Classical analysis of quantum phase transitions in a bilayer model

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In this Brief Report we extend the classical analysis performed on the schematic model proposed in [T. Moreira, G. Q. Pellegrino, J. G. Peixoto de Faria, M. C. Nemes, F. Camargo, and A. F. R. Toledo Piza, Phys. Rev. E **77**, 051102 (2008)] concerning quantum phase transitions in a bilayer system. We show that appropriate integrations along the classical periodic orbits reproduce with excellent agreement both the quantum spectrum and the expected mean value for the number of excitons in the system, quantities which are directly related to the observed boson-fermion quantum phase transition.

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Quantum entanglement has been an area of intense research in recent years. One reason for this might be the far-reaching possibilities advanced by quantum information science. Intimately associated with the search for results related to quantum computation was the possibility offered by quantum entanglement of a better understanding of the complex behavior shown by many-body systems, notably quantum phase transitions (QPTs). The first relation of QPT to quantum entanglement was established in the context of spin-1/2 models studied in the thermodynamic limit [1–3]. Given this $N\to\infty$ limit, a step further was the use of the so-called pseudospin collective operators which immediately connected QPT, quantum entanglement, and semiclassical analysis. Various many-body models were studied in this context, e.g., the models of Dicke [4–8], Lipkin [9], Jahn-Teller [10], and N-atom Jaynes-Cummings [11], the pairing model [12], as well as a giant spin model motivated by quantum computation [13], an integrable quantum dimer [14], and coupled quartic oscillators [15].

Even though the early definitions of QPT are based on ground-state properties of the energy spectrum, in the last few years it has been shown that QPT manifests itself also in excited states [excited-state QPT (ESQPT)]. Once again semiclassical analysis proved to be an important instrument of investigation. These issues were addressed in a variety of systems and situations, mostly related to nuclear physics as, for examples, the Lipkin model [16], collective vibrations [17], cusp and collective Hamiltonians [18], interacting boson models [19], and pairing interactions [12]. In the latter context, it was found that ESQPT is universal as concerning two-level models [20]. Finally, the maximization of decoherence induced on a single qubit by a two-level boson environment was conjectured in [21] and explicitly presented in [22]. Although semiclassical analysis was not actually performed in connection with decoherence, large-N cases were investigated, suggesting that related investigations could, in principle, be attempted in the semiclassical domain.

Much of that classical analysis was concentrated on fixed-point bifurcations occurring on the corresponding classical phase spaces [5,6,8–11,13–15]. Alternatives to this approach were the study of semiclassical spectra and their derivatives [12,18,20,23], WKB expansion around the minimum of energy in phase space [16], the association of the concept of classical monodromy with ESQPT [17], and also the study of degeneracies in a complex-extended parameter space [19]. Despite the fact that a firm connection was established between quantum entanglement (and phase transitions) and classical properties, no general analytical proof of that connection has yet been offered. It seems therefore of great relevance to analyze other aspects of the classical dynamics of such models in the search for an analytical link between quantum properties of QPT and their possible classical analogs.

In a previous paper [24], the dynamics for the creation and annihilation of excitons from electron-hole pairs, as suggested by experiments in a bilayer system [25], was modeled by the Hamiltonian

$$H = g\sum_{\alpha=1}^{N/2}(a_{1\alpha}^{\dagger}a_{2\alpha}^{\dagger}b + b^{\dagger}a_{1\alpha}a_{2\alpha}) + \delta b^{\dagger}b. \tag{1}$$

In this expression $a_{i\alpha}^{\dagger}$ ($a_{i\alpha}$) is the creation (annihilation) operator associated with the αth fermion in layer i ($i=1,2$) and $b^{\dagger}$ (b) is the creation (annihilation) operator for an exciton. In that paper, as well as here, the coupling parameter is taken to be the ratio δ/g between the total energy difference δ, from fermion pairs to formed excitons, and the rate g at which excitons are created.

Since the total number of fermions N is a constant of motion, measured by the operator

$$\aleph \equiv \sum_{i=1}^{2}\sum_{\alpha=1}^{N/2} a_{i\alpha}^{\dagger}a_{i\alpha} + 2b^{\dagger}b, \tag{2}$$

it was convenient to rewrite Hamiltonian (1) in terms of SU(2) spin operators

$$J_z \equiv b^{\dagger}b - \frac{\aleph}{4}, \tag{3}$$

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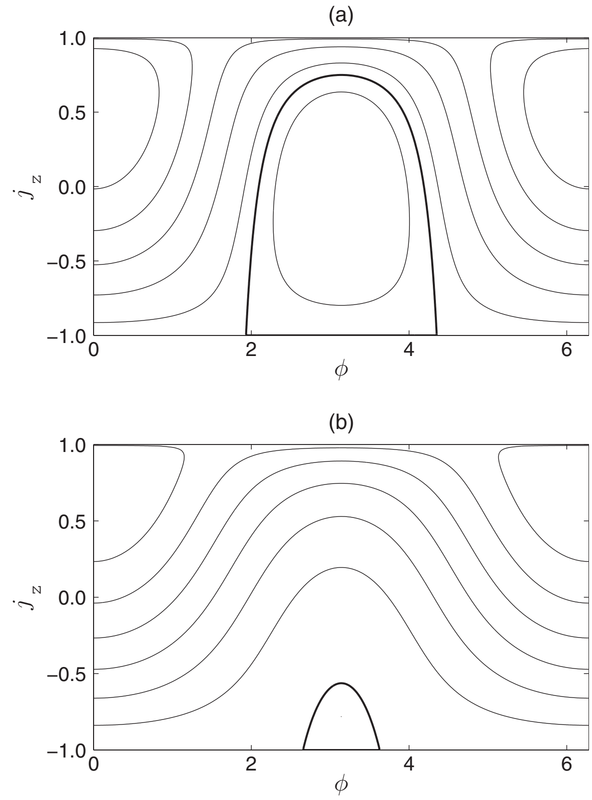

FIG. 1. Classical phase spaces for values (a) $\delta'/g'=1.0$ and (b) $\delta'/g'=2.5$. The separatrix orbit is shown as the thick curve corresponding to energy zero.

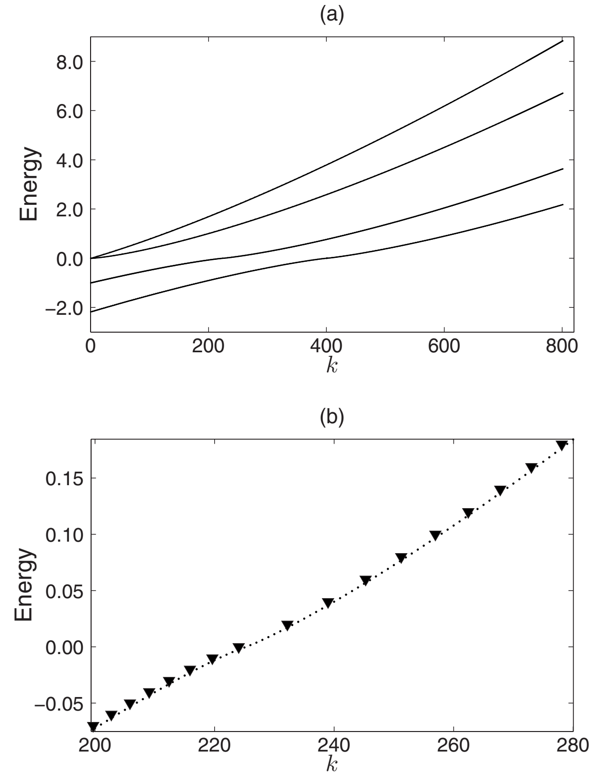

FIG. 2. (a) Quantum spectra $E_k \times k$ for different values of δ/g, and semiclassical spectra $\mathcal{E} \times k$ for the corresponding values of δ'/g' with k calculated following relation (11). From bottom to top, curves are drawn for values $\delta/g=0,20,20\sqrt{8},80$. (b) Magnification of part of the curves for $\delta/g=20$. Triangles refer to the classical estimate.

$$J_+ = J_-^\dagger = \frac{1}{\sqrt{b^\dagger b}} \sum_{\alpha=1}^{N/2} a_{1\alpha} a_{2\alpha} b^\dagger, \tag{4}$$

which give

$$H = g(J_- \sqrt{J_z + J} + \sqrt{J_z + J} J_+) + \delta(J + J_z), \tag{5}$$

where $J=N/4$.

The classical limit for Hamiltonian (1) or (5) was obtained as

$$h = 2g' \sqrt{(1-j_z)}(1+j_z)\cos\phi + \delta'(1+j_z) \tag{6}$$

after rescaling Hamiltonian H by the density of particles in the system, in the thermodynamic limit $N \to \infty$ and $V \to \infty$ with N/V being kept constant. In this expression the classical conjugate variables j_z and ϕ are given by standard definitions [26]

$$j_k = \lim_{J\to\infty} \frac{J_k}{J} \quad (k=+,-,z), \tag{7}$$

$$j_x = \tfrac{1}{2}(j_+ + j_-) = \sqrt{1-j_z^2}\cos\phi, \tag{8}$$

with $-1 \le j_z \le 1$ and h periodic in ϕ. In order to facilitate the comparison between quantum and classical results the parameters g and δ were rescaled to $g' = gV\sqrt{N}/8$ and $\delta' = \delta V/4$.

Classical phase-space pictures for two values of the coupling parameter δ'/g' are reproduced in Fig. 1. In this figure we have a minimum-energy critical point at coordinate $\phi=\pi$, maxima at $\phi=0$ (or 2π), and a separatrix orbit (thick curve) with energy zero for $0 \le \delta'/g' \le \sqrt{8}$. Above this value of δ'/g' the separatrix does no longer exist and the minimum energy is fixed at the line $j_z=-1$.

The expected quantum phase transition in this model is signalized by a sudden decrease in the linear entropy of the ground state when the ratio δ/g exceeds the approximate value of 56.6, as well as by a rapid decrease in the expected number of bosons for that state, which is interpreted as a boson-fermion transition from a collective excitonic state to an unpaired fermionic one. It was shown further that these aspects of the QPT are exhibited not only by the ground state with energy E_1 but also by all the excited states with energy E such that $E_1 < E < 0 = E_{ip}$, where E_{ip} marks the presence of an inflection point in the quantum spectra at energy zero, which occurs as long as $\delta/g \le 56.6$. For each of these excited levels the QPT is signalized at a corresponding value for δ/g, up to $\delta/g=56.6$ when $E_1=E_{ip}=0$. Above this value of δ/g the inflection point does no longer exist and the ground-state energy level E_1 is fixed at $E_1=0$. This QPT is shown to be intimately related to the properties of the classical phase space generated by Hamiltonian h [Eq. (6)]. In fact, the presence of the inflection point in the quantum spectra is connected with the permanence of the separatrix orbit in the classical phase space for $\delta'/g' \le \sqrt{8}$. Moreover, the rescaled ratio δ'/g' fixes a precise value of $\delta/g = \sqrt{2N}$ for the critical

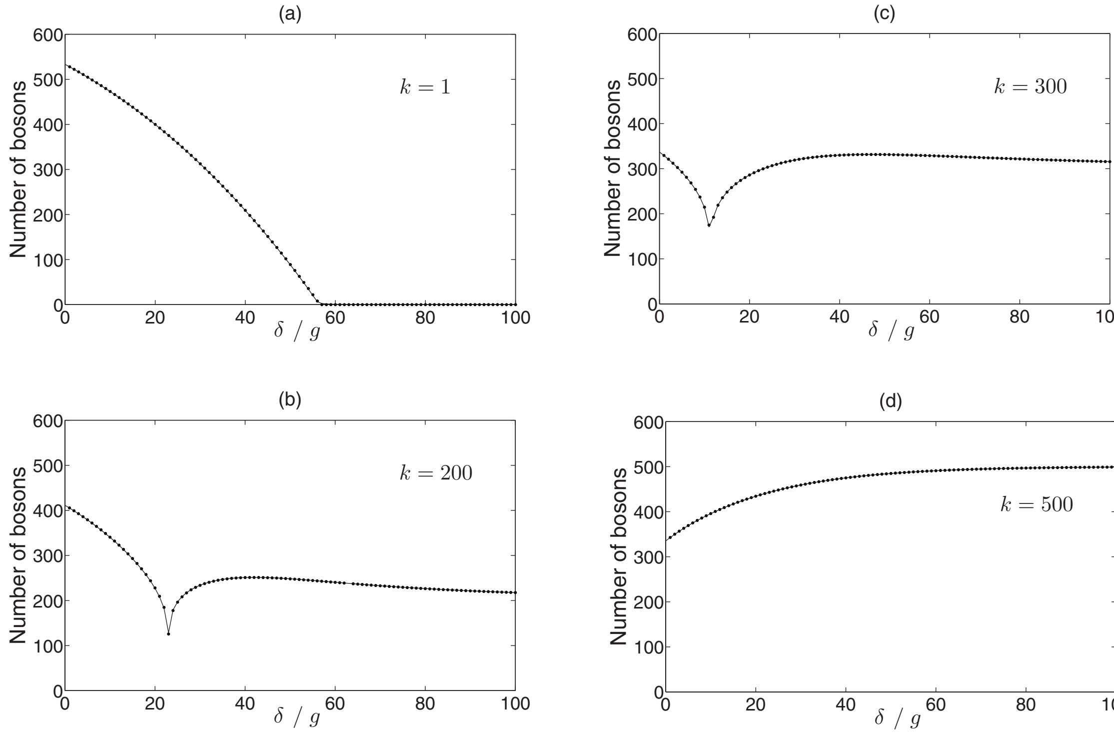

FIG. 3. Quantum expectation value for the number of bosons $\langle n_b(k)\rangle$ (solid curves) and semiclassical estimate for its classical analog $n_b(\mathcal{E}) \equiv \frac{N}{4}(1+\bar{j}_z)$ (points), as a function of the coupling parameter δ/g. In both cases, states E_k are chosen for (a) $k=1$, (b) $k=200$, (c) $k=300$, and (d) $k=500$.

parameter at the QPT, which for $N=1600$ particles—as used in the quantum calculations—gives $\delta/g=20\sqrt{8}=56.5685\ldots$. As one raises δ'/g' from zero to $\sqrt{8}$, the closed orbits around the minimum turn into open ones when the border line $j_z=-1$ is reached until the last closed orbit, the minimum itself, disappears and the dynamical regime given by the closed orbits is no longer supported. The system suffers then a transition to the (now mandatory) regime given by the open orbits.

In this Brief Report we extend this quantum-classical correspondence to the energy spectra E_k and also to the expected mean value for the number of bosons $\langle n_b(k)\rangle$ in state k. This will be done by evaluating appropriate integrals along the classical orbit corresponding to the energy of the chosen quantum state. We start with the semiclassical spectra.

In the limit $N\to\infty$, the quantum spectrum E_k for model (1) can be obtained by semiclassical methods as follows. It was already seen in Ref. [24] that quantum and classical energies are related as

$$\frac{E_k}{\left(\frac{gN^{3/2}}{8}\right)} = \frac{\mathcal{E}}{g'}. \tag{9}$$

The quantum index k can also be estimated semiclassically after the calculation of the action $\mathcal{A}(\mathcal{E})$ of the periodic orbit with energy $\mathcal{E}$ corresponding to the quantum energy E_k. The action $\mathcal{A}(\mathcal{E})=\oint_{\mathcal{O}(\mathcal{E})} j_z d\phi$ is obtained as the area of the phase space enclosed by orbit $\mathcal{O}(\mathcal{E})$, if it is a closed orbit with energy $\mathcal{E}<0$, or as the area between the open orbit and the lower border of the phase space at $j_z=-1$.

In Ref. [27] it is shown that the quantum index k is related to $\mathcal{A}(\mathcal{E})$ as

$$\mathcal{A} = \nu k + \gamma, \tag{10}$$

where ν is a constant depending on N and γ is an eventual correction to the direct proportionality, due to the Maslov index associated with the orbit. It is seen that for our model γ tends to zero as $1/N$; therefore, in the limit $N\to\infty$ we have simply $\mathcal{A}=\nu k$. Since the maximum area is achieved for the maximum energy as the full phase-space area, we have $\mathcal{A}(\mathcal{E}_{max})=4\pi$, which should correspond to the highest quantum level $k_{max}=N/2+1$. In this way we obtain the relation

$$k = \frac{N+2}{8\pi}\mathcal{A}(\mathcal{E}). \tag{11}$$

In Fig. 2 we plot both quantum and semiclassical spectra for different values of the parameter δ/g (and correspondingly for δ'/g'). The agreement is excellent.

It is interesting to note that this accordance between quantum and classical correspondences can be extended even to the expected number of excitons in the system. In fact, the quantum operator $b^\dagger b$, which counts the number of bosons, has the function $\frac{N}{4}(1+j_z)$ as its classical analog.

A classical estimate $n_b(\mathcal{E})$ for the expected mean value $\langle n_b(k)\rangle$ of the number of bosons in state k of energy E_k can be evaluated by averaging j_z over the orbit $\mathcal{O}(\mathcal{E})$ with the corresponding energy $\mathcal{E}$. Different expressions can be written for this estimate

$$n_b(\mathcal{E}) \equiv \frac{N}{4}(1+\bar{j}_z), \tag{12}$$

with

$$\bar{j}_z(\mathcal{E}) = \frac{1}{T}\oint_{\mathcal{O}(\mathcal{E})} j_z\, dt = \frac{\oint_{\mathcal{O}(\mathcal{E})} j_z \frac{ds}{|v|}}{\oint_{\mathcal{O}(\mathcal{E})} \frac{ds}{|v|}} = \frac{\oint_{\mathcal{O}(\mathcal{E})} j_z \frac{dj_z}{|j'_z|}}{\oint_{\mathcal{O}(\mathcal{E})} \frac{dj_z}{|j'_z|}}, \tag{13}$$

where T is the period of orbit $\mathcal{O}(\mathcal{E})$ and $v=\frac{ds}{dt}$ is the velocity over $\mathcal{O}(\mathcal{E})$. Any of these forms can be used for numerical integration but the last one seems to be the simplest one since j'_z is directly written as one of the Hamilton equations of motion $j'_z=-\frac{\partial h}{\partial \phi}$ generated by Hamiltonian h [Eq. (6)]. Figure 3 shows both quantum and classical evaluations of $\langle n_b(k)\rangle$ and $n_b(\mathcal{E})$ for various values of the parameter δ/g and for some quantum states E_k chosen along the spectra. Once again, the agreement is surprisingly good all along the range of the index k.

In these figures, the classical estimate for the number of bosons for state E_k shows a pronounced decrease at a specific value of the parameter δ/g. This change occurs at the value of δ/g at which the observed closed classical orbit becomes the separatrix and the classical system undergoes a transition to a different dynamical regime, as an open classical orbit. Correspondingly, the quantum energy level becomes the inflection point in the spectrum and the quantum system undergoes a phase transition. This behavior is observed for any state with energy less than $E_{ip}=0$. For $\delta/g=0$, the energy zero occurs at level $k=400$ (for $N=1600$); for $k>400$, E_k is already above the inflection point and no such indication of the QPT is seen in a curve for the number of bosons, as illustrated in Fig. 3(d) for $k=500$. Therefore, each excited state, and the corresponding classical orbit, with energy below $E_{ip}=0$ will offer evidence of the observed QPT.

In Ref. [24] it was seen that the presence of an inflection point in the quantum spectrum, where the density of energy levels is maximal, is directly related to the boson-fermion QPT. This QPT manifests itself as sudden changes in the number of excitons. We have seen that both these quantities can be obtained from the classical orbits, suggesting that in this particular model the observed QPT could in a sense be anticipated by an analysis of the corresponding classical phase space. More important, the results shown here and in Ref. [24] are meant to serve as a point of argument, besides fixed-point analysis, in the construction of a more consistent analytical connection between QPT and classical properties.

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