Semiclassical density of states at symmetric pitchfork bifurcations in coupled quartic oscillators

K. M. Atkins and G. S. Ezra
Baker Laboratory, Department of Chemistry, Cornell University, Ithaca, New York 14853
(Received 7 January 1994)

We analyze the quantum density of states for a system of coupled quartic oscillators in the vicinity of symmetric isochronous or pitchfork bifurcations of the primary oscillator modes. A uniform semiclassical expression for the contribution to the density of states from the set of periodic orbits involved in the bifurcation is derived following the approach of Ozorio de Almeida and Hannay [J. Phys. A **20**, 5873 (1987)] and Ozorio de Almeida and Aguiar [Physica D **41**, 391 (1990)].

PACS number(s): 03.65.Sq, 05.45.+b

I. INTRODUCTION

There has been much recent interest in the classical-quantum correspondence for nonintegrable systems [1,2]. A central tool in this field is the Gutzwiller trace formula (GTF), which expresses the quantum-mechanical density of states for chaotic systems in the semiclassical ($\hbar \to 0$) limit as a sum over contributions from isolated classical periodic orbits [1]. The GTF is not absolutely convergent for real values of the energy E [1], and much effort has been devoted to developing effective resummation methods for direct computation of the level density via the GTF [2]. The GTF can also be used in reverse; that is, Fourier transformation of the measured or computed density of states with respect to a suitable scaled energy variable (for scaling systems) or with respect to $\hbar^{-1}$ for general Hamiltonians yields a power spectrum consisting of peaks associated with classical periodic orbits (see, for example, Refs. [3–8]).

In the primitive semiclassical version of the GTF, the contribution of a given isolated periodic orbit p to the density of states is proportional to $\det|\mathbb{1} - \mathbf{M}_p|^{-\frac{1}{2}}$, where $\mathbf{M}_p$ is the associated monodromy matrix describing linearized motion in the vicinity of the periodic orbit. The GTF then predicts a divergent contribution from periodic orbit p when $\mathbf{M}_p$ (or powers thereof) has a unit eigenvalue, i.e., at bifurcations [9,10]. To repair this deficiency, it is necessary to go beyond the usual simple stationary phase approximation in evaluating the relevant integrals in the theory [9], and several efforts have been made along these lines [11–14].

The failure of the primitive GTF is also manifest in the appearance of "ghost" peaks in the power spectrum of density of states at actions for which there are no *real* classical periodic orbits [7,13,15].

We have recently investigated the classical-quantum correspondence for the coupled quartic oscillator system

$$H = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 + \eta_1 q_1^4 + \eta_2 q_2^4 + \gamma q_1^2 q_2^2 \qquad (1)$$

as a function of coupling parameter γ with $\eta_1 > \eta_2$ fixed [16]. Although this system has been widely studied in the chaotic limit $\gamma \to \infty$ [17–19], we have focused attention on the transition between the integrable $\gamma = 0$ and chaotic limits.

In the present paper, we analyze the quantum density of states for system (1) in the vicinity of γ values at which symmetric isochronous [12] or pitchfork [20] bifurcations of important low action orbits occur, and derive a uniform semiclassical expression for the contribution to the density of states from the set of periodic orbits involved in the bifurcation following the approach of Ozorio de Almeida and Hannay [11] and Ozorio de Almeida and Aguiar [12].

II. PERIODIC ORBITS AND PITCHFORK BIFURCATIONS

In addition to the two primary oscillator periodic orbits (i.e., orbits for which $q_i = p_i = 0$ for $i = 1$ or 2 for all time), over a range of values of γ, there also exist periodic orbits of the form

$$p_1 = \alpha p_2, \qquad q_1 = \alpha q_2, \qquad (2)$$

where

$$\alpha = \pm\left(\frac{2\eta_2 - \gamma}{2\eta_1 - \gamma}\right)^{\frac{1}{2}}. \qquad (3)$$

We refer to these solutions as "diagonal" periodic orbits. The $i = 2$ primary oscillator periodic orbit and the pair of diagonal periodic orbits are shown in Fig. 1 for $\eta_1 = 1.2$, $\eta_2 = 0.8$, and $\gamma = 1.4$. Clearly α is real except in the range $2\eta_2 < \gamma < 2\eta_1$.

The action S_i of a one dimensional quartic oscillator $H = \frac{1}{2}p^2 + \eta_i q^4$ as a function of energy E is

$$S_i = \frac{1}{2\pi}\oint \mathbf{p}\mathbf{dq} = \left(\frac{4K}{3\pi}\right) E^{\frac{3}{4}} \eta_i^{-\frac{1}{4}}, \qquad (4)$$

where $K = 1.854\ldots$ is the complete elliptic integral $K(\frac{1}{2})$ [21]. Expression (4) gives the action of the primary oscillator periodic orbits. Moreover, substituting

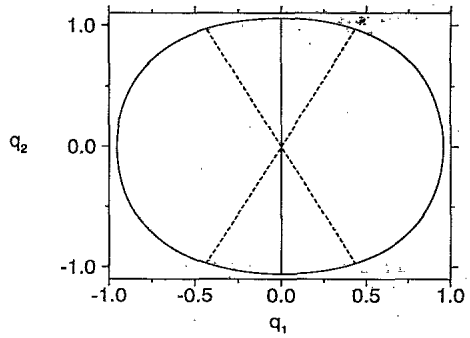

FIG. 1. The $i = 2$ primary oscillator mode and the two diagonal periodic orbits for the coupled quartic oscillator system of Eq. (1) at energy $E = 1.0$. Parameter values: $\eta_1 = 1.2, \eta_2 = 0.8, \gamma = 1.4$.

Eqs. (2) and (3) into (1) yields a quartic oscillator form for the Hamiltonian describing motion along the diagonal orbits, whose actions are given by

$$S_D = \left(\frac{4K}{3\pi}\right) E^{\frac{3}{4}} \left[\frac{4(\eta_1+\eta_2-\gamma)}{4\eta_1\eta_2-\gamma^2}\right]^{\frac{1}{4}}. \tag{5}$$

Note that this action is complex over a smaller range of γ than for α, S_D being real except in the range $2\sqrt{\eta_1\eta_2} < \gamma < \eta_1 + \eta_2$.

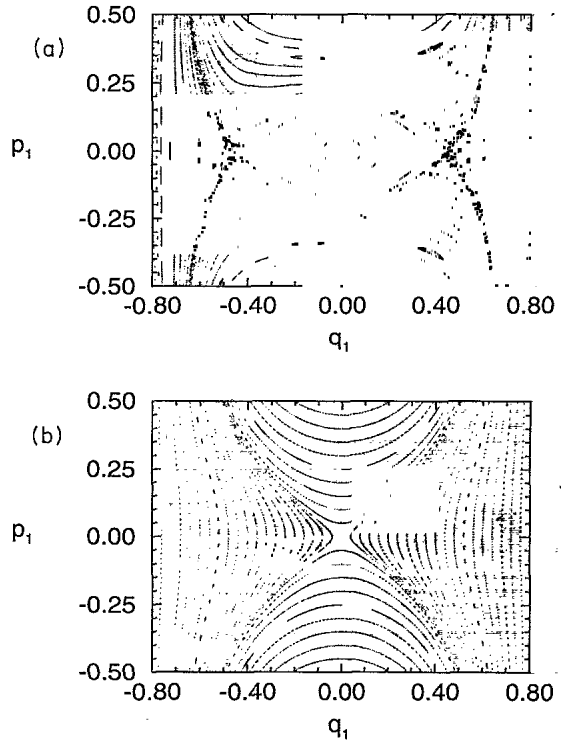

FIG. 2. Surfaces of section with $p_2 = 0$, $E = 1.0$. (a) The central periodic orbit is stable, and is flanked by two unstable diagonal periodic orbits ($\gamma = 1.4$). (b) The diagonal orbits have merged with the central orbit leaving the unstable primary oscillator mode ($\gamma = 1.8$). The classical bifurcation occurs at $\gamma = 1.6$.

From Eq. (3), we see that as γ approaches $2\eta_2$ from below, α approaches zero and the two diagonal orbits approach the $i = 2$ primary oscillator mode. At $\gamma = 2\eta_2$, the two unstable diagonal orbits merge with the oscillator mode. Equations (4) and (5) provide an analytic description of the actions of three periodic orbits as they merge in an "anti-pitchfork" bifurcation [20]. The surfaces of section in Fig. 2 show the effect of the bifurcation on the phase space structure in the vicinity of the primary oscillator periodic orbit. For the coupling parameter value of Fig. 2a, $\gamma = 1.4$, the central orbit is stable and is flanked by two unstable diagonal periodic orbits ($p_1 = 0, q_1 = \pm 0.434$). In Fig. 2b, $\gamma = 1.8$, the diagonal orbits have merged with the central orbit leaving an unstable primary oscillator mode. The classical bifurcation occurs at $\gamma = 2\eta_2 = 1.6$.

Similarly, as γ tends towards $2\eta_1$ from above, α goes to $\pm\infty$ as the diagonal orbits merge with the $i = 1$ primary oscillator mode. At $\gamma = 2\eta_1$ the two stable diagonal orbits merge with the single unstable primary oscillator mode to produce a single stable primary oscillator mode. In the range $2\eta_2 < \gamma < 2\eta_1$ real diagonal orbits do not exist (though they do exist in the complex phase space).

III. SEMICLASSICAL DENSITY OF STATES

The usual derivation of the GTF involves the integration of the semiclassical Green's function over configuration space [1]:

$$\rho(E) \propto \mathrm{Im}[g_{SC}(E)] = \mathrm{Im} \int d\mathbf{q} \quad G_{SC}(\mathbf{q},\mathbf{q};E), \tag{6}$$

with the semiclassical Green's function G_{SC} having the form [1]

$$G_{SC}(\mathbf{q}'',\mathbf{q}';E) = \sum_r \mathcal{A}_r(\mathbf{q}'',\mathbf{q}';E) e^{\frac{2\pi i}{h} S(\mathbf{q}'',\mathbf{q}';E) - \frac{i\mu_r\pi}{2}}, \tag{7}$$

where the sum is taken over classical trajectories r connecting $\mathbf{q}'$ and $\mathbf{q}''$ at energy E. The usual method of taking the trace involves the stationary phase approximation: the only points $\mathbf{q}$ that give a significant contribution to the integral are those points for which the action $S(\mathbf{q},\mathbf{q};E)$ is stationary with respect to variation of $\mathbf{q}$. This stationarity condition implies that the initial and final momenta of the closed trajectory connecting $\mathbf{q}$ with $\mathbf{q}$ are equal, i.e., it is a periodic orbit. The action function $S(\mathbf{q},\mathbf{q};E)$ in the vicinity of the periodic orbit is then expanded up to terms quadratic in small displacements from the orbit, leading to a Fresnel integral and the usual form of the GTF [1].

This primitive semiclassical method, however, breaks down when the periodic orbits are not well separated, as in the vicinity of a pitchfork bifurcation. Close to points in parameter and configuration space where the eigenvalues of the monodromy matrix pass through unity the prefactor $\det|\mathbb{1} - \mathbf{M}_p|^{-\frac{1}{2}}$ diverges, and a higher order approximation to the function $S(\mathbf{q},\mathbf{q};E)$ must be taken [11].

Starting directly with the semiclassical propagator, and using a coordinate system appropriate for describing motion in the vicinity of a given periodic orbit, Ozorio de Almeida and Hannay [11] have derived an expression for the contribution to the density of states from a periodic orbit that may be undergoing a bifurcation. Applying their result to the first occurrence of the $i = 2$ primary oscillator mode we have

$$g_{SC}(E) = (2\pi i\hbar)^{-\frac{3}{2}}\tau A_2 \exp\left[i\left(\frac{2\pi}{\hbar}S_2 - \mu\frac{\pi}{2}\right)\right], \tag{8}$$

where $\tau(E) = \tau^0 E^{-\frac{1}{4}}$ is the period of the orbit, μ is an appropriate index and the orbit amplitude A_2 is defined by

$$A_2 = \int \mathrm{d}Q \left|\frac{\partial^2 S}{\partial Q \partial Q'}\right|^{\frac{1}{2}} \exp\left[\frac{i}{\hbar}S(Q,Q)\right]. \tag{9}$$

Here, $S(Q,Q')$ is the generating function for the Poincaré map $(P,Q) \to (P',Q')$, where the coordinates (P,Q) describe displacements transverse to the central periodic orbit. We define the Poincaré section for motion in the vicinity of the $i = 2$ primary mode by the condition $p_2 = 0$ (this is the condition used to generate the surfaces of section of Fig. 2). With this sectioning condition, the diagonal orbits appear as fixed points at

$$P_D = 0, \tag{10a}$$

$$Q_D = Q_D^0 E^{\frac{1}{4}} = \pm\alpha E^{\frac{1}{4}}\left(\eta_1\alpha^4 + \eta_2 + \gamma\alpha^2\right)^{-\frac{1}{4}}. \tag{10b}$$

A normal form [9] for the generating function $S(Q,Q')$ that gives rise to such a pattern of fixed points is [12]

$$S(Q,Q') = \frac{1}{2}(Q-Q')^2 + aQ^4 + bQ^2, \tag{11}$$

where $4aQ_D^2 + 2b = 0$ from the positions of the fixed points and $aQ_D^4 + bQ_D^2 = 2\pi(S_D - S_2)$ from the actions of the outer periodic orbits. This gives us

$$a = 2\pi\frac{S_2 - S_D}{Q_D^4}, \tag{12a}$$

$$b = 2\pi\frac{2(S_D - S_2)}{Q_D^2}. \tag{12b}$$

The orbit amplitude is then

$$A_2 = \int \mathrm{d}Q \exp\left[\frac{i}{\hbar}(aQ^4 + bQ^2)\right]$$
$$= \frac{\pi}{2}|Q_D| e^{\frac{2\pi i}{2\hbar}(S_D - S_2)}\left[J_{-\frac{1}{4}}\left(2\pi\tfrac{|S_2-S_D|}{2\hbar}\right)e^{\sigma_a\frac{i\pi}{8}}\right.$$
$$\left. -\sigma_a\sigma_b J_{\frac{1}{4}}\left(2\pi\tfrac{|S_2-S_D|}{2\hbar}\right)e^{-\sigma_a\frac{i\pi}{8}}\right], \tag{13}$$

where $\sigma_a = \mathrm{sgn}(a)$, $\sigma_b = \mathrm{sgn}(b)$, and $J_\nu(x)$ is the Bessel function of order ν. The contribution to the density of states due to the first occurrence of this orbit is therefore

$$g_{SC}(E) = \frac{\pi}{2}(2\pi i\hbar)^{-\frac{3}{2}}\tau^0|Q_D^0| e^{i[\frac{\pi}{\hbar}(S_D+S_2)-\mu\frac{\pi}{2}]}$$
$$\times\left[J_{-\frac{1}{4}}\left(2\pi\tfrac{|S_2-S_D|}{2\hbar}\right)e^{\sigma_a\frac{i\pi}{8}}\right.$$
$$\left. -\sigma_a\sigma_b J_{\frac{1}{4}}\left(2\pi\tfrac{|S_2-S_D|}{2\hbar}\right)e^{-\sigma_a\frac{i\pi}{8}}\right]. \tag{14}$$

In the limit of well separated periodic orbits we have $|S_2 - S_D|$ large compared to $\hbar$, and we can take the asymptotic limits of the Bessel functions [21], $J_\nu(z) \to \left(\frac{2}{\pi z}\right)^{\frac{1}{2}}\cos(z - \frac{1}{2}\nu\pi - \frac{1}{4}\pi)$. With $\sigma_b = \sigma_a$, so that only one periodic orbit exists in the real phase space, we have

$$g_{SC}(E) = \sigma_a'\frac{\tau}{2\pi i\hbar\,(2|b|)^{\frac{1}{2}}}e^{i\left(\frac{2\pi}{\hbar}S_2 - \mu\frac{\pi}{2}\right)}. \tag{15}$$

However, from the form of the generating function, we have $|\det(M_2 - \mathbb{1})| = 2|b|$, where M_2 is the monodromy matrix for the $i = 2$ primary oscillator mode, so that

$$g_{SC}(E) = \sigma_a'\frac{\tau}{2\pi i\hbar\,|\det(M_2 - \mathbb{1})|^{\frac{1}{2}}}e^{i\left(\frac{2\pi}{\hbar}S_2 - \mu\frac{\pi}{2}\right)} \tag{16}$$

(where $\sigma_a' = 1$ for $a > 0$ and $\sigma_a' = -i$ for $a < 0$), which is the usual stationary phase result.

In the case $\sigma_b = -\sigma_a$, where the three periodic orbits exist, we have

$$g_{SC}(E) = \frac{\tau}{2\pi i\hbar\,|2b|^{\frac{1}{2}}}$$
$$\times\left[\sigma_{-a}' e^{i\left(\frac{2\pi}{\hbar}S_2 - \mu\frac{\pi}{2}\right)} + \sigma_a'\sqrt{2}e^{i\left(\frac{2\pi}{\hbar}S_D - \mu\frac{\pi}{2}\right)}\right]. \tag{17}$$

By expanding the generating function about the outer fixed points, we find that $|\det(M_D - \mathbb{1})| = \sqrt{4|b|}$ so that in this case

$$g_{SC}(E) = \frac{\sigma_{-a}'\tau}{2\pi i\hbar\,|\det(M_2 - \mathbb{1})|^{\frac{1}{2}}}e^{i\left(\frac{2\pi}{\hbar}S_2 - \mu\frac{\pi}{2}\right)}$$
$$+2\frac{\sigma_a'\tau}{2\pi i\hbar\,|\det(M_D - \mathbb{1})|^{\frac{1}{2}}}e^{i\left(\frac{2\pi}{\hbar}S_D - \mu\frac{\pi}{2}\right)}. \tag{18}$$

The factor 2 arises in the second term because there are two diagonal orbits. The period appearing in the second term is that of the single oscillator mode rather than the diagonal orbit, but otherwise the result is as for the stationary phase limit.

For completeness, we note that $S_2 = S_D$ and $Q_D = 0$ exactly at the bifurcation point, so that we must use a Taylor expansion of the terms a and b in $(2\eta_2 - \gamma)$ in order to obtain their limits. We find $b = 0$, $a = \frac{2}{3}(\eta_2 - \eta_1)K(E\eta_2)^{-\frac{1}{4}}$. Using the standard integral for $\int \exp(\frac{i}{\hbar}aQ^4)dQ$ we obtain

$$g_{SC}(E) = \frac{\tau}{(2\pi i\hbar)^{\frac{3}{2}}}\frac{\Gamma\left(\frac{1}{4}\right)}{2}\left(\frac{\hbar}{|a|}\right)^{\frac{1}{4}}$$
$$\times\exp\left(\frac{2\pi i}{\hbar}S_2 - \frac{\mu\pi}{2} + i\sigma_a\frac{\pi}{8}\right) \tag{19}$$

for the contribution to the density of states exactly at the bifurcation point.

IV. COMPARISON WITH NUMERICAL RESULTS

We now examine the manifestation of the pitchfork bifurcation in the quantum spectrum of system (1) by computing the Fourier transform of the density of states. The first 1000 energy levels of A_1 symmetry are calculated by matrix diagonalization for a range of γ values around the pitchfork bifurcation of the $i = 2$ primary mode, with $\eta_1 = 1.2$ and $\eta_2 = 0.8$. The power spectrum of the resulting density of states with respect to the scaled energy variable $\epsilon = E^{\frac{5}{4}}$ [17] is shown in Fig. 3(a). As a guide to the eye, the Fourier transform of the density of states at the actual bifurcation point is plotted as a thick line. With the chosen parameter values there are no other periodic orbits with action sufficiently close to S_2 to interfere with the bifurcation phenomenon under study. A peak does however appear at the high end of the action range in Fig. 3(a). This peak results from another (known) periodic orbit that is undergoing no bifurcations in this range of γ, and is well separated from the action region of interest.

For comparison, the Fourier transform of the functions (14) and (19) as appropriate are shown in Fig. 3(b)for the same parameter values with all terms being calculated analytically. The Fourier transform is taken over the same window as the computed quantum density of states with the same Blackman-Harris windowing function [22]. The numerical results have been scaled so that the maxima in Figs. 3(a) and 3(b) have the same value.

The numerical and theoretical figures are very similar, showing that the uniform semiclassical treatment gives an accurate description of the contribution to the density of states from those periodic orbits involved in the pitchfork bifurcation. Both the theoretical and numerical plots show clearly the coalescence of the peaks corresponding to the two action values associated with the

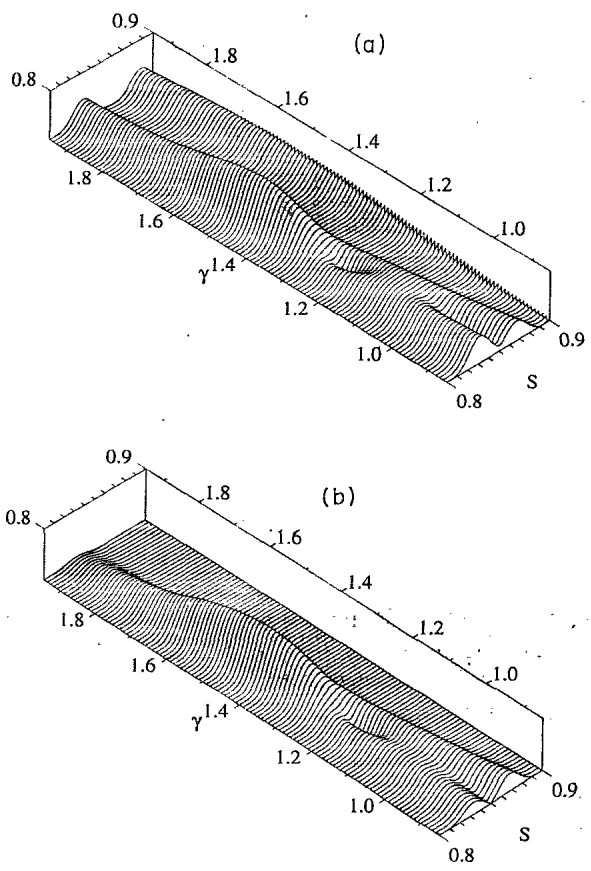

FIG. 3. Power spectra of the density of states for coupled quartic oscillator system Eq. (1) for S (reduced action) values close to that of the $i = 2$ primary mode periodic orbit, $S_2 = 0.832$, for a range of coupling parameter values in the vicinity of the classical bifurcation point, $\gamma = 1.6$. (a) Numerical result obtained by matrix diagonalization. (b) Analytical result obtained from Eqs. (14) and (19).

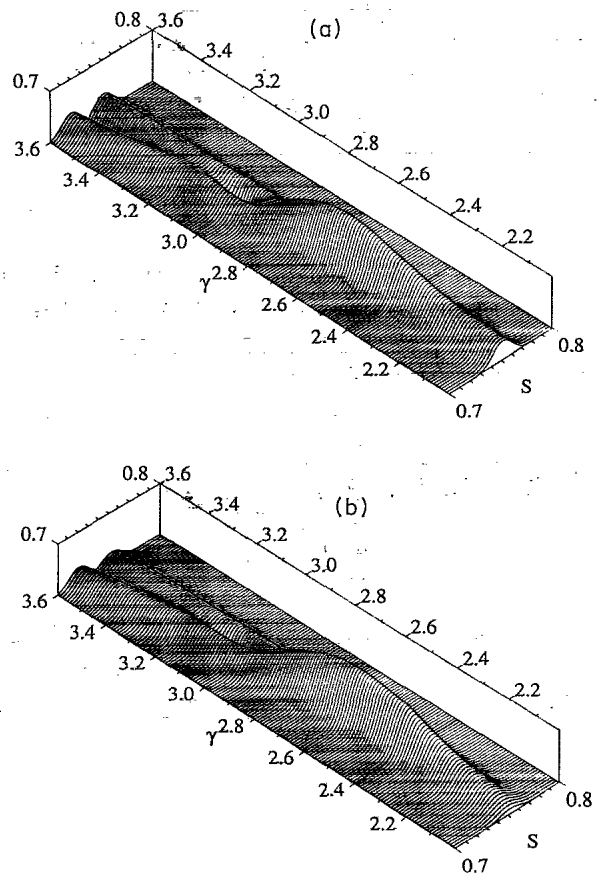

FIG. 4. Power spectra of the density of states for coupled quartic oscillator system Eq. (1) for S (reduced action) values close to that of the $i = 1$ primary mode periodic orbit, $S_1 = 0.752$, for a range of coupling parameter values in the vicinity of the classical bifurcation point, $\gamma = 2.4$. (a) Numerical result obtained by matrix diagonalization. (b) Analytical result obtained from Eqs. (14) and (19).

merging classical orbits. Note the "premature death" of the pair of action peaks, which merge at a γ value distinctly below the classical bifurcation value $2\eta_2$. Observe also that the absolute maximum in the Fourier transform is shifted away from the classical bifurcation point; this shift is analogous to the displacement of the rainbow maximum in elastic differential cross sections away from the classical rainbow angle [23]. Both theory and numerical results also show an interesting secondary rise in the peak heights further away from the bifurcation (note the filling up of the trough between the two major peaks), analogous to the existence of supernumerary rainbow peaks in elastic scattering differential cross sections [23]. For γ well below the bifurcation value, when the generating function (11) no longer provides a good approximation to the Poincaré section, the theoretical prediction is less accurate. On the single orbit side of the bifurcation, the quartic expansion of generating function (11) is only reasonable very close to the bifurcation, as the action of the imaginary periodic orbit goes rapidly to infinity as $\gamma \to 2\sqrt{\eta_1\eta_2}$.

Figure 4 shows analogous plots for the symmetric pitchfork bifurcation of the $i = 1$ primary mode, which occurs at $\gamma = 2.4$.

V. CONCLUSION

In this paper, using the general approach of Ozorio de Almeida and Hannay [9,11], we have quantitatively analyzed the effect of a classical pitchfork bifurcation on the quantum density of states in a simple case where the actions of all relevant periodic orbits could be calculated analytically. In the general case of a pitchfork bifurcation, the actions of the relevant periodic orbits and the parameters of the corresponding generating function would have to be determined numerically. Nevertheless, the general expressions derived here provide a functional form for the contribution to the density of states near a pitchfork bifurcation that can be fitted to numerical results at a small number of parameter values.

ACKNOWLEDGMENTS

We acknowledge helpful conversations with Dr. R.J. Hinde. K.A. has received financial support from NATO-SERC. This work was supported by NSF Grant No. CHE-9101357. Computations reported here were performed on the Cornell National Supercomputer Facility, which is supported in part by NSF and IBM Corporation.

[1] M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer-Verlag, Berlin, 1990).
[2] See, *Chaos and Quantum Physics*, edited by M.-J. Giannoni, A. Voros, and J. Zinn-Justin (Elsevier, New York, 1991); *Quantum Chaos*, Proceedings of the International School of Physics "Enrico Fermi" Course CX IX, Varenna, 1991, edited by G. Casati, I. Guarneri, and U. Smilansky (North-Holland, Amsterdam, 1993).
[3] D. Wintgen, Phys. Rev. Lett. **58**, 1589 (1987).
[4] M.L. Du and J.B. Delos, Phys. Rev. A **38**, 1896 (1988); **38**, 1913 (1988).
[5] J.-H. Kim and G.S. Ezra, in *Quantum Chaos*, Proceedings of the Adriatico Workshop, edited by H.A. Cerdeira, R. Ramaswamy, M.C. Gutzwiller, and G. Casati (World Scientific, Singapore, 1991).
[6] C.P. Malta and A.M. Ozorio de Almeida, J. Phys. A **23**, 4137 (1990).
[7] M. Kuś, F. Haake, and B. Eckhardt, Z. Phys. B **92**, 221 (1993).
[8] M. Baranger, M.R. Haggerty, B. Lauritzen, D.C. Meredith, and D. Provost (unpublished).
[9] A.M. Ozorio de Almeida, *Hamiltonian Systems: Chaos and Quantization* (Cambridge University, Cambridge, England, 1988).
[10] J.M. Mao and J.B. Delos, Phys. Rev. A **45**, 1746 (1992).
[11] A.M. Ozorio de Almeida and J.H. Hannay, J. Phys. A **20**, 5873 (1987); C.P. Malta, M.A.M. de Aguiar, and A.M. Ozorio de Almeida, Phys. Rev. A **47**, 1625 (1993).
[12] A.M. Ozorio de Almeida and M.A.M. de Aguiar, Physica D **41**, 391 (1990).
[13] M. Kuś, F. Haake, and D. Delande, Phys. Rev. Lett. **71**, 2167 (1993).
[14] M.W. Biems and G. Alber, Phys. Rev. A **48**, 3123 (1993).
[15] R. Scharf and B. Sundaram (unpublished).
[16] K. Atkins and G.S. Ezra (unpublished).
[17] B. Eckhardt, G. Hose, and E. Pollak, Phys. Rev. A **39**, 3776 (1989).
[18] C.C. Martens, R.L. Waterland, and W.P. Reinhardt, J. Chem. Phys. **90**, 2328 (1989).
[19] O. Bohigas, S. Tomsovic, and D. Ullmo, Phys. Rep. **223**, 43 (1993).
[20] K.R. Meyer, J.B. Delos, and J.-M. Mao (unpublished).
[21] M. Abramovitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).
[22] F.J. Harris, Proc. IEEE **66**, 51 (1978).
[23] M.V. Berry and K. Mount, Rep. Prog. Phys. **35**, 315 (1972).