



Figure 1. Sketch of the potential $V_N = 1/2 \tilde{x}^{2N}$, $\tilde{x} \equiv k^{1/2}x$, for $N = 1, 2, \dots$.

ON THE VALIDITY OF THE BOHR CORRESPONDENCE PRINCIPLE

par Richard L. LIBOFF^{*}

Laboratoire de Physique des Plasmas
Université de Paris-Sud
Centre d'Orsay
91405 ORSAY CEDEX

(manuscrit reçu le 21 Mai 1979)

Abstract : The notions of form and frequency correspondence for periodic systems are examined from the framework of quantization of action-angle variables. Systems with energy spectra which vary as n^α , where α is a finite number and n is quantum number, yield identical energy-frequency relations ("form correspondence") in both the quantum and classical domains in the limit of large quantum number, for all α . However, frequency spectra coalesce ("frequency correspondence") in the two domains, in the high quantum number limit if and only if $\alpha < 1$ (together with $\alpha = 1$ for the harmonic oscillator). Thus, energy spectra which vary as say, n^2 , fail to yield frequency correspondence, whereas for such systems the less physically relevant form correspondence is obeyed. For these cases the limits $\hbar \rightarrow 0$ and $n \rightarrow \infty$ are not equivalent.

Résumé : Les notions de forme et de correspondance en fréquence pour les systèmes périodiques sont examinées dans le formalisme de la quantification des variables angulaires d'action.

^{*}Perminant address : Cornell University, ITHACA, N.Y. 14853

Les systèmes avec un spectre d'énergie en n^α , où α est un nombre fini et n le nombre quantique, produisent des relations énergie-fréquence identiques ("correspondance de forme") dans les domaines quantique et classique considérés dans la limite $n \rightarrow \infty$, pour tout α . Cependant, les spectres se confondent ("correspondance en fréquence") lorsque $n \rightarrow \infty$ si et seulement si $\alpha < 1$ (et aussi $\alpha = 1$ pour l'oscillateur harmonique). Ainsi, le spectre en n^2 , ne donne plus la correspondance en fréquence, alors que la correspondance de forme (moins signifiante physiquement) est encore vérifiée. Dans ces situations, les limites $h \rightarrow 0$ et $n \rightarrow \infty$ ne sont plus équivalentes.

1. Introduction

In a previous work⁽¹⁾, it was established that two configurations fail to satisfy the high quantum number frequency correspondence principle due to Bohr⁽²⁾. This principle asserts that the emitted frequencies of a periodic system pass to the classical spectrum in the limit of large quantum numbers^(3,4). Hereafter we shall refer to this rule simply as the *frequency correspondence principle*. The two counter examples are : 1) A particle in a box with rigid walls and, 2) A rigid rotator. For both systems the quantum frequency spectrum is a discrete sequence separated by a constant interval. The separation frequency h/I , where h is Planck's constant, is independent of quantum number n . The moment of inertia constant I is dependent only on the mass and geometry of the system. Thus as $n \rightarrow \infty$, these spectra fail to collapse to the classical continuum. Whereas the first example is somewhat idealized, the uniformity of rotational spectra of many diatomic molecules in the rigid rotator phase is well established experimentally^(5,6).

In either of the two cases cited, the classical spectrum is obtained in Planck's limit, $h \rightarrow 0$ ⁽⁷⁾. In summary then, passing to the limit of large quantum numbers is *not* the same as passing to the limit of small h .

One also encounters the concept of *form correspondence*⁽¹⁾. This correspondence is obeyed when the form of frequency dependence on energy, $\nu = \nu(H)$, is the same in the quantum and classical prescriptions. Whereas frequency correspondence fails for the cases cited, form correspondence is satisfied in the limit of high quantum numbers. Form correspondence is often mistaken in the literature for frequency correspondence. Only the latter

guarantees the same frequency spectrum in the classical and quantum domains.

The purpose of this paper is to distinguish further between form and frequency correspondence. Specifically, criteria for the domains of validity of these components of the correspondence principle are developed from the formalism of action-angle theory and the Bohr-Sommerfeld quantization rules. Energy spectra asymptotic to n^α are examined, where α is a finite constant and n is an integer. Whereas form correspondence is obeyed for all α , frequency correspondence is satisfied only for $\alpha \leq 1$. Thus, the previously found counter examples of the box and rotator fall outside of the domain of validity for frequency correspondence, since for both these cases $\alpha = 2$. However, both examples satisfy form correspondence.

Also briefly reviewed in this paper is the notion of the classical continuum. It is found that a particle oscillating in the potential x^{2N} has frequency which depends on energy H , as $H^{(N-1)/2N}$. It follows that frequencies other than that of the harmonic oscillator ($N=1$) depend continuously on energy and therefore have a continuous spectrum.

2. Analysis

The frequency of a classical periodic system with one degree of freedom is readily obtained from Hamilton's equation of motion for the angle $\int v dt$,

$$1) \quad \frac{\partial H_C(J)}{\partial J} = \nu,$$

in action-angle variable representation^(8,9). Here H_C is the classical Hamiltonian and J is the action variable

$$2) \quad J = \oint p dq.$$

The coordinate q is conjugate to the momentum p and the integral is over a cycle of the periodic motion. The integral (2) represents an area in phase space. In classical physics this area may be continuously varied by varying the initial conditions.

2.1. Form Correspondence

In quantum mechanics the phase area (2) is restricted to multiples of h as stipulated by the Bohr-Sommerfeld quantization

rule⁽¹⁰⁾

3) $J = nh$

where n is an integer. The analogous formula to (1) in the quantum domain is given by Bohr's equation⁽²⁾,

4) $\frac{\Delta H_Q(J)}{\Delta J} = \nu$

where H_Q is written for the quantum mechanical Hamiltonian. It is apparent that for values of n for which $\Delta H_Q/\Delta J$ approximates the derivative dH_Q/dJ , Bohr's equation (4) will coincide with Hamilton's equation (1). When this coincidence of frequency dependence on energy occurs, form correspondence is satisfied.

To uncover the domain where one may expect this component of correspondence to be found, we examine energy spectra of the form

5) $H_Q = n^\alpha$

where n is an integer and α is a finite constant.

With the Bohr-Sommerfeld quantization rule (3) together with the preceding form (5) we may infer the classical Hamiltonian

6) $H_C = J^\alpha$

Here we are setting all constants equal to unity. The question now to be answered is as follows. For what values of n and α will the difference ration $\Delta H/\Delta n$ approximate a derivate ?

First we note that

7) $\frac{\Delta H_Q}{\Delta n} = \frac{(n+1)^\alpha - n^\alpha}{(n+1) - n} = n^\alpha \left(\left(1 + \frac{1}{n}\right)^\alpha - 1 \right)$

Expanding the bracketed term in the domain of large n gives

$$\frac{\Delta H_Q}{\Delta n} = \alpha n^{\alpha-1}$$

or equivalently,

8) $\frac{\Delta H_Q}{\Delta J} = \alpha J^{\alpha-1}$

With (6) we see that this is identical to the classical derivative

appropriate to Hamilton's equation (1),

9) $\frac{dH_C}{dJ} = \alpha J^{\alpha-1}$

irrespective of the value of α .

So we may conclude that for periodic systems with energy spectra n^α , the quantum frequency dependence on energy reduces to the classical expression, for large n, irrespective of α .

For example, for the case of a particle of mass m in a box of width d, the frequency-energy relation is given by

10.1) $\nu = \sqrt{E/2md^2}$

whereas for a rigid rotator with moment of inertia I,

10.2) $\nu = \frac{1}{\pi} \sqrt{E/2I}$

As is easily verified, these classical relations also emerge in quantum mechanics in the domain of high quantum number.

2.2. Frequency Correspondence

The Classical Continuum

Except for the harmonic oscillator, the frequency of a periodic system may be continuously varied by varying initial conditions. Let us establish the validity of this conjecture for symmetric potential wells. It suffices to consider potentials of the form (see Figure 1).

$$V_N(x) = \frac{k^N}{2} x^{2N}$$

With the substitution

$$x\sqrt{k} \equiv (2H)^{\frac{1}{2N}} \sin \theta$$

one readily obtains the result^(11, 12)

11) $\nu = \frac{dH}{dJ} = g_N^{-1} \sqrt{\frac{k}{m}} H^{\frac{N-1}{2N}}$

where g_N is the pure number

$$g_N = 2^{\frac{N+1}{2N}} \left(\frac{N+1}{2N}\right) \int_0^{\pi/2} \sin^{2N} \theta \cos \theta \sqrt{1 - \sin^{2N} \theta} \, d\theta$$

We may conclude from (11) that ν is energy dependent for all cases except that of the harmonic oscillator, $N=1$. For this case $g_1 = 2\pi$ and (11) yields the well known frequency

$$2\pi\nu = \sqrt{k/m}$$

which is independent of energy. Furthermore from the property that $V_N(k^{-1/2}) = \frac{1}{2}$ for all N , it is evident that $V_N(x)$ approaches a square well with increasing N , and (11) yields, $\nu \sim \sqrt{H}$, in agreement with the forms (10).

For $N \neq 1$, a charged particle oscillating in the potential V_N , radiates at the fundamental frequency (11) and subsequent harmonics. This is readily concluded from the observation that the orbit $x(t)$ is symmetric about $x = 0$ and has period ν^{-1} . Thus, Fourier expansion of $x(t)$ contains the fundamental frequency ν given by (11) together with subsequent harmonics of ν . These frequencies are dependent on initial conditions and yield a continuous spectrum. So in classical physics, periodic systems allow a continuum of frequencies. On the other hand, in quantum mechanics, frequencies are determined by the parameters of the system and *not* by initial conditions.

The Quantum Continuum

For a quantum frequency spectrum to collapse to the classical spectrum, frequencies must grow infinitesimally close and include the low frequency limiting value $\nu = 0$. Again examining the energy spectra (5), with the Bohr postulate for frequency emission we obtain, in the high quantum number domain

$$12) \quad \nu = \Delta H \sim \alpha n^{\alpha-1}.$$

For frequencies to grow close, the incremental change in ν ,

$$13) \quad \Delta\nu \sim \alpha(\alpha-1)n^{\alpha-2},$$

must approach zero. Apart from the case of the harmonic oscillator, $\alpha = 1$, the variation (13) implies that the classical continuum emerges in the high quantum number limit, for $\alpha < 2$. However for $1 < \alpha < 2$ one finds that this continuum is bounded away from $\nu=0$, in which case one cannot classify the frequency spectrum as being classical.

To establish this point consider the energy spectrum

$$H = n^{1+\epsilon}, \quad 0 < \epsilon < 1.$$

Then frequencies due to decay between successive energy levels are

$$14) \quad \nu = (n+1)^{1+\epsilon} - n^{1+\epsilon}.$$

Let us suppose that n is continuous. Then

$$\frac{d\nu}{dn} = (1+\epsilon)((n+1)^\epsilon - n^\epsilon) > 0.$$

If $d\nu/dn$ is positive, then ν as given by (14) is an increasing function of n . It follows that the minimum value of ν corresponds to the decay (for $n > 0$)

$$\nu = 2^{1+\epsilon} - 1^{1+\epsilon} > 0.$$

Therefore, we may conclude that for the energy spectra (5) to yield a continuous frequency spectrum which includes the $\nu=0$ value, one must have $\alpha < 1$. For $0 < \alpha < 1$, energies grow less rapidly with increasing n thereby securing the classical continuum in the limit of large n , whereas for $\alpha < 0$, this agreement in spectra is evident.

Harmonic Oscillator

The value $\alpha=1$ corresponds to the harmonic oscillator. For this configuration, frequency is not set by initial conditions, but rather as indicated previously, by the spring constant k and mass m . The Hamiltonian for this motion is ⁽⁹⁾

$$15) \quad H_C = \nu J.$$

The quantum mechanical Hamiltonian has the same form as (15) with $J = h(n + 1/2)$. This observation together with the selection rule $\Delta n = \pm 1$, indicates that the classical and quantum frequency spectrum agree for all n .

Criterion

Thus we may generalize the above finding to conclude that for the energy spectrum $H_Q = n^\alpha$ to yield the classical continuum of frequencies including $\nu=0$, in the limit of high quantum numbers it is necessary and sufficient that

$$16) \quad \alpha \leq 1.$$

In the aforementioned counter examples we find that for the infinite square well

$$H_Q = n^2$$

whereas for the rigid dumbbell

$$H_Q = n(n+1) \sim n^2.$$

These energy spectra clearly do not obey the criterion (16) and as stated previously, do not yield the classical continuum in the limit of high quantum numbers. Furthermore, the ideal rigidity of these counter examples is not a sufficient property to break the frequency correspondence principle. It may be shown that the ideal rigid walled spherical cavity does, in spite of its ideally impenetrable walls, satisfy all components of the high quantum number correspondence principle⁽¹⁾.

3. Conclusions

Within the framework of action-angle theory and the Bohr-Sommerfeld quantization rules we have examined the domain of validity of form and frequency correspondence for periodic systems. For energy spectra which vary as n^α , form correspondence is obeyed in the limit of large n , for all α . This result is established by examining conditions under which Bohr's equation reduces to Hamilton's equation. Both relations serve to relate frequency to energy. Classical and quantum frequency spectra agree in the limit of high quantum numbers if and only if $\alpha \leq 1$. For other values of α the limits $h \rightarrow 0$ and $n \rightarrow \infty$ are not equivalent.

The fact that the quantum frequency-energy relation $\nu = \nu(E)$ reduces to the classical form in the limit of high quantum numbers merely guarantees that quantum frequencies *fall on this curve*. Form correspondence does not imply that quantum frequencies densely populate the curve, as do the classical frequencies.

Acknowledgements

I am indebted to my colleagues Terrence Fine, Edward Ott, Drew Copeland and Kurt Gottfried for clarifying discussions on these topics.

REFERENCES

- (1) Liboff R., *Found. Phys.* 5, 271 (1975).
- (2) Bohr N., *Fysisk Tidsskrift* 12, 97 (1914).
Bohr N., *Z. Physik* 2, 423 (1920).
- (3) Jammer M., *The Conceptual Development of Quantum Mechanics*, McGraw Hill, New York (1966).
- (4) Waerden B. van der, *Sources of Quantum Mechanics*, Dover, New York (1968).
- (5) Czerny A., *Z. Physik* 34, 227 (1925).
- (6) Herzberg G., *Molecular Spectra and Molecular Structure*, Prentice Hall, New York (1939).
- (7) Planck M., *Vorlesungen über die Theorie der Wärmestrahlung*, Barth, Leipzig (1906).
- (8) Born M., *The Mechanics of the Atom*, G. Bell and Sons, London (1927).
- (9) Goldstein H., *Classical Mechanics*, Addison Wesley, Reading, Mass. (1950).
- (10) Sommerfeld A., *Münchener Berichte*, 425 (1915).
- (11) Haar D. ter, *Selected Problems in Quantum Mechanics*, Academic Press, New York (1964).
- (12) Liboff R., *Int. J. Th. Phys.* 185 (1979).