classical approximation for $G(E)=(E-QHQ)^{-1}$. This propagator involves the 'Hamiltonian' QHQ which we created to describe the dynamics of the classically allowed region. Thus it is quite satisfactory to apply a classical approximation to the Green function of this Hamiltonian. Still the classically forbidden region will be taken into account quantum mechanically through the self-consistent diagonalisation of $H'(E)$.

We sketch rapidly the stationary phase approximation (well known) for the phase-space functional integral representation of the propagator (Orland 1980, Faddeev 1976, Klauder 1978). First it is well known that the principal part (PP) of the Green function, $G(E)$, is related to the partial Fourier transform of the time dependent propagator

$$\mathrm{PP}(E-QHQ)^{-1}-\mathrm{i}\pi\delta(E-QHQ)=\mathrm{i}\int_0^\infty \mathrm{d}t\,\exp[\mathrm{i}(E+\mathrm{i}\varepsilon-QHQ)t]. \tag{10}$$

We are interested in computing complex wavepacket matrix elements of such a quantity. One notes that in the continuous limit of the functional integral, one finds

$$\langle z_i|\exp(-\mathrm{i}\,QHQt)|z_j\rangle=\int \mathscr{D}[z(\tau)]\exp\left(\mathrm{i}\int_0^t \mathrm{d}\tau[\mathrm{i}\langle z|\dot z\rangle-H(z)]\right), \tag{11}$$

where $z(\tau)=(q(\tau),\,p(\tau))$. The quantity $H(z)$ is simply

$$H(z)=\langle z|QHQ|z\rangle \tag{12}$$

and $|\dot z\rangle$ is defined as $\mathrm{d}|z(\tau)\rangle/\mathrm{d}\tau$.

As usual in functional integrals, $\int\mathscr{D}[z(\tau)]$ signifies a sum over all trajectories satisfying the boundary conditions

$$|z(0)\rangle=|z_j\rangle \qquad \text{and} \qquad \langle z(t)|=\langle z_i|. \tag{13}$$

The stationary phase approximation selects among all these trajectories those which make the phase of the integrand remain stationary i.e. which obey

$$\delta S=\delta\int_0^t \mathrm{d}\tau[\mathrm{i}\langle z|\dot z\rangle-H(z)]=0. \tag{14}$$

If the index ν counts the trajectories which satisfy (14) and (13), the stationary phase (SP) approximation reads

$$\langle z_i|\mathrm{e}^{-\mathrm{i}QHQt}|z_j\rangle_{\mathrm{SP}}=\sum_\nu C_\nu\exp(\mathrm{i}S_\nu(q_j,q_i;t)), \tag{15}$$

where

$$S_\nu(q_j,q_i;t)=\int_0^t \mathrm{d}\tau(\mathrm{i}\langle z_\nu|\dot z_\nu\rangle-\langle z_\nu|QHQ|z_\nu\rangle). \tag{16}$$

Although (14) reminds us of Hamilton's principle in classical mechanics, the analogy is not complete until we impose the stationary phase approximation to the integral in (10). Here, in the limit $\varepsilon\to 0$, the stationarity condition reads

$$E=-\partial S_\nu(q_j,q_i;t)/\partial t. \tag{17}$$

With (14) and (17), S can be fully identified with a classical action. For the problem

at hand (17) identifies a set of values for t, the $t_{\nu n}$, for which it is satisfied. Hence our classical approximation reads (for $E \neq H(z)$)

$$\langle z_i|(E-QHQ)^{-1}|z_j\rangle_{\rm cl} = \mathrm{Re}\Big(\mathrm{i}\sum_{n,\nu} d_{\nu n}\exp[\mathrm{i}(E+\mathrm{i}\varepsilon)t_{\nu n}+S_{\nu n}]\Big), \tag{18}$$

where $S_{\nu n} = S_\nu(q_j, q_i; t_{\nu n})$. The C_ν and $d_{\nu n}$ are the Jacobians which take into account the quadratic fluctuations of the integrands in (11) and (10). Following our choice of state vectors, $\{|z_i\rangle\}$, to span $\mathcal{Q}$, $H(z)$ has a value $E+\varepsilon_0$ where ε_0 is a zero-point energy. Consequently the δ-function term of (10) plays no role in practice.

The analogy with WKB is obvious since the latter rests essentially upon (18), along with (14) and (17). At the same time, the difference with the standard use of WKB is also obvious since it applies to the full H whereas we apply the semi-classical approximation to QHQ which is, by construction, responsible for the dynamics in the classical region. This seems more coherent, specially since the classically forbidden region is taken into account by the diagonalisation of H'. Due to the self-consistent condition (4) and the fact that the Bloch–Horowitz method is intrinsically exact, the classically forbidden region plays a non-perturbative role. Yet its introduction is not overwhelming in technical or computational terms since the finite range of H provides a manageable tool to reduce the rank of P.

3. The model

We present a model calculation to illustrate numerically the properties of the theory. It is based on the one-dimensional harmonic oscillator

$$H = \frac{\omega}{2}(p^2+q^2). \tag{19}$$

Its spectrum is well known

$$E_n = (n+\tfrac{1}{2})\omega, \qquad n = 0, 1, 2, \ldots, \tag{20}$$

and its bound state wavefunctions are also well known with

$$\psi_0 = \pi^{-1/4}\,\mathrm{e}^{-q^2/2}. \tag{21}$$

We note that the width is one.

In figure 2(b) the circle marks the classical equi-energy E in phase space. The discrete wavepackets $|z_i\rangle$ which span $\mathcal{Q}$ are indicated by ● and are centred on this equi-energy. We use Klauder's method to construct the $|z_i\rangle$ starting from a fiducial vector $|\phi_0\rangle$ (Klauder 1963, 1978).

$$\langle q|\phi_0\rangle = \pi^{-1/4}\beta^{-1/2}\,\mathrm{e}^{-q^2/2\beta^2}. \tag{22}$$

This yields

$$\langle q|z_i\rangle = \pi^{-1/4}\beta^{-1/2}\exp[-(q-q_i)^2/2\beta^2 - \mathrm{i}p_i(q-q_i)]. \tag{23}$$

The width, β, will turn out to be a variational parameter although a rather soft one in the present case.

It is straightforward to compute the overlap matrix N of elements

$$N_{ij} = \langle z_i|z_j\rangle. \tag{24}$$

The construction of the projector Q requires that we compute W, the inverse of N

$$W = N^{-1}, \tag{25}$$

and the diagonalisation of QHQ is made easier by knowing the matrix X

$$X = N^{-1/2} \tag{26}$$

which allows the construction from the $\{|z_i\rangle\}$ of an orthonormal basis $\{|Z_i\rangle\}$. In matrix notation

$$|Z\rangle = X^{\mathrm{T}}|z\rangle. \tag{27}$$

We diagonalise $\langle Z_i|QHQ|Z_j\rangle$ to obtain the eigenvalues, ε_k, and eigenvectors $|\chi_k\rangle$ of QHQ, required to calculate $G(E) = (E - QHQ)^{-1}$

$$G(E) = \sum_k |\chi_k\rangle (E - \varepsilon_k)^{-1} \langle \chi_k|. \tag{28}$$

The projector Q is simply

$$Q = \sum_i |Z_i\rangle\langle Z_i| \equiv \sum_{ij} |z_i\rangle W_{ij} \langle z_j|. \tag{29}$$

To span the $\mathscr{P}$-subspace, we first construct null momentum wavepackets centred on the crosses ($\times$) of figure 2(b). We elected to place them at $2E$, $3E\ldots$ and they are constructed according to Klauder's formula, as we did for the $|z_i\rangle$. They are labelled $\{|\gamma_n\rangle\}$. We do not use these $\{|\gamma_n\rangle\}$ since we must satisfy $PQ = 0$. They are replaced by the $\{|\bar{\gamma}_n\rangle\}$

$$|\bar{\gamma}_n\rangle = \mathscr{N}_n (1 - Q)|\gamma_n\rangle, \tag{30}$$

where $\mathscr{N}_n$ is a suitable normalisation factor. One can compute their overlap matrix

$$N_{nm} = \langle \bar{\gamma}_n | \bar{\gamma}_m \rangle, \tag{31}$$

with its inverse of elements W_{nm} and its square root matrix denoted Y. Then we construct an orthonormal set $\{|\Gamma_n\rangle\}$ according to

$$|\Gamma\rangle = Y^{\mathrm{T}}|\bar{\gamma}\rangle. \tag{32}$$

The projector P on $\mathscr{P}$ is simply

$$P = \sum_n |\Gamma_n\rangle\langle\Gamma_n| \equiv \sum_{n,m} |\bar{\gamma}_n\rangle W_{nm} \langle \bar{\gamma}_m|. \tag{33}$$

The computation of the inside–outside coupling terms of H', the QHP and PHQ, is now possible and so is the trivial Born term, PHP. Next we diagonalise $H'(E)$ in the $\{|\Gamma_n\rangle\}$ representation for various values of E until the self-consistent condition

$$E = \mathrm{eigen}(H'(E)) \tag{34}$$

is met for one eigenvalue of H' at a time.

We repeat the operation for various values of β since, strictly speaking, $E = E(\beta)$. By the Rayleigh–Ritz principle, β is a variational parameter and we seek $\bar{\beta}$ for which

$$\partial E(\beta)/\partial\beta|_{\bar{\beta}} = 0, \tag{35}$$

at which point $E(\bar{\beta})$ is identified with an eigenvalue of the original Hamiltonian H.

4. Some illustrative numerical results

We set $\omega = 15$ so that the spectrum of H is simply

$$E_0 = 7.5, \qquad E_1 = 22.5 \ldots .$$

First we make a search for $E_0 = 7.5$ using only four packets to span $\mathcal{Q}$, with their centres on the full dots (●) in figure 2(b). Similarly the rank of P is kept at four, with the packets centred on the crosses of figure 1(b). We repeat the sequence of operations outlined in § 3 for various values of β. The typical result of a sequence is shown in figure 3 for $\beta = 1.20$ which gives (full lines) the spectrum of H' as a function of E. The asymptote is due to the pole of $G(E)$ at ≈ 7.63. The self-consistent condition, $E = \text{eigen}(H'(E))$, yields $E = 7.5003$, essentially the exact result. The high level of precision is illustrated in figure 4 which reproduces a portion of figure 3 at a different scale to isolate the lowest level of $H'(E)$ around $E = 7.5$ for $\beta = 1.20$. In terms of percentage, the improvement is small between 7.63 and 7.5003. It is more significant that the final result be essentially exact. The broken line in figure 3 gives the spectrum of *PHP* which is very little dependent upon E and illustrates clearly the attraction toward the correct eigenvalue induced in H' by $G(E)$ correctly weighted by *PHQ* and *QHP*. The result may appear trivial, considering the simplicity of the illustrative model. Not quite so, if one consults figure 5 where we plotted the self-consistent value of E as a function of the parameter β. Albeit a soft one, β clearly appears as a variational parameter. More important is the fact that the stationary point lies at a value of $\beta \approx 1.20$ different from 1.00 the natural width of ψ_0, the eigenfunctions of H. In fact β is here a soft variational parameter and the minimum region extends from $\beta \approx 1.15$ to $\beta \approx 1.3$ with $E = E'$ in that region varying between 7.5007 and 7.5003, not a significant difference. It is nonetheless clear that $\beta = 1.0$ is not on the minimum plateau.

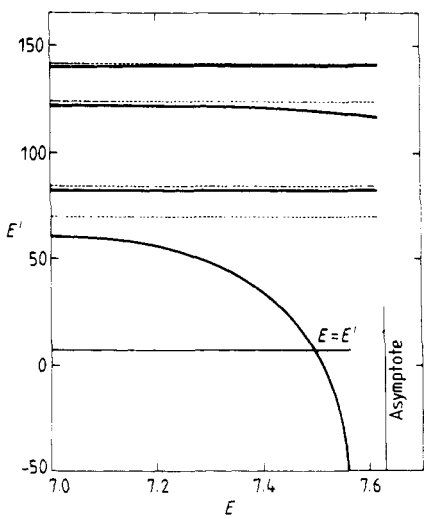

Figure 3. Spectrum of *PHP* (broken lines) and of H' (full lines) as a function of the trial energy E, around $E = 7.5$, with $\beta = 1.20$ and $N_Q = 4$.

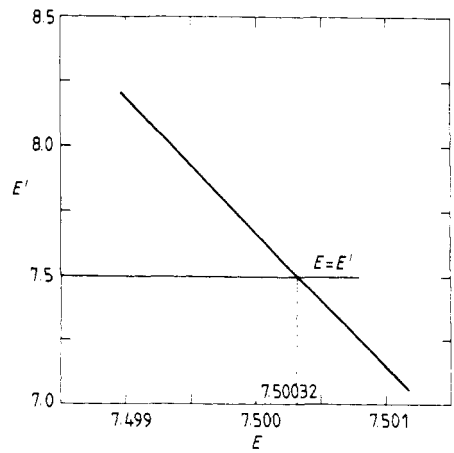

Figure 4. Small scale remake of figure 3 around $E = 7.5$ to illustrate the self-consistent convergence.

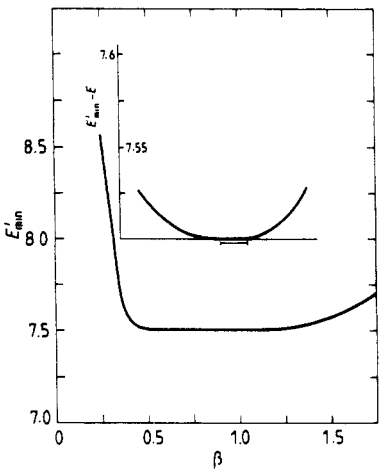

Figure 5. Large and small case of the self-consistent value of E as a function of β for the $E = 7.5$ level to illustrate the variational character of β.

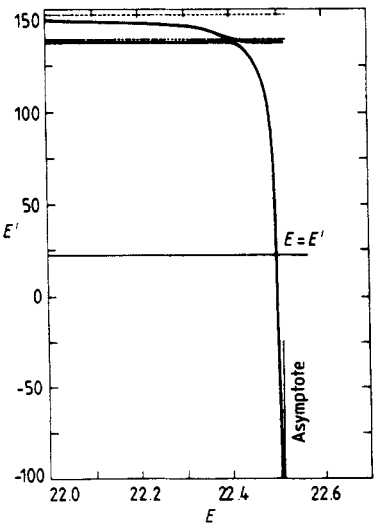

Figure 6. Spectrum of *PHP* (broken line) and of H' (full lines) as a function of the trial energy E, around $E = 22.5$, with $\beta = 1.20$ and $N_Q = 8$.

Next, keeping the rank of P and Q at 4 we seek the next level of H at 22.5. It proves simply impossible to achieve. On the other hand, raising the rank of Q to 8 while retaining that of P at 4 yields, for $\beta = 1.20$, the results of figures 6 and 7. Now the search proves not only possible but the numerical result obtained under the self-consistent condition, $E = E' = 22.5003$, is once again very accurate. How this comes into being, and the reason for this special role of the rank of Q, while $H'(E)$ is diagonalised in P, will become quite clear in § 5.

5. The classical limit for $G(E)$ and the rank of $\mathcal{Q}$

In § 2 we rapidly rederived a classical limit for the matrix element $\langle z_j|G(E)|z_i\rangle$ of the time independent propagator $G(E)$. The final result appears in (18). The phase of each contribution to this matrix element is $(E+i\varepsilon)t_{\nu n} + S_{\nu n}$ where

$$S_{\nu n} = \int_0^{t_{\nu n}} [i\langle z|\dot{z}\rangle - H(z)]\,dt. \tag{36}$$

Here $t_{\nu n}$ is the time required, for the classical system described by the Hamiltonian

$$H(z) = \langle z|QHQ|z\rangle, \tag{37}$$

with z the continuous label, $z = (\boldsymbol{q}, \boldsymbol{p})$, to join the 'points' z_i and z_j. Typically

$$H(z) = E + \varepsilon_0$$

where ε_0 is a zero-point energy. Although ε_0 finds its origin in quantum fluctuations it appears here, even if we are working in a 'classical' approximation since $H(z)$ is a classical quantity.

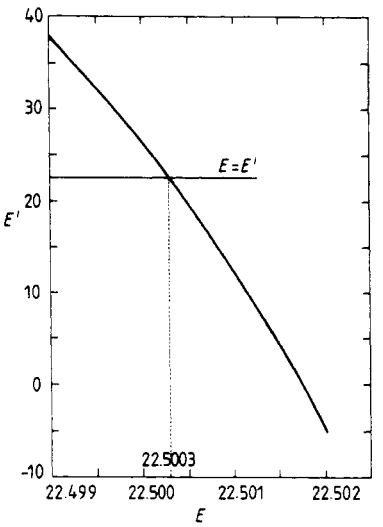

Figure 7. Small scale remake of figure 6 around $E = 22.5$ to illustrate the self-consistent convergence (convergence at 22.5003).

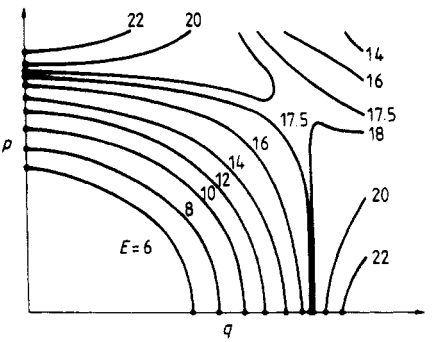

Figure 8. Trajectories, in the first quadrant of phase space, of $Q(E)HQ(E)$ for various values of E with $\beta = 1.15$ and $N_Q = 4$.

For $S_{\nu n}$ to exist in (36), there must exist at least one simply connected trajectory between z_i and z_j. In our simple example it would appear that such a trajectory must follow the circle in figure 2(b). This is not quite so because this circle is an equi-energy (value E) of H (classical) while we are interested here, in order to be coherent, in a trajectory of QHQ at a value $E + \varepsilon_0$. Because the projector Q is itself a function of E it follows that $H(z) = \langle z|Q(E)HQ(E)|z\rangle$ is itself dependent upon E. First we study the trajectories of $H(z)$ in z or (q, p) space for different values of E. Figure 8 shows the result of this investigation (limited to the first quadrant as it is symmetrical). Clearly for $N_Q = 4$ there exist no simply connected trajectories between z_1 and z_2 for $E \geqslant 18$. Now, because QHQ is of finite rank, it can be quantum mechanically diagonalised exactly and the matrix elements of $G(E)$ also calculated exactly between the various z. The same holds true for the time dependent propagator (15). The exact and classically approximated phases of this time dependent propagator $\exp(-\mathrm{i}QHQ)t$ between z_1 and various z_i are compared in table 1 as a function of E for $N_Q = 4$. With $z_i = z_1$ and $z_j = z_2$, the difference between these two phases is plotted in figure 9. Clearly this is an even more stringent test as the agreement starts breaking down at $E \approx 12.4$. Both tests agree that $E \approx 22.5$ is beyond the possibilities of $G(E)$ for a QHQ constructed from a Q-subspace of rank four. Simply put, the set of four packets $|z_i\rangle$ to span $\mathcal{Q}$ does not cover sufficiently the region of phase space involved to allow a good simply connected trajectory for $E \geqslant 12.4$ and in fact it does not allow any such trajectory for $E \geqslant 18$.

This problem disappears if we push the rank of $\mathcal{Q}$ to 8 by adding the full circles of figure 2(b) as sites to centre the $|z_i\rangle$ which span $\mathcal{Q}$. Now the search for the level at $E \approx 22.5$ becomes successful indeed as already shown in figure 6. This is quite coherent with the data collected in figure 10 where we plot the trajectories of $H(z)$ for various E and is further illustrated in table 2 where the exact and the classical phases of $\exp(-\mathrm{i}QHQt)$ are tabulated for $N_Q = 8$ as a function of E. Under both criteria the region around $E = 22.5$ is now clearly available to $G(E)$. Interestingly, it was not

Table 1. Calculated against expected values of $\arg(\langle z_j|e^{-iQHQt}|z_1\rangle)$ for various values of E for $\beta = 1.15$ and $N_Q = 4$. The expected value appears in the column labelled 'correct'.

E/β	N_Q	i/j	$(\varphi_{class}-\varphi_{quant})/\pi$	Correct
6/1.15	4	1/2	0.003	0
		1/3	1.002	1.0
		1/4	1.009	1.0
8/1.15	4	1/2	−0.003	0
		1/3	0.991	1.0
		1/4	0.995	1.0
10/1.15	4	1/2	−0.012	0
		1/3	0.978	1.0
		1/4	0.981	1.0
12/1.15	4	1/2	−0.026	0
		1/3	0.974	1.0
		1/4	1.002	1.0
14/1.15	4	1/2	0.960	0
		1/3	1.051	1.0
		1/4	2.146	1.0
16/1.15	4	1/2	0.989	0
		1/3	2.288	1.0
		1/4	2.494	1.0
17/1.15		1/2	−0.904	0
		1/3	−2.636	1.0
		1/4	−3.985	1.0

The column $(\varphi_{class}-\varphi_{quant})/\pi$ must be compared with the column labelled 'correct' which gives the expected value of $(\varphi_{class}-\varphi_{quant})/\pi$ taking into account the correction on φ_{class} due to the fact that z_3 is a classical turning point.

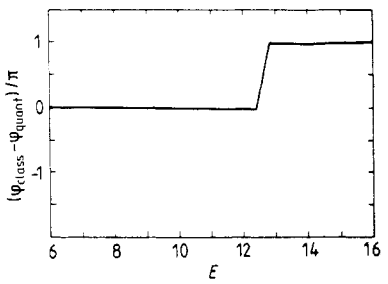

Figure 9. Plot of $(\varphi_{class}-\varphi_{quant})/\pi$ with $\beta = 1.15$ and $N_Q = 4$ where $\varphi = \arg(\langle z_2|e^{-iQHQt}|z_1\rangle)$.

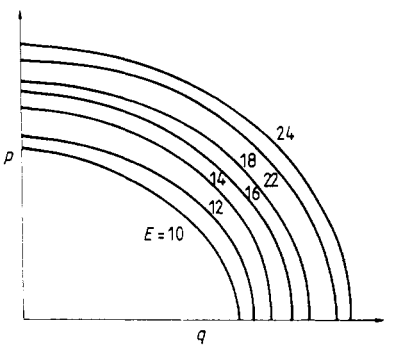

Figure 10. As figure 8 but with $N_Q = 8$.

necessary to increase the rank of P nor the way to define the packets $\{|\gamma_n\rangle\}$ which span it in order to restore order. The whole argument is based on the classical approximation to the propagator in the integral representation. This was made possible because, by construction, one restricted the role of this propagator to the classically allowed region. Nonetheless, there does not seem to be any *a priori* reason why the purely quantum treatment of the level at $E = 22.5$ should fail where it works so well

Table 2. Calculated against expected values of $\arg(\langle z_j|e^{-iQHQt}|z_1\rangle)$ for various values of E for $\beta = 1.15$ or 1.20 and $N_Q = 8$. The expected value appears in the column labelled 'correct'.

E/β	N_Q	i/j	$(\varphi_{class}-\varphi_{quant})/\pi$	Correct
10/1.15	8	1/2	0.004	0
		1/3	1.008	1.0
		1/4	1.013	1.0
12/1.15	8	1/2	0.003	0
		1/3	1.006	1.0
		1/4	1.010	1.0
14/1.15	8	1/2	0.002	0
		1/3	1.003	1.0
		1/4	1.006	1.0
16/1.15	8	1/2	0.001	0
		1/3	1.000	1.0
		1/4	1.003	1.0
17/1.15	8	1/2	0	0
		1/3	0.999	1.0
		1/4	1.001	1.0
18/1.20	8	1/2	0.007	0
		1/3	1.009	1.0
		1/4	1.019	
20/1.20	8	1/2	0.005	0
		1/3	1.005	1.0
		1/4	1.015	1.0
22/1.20	8	1/2	0.003	0
		1/3	1.001	1.0
		1/4	1.010	1.0
24/1.20	8	1/2	0.001	0
		1/3	0.997	1.0
		1/4	1.004	1.0
30/1.20	8	1/2	−0.008	0
		1/3	0.977	1.0
		1/4	0.980	1.0

As for table 1, $(\varphi_{class}-\varphi_{quant})/\pi$ must be compared with 'correct'.

at $E = 7.5$ for $N_Q = 4$. Since the evaluation of the propagator rests heavily on the spectrum of QHQ, equation (28), we study this spectrum in figure 11. The behaviour of the levels is smooth and continuous. Setting aside the case of the level at 7.5, the level which starts at 22.5 rises very smoothly. The straight line corresponds to $E = \text{eigen}(Q(E)HQ(E))$. Of course the second level of QHQ never gets close enough to this line for the Bloch–Horowitz diagonalisation to work. One must pursue the search to relatively high values of E for this test to work. The classical test told us in advance that the search for the 22.5 level for $N_Q = 4$ was doomed to fail.

Curiously enough it is the classical limit for $G(E)$ which succeeds in shedding some light on the situation. Clearly this is no accident and it points to the great significance of this classical approximation. At the same time it circumscribes its application which is made possible here only because we constructed the propagator of QHQ to cover the classically allowed region where a classical approximation makes sense. This raises new questions on the use of such an approximation for the propagator of a full

Hamiltonian H which, quantum mechanically, covers both classically allowed and forbidden regions. Here we kept the classically forbidden region under a purely quantum mechanical treatment, the self-consistent diagonalisation of $H'(E)$ in the $\mathcal{P}$-subspace. It is remarkable that the rank of P could be kept at a minimum.

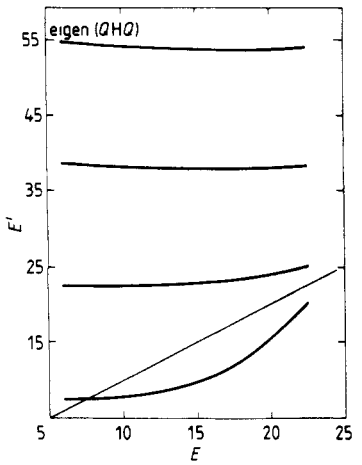

Figure 11. Spectrum of $Q(E)HQ(E)$ as a function of E with $\beta = 1.15$ and $N_Q = 4$. The straight line indicates simply where $E = \text{eigen}(Q(E)HQ(E))$.

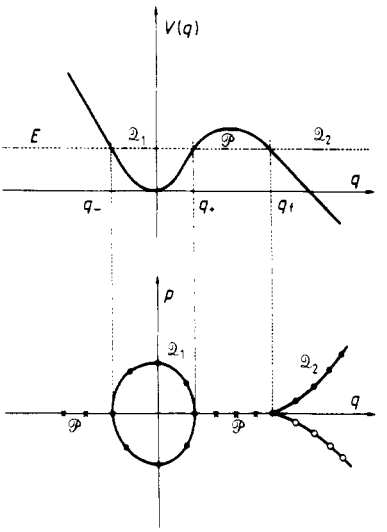

Figure 12. Schematic illustration of (a) a potential, $V(q)$ and (b) the phase space involved in the extension of the method to the problem of a barrier penetration.

6. Barrier penetration

This section is purely formal as calculations will be reported later. Schematically the problem is shown in figures 12(a) and (b). The $\mathcal{Q}$-subspace is now made up of $\mathcal{Q}_1 \oplus \mathcal{Q}_2$ with $Q = Q_1 + Q_2$. If we are interested in the decay of a quasi-bound state through penetration of the barrier then Q_2 will be built from wavepackets centred on the full dots (●) for $p > 0$. This way we restrict ourselves to purely outgoing wavepackets in the free region, beyond q_f. This is appropriate to describe disintegration. This restriction to purely outgoing Gamov-like packets and the appropriate definition of the matrix elements which involve them (Giraud *et al* 1982, Romo 1968) will generate a symmetric but non-Hermitian matrix. Hence the eigenvalues of $H'(E)$ will become complex. The imaginary part of E is readily turned into the half-life of the quasi-bound level.

Because of the high accuracy in the calculations, as suggested by our simple model calculation and because we have no problem of matching wavefunctions at q_-, q_+ and q_f, it is hoped that the present method can prove a useful tool to study barrier penetration. We also stress that the multidimensional generalisation is fairly straightforward.

7. Conclusion

We have proposed a new method which introduces simple classical mechanics elements in order to simplify the search for the spectrum of an operator H. Classically allowed and forbidden regions are effectively separated. Yet we avoid the problem of matching wavefunctions at the boundary, a problem which besets WKB, specially when trying to generalise to systems of more than one dimension. Here this generalisation is fairly straightforward, the price to be paid being purely technical. We single out the propagator of QHQ in the classically allowed region and successfully apply criteria based on the semi-classical approximation to this propagator in order to explain the breakdown of the purely quantum scheme in the search for the $E = 22.5$ level. Because QHQ is limited to the classically allowed region (up to the spread of the packets responsible for the zero-point energy of $H(z)$), it is coherent to apply semi-classical approximations to its propagator. We feel this is a significant improvement in the study of the meaning of this semi-classical approximation.

Evidently the example given is trivial but the results are not trivial, specially figures 5, 8 and 9. The latter shows a sharp breakdown between the classical and the quantum estimates of the phase of the time dependent propagator for QHQ with $N_Q = 4$. Indeed for $E \geqslant 18$, the former does not even exist whereas the latter can still be calculated but to no avail since we remain incapable of reaching the $E = E' = 22.5$ level even through a purely quantum mechanical procedure. Since the spectrum of QHQ plays a major role in $G(E)$ it is significant that this spectrum, see figure 11, shows no dramatic change around $E \approx 12.4$ where the discontinuity appears in figure 9, nor around $E \approx 18$, where the simply connected classical trajectory disappears ($N_Q = 4$). It is the semi-classical estimate of the propagator of QHQ, not H, which tells us why there is a breakdown.

Contrary to WKB this method is easily generalised to multidimensional systems, essentially because it is not beset by wavefunction matching. Consequently we feel that it can develop into a useful tool to study barrier penetration.

Acknowledgments

One of us (PA) wants to thank all the members, supporting staff and the director, R Balian, of the Division de Physique Théorique, CEN Saclay, for providing a warm welcome and a very professional atmosphere during his sabbatical stay. A travel grant from NSERC (Canada) is gratefully acknowledgeed.

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