Semiclassical periodic-orbit theory for identical particles

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Gutzwiller's semiclassical approximation is applied to systems of identical particles. The special case of antisymmetry under particle exchange is treated as an example. The Pauli principle is shown to cause a modification of Gutzwiller's periodic-orbit sum: The amplitude with which a periodic orbit contributes to the sum is changed, but new orbits do not arise in the sum. The case of noninteracting particles is used for purposes of illustration of the procedure.

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I. INTRODUCTION

The semiclassical method, based on Gutzwiller's trace formula and its generalizations, has become an invaluable tool in the study of quantum manifestations of classical chaos [1]. It has been very successfully applied to the analysis of systems with few degrees of freedom [2,3].

Quantum systems are typically composed of identical particles (fermions or bosons), and the wave functions must be antisymmetric (or symmetric) under an exchange of these particles. How can such symmetry requirements be accommodated in the framework of the semiclassical method? Which modifications arise in the sum over periodic orbits as a consequence of these symmetries? In the present paper, we give a general answer to these questions.

It may be argued that this effort is futile: Interacting many-body systems are too complex anyway to be accessible to the semiclassical approximation; the construction of periodic orbits is a nearly hopeless task. We do not share this view, for the following reasons: First, understanding the influence of symmetries on periodic-orbit theory is an important issue in its own right; it must be seen as an integral part of semiclassical theory. Second, given the intractability of the many-body system, there are questions which semiclassical theory hopefully can answer. We have in mind, for instance, the determination of the characteristic energy scale where the Δ_3 statistic for the two-level correlation function in classically chaotic systems becomes constant [4], or the occurrence of shell structure as a generic feature of self-bound quantum systems, or the modifications caused by electron-electron interaction and the exclusion principle in the application of semiclassical methods to mesoscopic physics [5].

The role of symmetries in the semiclassical approach has been dealt with in papers on molecular physics [6]. We mention, in particular, the work by Robbins [7]. There, a general group-theoretical method for Hamiltonians with special symmetries has been developed, and applied to several problems. In this method (the "reduced-phase-space method"), the entire phase space is generated by repeated application of the symmetry operation to part of the phase space, and the periodic orbits are constructed in this reduced phase space. It seems that this method does not apply to permutation symmetry; in any case the physically very relevant case of particle identity has not been dealt with.

In the present paper, we follow another route. Starting from an explicit expression [8] for the relevant projection operator $\mathbf{1}_A$ defined below, we construct semiclassical periodic-orbit theory directly and without using the reduced phase space of Ref. [7]. We arrive at a geometrically very appealing description of the influence of particle symmetry on the periodic-orbit sum.

For definiteness and for simplicity of notation, we consider a system of f interacting spinless fermions in one dimension with coordinates $q_1,\ldots,q_f$. We emphasize, however, that the method employed in this paper applies to more general situations. An extension to three dimensions would require vector notation throughout. Bosons would require trivial changes of signs. Spin can be included by extending the trace in Eq. (1) below to spin degrees of freedom, by replacing the operator $\mathbf{1}_A$ defined in Eq. (2) by a suitable generalization, and by dealing with the ensuing Young tableaux in coordinate space in a manner analogous to what follows.

In Sec. II we introduce the projection operator which imposes antisymmetry, and derive the periodic-orbit sum. In Sec. III we use properties of the symmetric group to elucidate the structure of the terms contributing to the sum. In Sec. IV we apply the method to the special case of noninteracting fermions. Section V contains a brief summary.

II. PERIODIC-ORBIT SUM FOR FERMIONS

In the present section, we follow closely Ref. [1]. We therefore only sketch the main steps, emphasizing those points where the presence of the projection operator leads to modifications.

Let $\rho(E)$ be the energy-level density of the quantum Hamiltonian $H(q_1,\ldots,q_f)$, an operator which is symmetric in the variables $q_1,\ldots q_f$, and let $G(E)=(E^+-H)^{-1}$ be the advanced Green's function. Then,

$$\rho(E)=\frac{(-1)}{\pi}\,\mathrm{Im}\,\mathrm{tr}G(E)\ . \tag{1}$$

For fermions, the trace extends only over that part of Hilbert space which is spanned by totally antisymmetric wave functions. With 1_A the projection operator onto this part, we have [8]

$$\langle q_1', \ldots, q_f' | 1_A | q_1'', \ldots, q_f'' \rangle = (f!)^{-1} \det(D_{ij}) . \quad (2)$$

Here, D is a matrix of dimension f with elements $D_{ij} = \delta(q_i' - q_i'')$. Equation (2) can easily be derived [8] by writing the projection operator 1_A explicitly in an (arbitrary) single-particle basis. Using the Laplace expansion for $\det(D_{ij})$ and substituting the result into Eq. (1), we obtain

$$\rho(E) = \frac{(-1)}{\pi f!} \sum_P (-1)^P \int dq_1' \cdots dq_f' dq_1'' \cdots dq_f'' \mathrm{Im} \langle q_1'', \ldots, q_f'' | G(E) | q_1', \ldots, q_f' \rangle P \prod_{j=1}^{f} \delta(q_j' - q_j'') . \quad (3)$$

The sum runs over all $f!$ permutations P acting on the variables $(q_1'', \ldots, q_f'')$ with $(-1)^P$ the sign of P. Equation (3) differs in two ways from the corresponding expression obtained in the absence of symmetry requirements: (i) The factor $(f!)^{-1}$ reduces overall phase space in an obvious fashion and (ii) the terms with $P \neq 1$ express the additional constraint that two particles may not occupy the same point in single-particle phase space, i.e., may not have the same coordinates [8]. We shall see that the terms with $P \neq 1$ cause a substantial modification of the standard sum over periodic orbits.

Writing $G(E)$ as the Laplace transform of the time-evolution operator $\exp(-iHt/\hbar)$, we express the latter as a Feynman path integral. The stationary-phase approximation for all paths connecting $q' = (q_1', \ldots, q_f')$ with $q'' = (q_1'', \ldots, q_f'')$ at time t is met by all classical trajectories connecting q' with q'' at time t; the same approximation with regard to the time integration is met by all classical trajectories of energy E which lead from the $2f$-dimensional phase-space point (q', p') to the $2f$-dimensional phase-space point (Pq', p''). Here, we made use of the factor $P \prod_{j=1}^{f} \delta(q_j' - q_j'')$ in Eq. (3) and wrote Pq' for the result obtained by P acting on q'. The values of p' and p'' are as usual given by partial derivatives of the action at q' and q'', respectively. The remaining integrals over q' in the directions perpendicular to the trajectory are again evaluated with the help of the stationary-phase approximation. This yields $p'' = Pp'$ and

$$\int dq' dq'' \langle q'' | G(E) | q' \rangle P \prod_{j=1}^{f} \delta(q_j' - q_j'') = \sum_{\text{classical trajectories}} \int \frac{dq}{q} \frac{2\pi}{(2i\pi\hbar)^{(f+1)/2}} F^{-1/2} \exp\left[\frac{iS(E)}{\hbar} - \frac{i\pi\mu}{2} \right] . \quad (4)$$

Here, $S(E)$ is the action along the trajectory from (q', p') to (Pq', Pp'), μ is the Maslov index (an integer), and F is the determinant of the monodromy matrix. This matrix has the form $1 - A$, where A describes the map of the infinitesimal area perpendicular to the trajectory at q' onto the corresponding area at Pq'. The integral over dq extends along the trajectory. In these steps, we have assumed that the points of stationary phase are isolated. In general, this condition will not be met unless the system is chaotic.

The right-hand side of Eq. (4) can be simplified by noticing that the trajectory connecting (q', p') with (Pq', Pp') is a piece of a periodic orbit [7]. This is seen as follows: As a consequence of the symmetry of the Hamiltonian under permutations of the variables q_j, $j = 1, \ldots, f$, the simultaneous substitutions $q' \to Pq'$ and $q'' \to Pq''$ leave Eq. (3) invariant. Using these substitutions and repeating the argument leading to Eq. (4), we arrive at a formally identical expression, the only difference being that the trajectory now connects the point (Pq', Pp') with the point $(P^2 q', P^2 p')$. The above-mentioned symmetry of the Hamiltonian guarantees that the values of F, $S(E)$, and μ on this new trajectory (which is but the continuation of the old one in the direction of increasing time) coincide with their counterparts on the old one. Let m be the smallest positive integer for which $P^m = 1$; such an integer always exists. Repeating the procedure described above m times, we generate [9] m trajectories. The jth trajectory connects the phase-space points

$$s_{j-1} = (P^{j-1} q', P^{j-1} p')$$

and $s_j = (P^j q', P^j p')$, with $j = 1, \ldots, m$. Obviously, the jth trajectory is the continuation of the $(j-1)$st in the direction of increasing time. Moreover, the last point s_m and the first point $s_0 = (q', p')$ coincide. We have thus shown that all the m trajectories defined above lie on a periodic orbit M.

Having shown that all the trajectories contributing to the sum in Eq. (4) are pieces of periodic orbits, we now relate the quantities S, F, and μ appearing in Eq. (4) with the action S_0, the monodromy determinant F_0, and the Maslov index μ_0 defined for a single traversal of the associated periodic orbit M. To do so, we define n as the number of traversals of M realized by adding the m trajectories defined in the previous paragraph. In general, we have $n > 1$. Note that for each P and each periodic orbit M, the value of n is uniquely defined, although for P fixed, n may depend on M. By construction, each of the m trajectories defined in the previous paragraph yields the same values for $S(E)$, F, and μ. Hence, $mS(E) = nS_0$, $A^m = A_0^n$, and $m\mu = n\mu_0$. But S_0, F_0, and μ_0 are independent of the initial point on the trajectory. Therefore, the integration over dq in Eq. (4) can be carried out after S_0, A_0, and μ_0 have been substituted for $S(E)$, A, and μ. The integral yields T_0, the time for a single traversal of M. We obtain

$$\rho(E)=\frac{(-1)}{\pi f!}\sum_{P}(-1)^{P}\mathrm{Im}\sum_{\text{transversals}}\sum_{\text{periodic orbits}}\frac{2\pi T_0}{(2i\pi\hbar)^{(f+1)/2}}D(n,m)\exp\left[i\frac{n}{m}\left[\frac{S_0}{\hbar}-\frac{\pi\mu_0}{2}\right]\right]. \tag{5}$$

Here, $D(n,m)$ is the inverse of the square root of the determinant of $[1-(A_0)^{n/m}]$. The sum over periodic orbits extends only over those orbits for which, with (q',p'), (Pq',Pp') also lies on the orbit. The summation over (multiple) traversals keeps track of contributions where the point (Pq',Pp') is reached from the point (q',p') after one or more complete traversals of M, while the sum with subscript periodic orbits accounts only for contributions which do not involve a complete traversal of M; the additional factors arising in Eq. (5) from multiple traversals are not written down explicitly but will be given in Sec. III below. Equation (5) generalizes the canonical periodic-orbit sum for the level density to the case of identical particles (fermions).

III. SYMMETRIC GROUP AND PERIODIC ORBITS

The structure of the sum (5) can be elucidated further, and the possible values of m and n can be determined by using the symmetric group. We define classes of periodic orbits by the following equivalence relation: Let M be some (arbitrary) periodic orbit at energy E, and let (q,p) be a phase-space point on M. We write $M(q,p)$ for M to indicate that M is obtained by solving the equations of motion with (q,p) as initial point. We consider the set $\mathcal{S}=\{(Pq,Pp)\}$ of $f!$ phase-space points generated by all permutations P. These points are generically distinct [9]. Solving the equations of motion with each of these $f!$ points as initial points, we create $f!$ trajectories $M(Pq,Pp)$. The symmetry of H under permutations implies that with $M(q,p)$, all the $M(Pq,Pp)$ must be closed orbits and that the values of $S_0(E)$, F_0, and μ_0 must be the same on all these orbits. The set $\mathcal{M}=\{M(Pq,Pp)\}$ thus generated by the $f!$ permutations defines a class of periodic orbits. We now rewrite the sum over the $f!$ permutations in Eq. (5) as a sum over classes of periodic orbits and, within each class, calculate the contributions of all permutations.

The following possibilities exist.

(i) No two points in $\mathcal{S}$ lie on the same orbit in $\mathcal{M}$. Then $\mathcal{M}$ contains $f!$ distinct elements. Each element contributes only to the term with $P=1$ in the sum over P in Eq. (5). All $f!$ elements in $\mathcal{M}$ give the same contribution to the sum. $(f!)^{-1}$ times the sum over all elements in $\mathcal{M}$ is therefore equal to the contribution of a single element in $\mathcal{M}$; the latter has the canonical form for a single periodic orbit with $m=1$ and $n=1$.

(ii) At least two points in $\mathcal{S}$ lie on the same periodic orbit in $\mathcal{M}$. The permutation symmetry of H then implies that each periodic orbit in $\mathcal{M}$ carries the same number of points in $\mathcal{S}$. Let this number be k. The set $\mathcal{M}$ then consists of $f!/k$ distinct elements. Again, the permutation symmetry of H shows that each element in $\mathcal{M}$ yields the same contribution to the sum over P in Eq. (5); $(f!)^{-1}$ times the sum over the contributions of all elements of $\mathcal{M}$ is thus equal to k^{-1} times the contribution from a single element of $\mathcal{M}$. It remains to work out this contribution.

We do so for the periodic orbit $M(q,p)$ in $\mathcal{M}$ which contains the point $s_0'=(q,p)$ and $(k-1)$ further distinct points s_j', $j=1,\ldots,k-1$ in $\mathcal{S}$. The points s_j' are ordered in the manner in which they are met as we traverse the periodic orbit M in the direction of increasing time, starting at s_0'. It is convenient to put $s_k'=s_0'$. We note that the k points s_j', $j=1,\ldots,k$, are not identical to the points s_j, $j=1,\ldots,m$, introduced in Sec. II although we obviously may and do choose $s_0=s_0'$. The relation between the two sets of points will be clarified below.

Let t_j be the time it takes to reach point s_j' from point s_{j-1}' on M in the direction of increasing time without traversing M more than once, with $j=1,\ldots,k$. All t_j must be equal. Indeed, let us assume the contrary and let t_i be the smallest of the set $\{t_j\}$. If t_i is not unique, we take it such that $t_{i+1}>t_i$. Both s_{i-1}' and s_i' are by construction permutations of s_0. Therefore, there exists another permutation P' such that $s_i'=P's_{i-1}'$. With both s_{i-1}' and s_i' on M, it follows that $P's_i'$ is also on M and is reached from s_i' at a time $t=t_i<t_{i+1}$, in contradiction to the assumption that t_i is the smallest of the t_j. Hence, all t_j are equal.

Let P_0 be the permutation for which $s_1'=P_0s_0$. From the argument just given, it follows that all the points s_j' are given by $(P_0)^j s_0$, $j=1,\ldots,k$, and that $(P_0)^k=1$. The possible values of k are found by writing P_0 as a product of l cycles of length f_w, $w=1,\ldots,l$, with $\sum_{w=1}^{l}f_w=f$. Then k is given by the smallest common multiple of the numbers $f_1,f_2,\ldots,f_l$. The parity $(-1)^{P_0}$ of P_0 is given by $(-1)^{f-k}$.

What is the relation of the set of points

$$\mathcal{S}_M=\{s_j,\ j=1,\ldots,m\}$$

introduced in Sec. II and the set

$$\mathcal{S}_M'=\{s_j',j=1,\ldots,k\}$$

considered now? By construction, $\mathcal{S}_M$ is a subset of $\mathcal{S}_M'$, and therefore $k\geq m$. Inequality does occur under the following conditions: (i) The partition f_w of f defining $\mathcal{M}$ consists of more than one nontrivial cycle (i.e., a cycle of length larger than 1), and (ii) k is larger than the largest of the f_w. Consider, for instance, the class $\mathcal{M}$ for $f=5$ with $l=2$, $f_1=3$, $f_2=2$, and $k=6$, and take a permutation of five elements consisting of the three cycles $f_1=3$, $f_2=1=f_3$. This permutation and its powers connect only three of the six points on M. We conclude that for $k>m$, k must be an integer multiple of m. To determine n, we recall that for P, one of the permutations considered in Sec. II, and s_1, a point defined on M by $s_1=Ps_0$, the point s_1 must also be a point in the set $\mathcal{S}_M'$, say, $s_1=s_i'$. Then, $P=P_0^i$, and n is determined by the relation $mi=kn$.

Returning to Eq. (5), we carry out the summation over

permutations within class $\mathcal{M}$ by summing over the contributions from the k points in $\mathcal{S}'_M$. Each point in this set does correspond to a permutation of s_0 and therefore contributes; no other permutations contribute to the sum over P on M. Since $s'_j = P_0^j s_0$, the contribution from point s_j is given by the jth power of the contribution of $P_0 s_0$, and the latter is the k^{-1}st power of the contribution of a single traversal of the orbit $\mathcal{M}$. Hence, we have

$$\rho(E)=\frac{(-1)}{\pi}\sum_{\text{classes of periodic orbits}}\operatorname{Im}\left\{\frac{2\pi T_0}{k(2i\pi\hbar)^{(f+1)/2}}(-1)^{f-k}\sum_{n=1}^{\infty}D(n,k)\exp\left[i\frac{n}{k}\left[S_0(E)-\frac{\pi\mu_0}{2}\right]\right]\right\}. \tag{6}$$

The sum over n now also includes multiple traversals of the orbit M. In Eq. (6), each class is specified by a partition of f into l integers f_w with $\sum_{w=1}^{l} f_w = f$, and k is the smallest common multiple of the numbers f_w, $w=1,\ldots,l$. The sum over classes includes each class that actually occurs in a given problem; at this point we cannot make any general statement about whether and how often classes pertaining to the same partition of f will occur.

In comparison with Eq. (5), the new Eq. (6) has the following advantage: Given a single periodic orbit, we can—by traversing this orbit—determine to which partition of f it belongs. This knowledge enables us to write down the contribution to the sum in Eq. (6) of the entire class to which the orbit belongs. We believe that this may be helpful in answering some of the general questions raised in the Introduction.

The considerations in the present section were quite simple and allowed us to bypass the explicit use of group theory. There is, of course, a close relationship between the classes of orbits introduced above and defined in terms of a partition of f, on the one hand, and the conjugacy classes of the symmetric group, on the other.

IV. NONINTERACTING FERMIONS

It is instructive to apply our procedure to the special case of noninteracting particles where the many-body Hamiltonian $H(q_1,\ldots,q_f)$ is the sum of f identical one-body Hamiltonians $H_0(q_j)$, $j=1,\ldots,f$. The projector 1_A onto antisymmetric states allows us to express the f-body density of states as the sum of convolution integrals over products of the one-body densities of states, and the periodic-orbit sum provides a useful approximation to the latter in case the one-body problem is not integrable. (This case occurs, of course, only in two or three dimensions. For simplicity of notation, we continue to consider f particles in one dimension, however.) From a systematic point of view, the present section lies somewhat outside the main topic of this paper because a system of independent particles is (at least partially) integrable.

Let $K_0(q_j'',t;-1q_j',0)$ be the (quantum) time-evolution operator of particle j. The quantity K_0 is related to the single-particle Green's function $g_0(\varepsilon)$ by

$$\langle q_j''|g_0(\varepsilon)|q_j'\rangle=(i\hbar)^{-1}\int_0^{\infty}dt\exp\left[\frac{i\varepsilon^+ t}{\hbar}\right]K_0(q_j'',t;q_j',0). \tag{7}$$

We note that, by definition,

$$\int dq_j K_0(q_j'',t'';q_j,0)K_0(q_j,t';q_j',0)=K_0(q_j'',t''+t';q_j',0). \tag{8}$$

The matrix element of $G(E)$ in Eq. (3) takes the form

$$\langle q_1'',\ldots,q_f''|G(E)|q_1',\ldots,q_f'\rangle=(i\hbar)^{-1}\int dt\exp\left[\frac{iE^+ t}{\hbar}\right]\prod_{j=1}^{f}K_0(q_j'',t;q_j',0). \tag{9}$$

We substitute Eq. (9) into Eq. (3). Before we give the full result, it is useful to consider two simple cases which elucidate the structure of the full result. The two classes are the following: (i) P is the identity and (ii) P is the product of the two cycles $(1,2,3,\ldots,f_1)$ and $(f_1+1,f_2+1,\ldots,f)$. We use Eqs. (7) and (8) and find, for case (i),

$$(f!)^{-1}\prod_{j=1}^{f}\int d\varepsilon_j\prod_{l=1}^{f}\left[\frac{(-1)}{\pi}\operatorname{Im}\int dq_l g_0(q_l,q_l,\varepsilon_l)\right]\times\delta\left[\varepsilon-\sum_{l=1}^{f}\varepsilon_l\right], \tag{10}$$

and for case (ii),

$$\frac{(-1)^f}{f!f_1f_2}\int_{-\infty}^{\infty}d\varepsilon\left[\frac{(-1)}{\pi}\operatorname{Im}\int dq_1 g_0\left[q_1,q_1,\frac{\varepsilon}{f_1}\right]\right]\times\left[\frac{(-1)}{\pi}\operatorname{Im}\int dq_f g_0\left[q_f,q_f,\frac{(E-\varepsilon)}{f_2}\right]\right]. \tag{11}$$

The expressions (10) and (11) differ. While expression (10) contains a product of f single-particle Green's functions, expression (11) contains only two, albeit with modified energy arguments. The physical significance of this difference emerges when we replace the straight brackets containing g_0 by their exact quantum counterparts $\sum_j\delta(\varepsilon-\varepsilon_j')$, with ε_j' the eigenvalues of the single-particle Hamiltonian H_0. The expression (10) takes the form

$$(f!)^{-1}\sum_{j_1,\ldots,j_f}\delta\left[E-\sum_{l=1}^{f}\varepsilon'_{j_l}\right], \tag{12}$$

while expression (11) becomes equal to

$$\frac{(-1)^f}{f!}\sum_{j_1,j_2}\delta(E-f_1\varepsilon'_{j_1}-f_2\varepsilon'_{j_2})\ . \tag{13}$$

The term (13) obviously corrects the term (12) for the presence of f_1 (f_2) particles in equal single-particle orbits, as imposed by the choice (ii) of P.

We return to the general case and give the exact form of Eq. (3) for the case of f independent particles. We observe that every P in the sum (3) corresponds to a partition of f and that different permutations which correspond to the same partition of f give identical contributions to the sum. (This last point follows because we are free to relabel the integration variables $q_1,\ldots,q_f$.) The sum in Eq. (3) can thus be written as a sum over partitions of f. We find

$$\rho(E)=\sum_{l=1}^{f}(-1)^{f-l}\sum_{\substack{f_1,f_2,\ldots,f_l\\(f_1\geq f_2\geq\cdots\geq f_l)}}\delta\left[f-\sum_{w=1}^{l}f_w\right](f!)^{-1}c(f_1,\ldots,f_l)\prod_{w'=1}^{l}(f_{w'}^{-1})\prod_{k=1}^{l}\int d\varepsilon_k\rho_0\left[\frac{\varepsilon_k}{f_k}\right]\delta\left[E-\sum_{j=1}^{l}\varepsilon_j\right]\ . \tag{14}$$

Here, ρ_0 is short for the single-particle level density, and the δ function with the argument $(f-\sum f_w)$ stands for a Kronecker symbol. The coefficients $c(f_1,\ldots,f_l)$ give the number of permutations belonging to the same partition of f. These coefficients are well known; in the present context, they are given in Ref. [8]. These coefficients, incidentally, give the number of elements within a conjugacy class of the symmetric group.

V. SUMMARY

We have shown that the semiclassical approximation to quantum systems with classically chaotic dynamics can be extended in such a way that it applies to systems of identical particles. The symmetry requirement imposed by particle identity causes modifications in the periodic-orbit sum. A classification of periodic orbits in terms of the partitions of the number f of particles is a useful tool in reordering the periodic-orbit sum. Within each class of periodic orbits, the sum extends over multiples of a basic element, a fraction of a periodic orbit. For each class, we have given an explicit expression for the contribution of this basic element to the periodic-orbit sum. From the point of view of symmetry considerations, the theory presented in this paper appears reasonably complete. From the point of view of general dynamical theory, it is not: We are not in a position to say which of the possible classes of periodic orbits do occur in a given dynamical system, and with which multiplicity this happens.

In the special case of noninteracting particles, the many-body level density is written as a convolution integral involving products of one-body level densities. This expression displays very clearly the influence of the exclusion principle. For systems of noninteracting identical particles composed of nonintegrable one-body systems in two or three dimensions, our result may serve as a useful starting point for an approximation to the level density.

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