Revival times at quantum phase transitions

F. de los Santos^{1,2} and E. Romera^{1,3}

¹Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, Fuentenueva s/n, 18071 Granada, Spain ²Departamento de Electromagnetismo y Física de la Materia and Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, Fuentenueva s/n, 18071 Granada, Spain

³Departamento de Física Atómica, Molecular y Nuclear and Instituto Carlos I de Física Teórica y Computacional, Universidad de Granada, Fuentenueva s/n, 18071 Granada, Spain (Received 24 August 2012; published 22 January 2013)

The concept of quantum revivals is extended to many-body systems and the implications of traversing a quantum phase transition are explored. By analyzing two different models, the vibron model for the bending of polyatomic molecules and the Dicke model for a quantum radiation field interacting with a system of two-level atoms, we show evidence of revival behavior for wave packets centered around energy levels as low as the fundamental state. Away from criticality, revival times exhibit smooth, nonsingular behavior and are proportional to the system size. Upon approaching a quantum critical point, they diverge as a power law and scale with the system size, although the scaling is no longer linear.

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I. INTRODUCTION

The concept of a phase transition can be extended to zero absolute temperatures, when thermal fluctuations cease. Quantum fluctuations then take over and the system may undergo a quantum phase transition (QPT), which reflects in a dramatic change in its physical properties as illustrated by the dependence of many several observables on a suitable control parameter (other than the temperature, say λ) that determines the amplitude of quantum fluctuations [1]. It is a generic feature that at second-order QPTs the system will exhibit diverging quantities as the transition is approached. An important one is the correlation length, which, following notions and a nomenclature borrowed from classical critical phenomena, diverges as $\xi \sim |\lambda - \lambda_c|^{-\nu}$. Similarly, other quantities such as specific heats or susceptibilities diverge in the same manner, defining new critical exponents which are related through scaling relations. This is all well known and to date examples abound of quantum critical features of classical observables brought about by quantum fluctuations alone. Much less studied, however, is the influence of QPTs on purely quantal properties, lacking a classical counterpart. Here, we address the problem of wave-packet revivals in systems exhibiting QPTs.

The long-time evolution of propagating quantum wave packets may lead to unexpected periodic behavior. Initially, the wave packets evolve quasiclassically and oscillate with a classical period $T_{\rm cl}$, but eventually spread out and collapse. At later times, multiples of the *revival time* $T_{\rm R}$, wave packets regain their initial form and behave quasiclassically again. The classical period and the revival time of wave-packet evolution are embodied in the first coefficients of the Taylor expansion of the energy spectrum E_k around the energy E_{k_0} corresponding to the peak of the initial wave packet,

$$E_k = E_{k_0} + E'_{k_0}(k - k_0) + \frac{E''_{k_0}}{2}(k - k_0)^2 + \frac{E'''_{k_0}}{6}(k - k_0)^3 + \cdots,$$
(1)

the first-, second-, and third-order terms in the expansion providing the classical period of motion $T_{\rm cl}=2\pi/|E_{k_0}'|$, the

quantum revival scale time $T_{\rm R} = 4\pi/|E_{k_0}''|$, and the so-called super-revival time $T_{SR} = 12\pi/|E_{k_0}''|$, respectively. Revivals have received considerable attention over the last decades [2]. Both experimental and theoretical progress was made in, among others, Rydberg atoms, molecular vibrational states, electric currents in graphene, or Bose-Einstein condensates [3–9]. Recently, methods for isotope separation [10] and number factorization [11] as well as for wave-packet control [12–14] have been put forward that are based on revival phenomena, and the presence of effective multibody interactions in a system of ultracold bosonic atoms in a three-dimensional optical lattice was identified in time-resolved traces of quantum phase revivals [15]. Interestingly, the collapse and revival dynamics of ultracold atoms in optical lattices have been investigated and shown to be strongly sensitive to the initial many-body ground state [16].

In this article, we extend the concept of quantum revivals to many-body systems and explore the implications of traversing a quantum phase transition. By analyzing two different models, the U(3) vibron model for the bending dynamics of molecules and the Dicke model of two-level atoms interacting with a one-mode radiation field, we show that, as a consequence of the squeezing of the energy levels around the ground-state energy at the critical point, revival times of wave packets centered around quantum numbers as low as the fundamental state diverge as a power law upon approaching a quantum critical point. Interestingly, we find that the revival times diverge sufficiently close to the critical point even at finite system sizes.

II. THE U(3) VIBRON MODEL

The U(3) vibron model has been successfully applied to study the bending dynamics of linear polyatomic molecules [17]. Its Hamiltonian is constructed as a combination of invariant operators associated with the subalgebras of U(3) (see [17] for further details), and it reads

$$H = (1 - \chi)k + \frac{\chi}{N - 1}\hat{P},$$
 (2)

where $0 \le \chi \le 1$ and \hat{P} is the so-called pairing operator (see below). Here N and k are the total number of bound states and the number of vibrational quanta. The associated base has elements $|k,l\rangle$, l being the value of the angular momentum along the z axis perpendicular to the plane of vibrations. Their allowed values for a given N are $k = 0,1,2,\ldots,N$ and $l = \pm k, \pm (k-2),\ldots,\pm 1$ or 0 for k odd or even. In what follows we shall restrict ourselves to zero vibrational angular momentum, l = 0.

Four cases can be distinguished in terms of the value of the control parameter χ : bending vibrations of rigidly linear molecules ($\chi=0$); the quasilinear case ($0<\chi\leqslant0.2$) (including a quantum critical point at $\chi=0.2$; see below); the quasibent case ($0.2<\chi<1$); and the rigidly bent case ($\chi=1$). The Hamiltonian is U(2) invariant for $\chi=0$ and SO(3) invariant for $\chi=1$, and in these cases analytical solutions for the spectra exist [18]:

$$E_k(\chi = 0) = 2k,\tag{3}$$

$$E_k(\chi = 1) = \frac{4}{N-1} \left[\left(N + \frac{1}{2} \right) k - k^2 \right].$$
 (4)

The classical and revival times can be computed from the expressions above to give the exact, limiting values $T_{\rm cl}(\chi=0)=\pi$ and $T_{\rm R}(0)=\infty$ on the one hand, and $T_{\rm cl}(\chi=1)=(N-1)\pi/(2N+1-4k_0)$ and $T_{\rm R}(1)=(N-1)\pi/2$ on the other. The divergence of $T_{\rm R}$ is in accordance with the harmonic nature of the Hamiltonian when $\chi=0$, while $T_{\rm R}(\chi=1)$ being linear in N provides an example of the scaling of revival times in a many-body system, a scaling feature that is absent in the classical period.

For general $0 < \chi < 1$ the spectra are no longer analytically accessible and one has to resort to numerical methods. To diagonalize the Hamiltonian Eq. (2) we use the matrix elements of $\hat{P} = N(N+1) - \hat{W}^2$ [18],

$$\langle k_2, l | \hat{W}^2 | k_1, l \rangle = a \delta_{k_1, k_2} + b \delta_{k_1 - 2, k_2} + c \delta_{k_1 + 2, k_2},$$
 (5)

with

$$a = (N - k_1)(k_1 + 2) + (N - k_1 + 1)k_1 + l^2,$$

$$b = -\sqrt{(N - k_1 + 2)(N - k_1 + 1)(k_1 + l)(k_1 - l)},$$

$$c = -\sqrt{(N - k_1)(N - k_1 - 1)(k_1 + l + 2)(k_1 - l + 2)}.$$
(6)

We find the general feature (already reported in Ref. [19]) that on increasing the system size N, k/N becomes a quasicontinuous variable x and that the combination $\frac{E_{k/N}}{N}$ converges to a common spectrum e_x . This property alone implies that the revival times for a given x scale with N because

$$\frac{d^2e_x}{dx^2} = N\frac{d^2E_k}{dk^2}. (7)$$

For the purpose of illustrating this scaling, we construct initial wave packets as the linear combination

$$|\Psi(t=0)\rangle = \sum_{k} c_k |k,l=0\rangle \tag{8}$$

with Gaussian coefficients $c_k \propto \exp[-(k - k_0)^2/\sigma]$, $\sigma = 2$, and centered around $x_0 = k_0/N = 0.25$. Centering the wave packets around a common x_0 guarantees that the average

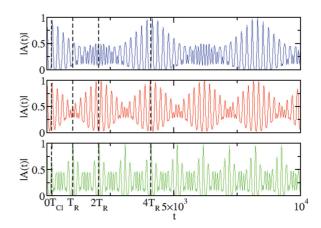


FIG. 1. (Color online) Time dependence of the modulus of the autocorrelation function |A(t)| for wave packets initially centered around $k_0/N=0.25$ with N=1000 (bottom), 2000 (center), and 4000 (top). Other parameter values are $\chi=0.5$ and $\sigma=2$. $T_R\simeq 1024$ denotes the revival time for N=1000, and $T_{\rm cl}\simeq 192$ the classical period. Times are given in dimensionless units.

energies are common in turn [20]. At later times, of course,

$$|\Psi(t)\rangle = \sum_{k} c_k |k, l = 0\rangle e^{-iE_k t}.$$
 (9)

Figure 1 shows the time evolution of the modulus of the autocorrelation function, $A(t) = \langle \Psi(0) | \Psi(t) \rangle$, which is the overlap between the initial and the time-evolving wave packets, of three wave packets corresponding to $\chi = 0.5$, N = 4000, 2000, and 1000. Given an initial state, |A(t)| decreases in time and the occurrence of revivals is reflected in its returning to its initial value of unity.

It can be clearly appreciated from the figure that $T_R(N=4000) \simeq 2T_R(N=2000) \simeq 4T_R(N=1000)$. For consistency, we have also verified that these revival times match those obtained by evaluating $4\pi/|E_{k_0}''|$, the second derivatives being simply computed through the numerical approximation $E_{k+1} + E_{k-1} - 2E_k$. The figure also shows the classical period $T_{\rm cl} \simeq 192$, which does not scale with N.

Revivals are also observed at energy levels as low as the ground state. As an example, Fig. 2 shows the time development of a wave packet with Gaussian-distributed population for $\chi=0.5$, centered around the ground state and with $\sigma=2$. The estimated revival time from the figure is approximately 2850, to be compared with $T_R/2=2\pi/|E_{k_0=0}''|=2853.5$. In this case, E_k'' is computed by fitting the first three levels of the spectrum to a parabola and then taking k=0. The results thus obtained are in perfect agreement with those observed by monitoring the wave packet's time evolution. Other values of χ , both above and below 0.2, yield again the behavior $T_R \sim N$.

Next, we study how the revival times are affected by the presence of the quantum critical point. At $\chi = \chi_c = 0.2$ this system undergoes a second-order quantum phase transition in the thermodynamic limit, $N \to \infty$, between two phases displaying anharmonicities of opposite signs. To compute the classical period and the revival time, notice that the former is simply related to the energy gap, $\Delta \equiv E_1 - E_0$, by $T_{\rm cl} \sim \Delta^{-1}$. Since this can be evaluated in the thermodynamic limit through $\Delta = \sqrt{(5\chi - 1)(1 + 3\chi)}$ (valid for $\chi > \chi_c$ [21]), this implies

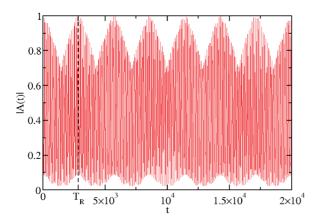


FIG. 2. (Color online) Time dependence of |A(t)| for a wave packet centered around the ground state and system parameters $\chi=0.5,\ N=2000,\ {\rm and}\ \sigma=2.\ T_{\rm R}\simeq2853.5$ denotes the revival time. Time is given in dimensionless units.

that the classical period of wave packets centered around the ground state diverges as the critical point is approached as $T_{\rm cl} \sim (\chi - \chi_{\rm c})^{-1/2}$. For the sake of consistency, we have verified this prediction numerically. As regards $T_{\rm R}$, a divergent behavior is also expected due to the squeezing of the energy levels around the ground-state energy at the critical point, what leads to the time evolution of the wave packet being basically controlled by a single autostate. In fact, we find $T_{\rm R} \sim (\chi - \chi_{\rm c})^{-1}$ at fixed N=1000 and $k_0=0$, with $\chi_c=0.205\,907\,075(3)$ (see Fig. 3). Supporting this image is the divergence of the super-revival time $T_{\rm SR}$, as shown in the inset of Fig. 3 with, in this case, $\chi_c=0.203\,904\,4(2)$ and the same scaling exponent -1. Notice that all time scales diverge at close but different χ , only to coincide at χ_c in the thermodynamic limit [for N=1000, $T_{\rm cl}$ peaks at $\chi_c=0.205\,305(5)$ rather than diverging].

Another interesting aspect is the dependence of T_R and T_{cl} on the system size N for a given k. Previous results for the energy gap yield the scaling form $\Delta \sim N^{-1/3}$ (see [18] and references therein), which is in perfect agreement with our own, $T_{cl}(k_0 = 0) \sim N^{1/3}$. Moreover, we find this same

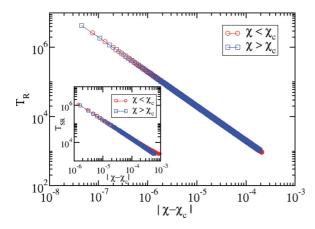


FIG. 3. (Color online) Revival and super-revival (inset) times at criticality as a function of χ for wave packets centered around the ground state and N=1000. The red circles and the blue squares correspond to, respectively, $\chi < \chi_c$ and $\chi > \chi_c$. Times are given in dimensionless units.

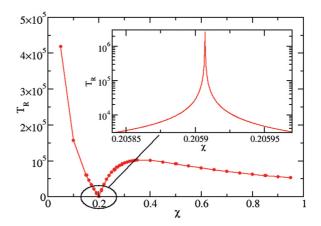


FIG. 4. (Color online) Revival time as a function of χ for wave packets centered around the ground state and N=1000. The inset is an enlargement of the delimited area and shows the divergence of T_R close to the critical point. Notice the logarithmic scale of the y axis. Time is given in dimensionless units.

scaling behavior for wave packets peaked at arbitrarily high k, i.e., $T_{\rm cl}(k_0>0)\sim N^{1/3}$. Turning to $T_{\rm R}$, we find that for any system size N there always exists a χ , the closer to $\chi_{\rm c}$ the larger N, such that $T_{\rm R}(k_0=0)$ diverges. This is illustrated in the inset of Fig. 4 which shows the behavior of $T_{\rm R}$ for N=1000 in the vicinity of $\chi_{\rm c}$. Similar divergences are found generically for any N, including values as low as 10, and for a different quantity in another model too, as discussed in the next section. To rationalize this behavior one can resort to analytical approximations to the spectra. In particular, a semiclassical approach at $\chi_{\rm c}$ gives [19]

$$\frac{E_k}{N} - \chi_c \sim \left(\frac{k}{N}\right)^{4/3},\tag{10}$$

which yields $T_{\rm R} \sim k_0^{2/3} N^{1/3}$ and $T_{\rm cl} \sim k_0^{-1/3} N^{1/3}$, k_0 being again the quantum number of the energy level the packet is centered around. However, this approximation seems to be valid only far from the ground state, as shown in Fig. 5 by plotting $\frac{E_k}{N} - \chi_{\rm c}$ vs k in double-logarithmic scale for several system sizes. Note that the spectra compare well with the

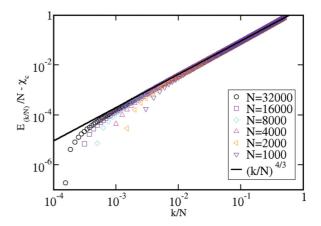


FIG. 5. (Color online) Numerical spectra at criticality for increasing system sizes N as compared with results of the semiclassical approximation. (Dimensionless units.)

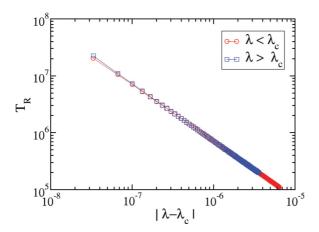


FIG. 6. (Color online) Log-log plot of the revival times for the Dicke model with j=10 in the vicinity of the critical point. The red circles and the blue squares correspond to, respectively, $\lambda < \lambda_c$ and $\lambda > \lambda_c$. The data can approximated by a straight line of slope -1. (Atomic units.)

power law $k^{1.36}$ only for sufficiently high k. This conveys the idea that the semiclassical formula might be asymptotically correct at very large values of both k and N.

III. THE DICKE MODEL

The Dicke model describes the interaction of a two-level atomic ensemble with a one-mode radiation field. It dates back to the 1950s [22], and to date several experimental realizations of the model have been proposed [23]. The Dicke model exhibits a quantum phase transition at zero temperature as embodied in the Hamiltonian [24]

$$H = w_0 J_z + w a^{\dagger} a + \frac{\lambda}{\sqrt{2j}} (a^{\dagger} + a)(J_+ + J_-).$$
 (11)

Here, J_z and J are the usual angular momentum operators for collective spin operators of length j=N/2, and a, a^{\dagger} are the bosonic operators of the field. The atomic level splitting is given by w_0 , w is the field frequency, and λ is the atom-field coupling. In the thermodynamic limit, $N, j \to \infty$, the system undergoes a second-order quantum phase transition at a critical coupling of $\lambda = \lambda_c = \sqrt{w_0 w}/2$. At this point the system changes from a normal phase to the so-called super-radiant one in which both the field and the atomic ensemble acquire macroscopic occupations. Revivals and fractional revivals in the Jaynes-Cummings model, a *single* (j=1/2) two-level atom interacting with one mode of the quantized radiation field, were studied in the past [25,26].

Proceeding along the same lines as in the previous section, that is, solving numerically for the spectra and populating the autostates around the ground state with Gaussian weights, a wave packet is constructed and its time development monitored. The parity has been taken into account as a symmetry in this system. (Variational approximations have been proposed in Refs. [27,28] to study the Dicke model in an analytical framework.) We have verified that our results for the classical time on scale resonance, i.e., $w_0 = w = 1$, follow those reported in Ref. [29], $\Delta \sim (\lambda_c - \lambda)^{1/2}$. As for T_R , we find $T_R \sim |\lambda_c - \lambda|^{-1}$ (see Fig. 6). Oddly enough, as in the vibron model, there is a value of λ at which T_R diverges irrespective of the system size. At this point, it may be in order to mention that it has been recently shown that the fidelity necessarily diverges at the critical point in the Dicke model [30], and, interestingly, divergent behavior has been observed to occur at finite system sizes [31].

IV. CONCLUSIONS

We have extended the concept of quantum revivals to manybody systems and explored the implications of traversing a quantum phase transition by analyzing the time development of wave packets centered around the fundamental state in two different models, namely, the U(3) vibron model and the Dicke model. Far from the quantum critical point, characteristic time scales such as the classical period and the revival and the superrevival times exhibit a smooth nonsingular behavior, and revival times are proportional to the system size. Upon approaching a quantum critical point, energy levels squeeze into the ground state, rendering the wave packet with a Gaussian-distributed population basically a combination of states with almost equal energies. We have shown evidence that under these circumstances, the above-mentioned quantities diverge as power laws with well-defined critical exponents. Interestingly, the revival and super-revival times were found to diverge on approaching the critical point even at finite system size. Should it be the case that all time scales in the Taylor expansion diverge, a statement we cannot confirm but that is suggested by the numerics and by the squeezing of the energy levels around the ground state as the transition point is approached, the time evolution of such wave packets at criticality would then be limited to phase changes, i.e., to rotations. Finally, we comment that quantum phase transitions can also influence the revival behavior of wave packets centered around excited states. This interesting effect, however, will be discussed elsewhere.

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