CHAPTER XII

GEOMETRICAL CONNECTION BETWEEN THE VFM AND THE JWKB METHOD

§.39. VFM and JWKB integrals for 1D systems with even potentials.

Previous paragraphs were devoted to discussing several functional energy representations of physical systems, through the generalization of semiclassical relationships, and the Heisenberg inequalities or the de Broglie hypothesis. It has been shown that all these approximations lead to eigenvalues depending on quantum numbers and parameters contained within the Hamiltonian, similarly to those obtained via the JWKB method and the variational theorem /1-13/ (see Chapter VI).

The aim of this section is to study the link between the JWKB method and the VFM from a different standpoint. The new formalism to be presented leads one to algebraic equations whose roots are the eigenvalues, and where one can introduce the information steming from RSPT.

The inspiring idea of this connection comes from the remarkable similarity between semiclassical and variational results. This suggests the existence of some kind of relation by which the semiclassical JWKB equations could be written in terms of some extreme functional.

In order to establish such a connection between the JWKB method and the VFM, let us consider a 1D problem with an even bounded from below potential, monotonously increasing for x>0:

$$H = p^2 + V(x) \quad ; \quad p \equiv -i\frac{d}{dx} \tag{39.1a}$$

$$V(x) = V(-x) \quad ; \quad \frac{dV}{dx} > 0 \ , \ x>0 \ ; \ V(0) = 0 \tag{39.1b}$$

where, without any loss of generality, we have chosen the potential minimum at the origin.

Within the first order JWKB approximation the energy associated with

the n-th bound state satisfies Eq. (5.21) ($\hbar$=m=1, as in the choice of units for Eq. (39.1a)):

$$S_1 = \oint p(x)dx = (2n+1)\pi;\ p = (E-V(x))^{1/2};\ n=0,1,2,... \qquad (39.2)$$

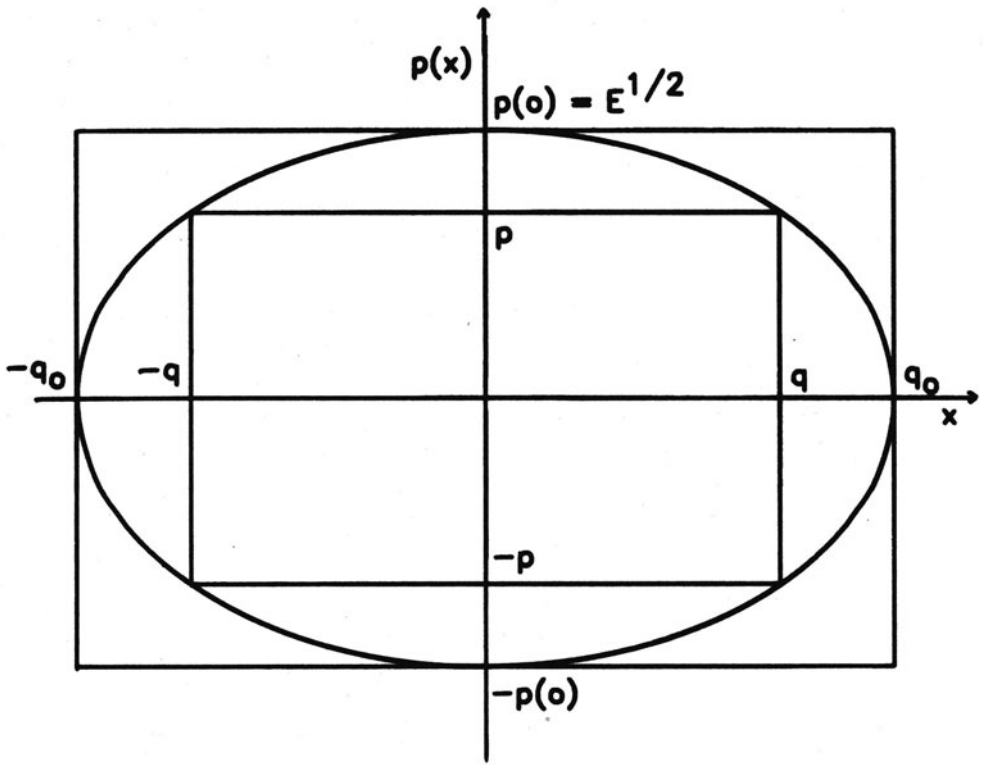

Fig. 12.1: Classical path $p(x) = (E-V(x))^{1/2}$ vs x for an arbitrary 1D system with an even, bounded from below and monotonously increasing potential function V(x).

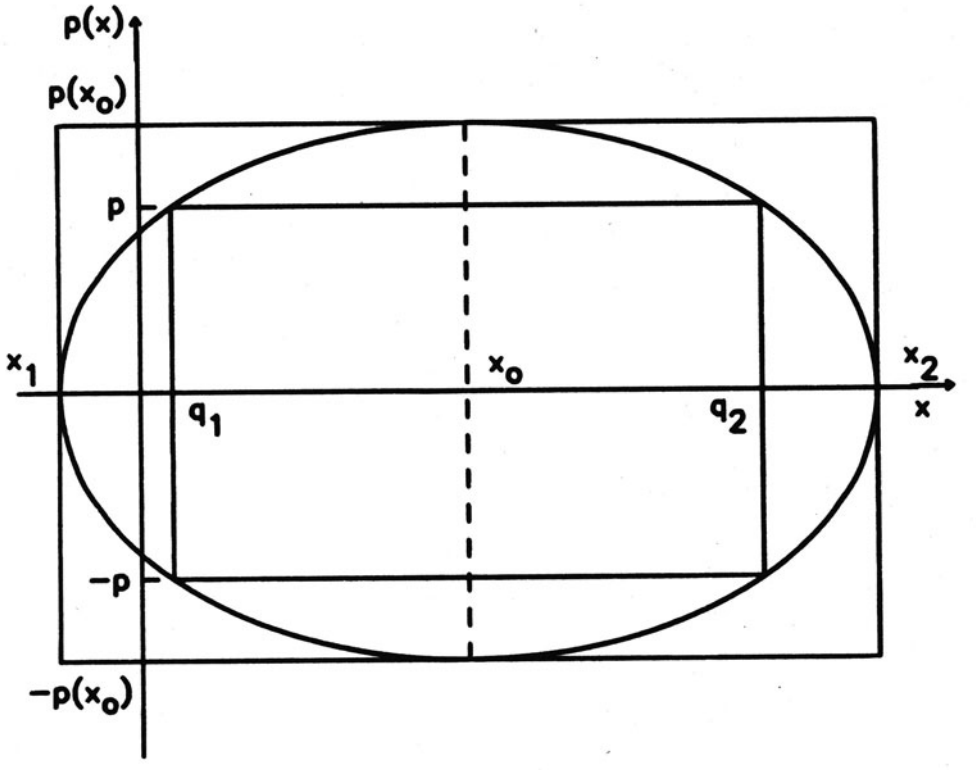

Fig. 12.2: Idem Fig. 12.1 for an odd V(x).

Fig. 12.1 shows a typical phase space trajectory p(x) vs x, for a quantum state with energy E. Obviously, the curve shape in Fig. 12.1 is ruled by the potential V(x) structure, which for the time being is irrelevant. Eq. (39.2) is a formula for the area enclosed within the phase space trajectory.

Our objective is to find out the semiclassical energy expression without solving explicitly the JWKB integral. For that purpose, let S(E) be the area of an rectangle inscribed in the trajectory (fig.12.1):

$$S(E) = 4pq, \tag{39.3}$$

where p is arbitrary and $\pm$ q are the roots of the algebraic equation $V(q) = E-p^2$. Then,

$$S(E) = 4q\ (E-V(q))^{1/2}\ , \tag{39.4}$$

and

$$E = \frac{S^2}{16q^2} + V(q)\quad . \tag{39.5}$$

Up to this moment S and q are indetermined. However, let us notice that Eq. (39.5) reveals the salient features of a variational functional. To make clearer this similarity, we choose the inscribed rectangle with maximum area:

$$\left(\frac{\partial S}{\partial q}\right)_E = 0\quad . \tag{39.6}$$

From Eqs. (39.5) and (39.6), and considering that E is constant, we derive the following relationship when S is maximum:

$$\frac{\partial E}{\partial q} = \left(\frac{\partial E}{\partial S}\right)_q \left(\frac{\partial S}{\partial q}\right) + \left(\frac{\partial E}{\partial q}\right)_S = \left(\frac{\partial E}{\partial q}\right)_S = 0 \tag{39.7}$$

Then, the final result makes clear that the semiclassical energy (E) may arise from the pair of Equations (39.5) and (39.7), instead of the integral (39.2). These two equations represent a functional and its extreme condition, and they make up the basic conditions existing in other variational methods previously studied /1-5,13/. This equivalence shows plainly why one gets the same (qualitative) results when using the JWKB method and the SVM /11,12,14,15/: both procedures carry to the same system of equations and they only differ about the S choice.

The geometrical condition represented by Eq. (39.6) totally determines S. For a potential like $V(x) = x^{2K}$, the following lemma is used to obtain the area:

Lemma 39.1: For $V = x^{2K}$, then

$$S = 2K^{3/2}(K+1)^{-(K+1)/2K}\Gamma\left(\frac{3K+1}{2K}\right) \frac{S_1}{\Gamma\left(\frac{3}{2}\right)\Gamma\left(\frac{1}{2K}\right)} \quad . \tag{39.8}$$

Proof. The calculation of S_1 for the proposed potential gives

$$S_1 = \oint (E-q^{2K})^{1/2} dq = 2\int_{-q_o}^{q_o} (E-q^{2K})^{1/2} dq = 4\int_{0}^{q_o} (E-q^{2K})^{1/2}\, dq \tag{39.9}$$

where $p(q_o) = 0$ defines the classical turning points changing the variable as in $z = q^{2K/E}$, (39.9) turns into a first class Euler integral:

$$S_1 = \frac{2}{K} E^{(K+1)/2K} \int_0^1 z^{(1-2K)/2K} (1-z)^{1/2}\, dz = \frac{2}{K} E^{(K+1)/2K} \beta\left(\frac{1}{2K};\frac{3}{2}\right) =$$

$$= \frac{2}{K} E^{(K+1)/2K} \frac{\Gamma\left(\frac{1}{2K}\right)\ \Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{3K+1}{2K}\right)} \quad . \tag{39.10}$$

On the other hand, the area of the inscribed rectangle is

$$S(q^*) = 4q^* \ (E-q^{*2K})^{1/2} \quad , \tag{39.11}$$

where

$$(\frac{\partial S}{\partial q}) \ (q=q^*) = 4(E-q^{*2K})^{1/2} - 4Kq^{*2K}(E-q^{*2K})^{-1/2} = 0 \quad , \tag{39.12}$$

and

$$q^* = (\frac{E}{K+1})^{1/2K} \quad . \tag{39.13}$$

Then, Eq. (39.12) allows one to show that $S(q^*)$ is a maximum area:

$$(\frac{\partial^2 S}{\partial q^2}) \ (q=q^*) = -8K^{1/2} \ (\frac{E}{K+1})^{(1-K)/2K} < 0 \ \forall K>0 \tag{39.14}$$

Finally, the substitution (39.13) in (39.11) yields

$$S = 4K^{1/2} \ (\frac{E}{K+1})^{(K+1)/2K} \tag{39.15}$$

The combination of Eqs. (39.10) and (39.15) completes the proof*.

Lemma 39.1 gives the constant S in the functional (39.5); applying Eq. (39.2), we get the result:

$$S = C_K \ (2n+1) \ ; \ C_K = \frac{2\pi K^{3/2}\Gamma((3K+1)/2K)}{(K+1)^{K+1/2K}\Gamma(\frac{3}{2})\Gamma(\frac{1}{2K})} \quad , \tag{39.16}$$

which whows that S is proportional to n, as discussed in Chapter VI.

It must be noted that the quotient between the phasic area and the inscribed rectangle area, S_1/S, is independent from n for a potential V(x) having just one term. For those potentials with two or more terms a relationship dependent on n should be expected. Notwithstanding, it must be remembered that the most important part of the E_n dependence with n is guaranteed by Eqs. (39.5) and (39.7).

For a potential having more than one term, a different alternative may be followed. One can maintain the S form given by lemma 39.1, and modify the functional (39.5):

$$E = \frac{S^2}{16q^2} + \hat{V}(q) \quad , \tag{39.17}$$

where $\hat{V}(q)$ is a function that can be chosen according to the VFM theory (Chapters VI and VII).

There exists another interesting energy expression, arising from geometric-like relationships. In order to discuss it, we start with:

Lemma 39.2: Let S_2 be the area of the smallest rectangle completely containing S_1 (as shown in Fig. 12.1), for $V = x^{2K}$. Then

$$S_2 = C'_K S_1 \; ; \; C'_K = 2K \frac{\Gamma(\frac{3K+1}{2K})}{\Gamma(\frac{3}{2})\Gamma(\frac{1}{2K})} \tag{39.18}$$

Proof: From Fig. 12.1 it follows at once that for S_2:

$$S_2 = 4p(0)q_0 = 4E^{1/2}E^{1/2K} = 4E^{(K+1)/2K} \tag{39.19}$$

The use of Eqs. (39.10) and (39.19) leads to (39.18)*.

Lemma 39.2 and Eq. (39.19) give the q_0 value at the classical turning point:

$$q_0 = \frac{\pi C'_K}{4} \frac{2n+1}{E^{1/2}} \quad . \tag{39.20}$$

Considering that $E = V(q_0)$, then we have the desired equation:

$$E = V\left(\{\frac{\pi C'_K}{4} \frac{2n+1}{E^{1/2}}\}\right) \quad . \tag{39.21}$$

Eq. (39.21) is a compact and elegant result for the approximate semiclassical eigenvalues, expressed as an algebraic equation. This formula adopts a peculiarly simple expression when the phase space curve is elliptical (from now on we will use the denomination elliptical approximation for such a case). In this case we get from lemma 39.2:

$$C'_1 = 4/\pi \quad . \tag{39.22}$$

Let us consider a simple example of application of Eq. (39.21), using again the anharmonic oscillator (see Appendices A and B):

$$H(g,\lambda) = p^2 + gx^2 + \lambda x^{2K} \quad . \tag{39.23}$$

Restricting ourselves to the elliptical approximation, Eqs. (39.23) and (39.21) give the following formula for the eigenvalues associated with $H(1,\lambda)$:

$$E = \frac{(2n+1)^2}{E} + \frac{(2n+1)^{2K}}{E^K} \lambda \quad . \tag{39.24}$$

Due to the elliptic approximation, the correct result is found when $\lambda \to 0$, although only a qualitative correct behavior with n and λ for $1/\lambda \to 0$:

$$E \simeq \lambda^{1/(K+1)} \, (2n+1)^{2K/(K+1)} \tag{39.25}$$

The iterative solution of Eq. (39.24) around $\lambda=0$ yields a power series in λ, whose first terms are:

$$E \simeq (2n+1) + \frac{1}{2} (2n+1)^{K} \lambda - \frac{1}{8} (2K-1)(2n+1)^{2K-1}\lambda^{2}+... \tag{39.26}$$

A comparison between Eq. (39.26) and Eqs. (36.20) (obtained by means of algorithms studied in §§.8 and 9) shows that, naturally, the power series deduced from (39.24) does not coincide with the RSPT. The result is by no means surprising since we have used the elliptical approximation corresponding to the harmonic potential, which is a very gross approximation. However, Eq. (39.26) possesses an interesting property: the dominant behavior for $n>>1$ in every perturbational correction is properly predicted.

If one wants to go beyond the elliptical approximation, then

$$E = \tau_{V} \left(\frac{2n+1}{E^{1/2}}\right) \tag{39.27}$$

where τ_{V} is some transform of the potential $V(x)$. A simple manner to make this extension consists of keeping up as far as possible the structure of Eq. (39.24).

Let us consider the generalization of Eq. (39.24) expressed in terms of the following equation

$$E^{K+1} = (2n+1)^{2} \, E^{K-1} + \lambda (2n+1)^{2K} \, D(E) \tag{39.28}$$

where $D(E)$ is an unknown function to be determined.

Eq. (39.28) makes up an alternative starting point to combine the RSPT with equations representing the qualitatively correct behavior of the energy eigenvalue. The geometrical considerations previously invoked allow one to obtain an algebraic equation whose roots are the eigenvalues.

To build D(E) one can follow a procedure as in §.38. According to the Symanzik theorem /16/ (Appendix A) the harmonic oscillator eigenvalue satisfies the following scaling law (Eq.(23.3)):

$$E(1,\lambda) = \lambda^{1/(K+1)}\, E(\lambda^{-2/(K+1)},1) = \lambda^{1/(K+1)} e \ , \qquad (39.29)$$

where E can be expanded in λ-series and e in $\lambda^{-2/(K+1)}$-series. Then, D(E) can be expanded in $\lambda(\lambda\to 0)$ power series as well as $\lambda^{-2/(K+1)}$ $(1/\lambda\to 0)$-power series in order to maintain the correct analytic structure in Eq. (39.28).

The following variables

$$u' = \lambda E^{-(K+1)} = e^{-(K+1)} \ , \qquad (39.30a)$$

$$v' = E^{-2} = \lambda^{-2/(K+1)}\, e^{-2} \ , \qquad (39.30b)$$

are a suitable pair to give an analytic representation of D(E), since any u' and v' power gives rise to λ and $\lambda^{-2/(K+1)}$ powers.

It is natural to represent D(E) as a power series expansion, viz.

$$D(E) = \sum_{i=0}^{\infty} D^{(i)}\, u'^{i} \qquad (39.31a)$$

$$D(E) = \sum_{i=0}^{\infty} D'^{(i)}\, v'^{i} \qquad (39.31b)$$

A simple analysis, similar to the one made in §.33, assures us that

the expansion (39.31a) is adequate to introduce the λ-expansion, while the v'-power series (39.31b) is suitable to employ the information regarding the anharmonic regime ($1/\lambda \to 0$).

Eq.(39.21) leads to alternative expressions with respect to those proposed by (39.28). Another possibility would be the following one

$$E^{K+1} = (2n+1)^2 E^{K-1} L(E) + \lambda \overset{\alpha}{C}_n (2n+1)^{2K} \qquad (39.32)$$

where $\overset{\alpha}{C}n$ is a constant introduced to achieve the correct result when $1/\lambda \to 0$ (Eq.(39.25)). Function L(E) can be written in terms of the variables u' and v' (Eqs.(39.30)):

$$L(E) = \sum_{n=0}^{\infty} L^{(n)} u'^n \quad , \qquad (39.33a)$$

$$L(E) = \sum_{n=0}^{\infty} L'^{(n)} v'^n \quad , \qquad (39.33b)$$

whose use is similar to that previously discussed for D(E).

A particularly simple and useful way to apply Eqs. (39.28) and (39.32) is the following: to introduce the $\lambda^{-2/(K+1)}$ power series expansion by means of (39.28) and (39.31b), and Eqs. (39.32) and (39.33a) to introduce the RSPT. The example below is an illustrative application.

Example. Let us to determine the first $\{D^{(i)}\}$ and $\{L^{(i)}\}$ coefficients so as to fit the $\{E^{(i)}\}$ and $\{e^{(i)}\}$ coefficients (Eq.(23.2)). Eq. (39.28) for $\lambda \to 0$ gives $E_n^{(0)}$ at once. Now, we incorporate the first two coefficients $e^{(0)}$ and $e^{(1)}$ by way of $D'^{(0)}$ and $D'^{(1)}$:

$$E^{K+1} \simeq (2n+1)^2 E^{K-1} + \lambda (2n+1)^{2K} \{D'^{(0)} + \frac{D'^{(1)}}{E^2}\} \quad . \qquad (39.34)$$

Substituting (39.30b) into (39.34), we get the result

$$e^{K+1} \simeq (2n+1)^{2K} \{D'^{(0)} + D'^{(1)} e^{-2} \lambda^{-2/(K+1)}\} + (2n+1)^{2} \lambda^{-2/(K+1)} e^{K-1} \quad . \tag{39.35}$$

Finally, taking into account that

$$e \simeq e_n^{(0)} + \lambda^{-2/(K+1)} e_n^{(1)} + \ldots \quad ,$$

we have the first two coefficients of the D(E) expansion

$$D'^{(0)} = e_n^{(0)K+1} (2n+1)^{-2K} \quad , \tag{39.36a}$$

$$D'^{(1)} = D'^{(0)} \{(K+1) e_n^{(1)} - (2n+1)^2 (e_n^{(0)})^{-1}\} \quad . \tag{39.36b}$$

Following the same steps for the other case, we rewrite Eq.(39.32) as

$$E^{K+1} = (2n+1)^2 E^{K-1} \{L^{(0)} + L^{(1)} E^{-(K+1)}\} + \lambda \tilde{C}_n (2n+1)^{2K} \tag{39.37}$$

It is possible to introduce the coefficients $E_n^{(0)}$ and $E_n^{(1)}$ through $L^{(0)}$ and $L^{(1)}$ and $e_n^{(0)}$ by way of $\tilde{C}_n$, in order to have an equation with the same number of adjustable constants as in (39.34). Thus, making

$$E \simeq E_n^{(0)} + \lambda E_n^{(1)} + \ldots$$

we find at once from (39.37) the following results:

$$L^{(0)} = 1 \tag{39.38a}$$

$$L^{(1)} = \{(K+1)\, E_n^{(1)} E_n^{(0)} K + (1-K) E_n^{(1)} E_n^{(0)} (K-2) - \tilde{C}_n\}\, E^{(0)2} \qquad (39.38b)$$

$$\tilde{C}_n = D'^{(0)} \qquad (39.38c)$$

As an example, we consider the ground state of the quartic anharmonic oscillator (K=2, n=0) and compare the numerical results obtained from Eqs. (39.34) and (39.37). Coefficients $E_n^{(0)}$ and $E_n^{(1)}$ are well known (Eqs.(36.20)) and coefficients $e_n^{(0)}$ and $e_n^{(1)}$ were determined from the published data in Ref./17/:

$$e_o^{(0)} = 1.060362090 \quad ; \quad e_o^{(1)} = 0.362022684 \qquad (39.39)$$

Table 12.1

Quartic anharmonic oscillator ground state as a function of the parameter λ.

λ	$E^{a)}$	$E^{b)}$	$E^{c)}$
10^{-5}	1.00000750	1.00000681	1.00000750
10^{-4}	1.00007499	1.00006813	1.00007499
10^{-3}	1.00074893	1.00068055	1.00074869
10^{-2}	1.00739525	1.00673406	1.00737367
10^{-1}	1.06638663	1.06140633	1.06528550
1	2.46022754	2.44711146	2.44917407
10	2.46022754	2.44711146	2.44917407
10^2	5.00609714	4.99872897	4.99941754
10^3	10.64308128	10.63950624	10.63978871
10^4	22.86315714	22.86148152	22.86160887

a) Eq. (39.37)

b) Eq. (39.34)

c) Exact results /18/

Computed results are compared with "exact" ones /13/ in Table 12.1. The agreement is quite acceptable in the whole range of λ, in spite of the simplicity of the employed expressions.

§. 40. VFM and JWKB integrals for 1D systems with potentials without defined parity and central field systems.

In this section the geometrial relations studied in §.39 are extended to potentials without defined parity and central field potentials.

Let $H = p^2+V(x)$ the Hamiltonian corresponding to a 1D system and $V(x)$ a potential bounded from below:

$$V(x_o) \leq (V(x) \; ; \; \frac{dV}{dx} \gtrless 0 \text{ whenever } (x-x_o) \gtrless 0 \quad . \tag{40.1}$$

The classical momentum take values $0 \leq p(x)^2 \leq E-V(x_o)$, for a given state with total energy E. For such a state, it is possible to build a rectangle of sides 2p and $q_2 - q_1$, where

$$V(q_1) = V(q_2) = E-p^2 \tag{40.2}$$

under the condition of being inscribed within the phase space trajectory (Fig.12.2). The rectangular area is

$$S = 2p(q_2 - q_1) \tag{40.3}$$

and has its maximum value when $\partial S/\partial p = 0$. Since E remains fixed, q_1 and q_2 are interdependent through p; then, it is possible to replace the difference $q_2 - q_1$ by $q - q_0$, where q describes the p-variation and q_0 is a constant(to be used in order to have a unique eigenvalue for each quantum number). On the basis of these considerations, we find the following functional

$$E = \frac{S^2}{4(q-q_0)^2} + \hat{V}(q), \tag{40.4a}$$

with the extreme condition

$$\left(\frac{\partial E}{\partial q}\right)_S = 0 \quad ; \quad \frac{\partial S}{\partial q} = \frac{\partial S}{\partial p} = 0 \quad . \tag{40.4b}$$

Function $\hat{V}(q)$ is, in general, a transform of the potential.

A similar functional form for the energy can be derived from quite different considerations /2,4,5/. Again, the approach presented here brings to light the relationship among variational and semiclassical methods.

Let us recall the attention to the way the condition (40.4b) was introduced within the functional. It has not been required the extreme condition for the functional, but a maximum area of the rectangle within the phase space trajectory. This choice is not arbitrary, because only under this condition the relation (lemma 39.1)

$$\frac{S}{S_1} = C(K) \tag{40.5}$$

is satisfied, independently of E, whenever $V(x) = (x-x_o)^{2K}$.

Let us consider now an equation analogous to (39.21) for potentials without definite parity. If x_1 and x_2 are the classical turning points ($p(x_1) = p(x_2) = 0$) and S_2 the area of inscribed the phase space trajectory (Fig.12.2):

$$S_2 = 2p(x_o)\ (x_2 - x_1) \quad ; \quad x_1 < x_2 \quad . \tag{40.6}$$

By extension of lemma 39.2, this latter area is proportional to the

phase space

$$\frac{S_2}{S_1} = C'(K) \tag{40.7}$$

with $C'(K)$ independent of E when $V(x) = (x-x_o)^{2K}$. Eqs.(40.6) and (40.7) lead us to

$$2x_2 = \frac{C'(K)S_1}{p(x_o)} + x_1 + x_2 \quad , \tag{40.8}$$

so that the energy E satisfies:

$$E = V(x_2) = V(\{\frac{C'(K)S_1}{2(E-V(x_o))^{1/2}} + \frac{x_1+x_2}{2}\}) \quad . \tag{40.9}$$

Eq.(40.9) turns, in general, into a trascendental equation for the energy, after x_o, x_1 and x_2 are determined. For an even potential (i.e., $x_1 = -x_2$), and choosing $V(x_o) = 0$, we meet again Eq. (39.21). Within the elliptical approximation for the trajectory, we have the result

$$\frac{C'(1)S_1}{2} = 2n+1 \quad . \tag{40.10}$$

Eqs. (40.4) and (40.9) are valid not only for 1D problems but they can be extended to 3D systems with central field potentials. In these latter cases our problem is to approach the eigenvalues associated with the Hamiltonian

$$H = p_x^2 + \frac{g^2}{x^2} + V(x) \quad ; \quad p_x \equiv -i\frac{d}{dx}, \; x \geq 0. \tag{40.11}$$

with $g^2 = \ell(\ell+1)$. In order to apply the geometric procedure developed before, it is necessary to consider as potential V(x) the effective

potential function U(x)

$$U(x) = g^2 x^{-2} + V(x) \quad . \tag{40.12}$$

When V(x) is supersingular and not bounded from below, i.e.

$$V(x) = -\lambda r^{-\nu} \quad ; \quad \lambda > 0 \quad , \nu > 2 \tag{40.13}$$

the effective potential (40.12) is not bounded from below either, for $\ell = 0$. In order to surmount this problem, it is necessary to introduce the Langer transformation /19/:

$$g = \ell + 1/2 \quad , \tag{40.14}$$

which is characteristic of the semiclassical approximation for radial potential problems. The JWKB quantization condition is

$$\oint p(x)dx = (2n_r+1)\pi \tag{40.15a}$$

$$p(x) = \{E - g^2 x^{-2} - V(x)\}^{1/2} \tag{40.15b}$$

where n_r is the number of radial zeros in the wave function.

In the following we present some simple examples illustrating the application of the equations derived in this paragraph.

Example I: Let us consider the 1D problem without defined parity

$$V(x) = \alpha x^2 + \beta x \quad . \tag{40.16}$$

The minimum potential value is at:

$$V'(x_o) = 0 \quad ; \quad x_o = -\beta/2\alpha \quad , \tag{40.17}$$

which gives the maximum impulse

$$V(x_o) = -\beta^2/4\alpha \quad , \tag{40.18a}$$

$$p(x_o) = \{E + \frac{\beta^2}{4\alpha}\}^{1/2} \quad . \tag{40.18b}$$

The classical turning points are

$$E - V(x) = E - \alpha x^2 - \beta x = 0 \quad , \tag{40.19a}$$

$$x_{1,2} = \frac{\beta \pm (\beta^2+4\alpha E)^{1/2}}{-2\alpha} \quad , \tag{40.19b}$$

where x_1 (x_2) corresponds to the sign choice +(-) in (40.19b).

Above equations give

$$\frac{x_1 + x_2}{2} = -\frac{\beta}{2\alpha} \quad . \tag{40.19c}$$

The replacement (40.13b) and (40.19c) in (40.9), and the application of the elliptical approximation (Eq.(40.10))yield the result

$$E = V(\frac{2n+1}{p(x_o)} - \frac{\beta}{2\alpha}) = \alpha\,[\frac{2n+1}{p(x_o)} - \frac{\beta}{2\alpha}]^2 + \beta[\frac{2n+1}{p(x_o)} - \frac{\beta}{2\alpha}] =$$

$$= \alpha[\frac{2n+1}{p(x_o)}]^2 - \frac{\beta^2}{4\alpha} = \alpha\frac{(2n+1)^2}{E+\frac{\beta^2}{4\alpha}} - \frac{\beta^2}{4\alpha} \quad . \tag{40.19d}$$

Finally, Eq. (40.19d) leads us to:

$$E = (2n+1)\ \alpha^{1/2} - \frac{\beta^2}{4\alpha} \quad , \tag{40.20}$$

which is the correct result. The procedure offers an alternative approach regarding that discussed in §.24 with respect the role played by the scaling in the VF theory.

Example II. Let us consider now the radial effective potential in a hydrogen-like atom:

$$V(x) = g^2x^{-2} - Zx^{-1} \quad , \tag{40.21}$$

whose minimum value is at

$$V'(x_o) = 0 \quad ; \quad x_o = 2g2Z^{-1} \quad . \tag{40.22}$$

The maximum impulse is

$$V(x_o) = -Z^2/4g^2 \tag{40.23a}$$

$$p(x_o) = \frac{1}{2g}\ (Z^2+4g^2E)^{1/2} \tag{40.23b}$$

From Eq. (40.23b) we find the appropriate condition to obtain bound states:

$$\frac{-Z^2}{4g^2} \leq E \leq 0 \tag{40.24}$$

This particular problem makes easier to use Eqs. (40.6) and (40.7)

instead of Eq. (40.9). The classical turning points are

$$x^2E + Zx - g^2 = 0 \tag{40.25a}$$

$$x_{\pm} = \frac{1}{4E}\{-Z^{\pm}(Z^2 + 4g^2E)^{1/2}\} \tag{40.25b}$$

and from (40.24) $x_- > 0$, $x_+ < 0$, so that

$$x_- - x_+ = x_2 - x_1 = -\frac{1}{E}(Z^2+4g^2E)^{1/2} \tag{40.25c}$$

The area of the rectangle inscribing the phase space trajectory (Eq.(40.6)) is

$$S_2 = 2p(x_o)\ (x_2 - x_1) = -\frac{Z^2+4g^2E}{gE} = C'S_1 \tag{40.26}$$

which determines the energy

$$E = -\frac{Z^2}{4g^2+C'gS_1} \tag{40.27}$$

The result makes clear the difficulties of the method to study radial potentials, since Eq. (40.7) presents an involved dependence on n_r and ℓ. In this regard, the geometrical approximation presented here has similar drawbacks as those shown by the JWKB method for radical problems. Such difficulties, closely related to the practical implementation of the formalism, do not occur when the geometric method is combined with the RSPT, as done in §.39 (Eqs. (39.28) and (39.32)).

§. 41. Generalization of geometrical relations and RSPT.

Classical trajectories for systems having an arbitrary number of degrees of freedom are quite complicated. The extension to these systems of the geometrical ideas developed in this chapter becomes thus cumbersome.

In order to apply the method to a greater number of systems it seems more appropriate to follow an alternative path. The generalization we propose below is the first attempt to introduce in a systematic manner the PT into a semiclassical functional, a subject to which is devoted the remaining of the book. Some results on this topic have been recently published /20/.

Let $E(1,\lambda)$ (using the notation as in §§. 23 and 24) be an eigenvalue of some Hamiltonian system, which can be expanded as follows:

$$E(1,\lambda) = \sum_{n=0}^{\infty} E^{(n)} \lambda^n \tag{41.1a}$$

$$E(1,\lambda) = \lambda^{\beta} e(\lambda) = \lambda^{\beta} \sum_{n=0}^{\infty} e^{(n)} \lambda^{\alpha n} , \quad \alpha<0 \tag{41.1b}$$

about $\lambda=0$ and $1/\lambda=0$, respectively.

We define now a couple of bounded variables and whose powers can be expanded both in λ-and λ^{α}-power series (by extension of (39.30)). The simplest choice is

$$u' = \lambda E^{-1/\beta} = e^{-1/\beta} \tag{41.2}$$

$$v' = E^{\alpha/\beta} = \lambda^{\alpha} e^{\alpha/\beta} \tag{41.3}$$

Eqs. (41.1) assure us that u'^m gives rise to λ^j ($j \geq m$) terms and all the λ^{α} powers. Analogously, we conclude that v'^m originates all the λ-powers and $\lambda^{\alpha j}$ ($j \geq m$) terms.

Using variables (41.2) and (41.3), Eqs. (39.23) and (39.32) can be generalized through the following relationship /20/:

$$E^{1/\beta} = E^{(\alpha+1)/\beta}\, L(E) + \lambda D(E) \quad . \tag{41.4}$$

This last equation includes as a particular case that in §.39 for anharmonic oscillators ($\alpha = -2/(K+1)$, $\beta = 1/(K+1)$).

Due to (41.2) and (41.3), the functions L(E) and D(E) may be constructed as follows:

$$L(E) = \sum_{n=0}^{\infty} L^{(n)}\, u'^{n} \quad , \tag{41.5a}$$

$$L(E) = \sum_{n=0}^{\infty} L'^{(n)}\, v'^{n} \quad , \tag{41.5b}$$

$$D(E) = \sum_{n=0}^{\infty} D^{(n)}\, u'^{n} \quad , \tag{41.5c}$$

$$D(E) = \sum_{n=0}^{\infty} D'^{(n)}\, v'^{n} \quad . \tag{41.5d}$$

The set of coefficients $\{D^{(n)}, D'^{(n)}\}$ and $\{L^{(n)}, L'^{(n)}\}$ can be determined using an arbitrary number of coefficients $\{E^{(n)}\}$ and $\{e^{(n)}\}$. Both power series expansions (41.1a) and (41.1b) may be added into Eq. (41.4) since, by construction, the solutions of these equations have expansions in λ-and λ^{α}-power series. Notwithstanding, from a practical standpoint it is convenient to use (41.5a) and (41.5c) into (41.4) if coefficients $\{E^{(n)}\}$ are introduced. In a similar manner, in order to introduce coefficients $\{e^{(n)}\}$ it is more suitable to employ Eqs. (41.5b) and (41.5d).

Let us stress on the meaning of the extension discussed in this paragraph: the original problem (Schrödinger formulation via a second-order differential equation) has been transformed into another quest of searching for the roots of an algebraic equation constructed from the power series expansions (41.1). Several open points in our ap-

proach can be mentioned:

i) Conditions for the existence of real roots in Eq. (41.4),

ii) Convergence of the solutions towards the eigenvalues, when the involved perturbation coefficients increase,

iii) Influence upon the results of Eq. (41.1) of possible spurious terms not considered within the expansion (41.1b) (see Appendix I).

These questions remain open to research. Our preliminary studies have shown that Eq. (41.1) may present in certain cases a multiplicity of real roots.

Although in the next sections we will present a more efficient formalism to sum RSPT, the basic principle is the same as the one discussed here: to develop non-numerical E-expressions, considering essential analytical properties of the function. In our present case, such properties correspond to the asymptotic expansions (41.1a) and (41.1b). The basic structure of such expansions of the energy of quantum systems is fixed by the VT and HFT.

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