Semiclassical analysis of spin systems near critical energies

Pedro Ribeiro[1] and Thierry Paul[2]

[1]*Laboratoire de Physique Théorique de la Matière Condensée, CNRS UMR 7600, Université Pierre et Marie Curie,*
4 Place Jussieu, 75252 Paris Cedex 05, France

[2]*CNRS, DMA, École Normale Supérieure, 45 rue d'Ulm, 75230 Paris Cedex 05, France*

The spectral properties of su(2) Hamiltonians are studied for energies near the critical classical energy ε_c for which the corresponding classical dynamics presents hyperbolic points. A general method leading to an algebraic relation for eigenvalues in the vicinity of ε_c is obtained in the thermodynamic limit, when the semiclassical parameter $n^{-1} = (2s)^{-1}$ goes to zero (where s is the total spin of the system). Two applications of this method are given and compared with numerics. Matrix elements of observables, computed between states with energy near ε_c, are also computed and shown to be in agreement with the numerical results.

PACS number(s): 03.65.Sq, 05.30.−d, 21.60.Ev

I. INTRODUCTION

Bohr-Sommerfeld (BS) rules determine the allowed quantized eigenenergies of integrable Hamiltonians by semiclassical analysis and are valid for energies corresponding to regular classical orbits. Nonregular orbits, usually called separatrix curves, correspond to a changing of topology of the orbits and to the appearance of hyperbolic fixed points (HP) of the flow equations, characterized in phase space by their stable and unstable manifolds.

BS quantization formulas for nonregular values of the energy parameter have been set up in [1,2] in the case of Schrödinger operators acting on spaces of square-integrable functions. They differ from the regular case and show a logarithmic accumulation of the spectrum near energies corresponding to hyperbolic fixed points. The phase-space version of such rules, obtained using the coherent-state representation, is better suited for generalizing such results to other cases as the one of collective su(2)-spin systems, a situation uncovered by earlier results.

su(2) Hamiltonians arise naturally in many areas of physics, in the study of mutually interacting spin-1/2 systems or due to symmetries present in collective bosonic and fermionic Hamiltonians. A typical example is given by the Lipkin-Meshkov-Glick (LMG) model proposed in 1965 to describe shape phase transition in nuclei [3]. This model is used to describe magnetic properties of molecules [4], interacting bosons in double-well structures [5] and to investigate the role of entanglement in quantum phase transitions (QPTs) [6]. The Hamiltonian of this system can be expressed in terms of the total spin operators $S_\alpha = \frac{1}{2} \sum_{i=1}^n \sigma_\alpha^i$, where σ^i's are the Pauli matrices,

$$H = -\frac{1}{n}(\gamma_x S_x^2 + \gamma_y S_y^2) - h S_z^2. \tag{1}$$

Considering only the fully symmetric sector ($s = n/2$), a semiclassical-like limit can be obtained when the number of interacting spin-1/2 subsystems n increases (thermodynamic limit). The role of the usual semiclassical parameter $\hbar$ is replaced by the inverse of the number of interacting subsystems n^{-1}, which fixes the dimension of the su(2) representation to $n+1$. This semiclassical-like approach coincides

with the usual mean-field approximation to zeroth order in n^{-1} and is similar to the WKB approximation [7]. It has permitted to derive the spectral properties for the LMG model in the large-n limit [8] as well as finite-size corrections in powers of n^{-1} and to compute mean values of observables characterizing the eigenstates within the spectrum [9].

QPT [10] arising at zero temperature are related to nonanalyticities of the ground state as a function of the Hamiltonian coupling constants. Since the nonanalyticities involved are generically algebraic, this kind of phase transitions are characterized by a set of critical exponents describing how physical quantities (density of states, excitation gap, observables) behave in the vicinity of such points. Recently, nonanalyticities arising within the spectrum have received much interest [8,9,11]; they can be viewed as QPT arising for excited states [12]. In the semiclassical limit, this phenomenon corresponds to a change in the topology of classical orbits and the appearance of HP. The nonanalyticities involved are generically found to be logarithmic [8,11,12], actually a general fact due to (features of) hyperbolicity [13].

In this paper a general method is constructed to overcome the breakdown of standard BS quantization near singular spectral points in the case of spins systems. Even if only leading-order results are derived, this method can be extended to compute higher-order corrections in the semiclassical parameter n^{-1} and should also be generalizable to Lie groups other than SU(2). Spectral analytical expressions are derived and tested numerically for two different situations arising within an LGM-like model (LMG plus a cubic term) where hyperbolic trajectories, homoclinic, and heteroclinic exist. Finally, matrix elements of observables are computed, both analytically and numerically, between states near critical energies. Their semiclassical behavior is discussed hoping to clarify critical phenomena arising at the so-called excited states QPT.

II. BS QUANTIZATION AND WKB

The non-normalized spin coherent states [14] for an su(2) representation of dimension $2s+1$ are defined by $|\alpha\rangle = e^{\alpha S_+}|s, -s\rangle$, $\bar\alpha \in \mathbb{C}$, with s, integer or half integer, being the

total spin (in the following we set $n=2s$). They form an overcomplete basis with a resolution of the identity given by $\int d\mu \frac{|\alpha\rangle\langle\alpha|}{\langle\alpha|\alpha\rangle}=1$, where $d\mu=\frac{d\,\mathrm{Re}(\alpha)d\,\mathrm{Im}(\alpha)}{\pi}\frac{n+1}{(1+\bar{\alpha}\alpha)^2}$ and $\langle\alpha|\alpha\rangle=(1+\bar{\alpha}\alpha)^n$. In the coherent states basis, the su(2) generators $(S_\pm=S_x\pm iS_y)$ act as differential operators

$$S_+ = n\bar{\alpha}-\bar{\alpha}^2\partial_{\bar{\alpha}}; \quad S_- = \partial_{\bar{\alpha}}; \quad S_z = -\frac{n}{2}+\bar{\alpha}\partial_{\bar{\alpha}}, \quad (2)$$

on the space of polynomial functions $\Psi(\bar{\alpha})=\langle\alpha|\Psi\rangle$ of degree n. To a generic operator,

$$\hat{A} = \sum_i p_i(\bar{\alpha})(n^{-1}\partial_{\bar{\alpha}})^i, \quad (3)$$

where the p_i's are polynomials in $\bar{\alpha}$, is associated with a function (symbol) $\mathcal{A}(\bar{\alpha},\zeta)=\Sigma_i p_i(\bar{\alpha})\zeta^i$.

In the framework of the WKB approximation, eigenstates of an Hermitian operator

$$\mathcal{H}(\bar{\alpha},n^{-1}\partial_{\bar{\alpha}})\Psi(\bar{\alpha})=\varepsilon\Psi(\bar{\alpha}) \quad (4)$$

are obtained considering $G(\bar{\alpha})=n^{-1}\partial_{\bar{\alpha}}\ln\Psi(\bar{\alpha})$, the logarithmic derivative of the wave function,

$$\Psi(\bar{\alpha}) = \exp\left[n\int_{\bar{\alpha}_I}^{\bar{\alpha}}G(\bar{\alpha}')d\bar{\alpha}'\right], \quad (5)$$

where $\bar{\alpha}_I\in\mathbb{C}$ fixes the normalization: $\Psi(\bar{\alpha}_I)=1$. The function G is obtained solving perturbatively the Riccati-like equation

$$\mathcal{H}[\bar{\alpha},G(\bar{\alpha})+n^{-1}\partial_{\bar{\alpha}}]=\varepsilon, \quad (6)$$

in powers of the semiclassical parameter n^{-1}, setting

$$\mathcal{H}(\bar{\alpha},\zeta) = \sum_{i=0}^{\infty}n^{-i}\mathcal{H}_i(\bar{\alpha},\zeta), \quad (7)$$

$$G(\bar{\alpha}) = \sum_{i=0}^{\infty}n^{-i}G_i(\bar{\alpha}); \quad \varepsilon = \sum_{i=0}^{\infty}n^{-i}\varepsilon_i. \quad (8)$$

The result is the WKB solution [7], given in terms of $\mathcal{H}_i[\bar{\alpha},G_0(\bar{\alpha})]$,

$$\Psi_{\mathrm{WKB}}(\bar{\alpha})$$
$$= \sqrt{\frac{\partial_\zeta\mathcal{H}_0[\bar{\alpha}_I,G_0(\bar{\alpha}_I)]}{\partial_\zeta\mathcal{H}_0[\bar{\alpha},G_0(\bar{\alpha})]}}\exp\left(n\int_{\bar{\alpha}_I}^{\bar{\alpha}}d\bar{\alpha}'\left\{G_0(\bar{\alpha}')\right.\right.$$
$$\left.\left.+\frac{1}{n}\frac{\varepsilon_1-\mathcal{H}_1[\bar{\alpha}',G_0(\bar{\alpha}')]+\frac{1}{2}\partial_\zeta\partial_{\bar{\alpha}}\mathcal{H}_0[\bar{\alpha}',G_0(\bar{\alpha}')]}{\partial_\zeta\mathcal{H}_0[\bar{\alpha}',G_0(\bar{\alpha}')]}\right\}\right)$$
$$\times[1+O(n^{-1})].$$

Quantization of the energies is obtained by imposing that $\Psi(\bar{\alpha})$ is a single-valued function of $\bar{\alpha}\in\mathbb{C}$, implying that

$$\mathcal{I}[\gamma] \equiv -\frac{1}{2\pi i}\oint_\gamma d\bar{\alpha}\,G(\bar{\alpha})=\frac{k}{n}, \quad (9)$$

with $k\in\mathbb{N}$, for all closed paths γ. In the semiclassical limit the probability amplitude $\langle\alpha|\alpha\rangle^{-1}|\Psi(\bar{\alpha})|^2$ of finding the system in the coherent state $|\alpha\rangle$ is exponentially localized on the classical trajectory $\mathcal{C}_0=\{\bar{\alpha}:\mathcal{H}_0(\bar{\alpha},\frac{\alpha}{1+\bar{\alpha}\alpha})=\varepsilon_0\}$, along which $G_0|_{\mathcal{C}_0}=\frac{\alpha}{1+\bar{\alpha}\alpha}$. Moreover, if $\mathcal{C}_0$ contains no singular point (fixed point of the flow), the WKB solution is an analytic function of $\bar{\alpha}$ in a neighborhood of $\mathcal{C}_0$: this is indeed a consequence of the implicit function theorem, as $\partial_\zeta\mathcal{H}_0(\bar{\alpha},\mathcal{C}_0)|_{\mathcal{C}_0}=\dot{\bar{\alpha}}\neq 0$. In this case $\mathcal{I}=\mathcal{I}[\mathcal{C}_0]$, given by Eq. (9), can be explicitly computed using the semiclassical expansion of G. The result is the Bohr-Sommerfeld quantization condition for a spin system,

$$\mathcal{I} = \mathcal{I}_0 + n^{-1}\mathcal{I}_1 + O(n^{-2})=n^{-1}k, \quad (10)$$

where

$$\mathcal{I}_0 = -\frac{1}{2\pi i}\oint_{\mathcal{C}_0}d\bar{\alpha}\frac{\alpha}{1+\bar{\alpha}\alpha}=\frac{1}{2\pi i}\int_\Sigma\omega \quad (11)$$

is the classical action obtained by integrating the symplectic two-form $\omega=(1+\bar{\alpha}\alpha)^{-2}d\bar{\alpha}\wedge d\alpha$ over the interior of the classical trajectory Σ, and

$$\mathcal{I}_1 = \frac{1}{2}-\frac{1}{2\pi i}\oint_{\mathcal{C}_0}d\bar{\alpha}\frac{\varepsilon_1-\mathcal{H}_1+\frac{1}{2}\partial_\zeta\partial_{\bar{\alpha}}\mathcal{H}_0}{\partial_\zeta\mathcal{H}_0}. \quad (12)$$

Different formulations of such Bohr-Sommerfeld formulas were obtained in several previous works [5,7,15,16]. They are valid for nonsingular values of the energy parameter where the action $\mathcal{I}$ can indeed be expanded in powers of n^{-1}. Section IV deals with the critical case where $\mathcal{I}$ can no longer be expanded in this simple form.

III. QUANTIZATION NEAR HP

The dynamics on the Riemann sphere can be understood in terms of the conjugated variables $\bar{\alpha}$ and $\zeta=\frac{\alpha}{1+\bar{\alpha}\alpha}$ for which the classical flow associated with the Hamiltonian function $\mathcal{H}_0(\bar{\alpha},\zeta)$ is simply given by

$$\dot{\bar{\alpha}} = i\partial_\zeta\mathcal{H}_0(\bar{\alpha},\zeta), \quad \dot{\zeta}=-i\partial_{\bar{\alpha}}\mathcal{H}_0(\bar{\alpha},\zeta). \quad (13)$$

The energy hypersurface, which is a flow invariant, is generically a smooth manifold except if it contains fixed points $(\dot{\bar{\alpha}}=0,\dot{\zeta}=0)$. Fixed points are said to be hyperbolic (or unstable) if their phase-space distance to a generic neighbor point increases exponentially along the evolution imposed by flow equations (for short times). The neighborhood of $(\bar{\alpha},\zeta)$ contains the so-called stable and unstable manifolds. It has been proven, in full generality and for any dimension, that the existence of HP (or manifolds of HP) is associated with a divergence in the density of states which is, most of the times, of logarithmic nature [13].

If an HP exists along classical trajectory for some $\bar{\alpha}_i\in\mathcal{C}_0$, $\mathcal{I}_1$ diverges and the quantization condition has to be
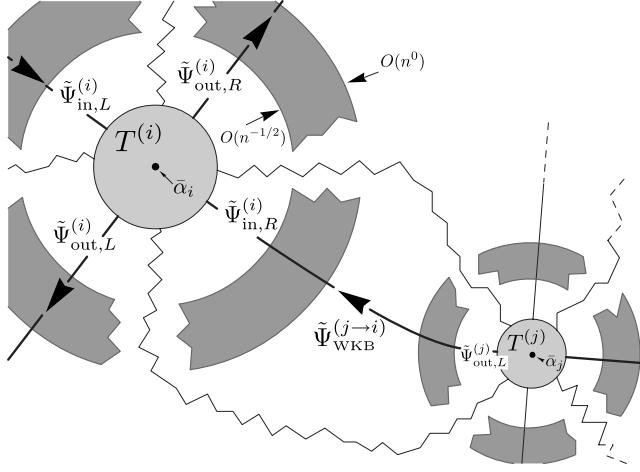
FIG. 1. Phase space portrait of a classical trajectory $\mathcal{C}_0$ (full lines) describing a critical orbit passing through two HP $\bar{\alpha}_i$ and $\bar{\alpha}_j$. For $O(n^{-1/2}) < |\bar{\alpha} - \bar{\alpha}_i| < O(n^0)$ both the linearized solutions around HP point and the WKB solutions coexist (dark gray region), permitting to identify both asymptotic behaviors. The "in" and "out" solutions are connected via the $T^{(i)}$ matrices. Branch cuts of the WKB solutions are displayed as broken lines.

modified for energies of order n^{-1} around the critical energy $\varepsilon_0 = \varepsilon_c$. The method used here to overcome this difficulty is the phase-space equivalent to the ones developed for standard Schrödinger operators [1,2]. It uses the WKB wave-function approximation away from HP and the solutions of a linearized version of Eq. (4) in their vicinity that are explicitly given in terms of special functions. Quantization follows by imposing the accordance of both asymptotic behaviors, from WKB and from the linearized Hamiltonian solutions, on the neighborhood of the HP since this accord is possible only for the values of the energy belonging to the spectrum of the Hamiltonian.

In the vicinity of an HP, setting $\bar{\beta} = \bar{\alpha} - \bar{\alpha}_i$, $\mathcal{H}$ can be linearized and brought to the form

$$\tilde{\mathcal{H}}(\bar{\beta}, \zeta) - \varepsilon = \tau_2 \zeta^2 + \tau_0 \bar{\beta}^2 + \frac{\tau_{00} - \varepsilon_1}{n} + O(|\bar{\beta}|^3), \quad (14)$$

by a simple transformation $\Psi(\bar{\alpha}) = \exp[np(\bar{\beta})]\tilde{\Psi}(\bar{\beta})$, where p is a second-order polynomial of $\bar{\beta}$. The constants τ_k depend on the parameters of the Hamiltonian around the HP. The solutions of $[\tilde{\mathcal{H}}(\bar{\beta}, n^{-1}\partial_{\bar{\beta}}) - \varepsilon]\tilde{\Psi}(\bar{\beta}) = 0$ are given explicitly by Parabolic Cylinder functions [17]. Let us mention that connection formulas for semiclassical approximations involving Parabolic Cylinder functions appeared already in the literature, although in a different context [18,19]. The following wave functions are linear combinations of the two independent solutions, having a well-defined behavior when $|\bar{\beta}|n^{1/2} \to \infty$, for $\bar{\beta}$ in a vicinity of $\mathcal{C}_0$ (see Fig. 1 for the directions along which each limit is taken),

$$\left.\begin{array}{r}\tilde{\Psi}_{\mathrm{out},R}(\bar{\beta}) \\ \tilde{\Psi}_{\mathrm{out},L}(\bar{\beta})\end{array}\right\} \to \exp(-\mathrm{i}n\rho^2\bar{\beta}^2)\bar{\beta}^{-1/2+\mathrm{i}\eta}[1 + O(|\bar{\beta}|^{-1}n^{-1/2})],$$

TABLE I. Regularized action integrals.

Heteroclinic	$2\pi\mathrm{i}S(\bar{\alpha}_i,\bar{\alpha}_j) = 2\pi\mathrm{i}S_{i,j} + \frac{1}{n}\{\nu_j \ln[(-1)^{\sigma_j}(\bar{\alpha}_i - \bar{\alpha}_j)]$ $\quad - \nu_i \ln[(-1)^{\sigma_i}(\bar{\alpha}_j - \bar{\alpha}_i)] + \sigma_i \mathrm{i}\pi\nu_i - \sigma_j \mathrm{i}\pi\nu_j\},$ $2\pi\mathrm{i}S_{i,j} = \int_{\bar{\alpha}_j}^{\bar{\alpha}_i} \frac{\alpha}{1+\bar{\alpha}\alpha}d\bar{\alpha} - \frac{1}{n}\int_{\bar{\alpha}_j}^{\bar{\alpha}_i} \partial_{\bar{\alpha}}[(\bar{\alpha} - \bar{\alpha}_i)(\bar{\alpha} - \bar{\alpha}_j)G_1]$ $\quad \times \frac{\ln[(-1)^{\sigma_i}(\bar{\alpha} - \bar{\alpha}_i)] - \ln[(-1)^{\sigma_j}(\bar{\alpha} - \bar{\alpha}_j)]}{\bar{\alpha}_i - \bar{\alpha}_j}d\bar{\alpha}$
Homoclinic	$2\pi\mathrm{i}S(\bar{\alpha}_i,\bar{\alpha}_i) = 2\pi\mathrm{i}S_i + \frac{\mathrm{i}\pi\sigma}{n},$ $2\pi\mathrm{i}S_i = \int_{\bar{\alpha}_j}^{\bar{\alpha}_i} \frac{\alpha}{1+\bar{\alpha}\alpha}d\bar{\alpha} - \frac{1}{n}\int_{\bar{\alpha}_j}^{\bar{\alpha}_i}\ln[(-1)^{\sigma}(\bar{\alpha} - \bar{\alpha}_i)]$ $\quad \times \partial_{\bar{\alpha}}[(\bar{\alpha} - \bar{\alpha}_i)G_1]d\bar{\alpha}$

$$\left.\begin{array}{r}\tilde{\Psi}_{\mathrm{in},L}(\bar{\beta}) \\ \tilde{\Psi}_{\mathrm{in},R}(\bar{\beta})\end{array}\right\} \to \exp(\mathrm{i}n\rho^2\bar{\beta}^2)\bar{\beta}^{-1/2-\mathrm{i}\eta}[1 + O(|\bar{\beta}|^{-1}n^{-1/2})],$$

where $\rho = |\frac{\tau_0}{4\tau_2}|^{1/4}$ and $\eta = \frac{\varepsilon_1 - \tau_{00}}{4\rho^2\tau_2}$. Being solutions of a second-order differential equation, these four functions are obviously not independent. The explicit form of the Parabolic Cylinder functions provides a "connection" between different asymptotic regions

$$\begin{pmatrix}\tilde{\Psi}_{\mathrm{out},L} \\ \tilde{\Psi}_{\mathrm{out},R}\end{pmatrix} = T\begin{pmatrix}\tilde{\Psi}_{\mathrm{in},R} \\ \tilde{\Psi}_{\mathrm{in},L}\end{pmatrix}, \quad (15)$$

$$T = \begin{pmatrix} c - \bar{c}^{-1}e^{-2\pi\eta} & \bar{c}^{-1}e^{-2\pi\eta} \\ \bar{c}^{-1} & -\bar{c}^{-1}\end{pmatrix} + O(n^{-1}), \quad (16)$$

with $c = \sqrt{\frac{2e^{-\pi\eta}}{\pi}}\cosh(\pi\eta)\exp\{-\mathrm{i}[\eta \ln(4n\rho^2) + \frac{\pi}{2}]\}\Gamma(\mathrm{i}\eta + \frac{1}{2})$.

Constrains of type (15) give a set of local relations between the "in" and "out" bases. A set of nonlocal relations is obtained by identifying the asymptotics of WKB solutions (see Fig. 1), leading to

$$\tilde{\Psi}_{\mathrm{out},L}^{(j)} = \exp[2\pi\mathrm{i}nS(\bar{\alpha}_i,\bar{\alpha}_j)]\tilde{\Psi}_{\mathrm{in},R}^{(i)}, \quad (17)$$

where $S(\bar{\alpha}_i, \bar{\alpha}_j)$ is the regularized action integral given in Table I, $\nu_j = (\pm \mathrm{i}\,\eta_j - \frac{1}{2})$ depending on the side R/L and j indexing HP. $\ln(x)$ is defined as having a branch cut along the negative real axes. $\sigma_k = 0, \pm 1$: 0 if the classical orbit does not cut the branch cut of $\ln(\bar{\alpha} - \bar{\alpha}_k)$ and ± 1 if it cuts it in the up-down or down-up directions, respectively. Summarizing the local and nonlocal basis relations

$$\boldsymbol{\Psi}_{\mathrm{out}} = \mathbf{T}\boldsymbol{\Psi}_{\mathrm{in}}; \quad \boldsymbol{\Psi}_{\mathrm{out}} = \boldsymbol{\Gamma}\boldsymbol{\Psi}_{\mathrm{in}}, \quad (18)$$

where $\boldsymbol{\Psi}_{\mathrm{out}}$ and $\boldsymbol{\Psi}_{\mathrm{in}}$ are column vectors collecting the in and out solutions for each HP (i), $\mathbf{T}$ and $\boldsymbol{\Gamma}$ are matrices, the first coupling states with the same (i) and the second coupling sates with (i) and (j) linked by the classical trajectory. Quantization is obtained by imposing the compatibility relation

$$D = \det(\mathbf{T} - \boldsymbol{\Gamma}) = 0. \quad (19)$$

We now apply the general method presented above to a particular spin Hamiltonian
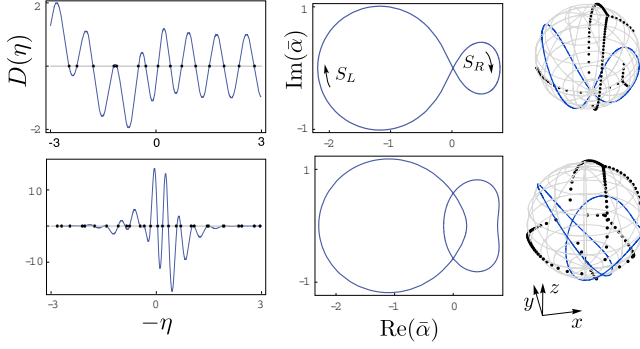
FIG. 2. (Color online) Homoclinic case (up): $h=1$; $\gamma_x=4$; $\gamma_y=1/4$; $\mu=5$. Heteroclinic case (down): $h=1$; $\gamma_x=5$; $\gamma_y=2$; $\mu=6$. Left: comparison between the zeros of D (blue line) and the eigenvalues of Eq. (20) computed numerically (black dots) for $n=500$. We define the renormalized energy $\eta=-\frac{h+\varepsilon_1}{2\sqrt{(\gamma_x-h)(h-\gamma_y)}}$; $\eta=\frac{\eta_1+\eta_2}{2}=\frac{-(\lambda+\gamma_y)\sqrt{\gamma_y}}{2\sqrt{(\gamma_x-\gamma_y)(\gamma_y^2-h^2)}}$, respectively, for the homoclinic and heteroclinic cases. Middle: stereographic projection of the critical classical orbit. Right: critical orbit on the Riemann Sphere, the zeroes of $\Psi(\bar\alpha)$ (black dots) are plotted for $n=120$, in the semiclassical limit they condense in branch cuts of G_0 [8,22].

$$\hat{H}=\frac{2}{n}\left(hS_z-\frac{\gamma_x S_x^2+\gamma_y S_y^2}{n}+\mu\frac{S_x^3}{n^2}\right). \qquad (20)$$

The LMG model [3] is obtained from Eq. (20) setting $\mu=0$. The cubic term in Eq. (20) is added to provide asymmetric orbits in order to test the quantization relations in a case as generic as possible. For the LMG model a detailed analysis of the phase space and the characterization of the critical points can be found in [8,9,20]. For small values of μ the phase diagram presented in [8] is kept invariant. In particular the system conserves a homoclinic HP at $\alpha=0$ for $\varepsilon_c=-|h|$ when $\gamma_x>|h|<|\gamma_y|$ and a heteroclinic caustic joining two HP for $\gamma_x>\gamma_y>|h|$ corresponding to $\varepsilon_c=-\frac{h^2+\gamma_y^2}{2\gamma_y}$. For the homoclinic case, one obtains

$$D=-\frac{\cos[\pi n(S_L+S_R)]}{\sqrt{1+e^{-2\pi\eta}}}-\sin\{\arg[\Gamma(1/2-i\eta)]$$
$$+\eta\log(4\rho^2 n)+\pi n(S_R-S_L)\}, \qquad (21)$$

as in the case of Schrödinger operators [2], where $S_{R/L}$ are given by S_i in Table I (directions of integration are given in Fig. 2). For the heteroclinic case the quantization condition is rather lengthy and will be given elsewhere [21]. The comparison of the semiclassical quantization conditions with numeric diagonalization of the Hamiltonian using a matrix representation of the spin operators is given in Fig. 2. In both cases the agreement between the numeric energies and the points where $D=0$ is remarkable, for the heteroclinic case one can see that the matching becomes worst as the modulus of the renormalized energy η increases.

IV. MATRIX ELEMENTS

In the semiclassical limit, the normalized matrix elements $f_k^A(\varepsilon^{(m)})=\frac{\langle\Psi_{m+k}|\hat{A}|\Psi_m\rangle}{\sqrt{\langle\Psi_{m+k}|\Psi_{m+k}\rangle\langle\Psi_m|\Psi_m\rangle}}$, of an observable $\hat{A}$ computed be-

tween eigenstates of an Hermitian operator H (with the energies $\varepsilon^{(m)}$ and $\varepsilon^{(m+k)}$), are known to be simply given as the amplitude of the kth Fourier mode of the observable symbol A, evaluated along the classical orbit of energy $\varepsilon^{(m)}$ [23],

$$f_k^A(\varepsilon^{(m)})=\frac{1}{T}\int_{-T/2}^{T/2}dt\exp\left(ik\frac{2\pi}{T}\right)\mathcal{A}[\bar\alpha(t),\zeta(t)], \qquad (22)$$

where T is the period of the classical orbit and the flow Eq. (13). This result holds for regular orbits and can be obtained by employing action-angle variables. Since f is the Fourier transform of an analytic function the matrix elements vanish exponentially with increasing k. This is a generalization of the result early obtained by Heisenberg for the harmonic-oscillator case.

For singular orbits containing HP the period T diverges; moreover no action-angle variables can be defined. Nevertheless it is still possible to estimate such matrix elements by analyzing local and global properties of the critical eigenstates [24]. Let us use the resolution of the identity in order to write matrix elements as integrals over Σ_i, a domain of size $O(n^{-1}\ln n)$ around the HP $\bar\alpha_i$, and $\Sigma_{i,j}$, a domain of order n^{-1} around $\mathcal{C}_0$. Within these two sets of domains the eigenstates are given, respectively, by special functions and WKB approximation,

$$\langle\Psi_{m+k}|\hat{A}|\Psi_m\rangle=\left[\sum_{(i)\to(j)}\int_{\Sigma_{i,j}}+\sum_{(i)}\int_{\Sigma_i}\right]$$
$$\times\frac{\langle\Psi_{m+k}|\alpha\rangle\langle\alpha|\hat{A}|\Psi_m\rangle}{\langle\alpha|\alpha\rangle}d\mu$$
$$=\sum_{(i)\to(j)}g_{i\to j}^A[n(\varepsilon^{(m+k)}-\varepsilon^{(m)})]$$
$$+\delta_{k,0}\sum_{(i)}\mathcal{A}(\bar\alpha_i,\zeta_i)\mu(i). \qquad (23)$$

The last equality follows from considering the symbol $\mathcal{A}$ constant on the domain Σ_i, by orthogonality of the eigenstates this term is nonzero only for $k=0$ where it gives the norm of the eigenstate inside the domain, $\mu(i)$. The regular functions $g_{i\to j}^A(\omega)=\int_{-\infty}^{\infty}dt\mathcal{A}(t)\exp(it\omega)$ are computed using the flow equations on the branch $i\to j$. Since $\mu(i)\propto\ln n$, we obtain at leading order,

$$f_{k=0}^A(\varepsilon^{(m)})=\frac{\sum_{(i)}\mathcal{A}(\bar\alpha_i,\zeta_i)\mu(i)}{\sum_{(i)}\mu(i)}, \qquad (24)$$

$$f_{k\neq0}^A(\varepsilon^{(m)})=\frac{\sum_{(i)\to(j)}g_{i\to j}^A[n(\varepsilon^{(m+k)}-\varepsilon^{(m)})]}{\sum_{(i)}\mu(i)}. \qquad (25)$$

Diagonal matrix elements (mean values of observables) are thus given as a sum of ponderate weights of the different HP and depend on local properties of eigenstates near this points. On the contrary, nondiagonal elements are given by the global properties of the classical orbit. Since g^A is ana-
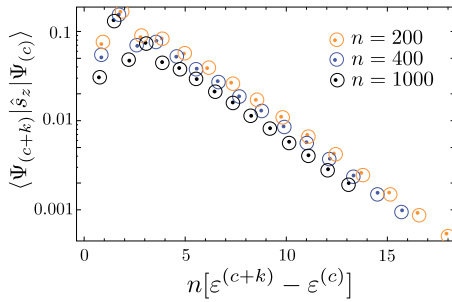
FIG. 3. (Color online) Matrix elements of the operator $\hat{s}_z = \frac{\hat{S}_z}{s}$ between two states near the critical energy. $\varepsilon^{(c)}$ is chosen to be the energy closest to the critical classical energy ε_c. The agreement of the numerical data (dots) with the predictions of Eq. (25) (circles) gets better for n big. The logarithmic downward shift as n increases is due to the fact that $\mu(i) \sim \ln^{-1} n$.

lytic, the matrix elements will decay exponentially as the energy difference increases, however, near the critical energy the mean energy spacing is of order $n(\varepsilon^{(m+k)} - \varepsilon^{(m)})$ $\propto k \ln^{-1} n$, meaning that the exponential decay in k becomes slower with increasing n (see Fig. 3). For an observable with $\mathcal{A}$ vanishing at the HP the amplitude of all matrix elements vanishes as $O(\ln^{-1} n)$, for fixed k (Fig. 3) [21]. This has a simple semiclassical explanation. In the critical case the volume of the phase space corresponding to an energy band of order n^{-1} around ε_c is $O(n^{-1})$ for regions of type $\Sigma_{i,j}$ and $O(n^{-1} \ln n)$ for Σ_i. However, for $\mathcal{A}$ vanishing at the HP, the relevant regions to compute the matrix elements are $\Sigma_{i,j}$, which, by Heisenberg inequalities, can carry only a finite number of states $O(n^0)$ and not the total $O(\ln n)$ eigenstates. The only way of conciliating these two facts is to take a

quantized observable described by an $O(\ln n) \times O(\ln n)$ matrix whose elements vanish in the classical limit.

V. CONCLUSION

We have presented a method for computing semiclassical spectra associated to any number of heteroclinic junctions. Not only the expected average spacing $\sim \ln^{-1} n$ is observed, but an algebraic relation is derived for eigenvalues near the critical energy. The method is fully general and applies to any su(2) Hamiltonian, it can be slightly improved to obtain corrections to all orders in n^{-1} (which will be presented in detail elsewhere [21]). In order to test it in full generality we have added a cubic term to the standard LMG model breaking the underlying quadratic symmetry. The agreement with numerics is remarkable, especially considering the fact that the formulas are algebraically quite heavy in the case of two hyperbolic fixed points linked by heteroclinic junctions. We have also computed the matrix elements of observables, and show that their semiclassical behavior is universal, and different from the one in the regular situation. Moreover we have given a physical argument for the logarithmic vanishing of these matrix elements in the classical limit.

[1] J. N. L. Connor, Chem. Phys. Lett. **4**, 419 (1969).
[2] Y. Colin de Verdière and B. Parisse, Commun. Math. Phys. **205**, 459 (1999).
[3] H. J. Lipkin, N. Meshkov, and A. J. Glick, Nucl. Phys. **62**, 188 (1965).
[4] D. A. Garanin, X. Martínez Hidalgo, and E. M. Chudnovsky, Phys. Rev. B **57**, 13639 (1998).
[5] V. V. Ulyanov and O. B. Zaslavskii, Phys. Rep. **216**, 179 (1992).
[6] J. Vidal, G. Palacios, and R. Mosseri, Phys. Rev. A **69**, 022107 (2004).
[7] J. Kurchan, P. Leboeuf, and M. Saraceno, Phys. Rev. A **40**, 6800 (1989).
[8] P. Ribeiro, J. Vidal, and R. Mosseri, Phys. Rev. Lett. **99**, 050402 (2007).
[9] P. Ribeiro, J. Vidal, and R. Mosseri, Phys. Rev. E **78**, 021106 (2008).
[10] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, New York, 1999).
[11] W. D. Heiss, F. G. Scholtz, and H. B. Geyer, J. Phys. A **38**, 1843 (2005).

[12] M. Caprio, P. Cejnar, and F. Iachello, Ann. Phys. (N.Y.) **323**, 1106 (2008).
[13] R. Brummelhuis, T. Paul, and A. Uribe, Duke Math. J. **78**, 477 (1995).
[14] A. Perelomov, *Generalized Coherent States and Their Applications* (Springer, New York, 1986).
[15] R. Shankar, Phys. Rev. Lett. **45**, 1088 (1980).
[16] A. Garg and M. Stone, Phys. Rev. Lett. **92**, 010401 (2004).
[17] I. Gradshteyn and I. Ryzhik, *Table of Integrals, Series and Product* (Academic, New York, 1980).
[18] W. G. Flynn and R. G. Littlejohn, Ann. Phys. **234**, 334 (1994).
[19] G. A. Hagedorn and A. Joye, Ann. Inst. Henri Poincare, Sect. A **68**, 85 (1998).
[20] O. Castanos, R. Lopez-Pena, J. G. Hirsch, and E. Lopez-Moreno, Phys. Rev. B **74**, 104118 (2006).
[21] T. Paul and P. Ribeiro (unpublished).
[22] S. Nonnenmacher and A. Voros, J. Phys. A **30**, 295 (1997).
[23] T. Paul and A. Uribe, Ann. Inst. Henri Poincare, Sect. A **59**, 357 (1993).
[24] J. R. Cary and P. Rusu, Phys. Rev. A **47**, 2496 (1993).