Entanglement and classical instabilities: Fingerprints of electron-hole-to-exciton phase transition in a simple model

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We propose a schematic model to study the formation of excitons in bilayer electron systems. The phase transition is signalized both in the quantum and classical versions of the model. In the present contribution we show that not only the quantum ground state but also higher energy states, up to the energy of the corresponding classical separatrix orbit, "sense" the transition. We also show two types of one-to-one correspondences in this system: On the one hand, between the changes in the degree of entanglement for these low-lying quantum states and the changes in the density of energy levels; on the other hand, between the variation in the expected number of excitons for a given quantum state and the behavior of the corresponding classical orbit.

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I. INTRODUCTION

One of the most interesting issues in condensed matter physics today is the phase transition from the unbound fermionic system, consisting of electron-hole pairs, to a coherent, mesoscopic one, composed of bosonic bound states of these pairs [1–3]. Recently, Eisenstein and MacDonald reported an experiment in a bilayer system under strong magnetic field [4], providing compelling evidence for such a transition. With this experiment in mind, we propose a model which allows for an exact numerical solution accounting for this (fermion-boson) phase transition and its classical limit. This schematic, physically motivated model proves to be rich enough to elucidate some of the basic features of this process.

A valuable tool to investigate quantum phase transition is the degree of entanglement of the ground state, as measured, e.g., by the linear or von Neumann entropies. Investigation along this line started in the context of spin-1/2 models [5,6] where it has been noted that the genuine character of a phase transition can be tested by entanglement [7]. Several other models were investigated and studies were also performed on the classical analogs of quantum phase transitions and on classical instabilities or bifurcations from equilibrium [8–15]. They are the fingerprint of a phase transition in the classical context. The first indications of a connection between qualitative changes in the ground-state entanglement properties and classical bifurcations were given in Refs. [12,13]. This connection was further developed in Refs. [14,15] and [10]. Up to now, there has been however no analytical proof of such a connection. In all numerical investigations the pattern is nevertheless the same. Here is how it works in the quantum case: At a certain value of the coupling strength there is a rapid decrease in the entropic measures of quantum correlations. This particular phenomenon has been investigated in connection with a larger class of so-called collective models [10]. Essentially all models in this class are of direct physical relevance, such as the Dicke maser model and its superradiant phase transition, the Lipkin model from nuclear physics describing the phase transition from spherical to deformed nuclei, and so on.

In this work we propose a schematic model for the fermion-boson phase transition in the context of the transition between a state characterized by electron-hole pairs and that involving excitons. We analyze both its spectral and classical properties. As expected, the entanglement of the ground state as a function of the coupling parameter signals the phase transition. The classical counterpart of the model exhibits a bifurcation from equilibrium. We also investigate the relation of a particularly interesting classical orbit—the separatrix—to the spectral structure around the corresponding energy eigenstate. In the classical limit this trajectory separates two kinds of motion and occurs at an energy which may be far from that of the ground state. At this energy the quantum spectrum presents an inflection point and the linear entropy also shows a decrease of almost one order of magnitude for the corresponding quantum state. We will show in what follows a class of phenomena involving not only the ground state but the entire spectrum and its classical counterpart.

In Sec. II, we present the model, its spectral properties and the linear entropy as a function of the coupling strength; we investigate the same property for several states with particular emphasis on the inflection point, which is related to the classical separatrix. Section III analyzes the classical analog of the model; concluding remarks are given in Sec. IV.

II. MODEL, SPECTRAL PROPERTIES AND THE LINEAR ENTROPY

We model the dynamics of the creation of an exciton from an electron-hole pair via the Hamiltonian

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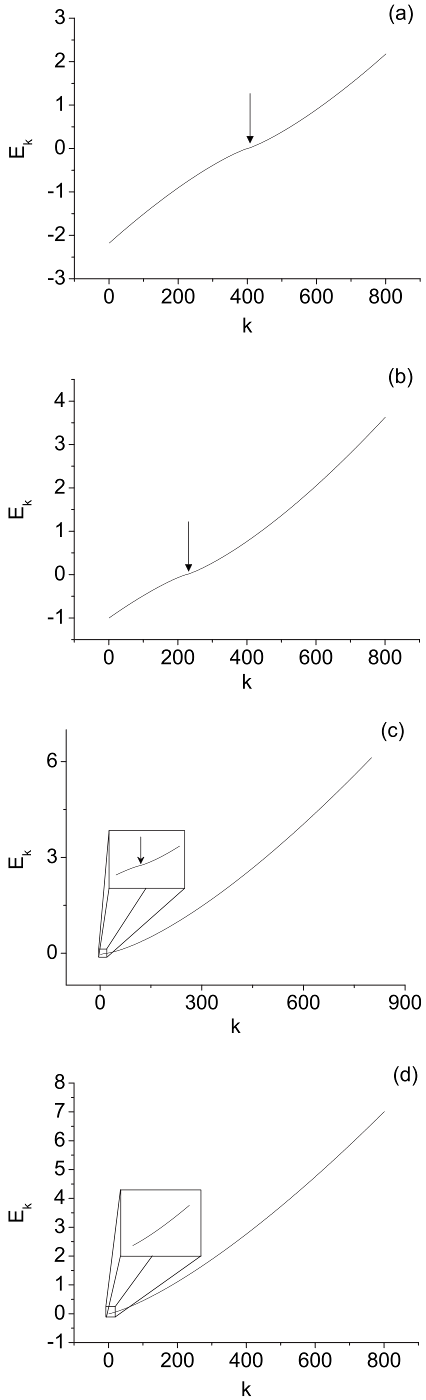

FIG. 1. Scaled energy spectra $E_k \times k$ for (a) $\delta/g=0$, (b) $\delta/g=20$, (c) $\delta/g=50$, and (d) $\delta/g=60$. The energies are scaled by the factor $8/(gN^{3/2})$ in order to be compared with the classical analog. The total number of fermions is $N=1600$ in all figures. The arrow indicates the position of the inflection point.

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

where $a_{i\alpha}^{\dagger}$ ($a_{i\alpha}$) is the creation (destruction) operator for the αth fermion in layer i ($i=1,2$) and $b^{\dagger}$ (b) is the creation (destruction) operator for an exciton. The coupling strength g measures the rate at which excitons are created. δ measures the energy difference between an exciton and a fermion pair. Since we have in mind the situation described in Ref. [4], in which one has electrons in both layers, we take $\delta>0$ and $g>0$ in what follows. Noting that the level of the fermion-pair-to-boson transition is inversely proportional to the ratio δ/g, we will use this ratio as the coupling parameter.

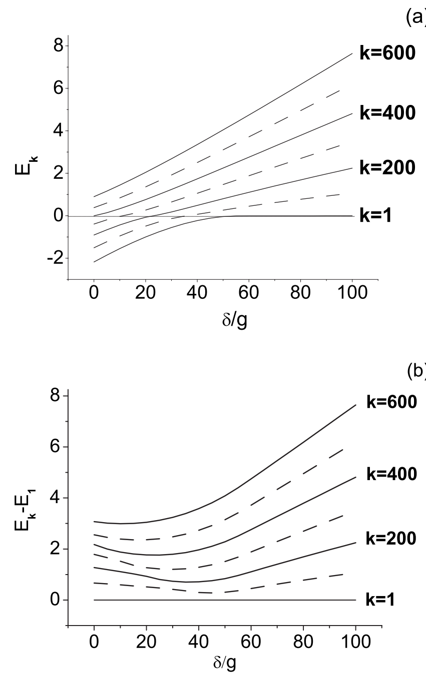

FIG. 2. Energy spectra as a function of the coupling parameter δ/g. In (b) the energies are rescaled, by setting the ground-state level equal to zero for all values of δ/g.

The operator

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

gives the total number of fermions N which is a constant of motion under the evolution given by Eq. (1). We can therefore diagonalize H in the basis $\{|n_a,(N-n_a)/2\rangle, n_a=2,4,6,\ldots,N\}$, where n_a is the number of fermions and $(N-n_a)/2$ is the number of bosons. In Fig. 1 we show the

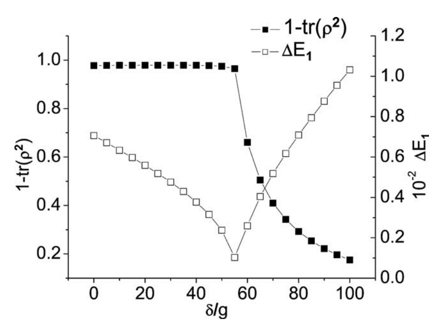

FIG. 3. Linear entropy (filled squares, left-hand axis) of the reduced fermionic state and level separation (open squares, right-hand axis) for the ground state.

scaled spectrum of the Hamiltonian for several values of δ/g as a function of the state label k. For values $\delta/g<56$ the spectra have an inflection point at energy zero. As the coupling parameter increases, the inflection point moves toward lower regions of the spectrum and disappears at a critical value $\delta/g\approx 56$. The energy at which this inflection point occurs is always zero and around this value the density of energy levels is maximal. This is illustrated also in Fig. 2(a), where we show the change in the quantum spectra as a function of δ/g. If one rescales the energy axis in this figure, by setting the ground-state level to a constant E_g for all values of δ/g, one can see a hollow in the region around $\delta/g=56$ [Fig. 2(b)]. The same behavior was observed by Heiss and Müller [13] in the Lipkin model, as an illustration of a phase transition. In Fig. 2 it is apparent that the difference between adjacent levels diminishes around the inflection points. Actually, this is the quantum counterpart of the fact that the period of classical orbits in this energy region increases (see Ref. [10]). Throughout this section we will call "separatrix" this particular state corresponding to the inflection point; the reason for this will become clear in the classical analysis, where we show a one-to-one correspondence between that quantum state and the classical separatrix, for each value of the coupling parameter.

Now we connect the entanglement properties with the states in the spectrum. In order to do this, consider the linear entropy given by

$$\Delta = 1 - \mathrm{tr}\,\rho_F^2, \tag{3}$$

where $\rho_F=\mathrm{tr}_B|\varphi_k\rangle\langle\varphi_k|$ is the reduced fermionic density operator and $|\varphi_k\rangle$ an eigenstate of Hamiltonian (1). Here, tr_B stands for the partial trace over the bosonic (excitonic) variables. Taking $|\varphi_1\rangle$ as the ground state, we see (Fig. 3) a rapid decrease in the linear entropy when the coupling parameter δ/g exceeds 56. In the same figure we show the energy separation between adjacent levels, $\Delta E_k=E_{k+1}-E_k$ for $k=1$. Note that this quantity follows closely the behavior of the linear entropy, indicating a correlation between level spacing and the sudden decrease in entanglement.

Higher states in the spectrum also appear to be sensitive to the phase transition although to a lesser degree, as can be seen in Fig. 4. Figures 3 and 4 show that the excited states behave in a way qualitatively similar to the ground state, as far as the linear entropy is concerned, albeit not so remarkably, since the left-hand scale $[1-\mathrm{tr}(\rho^2)]$ changes by one order of magnitude whereas the right-hand scale (ΔE_k) is the same. For any excited state in the spectrum with energy below the separatrix energy zero, the change in linear entropy always occurs when that state becomes the separatrix state, as δ/g is increased. In this sense, each excited state up to the separatrix evidences the phase transition at a corresponding critical value of the coupling parameter δ/g. The highest level for which this occurs, $k=400$, has the behavior shown in Fig. 4(c). For even higher lying states, as in Fig. 4(d), the effect disappears (as does the separatrix).

In order to understand what happens with bosons and fermions around the phase transition, we calculate the expectation value $\langle n_b(k)\rangle$ of the number of bosons in the system for a given state k. This is depicted in Fig. 5. For the ground

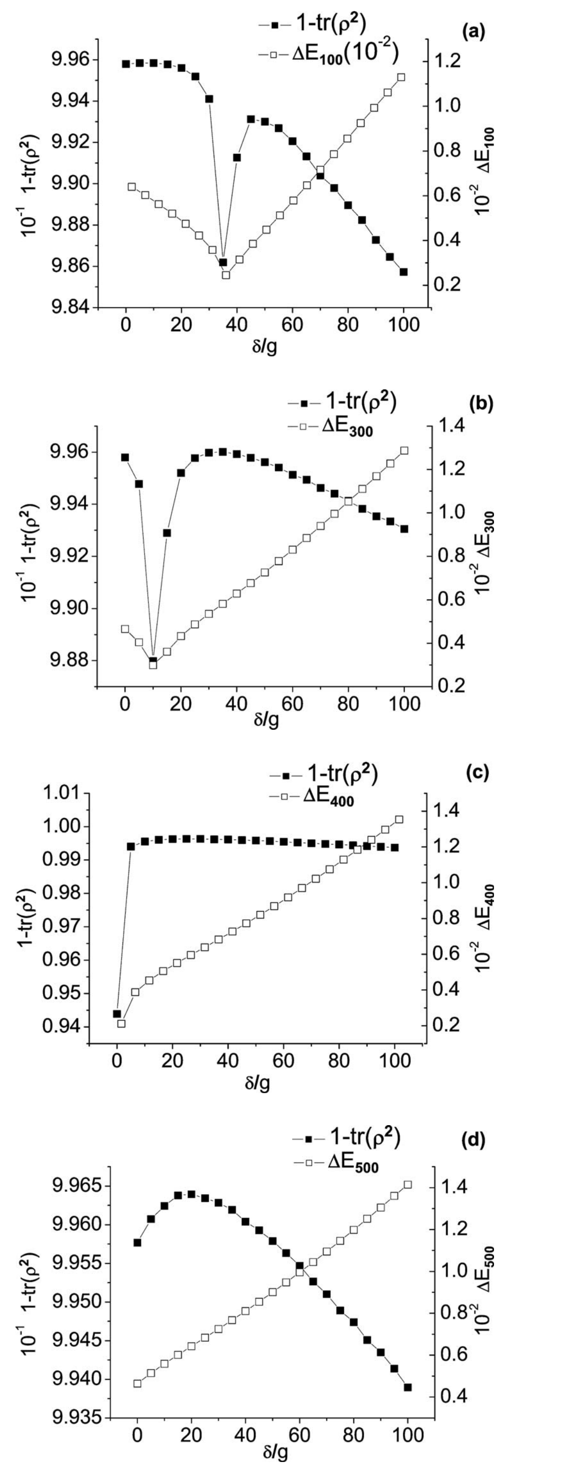

FIG. 4. Linear entropy (filled squares, left-hand axis) of the reduced fermionic state and level separation (open squares, right-hand axis) for excited states E_k with (a) $k=1$, (b) $k=300$, (c) $k=400$, and (d) $k=500$.

state, which exhibits the transition at $\delta/g\approx 56$, we expect to find a large number of bosons for values of δ/g below this critical value, while near the transition $\langle n_b(1)\rangle$ experiences a decrease, with an accompanying increase in the number of fermions, since the total number of particles is constant [see Fig. 5(a)]. The same observation can be made for every ex-

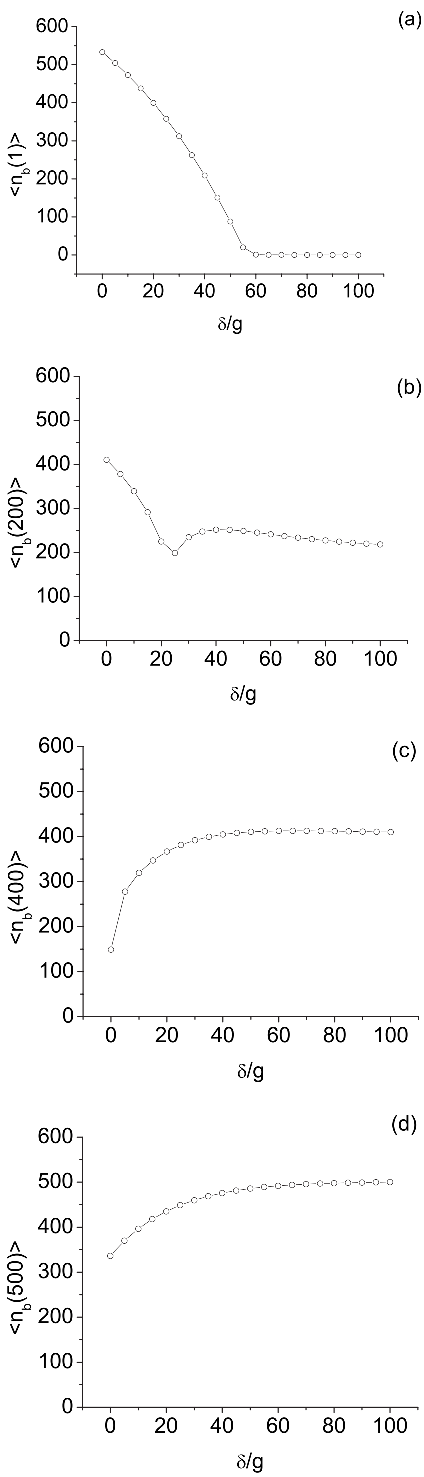

FIG. 5. Expectation value for the number of bosons $\langle n_b(k)\rangle$ as a function of the coupling parameter δ/g for states E_k with (a) $k=1$, (b) $k=200$, (c) $k=400$, and (d) $k=500$.

cited state below the separatrix state, although the effect is then less pronounced [see Figs. 5(b) and 5(c)]. Figure 5(d) illustrates the behavior for states above the separatrix, from where we expect large numbers of excitons for any value of δ/g.

III. CLASSICAL THERMODYNAMIC LIMIT OF THE MODEL

The classical analog of the model can be obtained as the thermodynamic limit of Hamiltonian (1). To this end we first map the creation and destruction operators into an SU(2) algebra by taking

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

and

$$J_+ = J_-^\dagger = \frac{1}{\sqrt{b^\dagger b}}\sum_{\alpha=1}^{n/2} a_{1\alpha}a_{2\alpha}b^\dagger . \tag{5}$$

In terms of these operators, Hamiltonian (1) is rewritten as

$$H = g(J_-\sqrt{J_z+J} + \sqrt{J_z+J}J_+) + \delta(J+J_z) \tag{6}$$

with $J=N/4$.

The thermodynamic limit is obtained by letting $N\rightarrow\infty$ and $V\rightarrow\infty$ with N/V, the density of particles in the system volume V, being kept constant, and finally by rescaling the Hamiltonian by N/V. In this classical limit variables are provided by the usual definitions [16]

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

and

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

where ϕ and j_z are canonical conjugate variables.

Finally a classical Hamiltonian is written as

$$h = 2g'\sqrt{(1-j_z)}(1+j_z)\cos\phi + \delta'(1+j_z) \tag{9}$$

with the rescaled constants $g'=gV\sqrt{N}/8$ and $\delta'=\delta V/4$.

Energy surfaces and the classical phase space are shown in Figs. 6 and 7 for various values of δ'/g', equivalent to δ/g for the quantum cases shown in the preceding section. As expected the phase space is periodic in the variable ϕ and j_z is restricted to $-1\leq j_z\leq 1$. In these figures we can see two different dynamical regimes: One is represented by closed orbits with negative energies encircling the central minimum at $\phi=\pi$; the other one is represented by closed orbits with positive energies around the lateral maxima. Separating these two dynamical regimes is a separatrix (dotted-dashed curve in Fig. 7) which is always at energy zero, when it exists.

These aspects can be settled analytically via investigation of the critical points of the function $h(\phi,j_z)$. These are of three kinds:

(i) Maxima localized at

$$(\phi,j_z)_{\max} = \left\{2n\pi, \frac{1}{18}\left[6-\left(\frac{\delta'}{g'}\right)^2 + \sqrt{\left(\frac{\delta'}{g'}\right)^4 + 24\left(\frac{\delta'}{g'}\right)^2}\right]\right\}. \tag{10}$$

(ii) Minima localized at

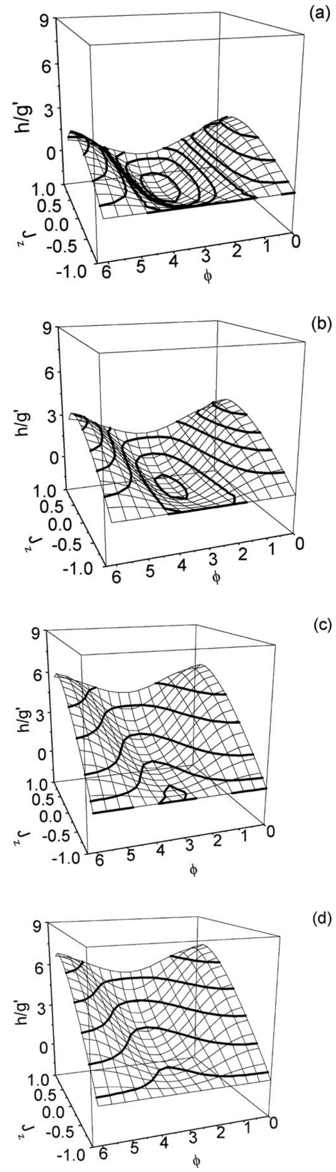

FIG. 6. Classical energy surfaces for some values of δ'/g' corresponding to the quantum cases shown in Fig. 1: (a) $\delta'/g'=0$, (b) $\delta'/g'=1.0$, (c) $\delta'/g'=2.5$, and (d) $\delta'/g'=3.0$.

$$(\phi,j_z)_{\min}=\left\{(2n+1)\pi,\frac{1}{18}\left[6-\left(\frac{\delta'}{g'}\right)^2-\sqrt{\left(\frac{\delta'}{g'}\right)^4+24\left(\frac{\delta'}{g'}\right)^2}\right]\right\} \qquad (11)$$

for $\delta'/g'<\sqrt{8}$. These minima turn into saddle points for $\delta'/g'>\sqrt{8}$.

(iii) Saddle points at

$$(\phi,j_z)_{\text{saddle}}=\left[\arccos\left(\frac{-1}{\sqrt{8}}\frac{\delta'}{g'}\right),-1\right]. \qquad (12)$$

As the ratio δ'/g' increases from zero, the energy surface is lifted and at the value $\delta'/g'=\sqrt{8}$ there are no more regions of negative energy. For increasing values of $\delta'/g'>\sqrt{8}$, the energy surface tends to become a vertical wall with basis at the line $j_z=-1$. The points $(\phi,j_z)_{\text{saddle}}$ mark the points in phase space where the separatrix touches the line $j_z=-1$ and restricts its existence to the interval $0\le\delta'/g'<\sqrt{8}$; the separatrix disappears for $\delta'/g'\ge\sqrt{8}$.

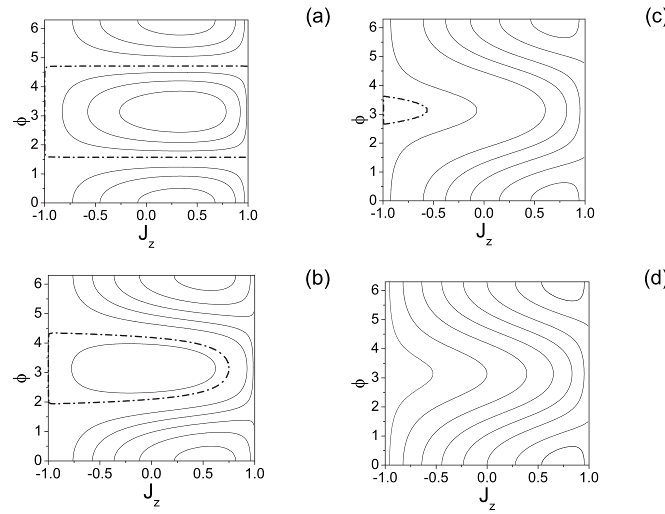

FIG. 7. Classical phase spaces for the same values of δ'/g' as shown in Fig. 6. The orbit associated to energy zero (dotted-dashed curve) is the separatrix.

The behaviors of the classical energy surface and phase space are in striking correspondence with the observations made in the preceding section concerning the quantum fermion-pair-to-boson phase transition.

The separatrix orbit at energy zero is associated with the quantum "separatrix" state given by the inflection point in the spectrum. In fact, the disappearance of the classical separatrix at $\delta'/g'=\sqrt{8}$ provides a more accurate value for the critical value δ/g at which the quantum ground energy level becomes the separatrix level, since $g=8g'/(V\sqrt{N})$ and $\delta=4\delta'/V$. For $N=1600$ particles, we have $\delta/g=20\sqrt{8}\cong 56.5685$.

The phase transition was seen to be associated to the rapid decrease, and even absence, of excitons in the system, once a critical value of the parameter δ/g is attained. Looking at the classical phase space, that transition can be anticipated and explained in the following way. As the ratio δ'/g' is increased from zero, the energy surface is gradually lifted until $\delta'/g'=\sqrt{8}$, when the minimum turns into a saddle point with energy zero at the line $j_z=-1$. On the other hand, the classical analog of the quantum operator $b^\dagger b$, which counts the number of bosons in the system, is nothing but the function $(1+j_z)$. A similar argument applies to the closed orbits around the minimum, which correspond to the excited quantum states with energy below zero.

The above correspondence between the quantum energy level and the classical energy surface, concerning the expected number of bosons, is verified not only for the separatrix energy but for the whole quantum spectrum. In this spirit, considering departures from the classical line $j_z=-1$, one can compare, for example, Fig. 5(d) at $\delta/g=60$ and Figs. 6(d) and 7(d) at $\delta'/g'\approx 4.0$.

IV. DISCUSSION

The model presented in this paper is motivated by an experiment, reported in Ref. [4], where a peak in electron tunneling in a bilayer system signalizes a boson-fermion transition, with a corresponding rapid decrease in the number of excitons. This quantum phase transition is seen when the interlayer separation is diminished and goes below a certain limiting distance, with the system always kept in a half-filling-per-layer condition, meaning equal number of electrons and holes. This condition can be broken by variations in field, temperature, or distance between layers, for example. In our work we deal with equal number of electrons and holes and, since our simple model does not account for factors such as fields nor temperature, it is reasonable to assume that the coupling parameter g reflects solely the interlayer separation. Concerning the above-mentioned experimental observations, this model shows correspondingly that, when δ/g exceeds the critical value $\sqrt{2N}$—here interpreted as the separation between layers being reduced below a critical value—the number of bosons expected for the ground state experiences a rapid decrease, eventually going to zero in the limit of vanishing values for g.

From the point of view of the classical analysis, it is conjectured in Ref. [15] that, whenever a fixed point in phase space undergoes a supercritical pitchfork bifurcation at some critical value of the coupling parameter, the corresponding quantum ground state shows maximum entanglement. Although in our work we do not see the emergence of two new fixed points for $\delta'/g' > \sqrt{8}$, characteristic of the pitchfork bifurcation, we indeed have a loss of stability, with the minimum [Eq. (11)] turning into a saddle point. As we observed, at this critical value the linear entropy Δ [Eq. (3)] for the quantum ground state attains a plateau approaching $\Delta=1$, its maximum possible value.

V. CONCLUDING REMARKS

We constructed a schematic physically motivated model to describe a fermion-boson phase transition in bilayer electron systems. The model allows for exact results and we explore the quantum-classical analogy.

The sudden decrease in the ground-state linear entropy has been discussed before in several contributions. We have shown in the present case that not only the ground state but every state, up to the separatrix energy, signals the phase transition at a corresponding coupling parameter. When the state becomes the separatrix state, it also shows a clear and sudden decrease of the linear entropy as well as the density of levels is maximized around its energy. The phenomenon is less pronounced than in the ground state but physically robust. These results are in accordance with those found in Refs. [13,17] for the Lipkin model and in Ref. [18] for collective vibrations of nuclei, and we believe similar results to be valid for others collective models [10,11] in which phase transitions have been studied.

Also the quantum-classical correspondence shows itself clear and wide ranging in this model, going from the role of the classical separatrix orbit as indicative of the phase transition to the direct representation of the number of bosons in the quantum system as one of the classical variables. Apart from particular aspects of the model, the classical analogy here presented suggests that the separatrix orbit can provide important information on the quantum transition and deserves a better understanding of its role.

From another point of view, it is clear that here we deal with noninteracting excitons. A repulsive interaction between these particles can be treated with no special difficulty with the inclusion of a term such as $(b^{\dagger}b)^2$ in the Hamiltonian. Work along these lines is presently in progress.

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[1] S. A. Moskalenko and D. W. Snoke, *Bose-Einstein Condensation of Excitons and Biexcitons* (CUP, New York, 2000).
[2] J. Kasprzak *et al.*, Nature (London) **443**, 409 (2006).
[3] M. Richard, J. Kasprzak, R. Andre, R. Romestain, L. S. Dang, G. Malpuech, and A. Kavokin, Phys. Rev. B **72**, 201301(R) (2005).
[4] J. P. Eisenstein and A. H. MacDonald, Nature (London) **432**, 691 (2004).
[5] T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002).
[6] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) **416**, 608 (2002).
[7] T. J. Osborne and M. A. Nielsen, Quantum Inf. Process. **1**, 45 (2002).
[8] G. Q. Pellegrino, K. Furuya, and M. C. Nemes, Chaos, Solitons Fractals **3**, 327 (1993).
[9] M. O. Terra, A. H. Blin, B. Hiller, M. C. Nemes, C. Providência, and J. da Providência, J. Phys. A **27**, 697 (1994).
[10] M. Reis, M. O. Terra Cunha, A. C. Oliveira, and M. C. Nemes, Phys. Lett. A **344**, 164 (2005).
[11] M. C. Nemes, K. Furuya, G. Q. Pellegrino, A. C. Oliveira, M. Reis, and L. Sanz, Phys. Lett. A **354**, 60 (2006).
[12] S. Schneider and G. J. Milburn, Phys. Rev. A **65**, 042107 (2002).
[13] W. D. Heiss and M. Müller, Phys. Rev. E **66**, 016217 (2002).
[14] A. P. Hines, C. M. Dawson, R. H. McKenzie, and G. J. Milburn, Phys. Rev. A **70**, 022303 (2004).
[15] A. P. Hines, R. H. McKenzie, and G. J. Milburn, Phys. Rev. A **71**, 042303 (2005).
[16] E. H. Lieb, Commun. Math. Phys. **31**, 327 (1973).
[17] W. D. Heiss, F. G. Scholtz, and H. B. Geyer, J. Phys. A **38**, 1843 (2005).
[18] P. Cejnar, M. Macek, S. Heinze, J. Jolie, and J. Dobes, J. Phys. A **39**, L515 (2006).