Quantum Signatures of The Classical Disconnection Border

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A quantum Heisenberg model with anisotropic coupling and all-to-all interaction has been analyzed using the Bose-Einstein statistics. In Ref.[1] the existence of a classical energy disconnection border (EDB) in the same kind of models has been demonstrated. We address here the problem to find quantum signatures of the EDB. An independent definition of a quantum disconnection border, motivated by considerations strictly valid in the quantum regime is given. We also discuss the dynamical relevance of the quantum border with respect to quantum magnetic reversal. Contrary to the classical case the magnetization can flip even below the EDB through Macroscopic Quantum Tunneling. We evaluate the time scale for magnetic reversal from statistical and spectral properties, for a small number of particles and in the semiclassical limit.

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The existence of an energy disconnection border (EDB) (previously called non-ergodicity threshold), in classical Heisenberg models with anisotropic coupling and infinite range of interaction has been recently found[1]. Below the EDB the energy surface is disconnected into two components with opposite sign of the total magnetization. The dynamical consequences of the EDB in classical Heisenberg models with infinite range coupling has also been investigated [2]. In particular, it has been shown that below the EDB the magnetization cannot change sign in time, while above it, in a fully chaotic regime, a time scale for the magnetic reversal (time needed for the total magnetization to flip) can be determined. Magnetic reversal times show an exponential growth with the number of spins and, as in standard phase transitions, a power law divergence at the EDB itself.

The existence of this border is not limited to the infinite range coupling case and can be in general related to the anisotropy of the coupling when it induces an easy–axis of magnetization (defined by the direction of the magnetization in the minimal energy configuration of the system). The relation between the EDB and the range of the interaction has also been studied: we have taken into account a Heisenberg models with an interaction potential among the spins which decays as $R^{-\alpha}$, where R is the distance among the spins. Defining as r, the ratio of the disconnected portion of the energy range with respect to the total energy range, it has been proved that for a $d-$dimensional system r tends to zero in the thermodynamic limit for $\alpha > d$(short range) while it remains finite for $\alpha < d$ (long range) [3].

The results found in the classical model guided our investigations on the quantum side. We are mainly interested here in the quantum signature of the classical EDB, and on its relevance with respect to the quantum reversal time of the magnetic moment.

We consider here an infinite-range interacting system since the explicit expression of the EDB has been obtained in this case only. Despite its unphysical character, magnetic systems can be realized, within modern experimental techniques [4], described by Heisenberg–like Hamiltonians with an infinite range term, which could induce the presence of the EDB. Moreover, when the range of the interaction is of the same order of the size of the system, the all-to-all coupling could be an important first order approximation in the understanding of their behavior [5, 6]. This could be the case for small systems used in present nano-technology which requires to deal with systems with a few dozens of particles[7], or for macroscopic systems with long range interactions.

We first analyze the spectral properties and we establish the existence of a quantum disconnection border in close correspondence with the classical one. An analytical estimate of this quantum threshold is given. We will then study the system from a dynamical point of view, analyzing the time scale for quantum magnetic reversal and comparing the quantum magnetic reversal times with the classical ones.

We consider a system of N particles of spin l, described by the following Hamiltonian,

$$\hat{H} = \frac{\eta}{2}\sum_{i=1}^{N}\sum_{j\neq i}\hat{S}_i^x\hat{S}_j^x - \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}\hat{S}_i^y\hat{S}_j^y, \qquad (1)$$

where $-1 < \eta \leq 1$ is the anisotropy constant. We define $\hat{M}_{x,y,z} = \sum_i S_i^{x,y,z}$ as the components of the total magnetization of the system. Due to the anisotropy of the coupling the system has an easy–axis of the magnetization along the $y-$direction. Quantization of the Hamiltonian follows the standard rules. According to the correspondence principle, the classical limit is recovered as $l \to \infty$. As in the classical case we fix the modulus of the spins to one. This can be achieved with an appropriate rescaling of the Planck constant, $\hbar \to \hbar/|S_i| = 1/\sqrt{l(l+1)}$. With this choice, in the classical limit, $l \to \infty$ ($\hbar \to 0$), the spin modulus remains equal to 1. Because of the infinite range nature

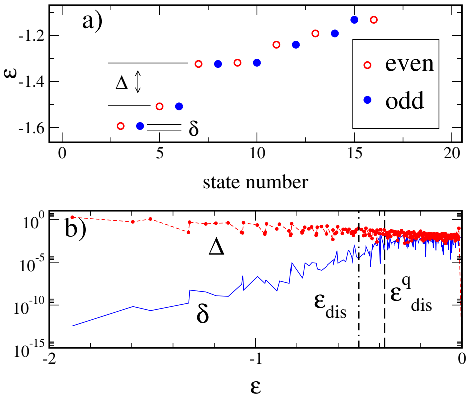

FIG. 1: (Color online) $N = 6$ $l = 3$ $\eta = 1$. a) Doublet structure of the low energy region of the spectrum. The different parity of the states constituting the doublets is shown. We also indicated the level distance among even eigenstates, Δ. b) the splitting of the doublets, δ, *vs* the specific energy, $\epsilon = E/N$ (blu line) and the nearest neighbor level spacing $\Delta(\epsilon)$ (red line). Also shown as vertical lines: the quantum disconnection border, ϵ^q_{dis} (dashed), computed analytically from Eq.(2), and ϵ_{dis} (dashed-dotted).

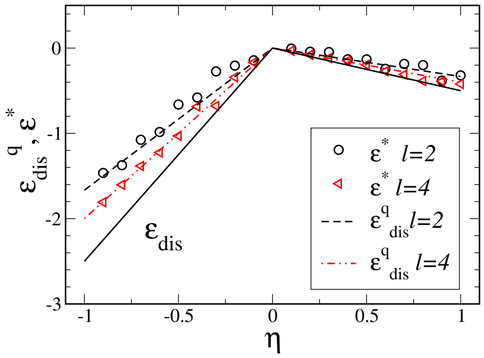

FIG. 2: (Color online) ϵ^q_{dis} (dashed lines) and ϵ^* (symbols) for different l values *vs* η. Data are $N = 6$, $l = 2, 4$. Also shown (as full line) ϵ_{dis} that showing, at the same time, the agreement between ϵ^q_{dis} and ϵ^* and their common semiclassical limit ϵ_{dis}.

of the interaction, the Hamiltonian (1) is a completely symmetric operator with respect to particle exchange. It is thus natural to limit ourselves to subspaces of definite symmetry. Specifically, we consider the bosonic case (an ensemble of integer spins), so we will limit our analysis in the subspace of all possible completely symmetric states, with dimension $\mathcal{N} = (N + 2l)!/(N!(2l)!)$. This choice reduces considerably the dimension of the Hilbert space, allowing to extend our analysis further in the classical limit. An important property of the Hamiltonian (1) is its invariance under a π rotation about the z-axis : the Hamiltonian commutes with the operator $\exp(i\pi \sum \hat{S}^z_i)$, and its eigenstates can be labeled as odd (-) or even (+) according to whether they change or do not change sign under such rotation.

The first aim of our analysis on the quantum system is to assess the quantum signature of the classical disconnection threshold, ϵ_{dis}. Numerical diagonalization of (1) gives rise to a quasi-degenerate energy spectrum with a energy splitting increasing with the energy. It is a standard result[8], that the infinite time average of any quantum operator is zero in presence of a non-degenerate discrete spectrum and if its quantum average over the energy eigenstates is zero. The operator $\hat{M}_y$ satisfies this conditions thus the total magnetization along the easy–axis, can change its sign for any energy. Also, the time scale at which this happens can be obtained by a detailed study of the energy difference between close eigenstates. Specifically, since the matrix elements of $\hat{M}_y$ between energy eigenstates of the same parity is zero, it will be important to study the characteristics of the energy distance between even and odd eigenstates. The possibility for the magnetization to reverse its sign also in the energy region where it would be classically forbidden, can be interpreted as a manifestation of Macroscopic Quantum Tunneling [9], (the total magnetization can be a macroscopic quantity). The evaluation of the tunneling rates becomes then crucial to obtain the time scale for the quantum magnetic reversal.

The most evident property of the energy spectrum is the presence, in the low energy region, of quasi degenerate doublets, see Fig. 1a. Each doublet is composed by an even and an odd eigenstate. Even if from Fig. 1a they seem degenerate, they are actually split by a small energy difference δ. At high energy the doublets are not well defined anymore. In Fig. 1a we have also indicated the level spacing between neighbor even states Δ. Note that the doublets are well defined only when $\delta \ll \Delta$.

The splittings of the doublets, δ, can be computed numerically for each even (or odd) eigenstate taking the energy difference from its closest odd (or even) state; δ can thus be considered as a degree of the spectrum degeneracy. In Fig. 1b we show how δ varies with the specific energy, $\epsilon = E/N$: a change of slope is clearly visible, from exponential to almost constant. Note that the energy at which the slope changes is close to the classical ϵ_{dis}, see Fig. 1b . It is possible to have a better estimate of the energy at which the slope changes, considering the energy ϵ^* at which the doublets disappear: $\delta(\epsilon^*) \simeq \Delta(\epsilon^*)$, see Fig 1b. Note that the value ϵ^*, distinguishes two regions of the spectrum, characterized or not by quasi-degenerate eigenvalues pairs. The behavior of ϵ^* for different l values as a function of the anisotropic coefficient η has been reported in Fig. 2. As one can see $\epsilon^* \to \epsilon_{dis}$ as l increases, which confirms the soundness of our definition.

ϵ^* can be thought as a quantum correction to the classical EDB. An hand-waving argument allows to evaluate this quantum correction: in the classical case, ϵ_{dis} has been obtained computing the minimum of $-(\eta/2)\sum(S^x_i)^2$ when $\eta > 0$, and of $(\eta/2)M^2_x - (\eta/2)\sum(S^x_i)^2$ when $\eta < 0$[1]. Thus, the lowest eigenvalue of the same operators could give an approximate quantum border. We will call this threshold the quantum

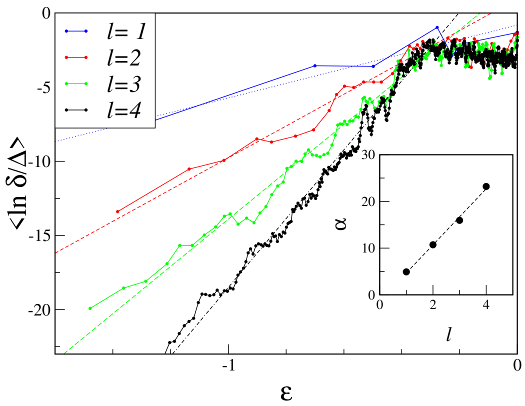

FIG. 3: (Color online) Average (over energy bins) of $\langle \ln(\delta/D) \rangle$ *vs* the specific energy ϵ, for $N = 6$, $\eta = 1$ and different l, as indicated in the legend. Here D is the average level spacing. Also shown (dashed and dotted style) the linear fit. Inset : the linear dependence of the slopes α with l. Linear fitting is $\alpha = -1.3 + 6l$.

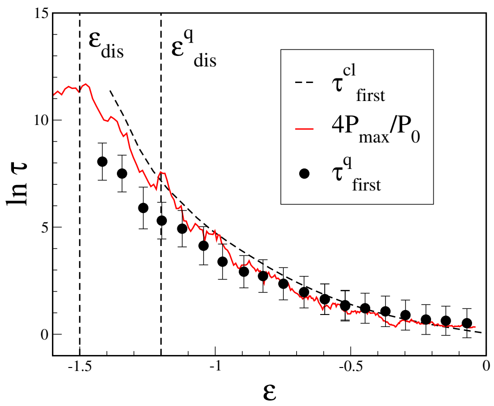

FIG. 4: (Color online) The quantum average reversal time, τ (circles), as a function of ϵ is are shown for the case $N = 6$, $\eta = 1$ and $l = 4$, are compared with the classical ones (dashed black line), showing a good agreement above ϵ^q_{dis} and a deviation near ϵ_{dis}. Also shown, as a full line $4P_{max}/P_0$ averaged over close eigenfunctions.

disconnection border ϵ^q_{dis}, and we have:

$$\begin{aligned} \epsilon^q_{dis} &\sim -\frac{\eta}{2}(\hbar l)^2 \ \text{ for } \ \eta > 0 \\ \epsilon^q_{dis} &\sim \frac{\eta}{2}(N-1)(\hbar l)^2 \ \text{ for } \ \eta < 0. \end{aligned} \tag{2}$$

The agreement between the numerical values ϵ^* and our analytical estimate ϵ^q_{dis} has been shown in Fig. 2 (compare symbols with dashed and dotted lines).

As shown in Fig. 3 the level splittings increase exponentially with the energy. Also, on increasing the semiclassical parameter l, the rate of growth becomes steepest. In Fig. 3 we show the average of $\ln\delta$ over suitable energy bins, and normalized to the average level spacing D (obtained dividing the energy range by the number of states). Linear fits have also been indicated as dashed lines. In the inset the exponent α, obtained from the fitting : $\langle \ln(\delta/D) \rangle = \alpha\epsilon + C$ has been shown to have a linear dependence on the semiclassical parameter l, so that $\delta(E) \approx 0$ for $\epsilon < \epsilon_{dis}$ when $l \to \infty$.

Let us now analyze the time scale for magnetic reversal in the quantum system, comparing the results with the classical ones[2]. Since in the classical case the reversal times have been determined at a fixed energy (microcanical approach), we adopt here the same procedure and compute the reversal time of the quantum average magnetization starting from an ensemble of initial states, $|\psi\rangle$, obtained choosing randomly energy eigenstates in a narrow energy interval: $|\psi\rangle = \sum_E^{E+\Delta E} C_E|E\rangle$. The coefficients C_E have been randomly chosen in modulus and phase and such that $\sum_E^{E+\Delta E} |C_E|^2 = 1$. Since the total magnetization along the easy–axis, $\hat{M}_y$, connects only energy eigenstates with different parity, we have:

$$\langle M_y(t) \rangle = 2\mathcal{R}e\{ \sum_{E_+,E_-=E}^{E+\Delta E} C^*_{E_+} C_{E_-} e^{-it/T} \langle E_+|\hat{M}_y|E_-\rangle \}, \tag{3}$$

where $T = \hbar/(E_- - E_+)$. From $\langle M_y(t) \rangle$ we compute the time of first passage through zero for each initial state of the ensemble. From these times we obtain the average magnetic reversal time τ. Before presenting the results of our analysis let us recall that in the quantum case, at variance with the classical one, we are legitimate to ask what is the time scale for magnetic reversal in the whole energy range. Indeed, since the energy spectrum is non-degenerate, from Eq.(3), the average magnetization will soon or later reverse its sign, even below the EDB.

In Fig. 4 we consider the energy region above ϵ_{dis}. As one can see there is good agreement between classical and quantum times above ϵ^q_{dis}. Note that the classical times diverge at ϵ_{dis} at variance with the quantum ones which are systematically smaller, in the region betwen ϵ_{dis} and ϵ^q_{dis} . This is not surprising since the possibility of tunneling will enhance the probability for the magnetization to reverse its sign. In the classical case we successfully evaluated the reversal times from the entropic barrier, ΔS, between the most probable value of the magnetization and its zero value, $\tau \sim e^{-\Delta S} = P_{max}/P_0$ [2]. Following the classical case we also computed P_{max}/P_0 from the quantum probability distribution of the magnetization, $P(M_y)$, and compared the dynamical times τ with the probabilistic ones given by cP_{max}/P_0 [2], where c is a constant. As one can see from Fig. 4 the agreement between probabilistic and dynamical times is fairly good where classical and quantum times agrees, while the agreement is less accurate in the crossover region, between ϵ_{dis} and ϵ^q_{dis}. Let us now discuss, in details, the behavior of the quantum reversal times below ϵ^q_{dis}.

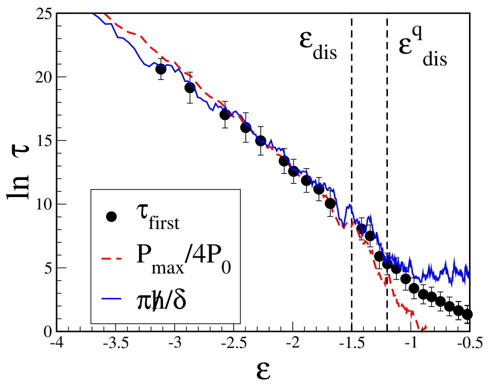

FIG. 5: (Color online). Comparison between dynamical and tunneling splittings in the classically forbidden energy region. Circles : dynamical quantum reversal times; Full (blu) line: tunneling splittings $\tau \sim \pi\hbar/(2\delta)$ for the case: $N = 6$, $l = 4$. Not surprisingly, the evaluation of τ through δ does not work above ϵ^q_{dis}, where the doublet structure disappear. As dashed (red) line $P_{max}/4P_0$.

In the low energy region of the spectrum, due to the intrinsic quasi-degeneracy the dynamics can be entirely characterized by the energy difference $|E_+ - E_-| = \delta$. This occurs if the energy bin ΔE of the initial state is sufficiently small so that one single doublet belongs to it. The dynamics is thus oscillatory with a period given by $2\pi\hbar/\delta$. Indeed under this condition, the magnetization oscillates coherently between states with opposite sign, a phenomenon known as Macroscopic Quantum Coherence[10]. This period also represents, within a numerical factor, the time for the first passage to zero of $\langle M_y(t)\rangle$. One thus can assume : $\tau \sim \pi\hbar/(2\delta)$. The agreement, over many orders of magnitude, has been shown in Fig. 5. Also below ϵ^q_{dis}, we checked the proportionality of the reversal times with P_{max}/P_0. It is surprising that P_{max}/P_0 turns out to be proportional to the tunneling rates and then, when properly defined, to the reversal times, even in the region classically forbidden (below ϵ_{dis}) where the only mechanism allowing the jumping of the barrier is through Macroscopic Quantum Tunneling, see Fig. 5. This suggests that the mechanism producing this proportionality can also have a non classical origin. One should also note that the constant of proportionality is different below ϵ_{dis} and above ϵ^q_{dis}. This explains the poor agreement between the statistical and dynamical times in the crossover region ($\epsilon_{dis} < \epsilon < \epsilon^q_{dis}$).

From the results presented here we can address the problem of the dynamical signature of the classical Energy Disconnection Border. In the semiclassical limit the crossover region becomes very narrow, ($\epsilon^q_{dis} \to \epsilon_{dis}$), thus we can expect a crossover from of the reversal time from a power law dependence on the energy, like in the classical case[2], to and exponential dependence on the energy. Moreover Fig. 3 suggests how the classical limit is recovered: indeed $\delta \approx 0$ as $l \to \infty$, for energies below ϵ_{dis}, which is consistent with the fact that the magnetization cannot reverse its sign below ϵ_{dis} in the classical system.

In conclusion we have found a quantum signature of the classical EDB in the spectral properties of the system leading to the definition of a quantum disconnection threshold, ϵ^q_{dis} with the correct classical limit. Below ϵ^q_{dis} the spectrum is characterized by the presence of quasi degenerate doublets, whose energy difference $\delta(\epsilon)$ depends exponentially on ϵ. The quantum reversal times of the total magnetization have been studied and compared with the classical ones above ϵ_{dis}. We have also shown that the total magnetization can flip in the energy region classically forbidden. Quite surprisingly, quantum reversal times (and thus the tunneling rates) are still proportional to P_{max}/P_0 even below ϵ_{dis}.

The existence of the classical EDB allows to address an energy region where to look for Macroscopic Quantum Phenomena, which have recently raised much interest[11]. Indeed the fact that the total magnetization can reverse its sign even below the EDB can be seen as a manifestation of Macroscopic Quantum Tunneling, a well known phenomenon in micromagnetism, also found experimentally[12, 13]. Nevertheless Macroscopic Quantum Tunneling of magnetization arises in literature [9, 10], from phenomenological Single–Spin Hamiltonians, where the single spin describes the total magnetic moment of the system, and no reference to the range of the interaction has been explicitly pointed out. On the other hand we presented here a multiparticle system in which this phenomenon clearly arises, in connection with the existence of the disconnection border and with the long range nature of the interaction.

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