Semiclassical quantization of multidimensional systems

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(Received 19 June 1980; accepted 5 August 1980)

The semiclassical quantization of nonlinear systems with two or more degrees of freedom has long been of interest.[1,2] Trajectory based methods[1] that were initially developed for nonintegrable (and nonseparable) Hamiltonians with $N=2$ degrees of freedom have recently been extended[3] to $N=3$ dimensions, in the quantization of the region of classically regular (quasiperiodic) behavior. Other semiclassical methods,[2] based on one form of classical perturbation theory or the other, have been seen to be complementary to trajectory methods,[1] and have been useful in the computation of semiclassical eigenvalues in two and more dimensions.

In recent investigations on the onset of chaotic behavior in nonintegrable systems, we have suggested that the simple perturbation methods may be useful when the eigenstates are not involved in avoided crossings.[4,5] Experience with multidimensional systems in general shows that the eigenvalue spectrum is discrete at low energies but with increasing energy, rapidly becomes dense—a quasicontinuum. Given the higher density of states in the quasicontinuum, overlapping avoided crossings[5] are the rule. Since the extensive overlapping avoided crossings give rise, we believe, to chaos,[4,5] trajectory and perturbation methods become difficult to apply and inaccurate, respectively. In this latter region, simple phase-space volume quantization[6] is likely to be more than adequate. For the low energy region, the perturbation results are usually accurate due to the lack of avoided crossings.

We illustrate the latter by application to a model three dimensional Hamiltonian,[3]

$$H=\frac{1}{2}\sum_{i=1}^{3}(p_i^2+\omega_i^2 q_i^2)+\lambda(q_1 q_2^2+\eta q_1^3)+\mu(q_2 q_3^2+\zeta q_2^3)$$

where p_i, q_i, ω_i, $i=1, 2, 3$ are the momenta, coordinates, and zeroth order angular frequencies, respectively. The perturbation method of choice here is that of the Lie-transform,[7] which, for the case of no internal

0021-9606/80/225400-02$01.00

TABLE I. Comparison of exact quantum and semiclassical perturbation method results for the lowest eigenvalues ($\hbar = 1$).

n_1	n_2	n_3	E_0[a]	E_q[b]	E_p[c]
0	0	0	1.5	1.494	1.493
1	0	0	2.2	2.185	2.185
0	0	1	2.5	2.486	2.486
0	1	0	2.8	2.771	2.772
2	0	0	2.9	2.873	2.873
1	0	1	3.2	3.177	3.177

[a]Unperturbed eigenvalues.
[b]Exact quantum result from Ref. 3.
[c]Present perturbation result.

resonances, gives the result

$$\begin{aligned}E_{n_1,n_2,n_3} = {} & \sum_{i=1}^{3}(n_i+\tfrac{1}{2})\hbar\omega_i - \frac{15}{4}\left\{\frac{\lambda^2\eta^2}{\omega_1^4}\hbar^2(n_1+\tfrac{1}{2})^2 + \frac{\mu^2\zeta^2\hbar^2}{\omega_2^4}(n_2+\tfrac{1}{2})^2\right\} \\ & + \hbar^2\omega_1\omega_2(n_1+\tfrac{1}{2})(n_2+\tfrac{1}{2})\left\{\frac{2\lambda^2}{\omega_1^2\omega_2^2(\omega_1^2-4\omega_2^2)} - \frac{3\lambda^2\eta}{\omega_1^4\omega_2^2}\right\} \\ & + \hbar^2\omega_2\omega_3(n_2+\tfrac{1}{2})(n_3+\tfrac{1}{2})\left\{\frac{2\mu^2}{\omega_2^2\omega_3^2(\omega_2^2-4\omega_3^2)} - \frac{3\mu^2\zeta}{\omega_2^4\omega_3^2}\right\} \\ & + 2\left\{\hbar^2\omega_2^2(n_2+\tfrac{1}{2})^2\frac{\lambda^2(\omega_2^2-3\omega_1^2/8)}{\omega_1^2\omega_2^4(\omega_1^2-4\omega_2^2)}\right. \\ & \left. + \hbar^2\omega_3^2(n_3+\tfrac{1}{2})^2\frac{\mu^2(\omega_3^2-3\omega_2^2/8)}{\omega_2^2\omega_3^4(\omega_2^2-4\omega_3^2)}\right\} \qquad (1)\end{aligned}$$

for the eigenvalues, up to terms of order λ^2, μ^2, ζ^2, η^2. The n_i's are the quantum numbers for the three degrees of freedom; the details of the semiclassical quantization are straightforward (through reduction to the Birkhoff normal form) and have been given elsewhere.[2(c),4] For the choice of parameters, $\omega_1 = 0.7$, $\omega_2 = 1.3$, $\omega_3 = 1.0$, $\lambda = \mu = -0.1$, $\zeta = \eta = 0.1$, the results of the simple second order perturbation theory are presented in Table I, and compared with exact quantum results. [It may be pointed out that since the perturbation expressions can be used to locate[8] the avoided crossings in such systems, the above method can itself detect its region of validity. On that basis, for the example here one would expect the expression (1) to hold for all states with energy less than ~6 units; above this energy we find that avoided crossings proliferate and the quasicontinuum effectively sets in.] The agreement is seen to be excellent for these lowest few eigenvalues. The semiclassical trajectory quantization also gives eigenvalues which agreed well with the quantum ones.[3]

For molecular systems that are close to normal form, and thus are almost separable, the application of the perturbation methods to low orders is straightforward and gives good results. (The perturbation is fairly small in the present example.) For nonintegrable systems that are intrinsically nonseparable as well, as, for example, the split-mass Toda lattice,[9] it is probable that trajectory methods will be more useful.

We are pleased to acknowledge the support of the National Science Foundation.

[a)]Contribution No. 6254.
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