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Classical and semiclassical theory for the exchange symmetry of identical particles

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Abstract. The primitive semiclassical (EBK) theory of bound states is applied to finite non-relativistic systems with a discrete symmetry, particularly systems of identical particles. The symmetry properties of invariant tori are obtained, and illustrated for simple models with a pair of identical particles, each with one freedom. Examples without and with interaction between the particles, and with vibration and rotation are all considered. Particular care has to be taken with interacting particles that rotate around a ring.

1. Introduction

In recent years there has been a considerable development of the non-relativistic semiclassical theory of bound states, partly due to advances in classical dynamics, and stimulated by experiments on atoms and molecules of high quantum number. Systems of identical particles show the contrast between classical and quantum mechanics particularly clearly, so their semiclassical mechanics requires special treatment.

A proper treatment of identical particles and exchange is needed for a full semiclassical theory of the helium atom. Without this treatment, it is not possible to distinguish between singlet and triplet states, the principal failing of an earlier independent-particle model (Leopold and Percival 1980). However the helium atom is complicated, so this paper deals with relatively simple models, with a view to later extension to helium and other systems.

We concentrate on the problem of bound states and energy spectra of non-relativistic systems without spin, treating them as examples of systems where dynamics is invariant under a discrete symmetry group. The simple case of two identical particles of one freedom is treated in detail to illustrate the major features of more complicated systems.

We use the zero-order semiclassical theory of Einstein, Brillouin and Keller (EBK) and Maslov, that relates the bound states of quantum mechanics to the invariant tori of classical mechanics using quantised action integrals and Maslov indices (Maslov 1972). It is the modern corrected version of Bohr–Sommerfeld quantisation and is described with the notation of this paper in a review (Percival 1977, denoted I).

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In § 2 we introduce the relevant parts of the classical dynamics of systems with many degrees of freedom, in particular the theory of invariant tori. These are then classified for systems with a discrete symmetry group.

In § 3 we give a brief account of the canonical action and Maslov indices of these systems. Greater detail is provided by I. In § 4 we treat some very simple systems of identical particles in detail. Not all of these systems are bound. It is shown that the interaction between particles introduces new types of motion for which the symmetry properties are different than for non-interacting particles.

Section 5 contains the theory of two free particles on a ring, which presents some special problems. In § 6 the particles are allowed to interact, so that we have a simple model of the hindered rotation of two identical particles. The semiclassical theory with sinusoidal interaction is treated in detail semiclassically and quantally. As expected, the symmetry classification agrees for the two treatments, but its subtlety was not expected. The semiclassical energy levels are in reasonable agreement except near the separatrix, where uniformisation methods would be needed (Berry and Mount 1972, Child 1974). When the particles rotate relative to one another the simple semiclassical theory gives degenerate states, whose degeneracy is broken in quantum mechanics by barrier penetration. This also requires uniformisation for a semiclassical treatment.

As discussed in detail in I, and briefly in § 2, bounded classical motion can be regular or irregular, and for most systems of more than one freedom both are significant. We have considered only the regular motion. The semiclassical theory of irregular motion has recently been treated using periodic orbits instead of invariant tori by Berry (1981) and Gutzwiller (1980).

We do not yet know how to deal with discrete symmetries for irregular motion.

2. Discrete symmetry of classical motion

The classical state of a conservative system of one freedom with coordinate q and momentum p is represented by a phase point $X = (q, p)$ in the two-dimensional phase space. If for a particular motion the initial state of the system at $t = 0$ is $X^0 = (q^0, p^0)$ and

$$X(t) = (q(t), p(t)) \quad (X(0) = X^0) \quad (2.1)$$

represents the subsequent motion, then the function $X(t)$ may be considered as a parametric representation of the phase curve of the motion with the time t as the parameter. Clearly $(q(t), p(t))$ must be solutions of Hamilton's equations of motion.

We denote by $U(\tau)$ the evolution operator that turns a state at time t into the state at time $t + \tau$, so that for the above motion

$$U(\tau)X(t) = X(t + \tau) \quad (2.2)$$

and in general $U(t)X^0$ represents the motion with X^0 as initial condition, or the phase curve through X^0 .

Almost all the phase curves of bound conservative systems of one freedom are closed, and in the EBK theory of semiclassical quantisation a countable set of these closed phase curves correspond to the stationary quantal states as discussed in § 3.

The phase curve of a separable bound system of two degrees of freedom is not normally closed, and does not correspond to a quantal state. However, usually each phase curve occupies a two-dimensional region of the four-dimensional phase space,

known because of its shape as an invariant torus, and a countable set of these invariant tori do correspond to the quantal states.

If q_1, q_2 are separation coordinates and p_1, p_2 their conjugate momenta, then

$$X \equiv (X_1, X_2) \equiv (q_1, q_2, p_1, p_2) \tag{2.3}$$

is a phase point, representing a classical state of the system. X_1 and X_2 represent the states of subsystems, at least formally. Evidently X_1 and X_2 lie on phase curves of the subsystems if and only if X lies on an invariant torus of the whole system. The torus is a direct product of the invariant curves in a topological sense. Almost all the phase space is occupied by invariant tori.

For non-integrable systems some of the phase space may be occupied by invariant tori, though not always. The regions of phase space so occupied are known as regular regions (I) in contrast to the remaining irregular regions where the motion is chaotic and we do not attempt to quantise. The invariant tori of non-integrable systems have a similar shape to those of integrable systems, but they are not related to any phase curves of separated systems. The generalisation of invariant tori to systems of N freedoms is not difficult.

For a system of one freedom, if X^0 is any point on a closed phase curve, then the entire phase curve is traced out by the motion with X^0 as initial condition. Thus the invariant curve is defined uniquely by any phase point on it.

For systems of more freedom, a phase curve cannot occupy the whole of an invariant torus, as they are of different dimension, but normally a phase curve that lies in a torus approaches arbitrarily close to any point of it, an ergodic property. If this is true for any phase curve of an invariant torus, it holds for all of them and the torus is the closure of any one of its phase curves. Such a torus is defined uniquely by any one of its phase points and is known as a proper torus. For most systems almost all invariant tori are proper tori.

We can use this property to classify the proper tori of a system with a symmetric Hamiltonian $H(X)$. Suppose the Hamiltonian is unchanged by a discrete group G of M transformations g_i of the phase points. If $g_i X$ is the transformation of the phase point X , then we have

$$H(g_i X) = H(X) \quad (i = 1, \dots, M). \tag{2.4}$$

For if G is the permutation group of two identical particles, then it has only two elements, the identity, and the exchange operator e_{12} that interchanges the coordinates and momenta of the two particles. In that case

$$e_{12}(X_1, X_2) = (X_2, X_1) \tag{2.5}$$

and for the particles to be identical the Hamiltonian must be invariant under this exchange.

But this is a very special case. In general if t_A is an invariant torus of the system with Hamiltonian (2.4), then we write $g_i t_A$ for the torus made up of all the phase points $g_i X$ with X in t_A . From its definition $g_i t_A$ is congruent to t_A and we would expect it to be an invariant torus, as we now show.

If X^0 is in $g_i t_A$, then $g_i^{-1} X^0$ is in t_A , and since t_A is invariant $U(t) g_i^{-1} X^0$ is in t_A . But the Hamiltonian is invariant under the transformation g_i^{-1} , so the evolution operator $U(t)$ is also invariant under g_i^{-1} . It follows that for all X, g_i and t

$$U(t) g_i^{-1} X = g_i^{-1} U(t) X. \tag{2.6}$$

Thus $g_i^{-1}U(t)X^0$ is in T_A and $U(t)X^0$ is in g_iT_A , given our initial assumption. This shows that the phase curve through any point of g_iT_A lies in g_iT_A , which is therefore an invariant torus. The analogy with the stationary states of a quantal system with a discrete symmetry is clear.

The congruent invariant torus g_iT_A may or may not be the same as T_A . The group elements that leave an invariant torus T_A unchanged form a subgroup G' of G whose M' elements we denote by g'_j . The remaining elements of G produce distinct invariant tori congruent to T_A , making M/M' distinct tori altogether. Such sets of congruent tori are used in the semiclassical quantisation of systems with discrete symmetry. The intrinsic properties of all the congruent tori are the same, as we now demonstrate for action integrals.

Consider any closed curve \mathcal{C}_A which lies in the invariant torus T_A and which need not have any connection with motion on the torus. Suppose that it is represented parametrically by the function

$$X(s) = (q(s), p(s)) \quad (0 \leq s \leq 1). \tag{2.7}$$

Note that s ranges over the unit interval. This corresponds to a closed curve \mathcal{C}_B which lies in the invariant torus $T_B = g_iT_A$ and is represented parametrically by the function

$$g_iX(s) = (g_iq(s), g_ip(s)) \quad (0 \leq s \leq 1). \tag{2.8}$$

The action integral $I(\mathcal{C}_B)$ for the curve \mathcal{C}_B is defined by

$$\begin{aligned} 2\pi I(\mathcal{C}_B) &= \int_0^1 (g_ip(s)) \left(g_i \frac{dq(s)}{ds} \right) ds \\ &= g_i \int_0^1 p(s) \frac{dq(s)}{ds} ds \\ &= \int_0^1 p(s) \frac{dq(s)}{ds} ds = 2\pi I(\mathcal{C}_A). \end{aligned} \tag{2.9}$$

Now consider a torus T_A that is invariant under the evolution $U(t)$ and the elements g_j of a discrete symmetry group G . Let X^0 be a phase point of T_A and g_j an element of G of order R , so that g_j^R is the identity.

Then the set of points

$$g_j^r X^0 \equiv X^r \quad (r = 0, 1, \dots, R - 1) \tag{2.10}$$

lie on T_A and are invariant under the symmetry operation g_j .

For this case first consider a curve \mathcal{D}_0 joining X^0 and X^1 , which lies in the invariant torus T_A and which need not have any connection with motion on the torus. The curve \mathcal{D}_0 is clearly not closed, but we shall soon show how to construct a closed curve from it.

Suppose \mathcal{D}_0 is represented parametrically by the function

$$Y(s) \quad (0 \leq s \leq R^{-1}, Y(0) = X^0, Y(R^{-1}) = X^1). \tag{2.11}$$

Note that s ranges over the interval $[0, R^{-1}]$.

Then for every integer r with $0 \leq r \leq R - 1$ we can define a curve \mathcal{D}_r which is represented parametrically by the function

$$g_j^r Y(s) \quad (r/R \leq s \leq (r + 1)/R). \tag{2.12}$$

The curve \mathcal{D}_r has end points X^r and X^{r+1} , where $X^R = X^0$, so if we define the function

$$X(s) = g_j^r Y(s) \quad (r/R \leq s \leq (r+1)/R, r = 0, 1, \dots, R-1), \quad (2.13)$$

then the values of s in $[0, 1]$ define the closed curve \mathcal{C} obtained by joining all R of the \mathcal{D}_r together in a necklace, as illustrated in figure 1.

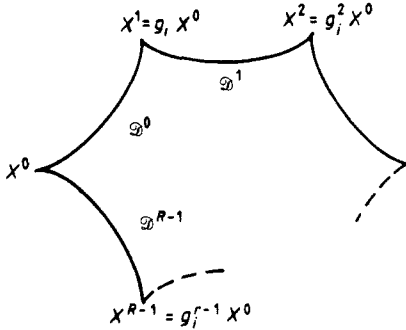


Figure 1. Phase points and phase curves on a symmetric invariant torus.

The canonical action for the closed curve \mathcal{C} is given by

$$\begin{aligned} I(\mathcal{C}) &= \frac{1}{2\pi} \int_{\mathcal{C}} p \, dq = \frac{1}{2\pi} \sum_{r=0}^{R-1} \int_{\mathcal{D}_r} p \, dq = R \frac{1}{2\pi} \int_{\mathcal{D}_0} p \, dq \\ &= RI(\mathcal{D}_0). \end{aligned} \quad (2.14)$$

The action integral from X^0 to $X^1 = g_1 X^0$ is R^{-1} times a canonical action for a closed curve on the torus. Since the canonical action for closed curves is constrained by quantisation conditions, this puts constraints on the action integrals between equivalent points on a symmetric torus.

The exchange symmetry of two identical particles is a particularly simple case. If T_A is an invariant torus of the two-particle system and $e_{12} T_A = T_A$, then T_A is named an exchange torus.

If T_B is a proper torus of the system, but is not an exchange torus, then T_B and $T_C = e_{12} T_B$ are distinct tori congruent under exchange.

For an exchange torus the action for a curve between two exchange points X and $e_{12} X$ is one half of a canonical action on the torus, and will be named a semi-action. Similarly the Maslov index will be named a semi-index.

3. Canonical action and Maslov index

We illustrate the EBK theory by the example of the oscillator, following I. The theory is based on the properties of those action functions that are solutions of the time-independent Hamilton–Jacobi (HJ) equation, supplemented by the Maslov index function. This index function depends on the topology of the motion and accounts for the behaviour of the system at turning points.

Consider a one-dimensional oscillator with Hamiltonian $H(q, p)$. To fix ideas we can suppose that $H(q, p)$ has the form

$$H(q, p) = V(q) + p^2/2m. \tag{3.1}$$

The motion may be represented by a curve in phase space like that illustrated in figure 2.

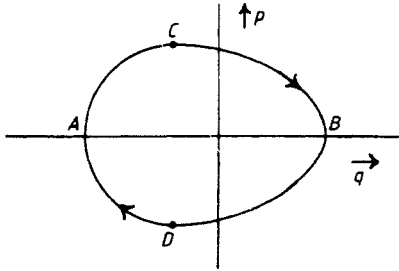


Figure 2. Phase space diagram of an oscillator.

The equations of motion in phase space are Hamilton's equations

$$\dot{q} = \partial H/\partial p, \quad \dot{p} = -\partial H/\partial q. \tag{3.2}$$

They implicitly define p as a two-valued function of q . The two values lie on different sheets analogous to the Riemann sheets of complex variable theory. They are joined at the turning points A and B of the phase curve, which we name the q -turning points. At these points p is a singular function of q and dp/dq becomes infinite.

The points $X = (q, p)$ on the phase curve are also two-valued functions of q . However, we may also consider the points X on the phase curve as functions of p , and these are also two-valued. The corresponding p -sheets are joined at the p -turning points C and D , where q is a singular function of p and dq/dp becomes infinite.

In q -representation the phase curve may be considered as the graph of p as a two-valued function of q , with ACB and ADB as the two sheets of this function. In p -representation the phase curve is the graph of q as a function of p , with two sheets CAD and CBD .

In q -representation the time-independent HJ equation for the action function $S(q)$ is

$$H(q, dS/dq) - E = 0, \tag{3.3}$$

where E is the energy. In the language of the textbooks, $S(q)$ is the characteristic function. For a given energy E , a solution of the HJ equation (3.3) defines part of a phase curve, made up of points $(q, dS/dq)$. But the equation can only be used to define the q -sheet, between the turning points A and B .

By the theory of canonical transformations the action function $\bar{S}(p)$ in momentum representation, defined on the phase curve as

$$\bar{S}(p) = S(q) - pq, \quad p = dS/dq, \tag{3.4}$$

satisfies the HJ equation

$$H(-d\bar{S}/dp, p) - E = 0 \tag{3.5}$$

everywhere on ACB except the point C . However, this equation may be used to continue $\bar{S}(p)$ into the complete p -sheet CBD , past the turning point at B , and the

relation (3.4) can then be used to define $S(q)$ in the segment BD of the second q -sheet. Continuation around the phase curve can be completed by successive transformations between q - and p -representation.

It is often convenient to use the point $X = (q, p)$ on the phase curve as the independent variable, so that

$$S_q(X) = S(q), \quad S_p(X) = \bar{S}(p), \quad (3.6)$$

where the suffixes q and p are not variables but labels for the representations. The phase points distinguish automatically between the sheets.

When the phase point X passes once around the phase curve in a negative (clockwise) sense, then either action function $S_q(X)$ or $S_p(X)$ gains an increment $[S]$. We use this to define the action integral or canonical action

$$I = \frac{1}{2\pi}[S] = \frac{1}{2\pi} \oint p \, dq. \quad (3.7)$$

For semiclassical quantisation the canonical action is not enough. We also need the Maslov index. This is obtained from the index function, which keeps a record of the singularities. Like the action function, the index function $\sigma_q(X)$ or $\sigma_p(X)$ depends on the representation, and is many-valued. It is defined up to an additive integer constant by the properties

$$\sigma_q(X) \text{ is an integer constant on any } q\text{-sheet}, \quad (3.8a)$$

$$\sigma_p(X) \text{ is an integer constant on any } p\text{-sheet}, \quad (3.8b)$$

$$\sigma_p(X) = \sigma_q(X) - \text{sgn}(dp/dq), \quad (3.8c)$$

where $\text{sgn}(dp/dq)$ is the sign of the slope of the phase curve at the point X .

We define the canonical Maslov index α in terms of $\sigma(X)$ by the relation

$$\alpha = [\sigma]/2 \quad (3.9)$$

where $[\sigma]$ is the increment of either σ_q or σ_p in one clockwise cycle of the phase curve. Using these relations, we find that for the oscillator of figure 2, $\alpha = 2$ and this is true for any oscillator. However for rotational motion there are no q -turning points and $\alpha = 0$.

In q -representation the EBK semiclassical wavefunction on the phase curve is defined by the equation

$$\psi_q(q, p) = \psi_q(X) = B_q(X) \exp[i\eta_q(X)], \quad (3.10)$$

where the phase function is

$$\eta(X) = S(X)/\hbar - \sigma(X)\pi/4 \quad (3.11)$$

and $B_q(X)$ is a positive amplitude factor.

The wavefunction for a particular value of q is given by

$$\psi(q) = \sum_p \psi_q(q, p), \quad (3.12)$$

where the sum is taken over those values of p for which (q, p) lies on the phase curve. If there is no such value, so that the motion never reaches q , then the sum is zero. This wavefunction satisfies the Schrödinger equation to zero order in \hbar except for the q -turning points. These are treated by transforming to p -representation, by analogy with the classical theory of § 3. The details are given in I.

The function $\eta_q(X)$ is not single-valued on the phase curve, but the wavefunction (3.10) is single-valued, so the increment in $\eta_q(X)$ around the phase curve must be a multiple of 2π , that is

$$[\eta_q(X)] = 2\pi n \quad (n = 0, \pm 1, \pm 2, \dots) \quad (3.13)$$

or

$$I = (n + \alpha/4)\hbar \quad (n = 0, \pm 1, \pm 2, \dots) \quad (3.14)$$

where

$$\alpha = 0 \text{ for rotation} \quad \text{and} \quad \alpha = 2 \text{ for vibration.} \quad (3.15)$$

This is the EBK quantisation condition for a single invariant torus of a system with one freedom.

For a system of N freedoms there is one such quantisation condition for each of the canonical actions I_k belonging to each of N independent closed curves \mathcal{C}_k on the invariant tori.

For systems with discrete symmetry the quantisation depends on the congruent invariant tori. Because they are congruent their quantisation conditions are identical and their semiclassical wavefunctions degenerate. If the number of congruent tori is equal to the number of elements of the symmetry group, then the semiclassical theory is formally no different from the quantum theory, symmetric wavefunctions being formed from linear combinations of the semiclassical wavefunctions of the congruent tori. There is nothing new for the primitive semiclassical theory.

However, if the number of congruent tori is less than this, the tori themselves possess a discrete symmetry and there are new features which are illustrated by examples in the next sections.

4. Semiclassical exchange for simple systems

We investigate some very simple systems of two identical particles with one freedom each. All of them are separable, but not all of them are bound, so instead of tori we sometimes have invariant planes or cylinders.

Our first system S1 consists of two identical non-interacting free particles 1 and 2, each moving in one space dimension, labelled q_j . The momentum P_j of each particle is conserved, and the action function $\tilde{S}(p_1, p_2)$ is singular. In q -representation the action function is

$$S(q_1, q_2) = P_1 q_1 + P_2 q_2, \quad (4.1)$$

corresponding to the invariant plane $p_1 = P_1$, $p_2 = P_2$ in the four-dimensional phase space. There are no turning points so the index function can be taken as zero.

A phase point $X = (q_1, q_2, P_1, P_2)$ is exchange equivalent to the point

$$e_{12}X = (q_2 q_1 P_2 P_1). \quad (4.2)$$

If $P_1 \neq P_2$ this lies on a different invariant plane. These classically distinct invariant planes are indistinguishable in quantum and semiclassical mechanics. The resulting degeneracy is removed in semiclassical mechanics as it is in quantum mechanics by the condition

$$\psi(q_1, q_2) = \pm e_{12} \psi(q_1, q_2) = \pm \psi(q_2, q_1), \quad (4.3)$$

for bosons and fermions respectively, leading to the wavefunction

$$\psi(q_1, q_2) = B\{\exp[(i/\hbar)(P_1q_1 + P_2q_2)] \pm \exp[(i/\hbar)(P_1q_2 + P_2q_1)]\}, \quad (4.4)$$

where B is a normalising factor. However for $P_1 = P_2$ there is a single invariant plane and $S(q_1, q_2) = S(q_2, q_1)$. The fermion state does not exist, leading to the Pauli exclusion principle for this degenerate case. For this example the probability that $P_1 = P_2$ is negligible, but this is not so for the next example.

The system S2 consists of two non-interacting particles in a potential well $V(q)$. In that case the phase curve for an individual particle has two q -sheets, labelled u for the upper sheet and l for the lower sheet. Following the prescription of § 2, the action functions for the particle 1 in q -representation are

$$\begin{aligned} S_u(q_1) &= (2m)^{1/2} \int_{q_-}^{q_1} dq (E_1 - V(q))^{1/2} & (q_- \leq q_1 \leq q_+) \\ S_l(q_1) &= S_u(q_+) - (2m)^{1/2} \int_{q_+}^{q_1} dq (E_1 - V(q))^{1/2} & (q_- \leq q_1 \leq q_+) \end{aligned} \quad (4.5)$$

and the index functions are

$$\sigma_u(q_1) = 0, \quad \sigma_l(q_1) = 2, \quad (4.6)$$

where q_{\pm} are the turning points. Taking into account the discontinuity in $\sigma(q_1)$ at q_- , the canonical action and index are

$$I_1 = \frac{(2m)^{1/2}}{\pi} \int_{q_-}^{q_+} dq (E_1 - V(q))^{1/2}, \quad \alpha_1 = 2. \quad (4.7)$$

The single-particle semiclassical wavefunction can be constructed only when the quantisation condition

$$I_1 = (n_1 + \frac{1}{2})\hbar \quad (4.8)$$

is satisfied. It is the normalised sum of the wavefunctions for the upper and lower sheets

$$\psi_1(q_1) = \psi_{u1}(q_1) + \psi_{l1}(q_1) = B_{u1}(q_1) \exp[i\eta_{u1}(q_1)] + B_{l1}(q_1) \exp[i\eta_{l1}(q_1)]. \quad (4.9)$$

For the two particles, the separated phase curves of the individual particles may or may not have the same canonical action. If they do not, $I_1 \neq I_2$ and the exchange operator produces a distinct congruent invariant torus. The symmetric and antisymmetric wavefunctions are formed from combinations of the semiclassical wavefunctions of the two congruent tori in the usual way.

If $I_1 = I_2$, then we have an exchange torus. This is represented in figure 3 in the separated phase spaces of the individual particles and on the θ_1, θ_2 plane of the angle variables. In this plane the torus is represented repeatedly by a square mesh of side 2π . The illustrated phase points A and B are exchange equivalent. The points B and B' are equivalent both classically and semiclassically. It can be seen from the figure that the operation e_{12} of exchange corresponds to a reflection in any of the diagonal dotted lines of figure 3. Illustrated also is the curve \mathcal{D}_0 joining A to B and the curve $e_{12}\mathcal{D}_0 = \mathcal{D}_1$ joining B to A . The combined closed curve \mathcal{C} can be deformed to a point, so the action integrals

$$I(\mathcal{C}) = I(\mathcal{D}_0) = 0, \quad (4.10)$$

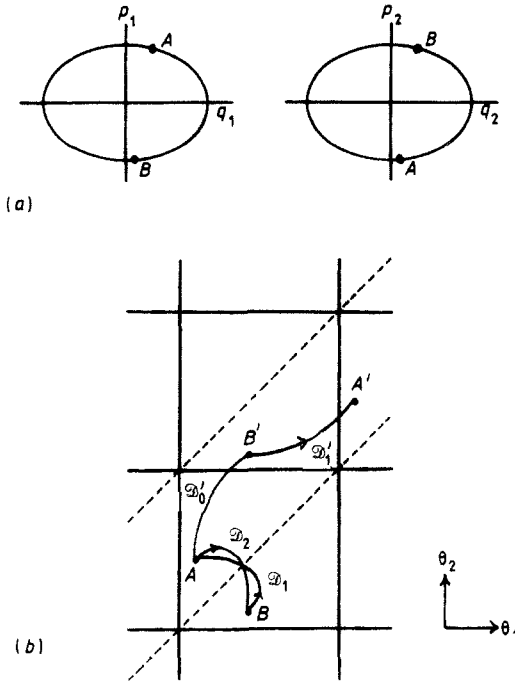


Figure 3. An exchange torus for two non-interacting oscillators: (a) representation in phase space, (b) representation in angle space.

where we have used the relation (2.14) to show that the semi-action $I(\mathcal{D}_0)$ is zero. Similarly the semi-index must be zero.

But when the semi-action and the semi-index are zero the semiclassical wavefunction is unchanged by the exchange e_{12} and cannot represent two fermions. This is the semiclassical statement of the exclusion principle for two particles.

For the curve \mathcal{D}'_0 joining A to B' we come to the same conclusion by a slightly different route. The curve $\mathcal{D}'_1 = e_{12}\mathcal{D}'_0$ joins B' to A' , so \mathcal{C} joins A to A' . The action $I(\mathcal{C})$ is not zero, but we see by inspection that $I(\mathcal{C}) = I_1 + I_2 = 2I_1$ because the separated phase curves are identical. Consequently the semi-action $I(\mathcal{D}'_0)$ is equal to I_1 and must be a multiple of 2π . The semiclassical wavefunction is unchanged by exchange and fermion states are excluded.

It might be thought that an exchange torus could never represent a state of two fermions, but that is not so if the particles can interact.

We give an example S3 in which they are bound by the potential

$$W(q_1, q_2) = \frac{1}{2}a(q_1 + q_2)^2 + V(|q_1 - q_2|). \tag{4.11}$$

This system is separable in centre-of-mass coordinates

$$Q = (q_1 + q_2)/2, \quad q = q_1 - q_2. \tag{4.12}$$

The centre of mass itself is a linear oscillator and is unaffected by exchange. All the properties of exchange appear in the relative coordinate and momentum, whose phase space is illustrated in figure 4.

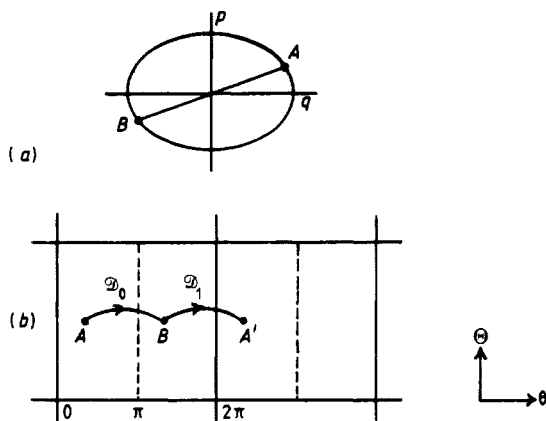


Figure 4. Exchange torus for interacting oscillators: (a) phase curve for relative coordinate, (b) representation in angle plane.

The exchange of particles corresponds to a change in the sign of both q and its conjugate momentum p , so the point B on the opposite side of the symmetric phase curve is exchange equivalent to A . All invariant tori are exchange tori. If θ, Θ are the angle variables corresponding to the relative and centre-of-mass motion, and θ_A, Θ_A and θ_B, Θ_B are the angle variables of the phase points A and $B = e_{12}A$ on an exchange torus, then

$$\theta_B = \theta_A \pm \pi, \quad \Theta_B = \Theta_A. \tag{4.13}$$

As will be seen from inspection of figure 4, the operation of exchange corresponds to a *translation* in the angle plane and not a reflection as in the previous case. As a result of the phase curve \mathcal{C} , made up of \mathcal{D}_0 joining A to B , and $\mathcal{D}_1 = e_{12}\mathcal{D}_0$ joining B to A , completes a cycle of the torus, and the semi-action is simply half the action integral of relative motion. Similarly for the semi-index so the phase

$$[\eta]_{\mathcal{D}_0} = \frac{1}{2}[\eta]_{\mathcal{C}}. \tag{4.14}$$

But

$$[\eta]_{\mathcal{C}} = 2\pi\nu, \tag{4.15}$$

so the phase change under exchange is $\pi\nu$, the sign of the semiclassical wavefunction remains the same for ν even, and it changes when ν is odd. The tori correspond to boson and fermion states respectively. This is consistent with the alternation of boson and fermion states in quantum theory.

Notice that in going from non-interacting to interacting particles there is no smooth transition in the behaviour under exchange. The changed topology of the motion changes the topology of the map from q, p representation to θ, I representation, so the effect of exchange is completely different. This also occurs for the more subtle case of two particles on a ring, as in § 5.

5. Two free particles on a ring

In § 4 we dealt with the simplest cases of vibration. In this section we consider two identical particles on a ring, the simplest case of rotation. Because of its simplicity it is

degenerate, and we can separate in either individual particle or relative motion coordinates, leading to different sets of invariant tori in either case. The relative motion coordinates lead to special problems that require careful consideration.

Suppose the ring is circular, and that φ_1 and φ_2 are the angular coordinates of the particles. If p_1 and p_2 are the conjugate momenta, then the Hamiltonian has the form

$$H(\varphi_1, \varphi_2, p_1, p_2) = (1/2m)(p_1^2 + p_2^2). \tag{5.1}$$

These are the individual particle coordinates, and because of the especially simple form of the Hamiltonian the physical angles φ_i are the same as the angle variables θ_i and their conjugate momenta p_i are the action variables I_i . The angle space (θ_1, θ_2) is the same as the configuration space (φ_1, φ_2) . We find it convenient, because of the subtleties associated with the change to relative motion coordinates, to consider the whole (φ_1, φ_2) plane, so that each configuration is represented any number of times on a square mesh of side 2π in the (φ_1, φ_2) plane. The points

$$(\varphi_1 + 2\pi\nu_1, \varphi_2 + 2\pi\nu_2) \quad (\nu_1, \nu_2 = 0, \pm 1, 2, \dots) \tag{5.2}$$

are classically equivalent to one another, since they represent the same configuration. This also applies to the angle plane. The points

$$(\theta_1 + 2\pi\nu_1, \theta_2 + 2\pi\nu_2) \quad (\nu_1, \nu_2 = 0, \pm 1, \pm 2, \dots) \tag{5.3}$$

are classically equivalent as they represent the same point on an invariant torus. For the special example of free particles on a ring (5.2) and (5.3) are equivalent, but in general they are not, and we need both relations.

In (φ_1, φ_2) representation the action function for an invariant torus with values of the action variables given by I_1^0, I_2^0 is

$$S(\varphi_1, \varphi_2) = I_1^0 \varphi_1 + I_2^0 \varphi_2. \tag{5.4}$$

It is this action function that determines the semiclassical phase and thus the quantisation of this system. There are no turning points so that the Maslov index is zero, and the quantisation gives $I_j = n_j \hbar$.

In figure 5(a) we illustrate the positions φ_1 and φ_2 of the two particles on the ring, and in 5(b) we illustrate the configuration space, which is the same as the angle space.

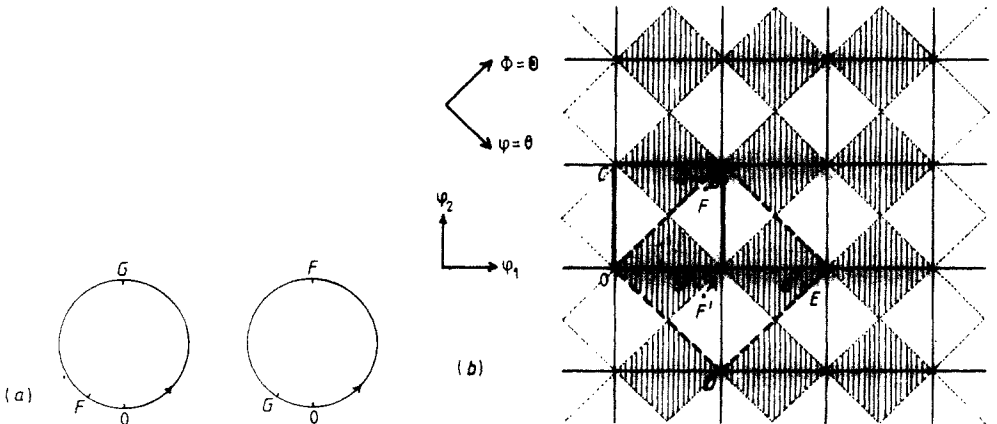


Figure 5. (a) Non-interacting particles on a ring and (b) the configuration and angle space.

The fundamental square $OABC$ of side 2π represents an invariant torus, and is repeated over the plane. The origin is at O . Horizontal or vertical translation by a multiple of 2π leaves the classical state unchanged.

Also illustrated is the fundamental square $ODEB$ for the coordinates

$$\varphi = (\varphi_1 - \varphi_2)/2, \quad \Phi = (\varphi_1 + \varphi_2)/2, \quad (5.5)$$

of relative motion.

The motion is separable in these coordinates, but the new fundamental square is twice as big as the old one. It contains two representations of each configuration instead of the standard one. For example F and F' are in the same fundamental square $ODEB$ of relative coordinates, but they represent the same configuration. The same applies to the points G' and G'' . They are classically equivalent. For this reason we refer to the (φ, Φ) representation as a *double* representation. Some aspects of this representation are considered by Born (1927, p 266).

We are now ready to consider some of the problems of exchange for this system. Two classical states that are obtained from one another by interchanging identical particles are said to be exchange equivalent. In our configuration space of figure 5(b) the effect of exchange is represented by interchanging φ_1 and φ_2 , or by changing the sign of the relative coordinate φ and leaving Φ unchanged. This corresponds to reflection in a diagonal through the origin, or any parallel diagonal through a point that is classically equivalent to the origin.

In figure 5(b) we have divided the (φ, Φ) space into a black and white chessboard, with four squares of the chessboard in the fundamental square of the (φ, Φ) representation. Corresponding points in white squares, like F and F' , are classically equivalent, as are corresponding points in black squares, like G' and G'' . However the points F and G are in different coloured squares and they are exchange equivalent, so all the points F, F', G', G'', G must be exchange equivalent, and quantally indistinguishable.

By the periodicity, all white squares are classically equivalent to one another, and so are all black squares. In (φ, Φ) coordinates all points

$$(\varphi + \mu\pi, \Phi + \nu\pi) \quad (\mu + \nu \text{ even}) \quad (5.6)$$

are classically equivalent for integer μ and ν . All points

$$(\pm\varphi + \mu\pi, \Phi + \nu\pi) \quad (\mu + \nu \text{ even}) \quad (5.7)$$

like F and G are exchange equivalent, and all black and white chessboard squares are exchange equivalent. They are indistinguishable in quantum mechanics.

We notice that in the angle space (θ_1, θ_2) we can use *relative* angle coordinates $\theta = \varphi, \Theta = \Phi$, but these are *not* standard angle variables, because the fundamental square contains two representations of each classical state, which is not normally allowed. We refer to them as *scaled* angle variables. The same difficulty occurs even when we introduce interactions and the angle variables (θ, Θ) are no longer the same as the physical angles (φ, Φ) .

We now consider the problem of semiclassical quantisation in the double representation, and denote the action variables conjugate to (θ, Θ) by (I_-, I_+) , where by the Poisson bracket relations for conjugate variables

$$I_- = p_1 - p_2, \quad I_+ = p_1 + p_2, \quad (5.8)$$

and the Hamiltonian function is

$$H(I_-, I_+) = (1/4m)(I_-^2 + I_+^2). \quad (5.9)$$

When the motion is separated in these coordinates the action function

$$S(\varphi, \Phi) = I'_- \varphi + I'_+ \Phi \quad (5.10)$$

satisfies the HJ equation for fixed values of I'_- , I'_+ . The invariant torus $T(I'_-, I'_+)$ with this action function is defined by the equations $I_- = I'_-$, $I_+ = I'_+$ in the $(\varphi, \Phi, I_-, I_+)$ coordinates of the phase space. The Maslov index is zero.

For the quantisation conditions we must take care because of the double representation of classical states within the fundamental square. In order that the wavefunction should be single-valued we have

$$\psi(\varphi, \Phi) = \psi(\varphi + 2\pi, \Phi) = \psi(\varphi, \Phi + 2\pi) = \psi(\varphi + \pi, \Phi + \pi). \quad (5.11)$$

The third equality is a consequence of the double representation.

The definition (5.8) of I_- and I_+ or the relation (5.11) leads to the quantisation conditions

$$I_- = n_- \hbar, \quad I_+ = n_+ \hbar \quad (n_- + n_+ \text{ even}), \quad (5.12)$$

where n_- and n_+ are integers.

The effect of exchange on the torus is

$$e_{12}T(I_-, I_+) = T(-I_-, I_+) \quad (5.13)$$

and unless $I_- = n_- = 0$ this is a distinct congruent torus. The boson and fermion states are formed from the appropriate linear combinations of the wavefunctions formed from the congruent tori. For $I_- = n_- = 0$ there is only one exchange torus for each I_+ and this represents a boson state only.

6. Two interacting particles on a ring

We introduce an interaction between the identical particles, so that the Hamiltonian now has the form

$$\begin{aligned} H(\varphi_1, \varphi_2, p_1, p_2) &= (1/2m)(p_1^2 + p_2^2) + V(|\varphi_1 - \varphi_2|/2) \\ &= H(\varphi, \Phi, p_-, p_+) = (1/4m)(p_-^2 + p_+^2) + V(|\varphi|), \end{aligned} \quad (6.1)$$

where the momenta are denoted p instead of I because they are no longer all action variables of the system. This problem has been treated classically by Born (1927, p 266). The interaction destroys the separability in (φ_1, φ_2) but retains it in (φ, Φ) . The Hamiltonian for relative motion is

$$H_-(\varphi, p_-) = (p_-^2/4m) + V(\varphi), \quad (6.2)$$

with $V(\varphi)$ even and periodic in φ of period π and independent of Φ .

Unlike the previous examples both rotation and vibration can take place, the former when the energy is greater than the maximum of the potential, and the latter when, as illustrated in figure 6, it is smaller. The two types of motion are divided by a separatrix

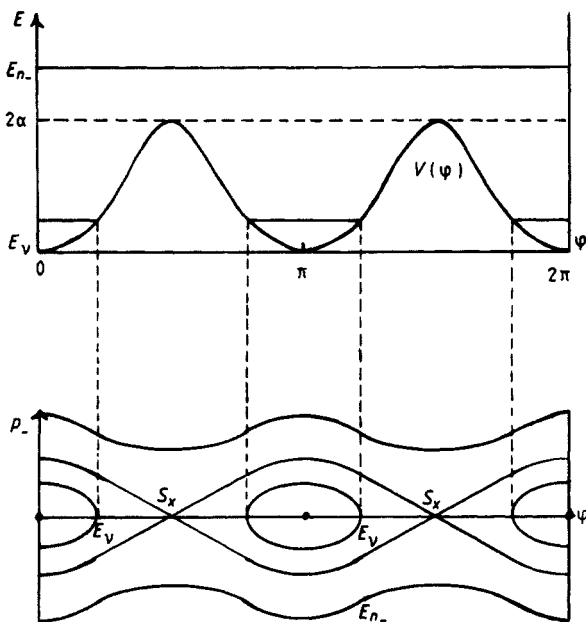


Figure 6. The potential $V(\varphi) = \alpha(1 - \cos 2\varphi)$ and the phase space with phase curves for the energies $E_v < 2\alpha$, $E_{n_-} > 2\alpha$ and the separatrix S_x .

in the (φ, p_-) phase plane. In the neighbourhood of this separatrix the primitive semiclassical EBK theory breaks down and uniformisation methods have to be used. These methods are clearly important for problems involving exchange, but we do not discuss them here.

We content ourselves with the comparison of the EBK and the exact quantal energy levels for a particular case in which the potential is

$$V(\varphi) = \alpha(1 - \cos 2\varphi), \tag{6.3}$$

where α is a perturbation parameter.

The potential and phase space are illustrated in figure 6. For any energy E except 2α there are two phase curves, but clearly they have a very different form for vibration and rotation.

(φ, Φ) are no longer scaled angle variables as they are for the free particles on a ring of § 5. In the rotational region ($E > 2\alpha$), though, the topology of the angle space (θ, Θ) is retained in the coordinate space (φ, Φ) and the identification of classically and exchange equivalent points is the same as in § 5. Thus, for rotational motion the effect of exchange (equation (5.13)) corresponds to going from an upper rotational curve to its respective lower one in figure 6. The quantisation condition (5.12) holds here too, so for n_+ even, n_- is even while for n_+ odd, n_- is odd. For either even or odd $n_- > 0$ the semiclassical boson and fermion wavefunctions are formed from the appropriate linear combinations of the wavefunctions on the two congruent tori. For any value of n_- there are two degenerate semiclassical states of $[+]$ and $[-]$ exchange symmetry. $[+]$ and $[-]$ denote respectively a symmetrical and an antisymmetrical semiclassical state with respect to exchange of identical particles.

For the rotational region at a given energy E of the Hamiltonian (6.2), the action integral is given by

$$I_- = \frac{1}{2\pi} \int_0^{2\pi} d\varphi (4mE - 8m\alpha \sin^2 \varphi)^{1/2}. \tag{6.4}$$

Here $E > 2\alpha$ and the integral (6.4) is given by

$$I_- = \frac{(4mE)^{1/2}}{2\pi} \int_0^{2\pi} d\varphi (1 - k^2 \sin^2 \varphi)^{1/2} = \frac{4(mE)^{1/2}}{\pi} E(k), \tag{6.5}$$

where we have chosen

$$k^2 = 2\alpha/E < 1 \tag{6.6}$$

and $E(k)$ is a complete elliptic integral of the second kind (Gradshteyn and Ryzhik 1965). Simple semiclassical quantisation gives

$$I_- = [4(mE)^{1/2}/\pi]E(k) = n_- \hbar \quad (n_- = 0, 1, 2, \dots) \tag{6.7}$$

and we have a degeneracy in $\pm n_-$ due to the double valuedness of p_- . For $k^2 \ll 1$ ($E \gg 2\alpha$) the system is very near to two free particles on a ring and we have $E(k) \approx \pi/2$,

$$I_- \approx (4mE)^{1/2} = n_- \hbar \tag{6.8}$$

and

$$E \approx n_-^2 \hbar^2 / (4m). \tag{6.9}$$

The energy levels can be obtained in general by inverting equation (6.7) so as to obtain E for a fixed integer value of n_- .

For the vibrational motion the physical angles (φ, Φ) are not related to angle variables in a simple manner. This is similar to the system S3 treated in § 4. Here an exchange corresponds to a translation of π in the angle variable θ as in equation (4.13), keeping Θ constant, as for the points A and B in figure 7(a). As φ goes to $-\varphi$ during an exchange operation, θ goes to $\theta + \pi$ (figure 7(b)). Note that here we are concerned with translations in the (θ, Θ) space and *not* the (φ, Φ) space. This reflects the equivalence of the two wells in our double representation. If for this region we change the coordinate φ to $\chi = 2\varphi$, the Hamiltonian separates in χ and Φ and for the χ motion it is now

$$H_\chi = p_\chi^2 / (2m/2) + \alpha(1 - \cos \chi) \tag{6.10}$$

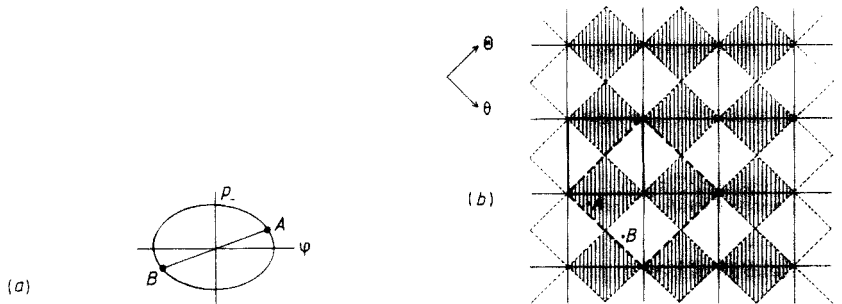


Figure 7. (a) Phase curve for a system of two interacting particles on a ring with vibrational motion in the relative angle and (b) the angle plane. An exchange operation is between points A and B , with $\theta_B = \theta_A + \pi$.

and the theory is identical to that of a vertical pendulum of mass $m/2$. The χ motion is quantised in the same manner as in § 4, equation (4.15), by the quantum number ν which is distinct from n_- and is independent of n_+ .

For even and odd ν we obtain semiclassical boson and fermion states alternately. For the vibrational motion we have $E < 2\alpha$ and we define

$$k'^2 = E/2\alpha < 1. \tag{6.11}$$

The required action integral is given by

$$I_\nu = \frac{1}{2\pi} \oint d\chi (mE - 2m\alpha \sin^2 \chi/2)^{1/2}. \tag{6.12}$$

Putting $k'^2 = \sin^2 \varphi_0$ and $\sin \varphi = \sin \varphi_0 \sin \beta$, we obtain

$$\begin{aligned} I_\nu &= \frac{4(2m\alpha)^{1/2}}{\pi} \int_0^{\varphi_0} d\varphi (\sin^2 \varphi_0 - \sin^2 \varphi)^{1/2} \\ &= \frac{4(2m\alpha)^{1/2}}{\pi} \int_0^{\pi/2} d\beta k'^2 \frac{\cos^2 \beta}{(1 - k'^2 \sin^2 \beta)^{1/2}} \\ &= [4(2m\alpha)^{1/2}/\pi][E(k') - (1 - k'^2)K(k')], \end{aligned} \tag{6.13}$$

where $K(k')$ is a complete elliptic integral of the first kind. For $k'^2 \ll 1$ (α large, very deep well, or E small, very low vibrational states) I_ν is given approximately by

$$I_\nu \approx (2\alpha/m)^{-1/2} E \tag{6.14}$$

or the energy by

$$E_\nu \approx (\nu + \frac{1}{2})(2\alpha/m)^{1/2} \hbar \quad (\nu = 0, 1, 2, \dots), \tag{6.15}$$

where we have used simple EBK quantisation for vibrational motion. (6.15) gives the energy levels of a harmonic oscillator of mass $m/2$. For higher k'^2 we can approximate the elliptic integrals by finite polynomials in k'^2 .

With this approximation the semiclassical energy levels of the system can be obtained by solving equations (6.13) for $k'^2 = E/(2\alpha)$ with

$$I_\nu = (\nu + \frac{1}{2})\hbar \quad (\nu = 0, 1, 2, \dots). \tag{6.16}$$

The classical equivalence puts constraints on the forms of both the semiclassical and quantal wavefunctions. For the quantal wavefunction there is no formal distinction between rotation and vibration and classical equivalence is valid all through. Because of the classical equivalence of the points (φ, Φ) and $(\varphi + \pi, \Phi + \pi)$, the separated quantal wavefunctions have the form

$$\begin{aligned} \Psi(\varphi, \Phi) &= \psi(\varphi)(2\pi)^{-1/2} \exp(in_+\Phi) \\ &= \Psi(\varphi + \pi, \Phi + \pi) = \psi(\varphi + \pi)(-1)^{n_+}(2\pi)^{-1/2} \exp(in_+\Phi). \end{aligned} \tag{6.17}$$

Therefore we have

$$\psi(\varphi + \pi) = (-1)^{n_+} \psi(\varphi). \tag{6.18}$$

The behaviour of $\psi(\varphi)$ under translation therefore depends on the parity of the 'centre-of-mass' quantum number n_+ . This applies to both bosons and fermions. The *quantal* exchange properties do not depend on the parity of n_+ but only on the sign change in $\psi(\varphi)$ going to $\psi(-\varphi)$.

The quantal wavefunction $\psi(\varphi)$ is a solution of the Schrödinger equation

$$\left(-\frac{\hbar^2}{4m} \frac{d^2}{d\varphi^2} + \alpha(1 - \cos 2\varphi) - E\right)\psi(\varphi) = 0. \tag{6.19}$$

This has the form of a Mathieu equation

$$\psi''(z) + (a - 2q \cos z)\psi(z) = 0, \tag{6.20}$$

where

$$z = \varphi + \pi/2, \quad a = (E - \alpha)4m/\hbar^2, \quad 2q = 4m\alpha/\hbar^2. \tag{6.21}$$

The Mathieu equation (6.20) has four types of periodic solutions (Gradshteyn and Ryzhik 1965) $ce_{2r}(z)$, $se_{2r+1}(z)$, $ce_{2r+1}(z)$, $se_{2r+2}(z)$ with $r = 0, 1, \dots$. The solutions with even subscript are of period π while those of odd subscript are of period 2π . The ce solutions are even functions while the se ones are odd. The first four solutions are sketched in figure 8(a). The eigenvalues of the Mathieu equation (6.20) are denoted a_r , associated with even solutions, and b_r , associated with odd solutions.

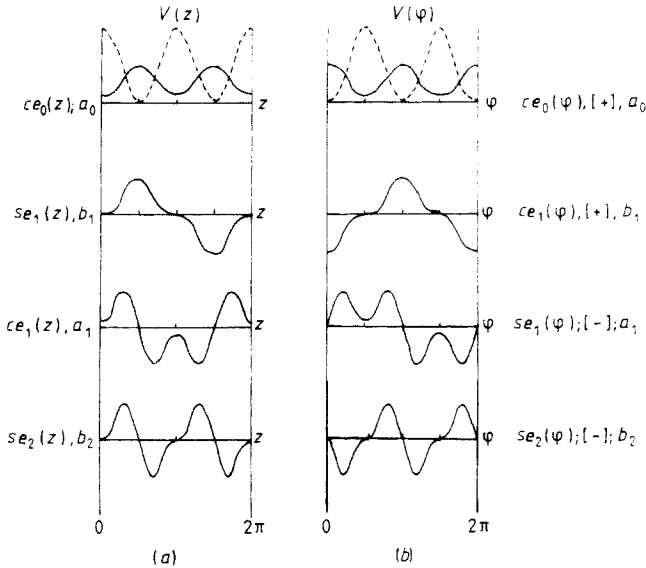


Figure 8. The potential V (dotted line) and the first four Mathieu functions in z and φ representation. Each function is denoted by its name ce_r or se_r and has a period 2π or π for even and odd r respectively. The signs in the square brackets are the corresponding exchange symmetries while a and b denote the eigenvalues.

The solutions of the Schrödinger equation (6.19) are related to the solutions of the Mathieu equation (6.20) in the following way (Gradshteyn and Ryzhik 1965, p 993):

$$\begin{aligned} ce_{2r}(z) &= (-1)^r ce_{2r}(\varphi), & se_{2r+1}(z) &= (-1)^r ce_{2r+1}(\varphi), \\ ce_{2r+1}(z) &= (-1)^r se_{2r+1}(\varphi), & se_{2r+2}(z) &= (-1)^r se_{2r+2}(\varphi). \end{aligned} \tag{6.22}$$

Clearly the $\pi/2$ shift in $z = \varphi + \pi/2$ leaves the periodicity of the solutions unchanged, but for the solutions of period 2π , this shift changes the parity of the

solutions. The eigenvalues of (6.19) a' , and b' , relate to those of (6.20) in the following way:

$$a_{2r} = a'_{2r}, \quad b_{2r+1} = a'_{2r+1}, \quad a_{2r+1} = b'_{2r+1}, \quad b_{2r+2} = b'_{2r+2}. \quad (6.23)$$

Table 1. Quantal (E_{QM}) and semiclassical (E_{SC}) energy levels for the system of two interacting identical particles on a ring. $E_{spk} = 2\alpha$ is the value of the energy at the classical separatrix. The signs in the square brackets are the corresponding exchange symmetries. a , and b , are the corresponding Mathieu eigenvalues.

α	E_{QM}		E_{SC}		$E_{spk} = 2\alpha$	ν (for $E < 2\alpha$) n_- (for $E > 2\alpha$)
	n_+ even	n_+ odd	n_+ even	n_+ odd		
10.	2.171 65[+], a_0	2.171 65[+], b_1	2.205[+]		20.	0
	6.377 24[-], b_2	6.377 18[-], a_1	6.414[-]			1
	10.288 57[+], a_2	10.290 18[+], b_3	10.332[+]			2
	13.873 49[-], b_4	13.848 95[-], a_3	13.915[-]			3
	16.898 65[+], a_4	17.117 06[+], b_5	17.087[+]			4
		19.161 24[-], a_5	19.652[-]		5	

		20.147 42[-], b_6	20.590[+-]		6	
		21.015 74[+], a_6		23.333[+-]	7	
		23.276 62[+], b_7				
	23.466 12[-], a_7					
	26.813 06[-], b_8		26.820[+-]	8		
	28.836 47[+], a_8					
		30.888 05[+], b_9		30.888[+-]	9	
		30.890 06[-], a_9				
5.	1.515 76[+], a_0	1.515 86[+], b_1	1.5492[+]		10.	0
	4.404 46[-], b_2	4.400 21[-], a_1	4.4425[-]			1
	6.929 34[+], a_2	6.996 52[+], b_3	7.018[+]			2
	9.345 35[-], b_4	8.875 69[-], a_3	-----			
		10.276 16[+], a_4				
			11.691 61[+], b_5		11.779[+-]	5
			11.925 94[-], a_5			
		14.354 96[-], b_6		14.355[+-]	6	
		14.383 40[+], a_6				
		17.513 54[+], b_7		17.510[+-]	7	
		17.515 67[-], a_7				
0.5	0.386 22[+], a_0	0.472 44[+], b_1	0.46630[+]		1.0	0
		0.964 78[-], a_1	-----			
		1.479 26[-], b_2		1.5319[+-]		2
		1.592 83[+], a_2				
			2.761 93[+], b_3		2.7639[+-]	3
			2.769 59[-], a_3			
		4.508 24[-], b_4		4.5085[+-]	4	
		4.508 46[+], a_4				
			6.755 21[+], b_5		6.756[+-]	5
		6.755 21[-], a_5				
	9.503 57[-], b_6		9.504[+-]	6		
	9.503 57[+], b_6					

From (6.18) we have that the solutions of period π are associated with even n_+ while those of period 2π are associated with odd n_+ . The functions $ce_r(\varphi) = ce_r(-\varphi)$ are symmetric [+] while $se_r(\varphi) = -se_r(-\varphi)$ are antisymmetric [-] with respect to exchange, as can be seen in figure 8(b). Thus, the quantal spectrum and exchange symmetry classification for this system can be represented in the following table:

n_+ even	n_+ odd
$a_0[+]$	$\leq b_1[+]$
	\wedge
$b_2[-]$	$\geq a_1[-]$
\wedge	
$a_2[+]$	$\leq b_3[+]$
\vdots	\vdots

where the inequality continues from line to line and the two columns correspond to different n_+ parities. The values of the corresponding energies E_{QM} are obtained using the second equation in (6.21) where a is replaced by the corresponding a_r or b_r .

In table 1 we summarise some of our numerical results for certain α . The comparison between the semiclassical and quantal energy levels is not too good in the neighbourhood of the classical separatrix, but a clear exchange symmetry matching is possible. In the vibrational region ($E < 2\alpha$) the semiclassical spectrum is independent of the parity of n_+ . This corresponds to the degeneracy $a_{2r}[+] \approx b_{2r+1}[+]$ and $a_{2r+1}[-] \approx b_{2r+2}[-]$ in the quantal spectrum for low r' and α not too small. In the semiclassical rotational region for n_+ even, n_- is even while for n_+ odd, n_- is odd and both [+] and [-] symmetries occur for any n_- . This corresponds to the degeneracy $a_{2r}[+] \approx b_{2r}[-]$ and $a_{2r+1}[-] \approx b_{2r+1}[+]$ in the quantal spectrum for high values of r . The semiclassical solution is not valid in the neighbourhood of the separatrix where the quantal tunnelling effect destroys the above degeneracy.

The classical separatrix divides the motion into two distinct regions. A uniformisation procedure can be used to pass smoothly from one region to the other. This has not been attempted in this work. The degeneracy displayed by the Mathieu functions in the two classical regions preserve the dynamical properties of the system.

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