

# Classical Trajectories and Quantum Spectra

Bogdan Mielnik<sup>a,b</sup>  
and  
Marco A. Reyes<sup>a</sup>

<sup>a</sup>*Departamento de Física  
Centro de Investigación y Estudios Avanzados del IPN  
Apdo. Postal 14-740, México D.F. 07000, México*

<sup>b</sup>*Department of Physics  
Warsaw University, Warsaw, Poland*

## Abstract

A classical model of the Schrödinger's wave packet is considered. The problem of finding the energy levels corresponds to a classical manipulation game. It leads to an approximate but non-perturbative method of finding the eigenvalues, exploring the bifurcations of classical trajectories. The role of squeezing turns out decisive in the generation of the discrete spectra.

## 1 The classical model of quantum systems.

The quantum theory devotes a lot of attention to the classical models of quantum phenomena. Much less attention to the quantum models of classical phenomena. Yet, such models exist. Some classical processes can mimic the quantum laws. One of the most provocative examples was given by Avron and Simon in 1986 by explaining the structure of the Saturn rings in terms of the band spectrum of the Schrödinger's operator [1](Fig.1). Their work shares some epic qualities of Jonathan Swift [2] (something so enormous imitating something so little!).

The analogy, though, is natural and has some antiquity [3]. Consider the 1-dimensional Schrödinger's equation:

$$-\frac{1}{2} \frac{d^2}{dx^2} \psi(x) + [V(x) - E] \psi(x) = 0 \quad (1)$$

with  $V(x)$ ,  $\psi(x)$  and  $E$  real. Suppose, we are interested in the solutions of (1) for arbitrary  $E \in \mathfrak{R}$ , *not necessarily belonging to the spectrum*. Denote now the variable  $x$  by  $t$  and call it *time* [3, 4, 5]; put also  $q = \psi(t)$ ,  $p = \psi'(t)$ . The equation (1) becomes:

$$\frac{dq}{dt} = p, \quad \frac{dp}{dt} = 2[V(t) - E]q \quad (2)$$

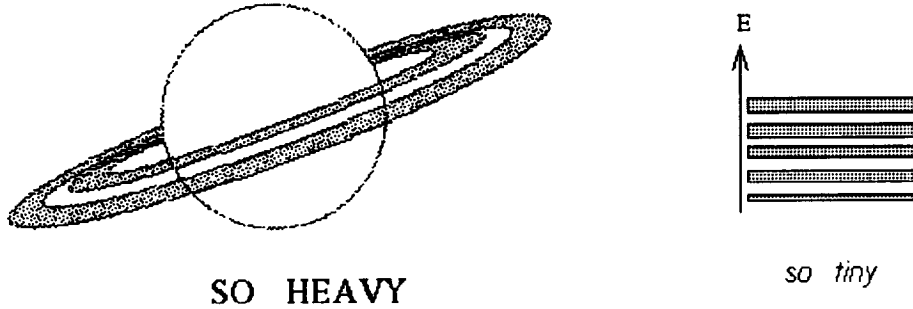
Note, that (2) is simply the pair of canonical equations for the classical variables  $q, p$  of a classical oscillator with a time dependent elastic constant. The Hamiltonian reads:

$$H(t) = \frac{p^2}{2} + g(t)\frac{q^2}{2}, \quad g(t) = 2[E - V(t)] \quad (3)$$

The canonical trajectories of (3):

$$\mathbf{q}(t) = \left\| \begin{array}{c} q(t) \\ p(t) \end{array} \right\| \quad (t \in \mathfrak{R}) \quad (4)$$

‘portrait’ every detail of the Schrödinger’s wave packet  $\psi(x)$  and its first derivative  $\psi'(x)$ . This includes the phenomenon of the “classical spectral bands”.



**Figure 1.** Saturn rings, the macroscopic imitation of the spectral bands (An imperfect image of Avron and Simon idea: the spectral bands of a quasi-periodic potential form a Cantor set).

Indeed, assume  $V(t)$  is periodic or quasi-periodic. If  $E$  belongs to a spectral band of the Schrödinger’s operator, the wave functions (1) are bounded in  $x \rightarrow \pm\infty$  and so are the trajectories of the classical oscillator (2-3). Thus, the spectral bands of  $V(t)$  define the stability bands (trapped motions) of the classical system (2-3). In turn, for  $E$  belonging to the resolvent set, the “act of creation” was incomplete on the quantum side: the wave functions (1) have no physical meaning. However, the classical trajectories have: they escape to  $\infty$  either for  $t \rightarrow +\infty$  or  $t \rightarrow -\infty$ , painting the picture of a parametric resonance. Hence, the resolvent set defines the instability regime (escape motions). This explains why the spectral gaps determine the empty spaces in the Saturn rings (Avron and Simon [1]). A tempting question arises: can there be a similar ‘classical portrait’ for the discrete spectrum?

## 2 “Classical point-spectrum”.

Consider again the classical system (2-3), with  $E < 0$  and with  $V(t)$  in form of a limited potential well:

$$V(t) = \begin{cases} \leq 0 & \text{for } a \leq t \leq b \\ = 0 & \text{for } t \leq a \text{ or } t \geq b \end{cases} \quad (5)$$

The corresponding classical Hamiltonian:

$$H(t) = \frac{p^2}{2} + [E - V(t)]q^2 \quad (6)$$

represents a rather simple mechanical system. The classical point is driven by a constant repulsive potential, corrected by an “attractive episode”  $-V(t)q^2$  (see Fig.2). The motion trajectory, in general, diverges either for  $t \rightarrow -\infty$  or  $t \rightarrow +\infty$  (as the result of a constant repulsive term  $Eq^2$ ). For some  $E$ , however, a very special dynamical phenomenon occurs: the trajectory, departing from  $q=0$  at  $t = -\infty$ , by a rare dynamical coincidence, returns asymptotically to 0 for  $t \rightarrow +\infty$ . This phenomenon, extremally unstable, as exceptional as an eclipse, is our classical equivalent of a bound state [ $\psi(x) \rightarrow 0$  for  $x \rightarrow \pm\infty$ ] i.e., the most stable motion form in quantum mechanics!

The “classical portrait”, this time, has no astronomic magnitude: it represents rather a kind of classical sport game. This aspect is specially visible if  $V(t)$  is a sum of  $\delta$ -peaks:  $V(t) = -a_1\delta(t-t_1) - \dots - a_n\delta(t-t_n)$ , with  $a_j > 0$  ( $j = 1, 2, \dots$ ). The classical Hamiltonian:

$$H(t) = \frac{p^2}{2} + Eq^2 + \sum_{j=1}^n a_j\delta(t-t_j)q^2 \quad (7)$$

then describes a point mass in a constant repulsive field, perturbed by a sequence of attractive pulses. Consider now a trajectory departing from  $q=0$  at  $t = -\infty$ . What typically happens when the attractive pulses are over, is that the point must escape either to  $q = -\infty$  or  $q = +\infty$ . Yet, for some exceptional  $E < 0$ , the kicks will provide to the mass point a momentum exactly sufficient to climb asymptotically to 0, against the repulsive forces. When this happens,  $E$  is an eigenvalue of (1). The whole phenomenon resembles a ping-pong game against the repulsive potential. The attractive kicks in (7) are an equivalent of the “ping-pong rocket” and the “goal” of the game is to collocate the point at the very repulsion center!

Note, that the picture permits one to guess the number of the bound states. Thus, e.g., for  $n = 1$  (one kick), there is only one way (modulo proportionality) to return the escaping point to zero. Henceforth, the single  $\delta$ -well has exactly one bound state. For  $n = 2$  (2 kicks), the point can be returned in two (qualitatively different) ways corresponding to two different values of  $E$  and two different bound states. For more peaks, or for continuous  $V(t)$ , the game complicates and to predict results, some geometry elements on the classical phase plane  $\mathcal{P}$  are necessary.

### 3 The bifurcations.

We shall assume below, that  $V(t)$  is a continuous real function, satisfying (5) [the  $\delta$  peaks (7) are included as limiting cases].

One of the oldest observations of quantum mechanics is that the eigenvectors of (1) are a kind of “recurrent phenomenon”, tending to repeat itself as  $E$  grows. This fact can be explained in several ways, but its simplest illustration is obtained in terms of the integral trajectories of (2-3).

Since the evolution equations (2) are linear, the phase point (4) depends linearly on the initial condition:

$$\mathbf{q}(t) = u(t, a)\mathbf{q}(a), \quad (8)$$

where  $u(t, a)$  is a real  $2 \times 2$  symplectic evolution matrix. The canonical equations (2) in terms of (8) read:

$$\frac{du}{dt} = \underbrace{\begin{vmatrix} 0 & 1 \\ -g(t) & 0 \end{vmatrix}}_{\Lambda(t)} u(t) \quad (9)$$

For  $V(t) \equiv 0$  ( $t \leq a$  and  $t \geq b$ ), (2) becomes an equation with constant coefficients which can be explicitly solved:

$$\mathbf{q}(t) = \begin{cases} e^{\Lambda(t-a)}\mathbf{q}(a) & \text{for } t \leq a \\ e^{\Lambda(t-b)}\mathbf{q}(b) & \text{for } t \geq b \end{cases} \quad (10)$$

where  $\Lambda$  is a constant  $2 \times 2$  matrix:

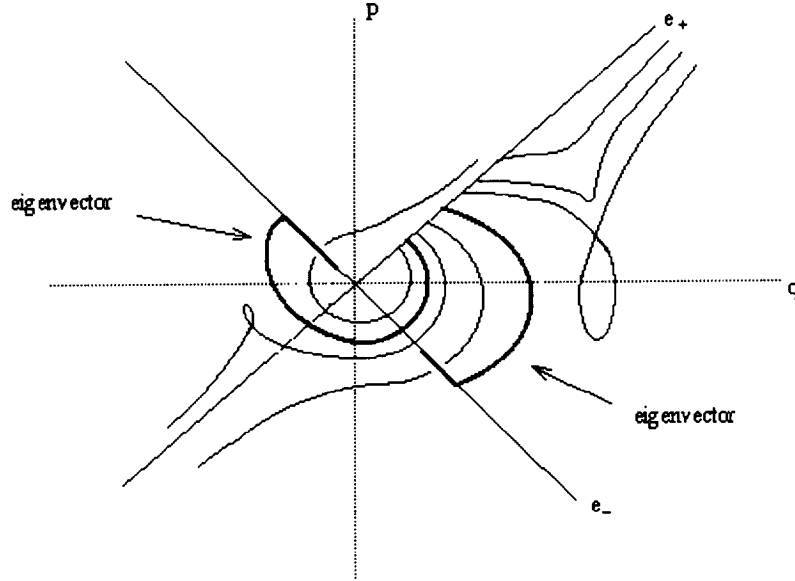
$$\Lambda = \begin{vmatrix} 0 & 1 \\ 2|E| & 0 \end{vmatrix} \quad (11)$$

Note that  $\Lambda$  has a pair of real eigenvalues:

<i>eigenvalues</i>	<i>eigenvectors</i>	
$\lambda_+ = +\sqrt{2 E }$	$\mathbf{e}_+ = \begin{vmatrix} 1 \\ +\sqrt{2 E } \end{vmatrix}$	(12)
$\lambda_- = -\sqrt{2 E }$	$\mathbf{e}_- = \begin{vmatrix} 1 \\ -\sqrt{2 E } \end{vmatrix}$	

Thus, in absence of  $V(t)$  (i.e. for  $t \notin [a, b]$ ), the motion on the phase plane  $\mathcal{P}$  amounts to a continuous squeezing: the direction  $\mathbf{e}_+$  expands while  $\mathbf{e}_-$  exponentially shrinks as  $t \rightarrow +\infty$  (inversely for  $t \rightarrow -\infty$ ). The typical phase trajectory (2) diverges for both  $t \rightarrow \pm\infty$ . However, exceptional cases exist. If  $\mathbf{q}(a) = \text{Const} \times \mathbf{e}_+$ , then  $\mathbf{q}(t)$  vanishes for  $t \rightarrow -\infty$ , and if  $\mathbf{q}(b) = \text{Const} \times \mathbf{e}_-$ , then  $\mathbf{q}(t)$  vanishes for  $t \rightarrow +\infty$ . The number  $E < 0$  is an *eigenvalue* of the Schrödinger's operator, *iff* there exists a canonical trajectory vanishing on both extremes  $t \rightarrow \pm\infty$ . This can happen if and only if the evolution between  $t = a$  and  $t = b$  brings the direction of  $\mathbf{e}_+$  into that of  $\mathbf{e}_-$ , i.e:

$$u(b, a)\mathbf{e}_+ = \text{Const} \times \mathbf{e}_- \quad (13)$$



**Figure 2.** The metamorphosis of the classical trajectory (2-3) for varying  $E$  and fixed  $V(t)$  (qualitative picture). As  $E$  raises to zero from below, the deformation due to the rotating term  $-V(t)q^2$  expands clockwise around the phase space origin, crossing several times the “shrinking axis”  $\mathbf{e}_-(E)$ . At each new intersection a bifurcation occurs, producing a new closed orbit interpretable as an eigenvector of the Schrödinger’s equation (1). The trajectory transformations are pictured in the moving frame of the ‘squeezing axis’ and represent as well the bifurcations which must occur for a fixed  $E < 0$  and variable  $V(t)$ .

To see the ‘recurrent nature’ of the phenomenon, consider an integral trajectory of (2) with  $\mathbf{q}(a) = C\mathbf{e}_+$  (i.e., departing from  $\mathbf{q}(-\infty) = 0$ ) and observe how does it change for varying  $E < 0$ . If  $V(t) \equiv 0$ , the trajectory escapes to infinity along the  $\mathbf{e}_+$  direction. If  $V(t) < 0$  in  $[a, b]$ , the escape is corrected by a rotation around the phase space origin (typically generated by the attractive oscillator Hamiltonians). For  $t > b$ , i.e., when the rotation ceases, the deformation is squeezed back to zero, and the trajectory returns asymptotically to the expanding axis  $\mathbf{e}_+$  (see Fig.2). Now, as  $E$  grows (approaching zero from below), the repulsion (squeezing) becomes weaker and the deformation caused by  $-V(t)q^2$  grows, typically drawing a loop, till  $\mathbf{q}(b)$  touches the  $\mathbf{e}_-$ -axis. When this happens, (13) is fulfilled and the trajectory, instead of escaping to infinity, falls to zero, forming a closed orbit (an

eigenvector of (1) ). As  $E$  still grows (and  $|E|$  decreases) the deformation caused by  $-V(t)q^2$  drives the phase point  $\mathbf{q}(b)$  across the  $\mathbf{e}_-$ -axis and the asymptotic picture suddenly changes: the trajectory escapes to  $\infty$  again, but this time in the direction  $-\mathbf{e}_+$  (not  $+\mathbf{e}_+$ ), meaning the bifurcation (discontinuous change of the asymptotic angle by  $-\pi$ ). If  $E$  still rises (tending to  $E = 0$ ), the deformation expands clockwise around the phase space origin, intersecting several times the shrinking axis  $\mathbf{e}_-$ . Each time this happens, a new bifurcation occurs (a discontinuous change of the asymptotic angle), giving birth to a new closed orbit (next eigenvector) at the exact bifurcation point (Fig.2).

Henceforth, the eigenvalues of (1) are the *bifurcation values* of  $E$  (i.e. the values for which the trajectories of (2) change their asymptotic type). In order to bifurcate, the trajectories must pass through a sequence of exceptional forms (closed orbits): this is why there exist spectra. Can this help to find the spectral values? The difficulty of finding the *bifurcation values*, of course, is the same as that of finding the point spectrum (the analytical sciences are empty!). Yet, an advantage of our model (2-3) is, that it turns attention to some new methods till now neglected.

## 4 The angular Schrödinger equation.

Since the vector norms are irrelevant, our condition (13) can be conveniently written in terms of an *angular coordinate*. Indeed, define:

$$q = \rho \cos \alpha, \quad p = \rho \sin \alpha \quad (14)$$

The canonical equations (2) become:

$$\dot{\rho} \cos \alpha - \dot{\alpha} \rho \sin \alpha = \rho \sin \alpha \quad (15)$$

$$\dot{\rho} \sin \alpha + \dot{\alpha} \rho \cos \alpha = 2[V(t) - E] \rho \cos \alpha \quad (16)$$

where  $\dot{\rho}$  and  $\dot{\alpha}$  mean the time derivatives. Curiously, the equation for the angular variable separates. In fact, multiplying (15) by  $-\sin \alpha$ , (16) by  $\cos \alpha$  and adding one gets the 1-st order differential equation for  $\alpha$  alone:

$$\dot{\alpha} = 2[V(t) - E] \cos^2 \alpha - \sin^2 \alpha \quad (17)$$

while permuting the operations, one arrives at:

$$\frac{\dot{\rho}}{\rho} = [V(t) - E + \frac{1}{2}] \sin 2\alpha \quad (18)$$

The angular equation (17) was found by Drukarev [6] and Franchetti [7] (though without the geometric interpretation) and used to evaluate the phase shifts. Note, that the squeezing directions  $\mathbf{e}_\pm$  too can be defined in terms of the angles:

$$\alpha_\pm(E) = \pm \arctan \sqrt{2|E|} \quad (19)$$

Now, our condition (13) means, that the evolution described by the 1st-order eq.(17) in the time interval  $[a, b]$  should transform the 'expansive direction'  $\alpha(a) = \alpha_+(E)$  into the

'shrinking direction'  $\alpha(b) = \alpha_-(E) + n\pi$  ( $n = 0, 1, 2, \dots$ ). Introducing the *defect angle*  $\Gamma(E)$  as a difference between the 'shrinking angle'  $\alpha_-(E)$  and the final angle  $\alpha(b, E)$  obtained by integrating (17), one can write the spectral condition (13) as:

$$\Gamma(E) = \alpha_-(E) - \alpha(b, E) = n\pi \quad (n = 0, 1, 2, \dots) \quad (20)$$

An immediate generalization of (20) is obtained for  $V(t)$  constant (though not necessarily vanishing) for  $t \notin (a, b)$ :

$$V(t) = \begin{cases} V(a) & \text{for } t \leq a \\ V(b) & \text{for } t \geq b \end{cases} \quad (21)$$

The trajectory (2) has then two constant generators  $\Lambda(a)$  and  $\Lambda(b)$  for  $t \leq a$  and  $t \geq b$  and the formula (20) holds after substituting  $|V(a) - E|$  or  $|V(b) - E|$  instead of  $|E|$  in the expressions (19) for  $\alpha_+$  and  $\alpha_-$  respectively. Two elementary facts make the bifurcation condition (20) specially efficient to determine the eigenvalues:

**Observation 1.** For a fixed  $V(t)$  and  $E < 0$ , the spectral angle  $\Gamma(E)$  is an increasing function of  $E$ . (This is an elementary consequence of the Cauchy equation (17); see also [8]). The monotonicity of  $\Gamma(E)$  permits one to interpolate easily, helping to find the points where  $\Gamma(E)$  intersects the critical values  $\Gamma = n\pi$  ( $n = 0, 1, 2, \dots$ ).

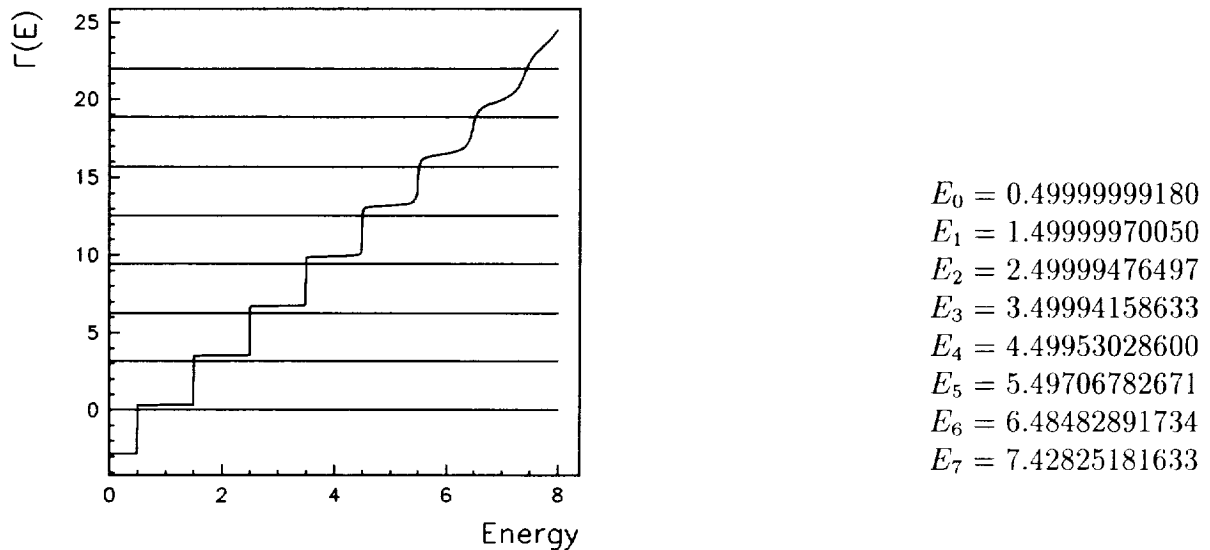
**Observation 2.** The function  $\Gamma(E)$  is unstable and changes very abruptly when crossing the sequence of critical values  $\Gamma = n\pi$  ( $n = 1, 2, \dots$ ) (i.e. when  $E$  crosses spectral points). Thus, even a little error in  $E$  in vicinity of an eigenvalue traduces itself into a visible effect in  $\Gamma$ , improving the accuracy. This instability is caused by the fact that the energy eigenvalues correspond to the orbit bifurcations where the final integration point  $\alpha(b, E)$  deflects fast when  $E$  crosses a bifurcation value. If the integration could yield  $\alpha(+\infty, E)$ ,  $\Gamma(E)$  would be an exact step function (see also the observation in [9, p.274]).

As an example, we have considered the energy levels for the truncated 1-dimensional oscillator potential:

$$V(x) = \begin{cases} \frac{1}{2}\omega^2 x^2 & \text{for } |x| \leq \frac{a}{2} \\ \frac{1}{8}\omega^2 a^2 & \text{for } |x| \geq \frac{a}{2} \end{cases} \quad (22)$$

We have determined the angular function  $\Gamma(E)$ ,  $0 < E < V(\frac{a}{2})$ , for  $w = 1$ ,  $a = 8$  integrating numerically (17) (see Fig.3), and obtaining the 8 energy levels for the oscillator truncated at  $a = 4$ , all calculated with accuracy up to  $10^{-10}$ . The obtained eigenvalues are very close to the first 8 levels of the exact oscillator,  $E_n = n + \frac{1}{2}$  (indeed, even the highest, and last eigenvalue of the truncated potential (22) differs rather little from the orthodox  $E_7 = 7.5$ ).

Note the characteristic shape of  $\Gamma(E)$ , with sharp steps helping to localize the energy eigenvalues! The same spectral problem would be much more troublesome if approached by the conventional perturbation calculus. (Even compared to Ritz method, our algorithm shows some simplicity as there is no need to invent adequate classes of test functions!). Moreover, the same method can be used without difficulty to find the eigenvalues of arbitrarily deformed wells.



**Figure 3.** The defect angle  $\Gamma(E) = \alpha_+ - \alpha(4, E)$ . The intersections of this “stepping” function with the lines  $n \times \pi$  give the eigenvalues of the Schrödinger problem.

The method, till now, concerns the limited potential wells. However, the generalization for unlimited and/or singular wells is already reported (it involves the substitution of the constant angles  $\alpha_{\pm}(E)$  by their variable analogues [5, 8]). The (generalized) spectral function  $\Gamma(E)$  shows the same “step behaviour” permitting to determine spectra with a high accuracy.

It is interesting to notice that all the structure elements which we have introduced were basically known since long time, though very seldom used. Thus, the idea about the classical model of (1) (with  $x$  substituted by  $t$ ) was considered as far back as 1970 (or even earlier; see the discussion in [3]). The angular equation (17) was found by Drukarev [6] and then by Franchetti [7] (though without geometric pictures) and was used to examine the phase shifts. The idea that the *angles* determine the *discrete spectra* is quite old (see e.g. discussions in [10]) though is usually focused on the *phase of the complex wave function*, and mixed up with the WKB approximation. The implications of the classical angle were known to Calogero (see [11, p.82] and [9, p.274]), though Calogero was not interested in the numerical algorithms! The idea that the eigenvalues are bifurcations is as old (though usually contemplated without paying attention to the geometry of  $\mathcal{P}$ , and the role of squeezing in producing the bifurcation).

It seems also worth noticing, that the definition of the *bifurcation* does not require the *linearity* of the evolution equations (2). Hence, the definition of the spectrum via *bifurcations* might be a natural answer to the intriguing problem of how to extend the concept of spectrum to non-linear variants of the Schrödinger’s operator (see, e.g. discussions in [12]). Some work in this direction is being recently carried [13].



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