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Classification of excited-state quantum phase transitions for arbitrary number of degrees of freedom

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ABSTRACT

Classical stationary points of an analytic Hamiltonian induce singularities of the density of quantum energy levels and their flow with a control parameter in the system's infinite-size limit. We show that for a system with f degrees of freedom, a non-degenerate stationary point with index r causes a discontinuity (for r even) or divergence (r odd) of the $(f-1)$ th derivative of both density and flow of the spectrum. An increase of flatness for a degenerate stationary point shifts the singularity to lower derivatives. The findings are verified in an $f=3$ toy model.

1. Introduction

Excited-State Quantum Phase Transitions (ESQPTs) are singularities observed in discrete energy spectra of some bound quantum systems in the infinite-size limit [1–3]. They show up as non-analyticities in the density of quantum energy eigenstates as a function of energy E and in the flow of the excited spectrum with a suitable control parameter λ. The ESQPT critical borderlines in the $\lambda \times E$ plane are usually terminated by critical points of the ground-state Quantum Phase Transitions (QPTs) [4,5], so they can be seen as extensions of the QPTs to the excited domain. Thermodynamical and dynamical consequences of ESQPTs, as well as their experimental evidence in some synthetic quantum systems are currently focus of intense research, see *e.g.* Refs. [6–9].

The ESQPT singularities in systems with a single effective degree of freedom, $f=1$, are most dramatic and have been known for long, see *e.g.* Refs. [10–13]. For increasing numbers of degrees of freedom f, the ESQPTs affect higher and higher derivatives of the level density and flow of the spectrum. Their effects in systems with $f=2$ have been thoroughly studied in our recent works [14, 15]. These analyses contain the prerequisites for an ESQPT theory in an arbitrary number of degrees of freedom, but only for systems whose Hamiltonian is of the form

$$H = \frac{\boldsymbol{p}^2}{2} + V(\boldsymbol{q}), \tag{1}$$

where $V(\boldsymbol{q})$ is an analytic potential depending on coordinates $\boldsymbol{q}$ and $\boldsymbol{p}^2/2$ is a coordinate-independent kinetic energy, which is quadratic in momenta $\boldsymbol{p}$. In this case, ESQPTs appear at energies corresponding to stationary points of $V(\boldsymbol{q})$ above the main minimum, the corresponding defects in the spectrum being related to the stationary-point types.

The aim of the present paper is to develop a general-f ESQPT theory for systems with unrestricted forms of the Hamilton function $H(\boldsymbol{q}, \boldsymbol{p})$. It should be stressed that Hamiltonians with nontrivial couplings between coordinates and momenta are common in algebraic models of many-body collective dynamics because generators of the corresponding dynamical groups are usually formed by combinations of coordinate and momentum operators [16]. We develop a full classification of ESQPTs caused by non-degenerate (quadratic) stationary points of a general Hamiltonian. Although our approach is rooted in the evaluation of the system's level density, we show that non-analyticities in this quantity affect correspondingly the flow properties of the spectrum with a variable parameter (the "level dynamics"). Our conclusions are illustrated by a simple model. An example of an ESQPT due to a degenerate stationary point is also analyzed, although for such higher-order stationary points no general classification exists.

The paper is organized as follows: Section 2 analyzes the semiclassical level density in a vicinity of a non-degenerate stationary point and exemplifies a degenerate case. Section 3 aims at the impact of stationary points on flow properties of the spectrum. Section 4 presents a toy model with $f=3$. Section 5 brings a brief summary.

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2. Level density

The quantum level density for a system with discrete energy spectrum is defined by

$$\rho(E) = \sum_l \delta(E - E_l)\,, \tag{2}$$

where δ stands for the Dirac function and $E_0 \le E_1 \le E_2, \dots$ denote individual energy eigenvalues. The level density can be decomposed into a sum of smooth and oscillatory components:

$$\rho(E) = \bar{\rho}(E) + \widetilde{\rho}(E)\,. \tag{3}$$

The smooth component $\bar{\rho}$ captures the mean energy dependence of the level density (obtained, *e.g.*, by a convolution of ρ with a sufficiently wide smoothening function), while the oscillatory component $\widetilde{\rho}$ has a zero mean and collects fluctuations (the balance between the smoothed dependence and the full discrete spectrum).

In the limit $\hbar \to 0$, which in systems with finite numbers of degrees of freedom f is equivalent to the infinite size limit [14,17], the fluctuations of the level density become infinitely dense and the oscillatory component gets washed out even by smoothening over an infinitesimal energy interval. We shall therefore focus on the smooth component only. It can be determined from the size of the accessible phase space at a given energy:

$$\bar{\rho}(E) = \left(\frac{1}{2\pi\hbar}\right)^f \underbrace{\int d^{2f}\boldsymbol{x}\,\delta(E - H(\boldsymbol{x}))}_{\frac{\partial}{\partial E}\underbrace{\int_{H(\boldsymbol{x})\le E} d^{2f}\boldsymbol{x}}_{\Omega(E)}}\,, \tag{4}$$

where $\boldsymbol{x} \equiv (\boldsymbol{p}, \boldsymbol{q})$ is a $2f$-dimensional vector containing f-dimensional vectors of coordinates $\boldsymbol{q}$ and momenta $\boldsymbol{p}$, and $H(\boldsymbol{x})$ is the classical Hamiltonian of the system. Note that Eq. (4) can be derived by the Feynman integration over the orbits of zero length, while the oscillatory component is analogously linked to classical periodic orbits [18].

2.1. Effects of stationary points

As seen in Eq. (4), the smooth component of the level density is proportional to the energy derivative of the volume function $\Omega(E)$ associated with the Hamiltonian $H(\boldsymbol{x})$. The function $\Omega(E)$ measures the $2f$-dimensional volume of the phase–space region satisfying $H(\boldsymbol{x}) \le E$. Even for analytic classical Hamiltonian forms $H(\boldsymbol{x})$ it develops singularities at the points where the $(2f-1)$-dimensional hypersurface determined by the constant energy condition $H(\boldsymbol{x}) = E$ crosses a stationary point of H. Indeed, using the substitution formula $\delta(\chi(\boldsymbol{x})) = \sum_i \delta(\boldsymbol{x} - \boldsymbol{x}_{0i})/|\nabla_n \chi(\boldsymbol{x}_{0i})|$, where χ is any function satisfying $\chi(\boldsymbol{x}_{0i}) = 0\ \forall i$ and ∇_n stands for n-dimensional gradient, we express Eq. (4) via integration of the reciprocal gradient $1/|\nabla_{2f} H|$ over the constant-energy hypersurface. Therefore, the smooth component of the level density has non-analyticities at energies $E_{\boldsymbol{w}} \equiv H(\boldsymbol{w})$ corresponding to points $\boldsymbol{w}$ where $\nabla_{2f} H(\boldsymbol{w}) = 0$.

The impact of a stationary point of a given type on the level density has a universal character—it depends only on the local behavior of $H(\boldsymbol{x})$ near $\boldsymbol{w}$, and not on the global, system-specific features of dynamics. This conclusion can be verified by a splitting of the integral in Eq. (4) near the stationary-point energy $E_{\boldsymbol{w}}$ into a sum of regular and irregular parts:

$$\bar{\rho}(E) = \bar{\rho}^{(0)}_{\boldsymbol{w}}(E) + \bar{\rho}_{\boldsymbol{w}}(E)\,. \tag{5}$$

The irregular part $\bar{\rho}_{\boldsymbol{w}}$ contains integration over a small phase–space neighborhood of the stationary point and captures all non-analytic behavior of $\bar{\rho}$ due to the stationary point. The regular part $\bar{\rho}^{(0)}_{\boldsymbol{w}}$ contains the integration over the rest of the accessible phase space and yields an analytic contribution to $\bar{\rho}$. To classify the singularity in the level density caused by the stationary point, it is sufficient to analyze properties of the irregular part.

Singularities of various volume functions have been studied in rather different contexts. For instance, the so-called level set method of computational geometry and image processing (see *e.g.* Ref. [19]) describes the motion of a general interface Γ in an n-dimensional space of variable $\boldsymbol{x}$ via a suitably determined function $\varphi(\boldsymbol{x}, t)$ such that $\Gamma(t)$ at any time t coincides with the set of $\boldsymbol{x}$ with $\varphi = 0$. In this method, an expression analogous to Eq. (4) represents time derivative of the volume Ω bounded by Γ. Non-differentiability of the volume function at the places where the interface crosses a non-degenerate stationary point of φ has been analyzed by Hoveijn [20]. A similar problem has been addressed also by Kastner et al. [21–23] in the framework of statistical mechanics, namely in connection with the so-called configurational state density defined by $\omega(E) = \int d^f\boldsymbol{q}\,\delta(E - V(\boldsymbol{q}))$, in analogy to Eq. (4), for systems with Hamiltonians of the type (1). Mathematical conditions have been formulated for the occurrence of a thermodynamic phase transition caused by stationary points of the potential energy landscape [22].

Our aim in this paper is to analyze the link of various classical stationary points to the ESQPT singularities in quantal spectra of general Hamiltonian systems. At first we show (Sec. 2.2) that there exists a finite classification of ESQPTs corresponding to non-degenerate (quadratic) stationary points of various types, where "classification" means typology of discontinuities or singularities that for a given number of degrees of freedom f appear in the $(f-1)$th energy derivative of $\bar{\rho}$. The results in this part are mathematically equivalent to those derived previously in other contexts [20–23]. Second, although a classification of ESQPTs caused by higher-order stationary points does not exist, we give an illustrative example of this kind (Sec. 2.3) and discuss conditions for descending the ESQPT signatures to lower derivatives of $\bar{\rho}$. Third, we analyze (Sec. 3) generic effects of stationary points on the flow of quantum spectrum with the Hamiltonian control parameters, showing that a smoothed flow is generally expected to exhibit the same type of singularity as level density.

2.2. Singularities caused by non-degenerate stationary points

The analysis presented in this section is based on the Morse theory [24]. Let $\mathcal{M}$ be an n-dimensional manifold of points $\boldsymbol{x} = (x_1, \dots, x_n)$ and $H(\boldsymbol{x})$ a smooth function $H : \mathcal{M} \to \mathbb{R}$. Consider a stationary point $\boldsymbol{w}$ satisfying $\nabla_n H(\boldsymbol{w}) = 0$. The stationary point is called non-degenerate if the Hessian matrix $\mathcal{H}(\boldsymbol{w})$ with elements $\mathcal{H}_{ij}(\boldsymbol{w}) = \partial^2 H(\boldsymbol{x})/(\partial x_i \partial x_j)|_{\boldsymbol{x}=\boldsymbol{w}}$ has only non-zero eigenvalues. This means that the function $H(\boldsymbol{x})$ is locally quadratic in all directions at the point $\boldsymbol{w}$. According to the Morse lemma [24], close to any non-degenerate stationary point $\boldsymbol{w}$ one can choose coordinates $\boldsymbol{y}$ such that the following equality holds up to the $\mathcal{O}(y_i^3)$ terms:

$$H_{\boldsymbol{w}}(\boldsymbol{y}) = H(\boldsymbol{w}) \underbrace{-y_1^2 - \cdots - y_r^2}_{-R_-^2} \underbrace{+y_{r+1}^2 + \cdots + y_n^2}_{+R_+^2}\,. \tag{6}$$

The integer r, called the *index* of stationary point, is equal to the number of negative eigenvalues of $\mathcal{H}(\boldsymbol{w})$. Variable R_- is a radial coordinate in the r-dimensional subspace connected with negative eigenvalues of the Hessian matrix, while R_+ is a radial coordinate in the adjunct s-dimensional subspace $(s = 2f - r)$ connected with the positive eigenvalues.