On the Direction of Decoherence in the Morse Potential

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Abstract. The Markovian master equation that describes the dynamics of the anharmonic Morse potential under the influence of a thermal environment is analogous to the amplitude damping of the harmonic oscillator, but the result is qualitatively different. We show that the environment induced decoherence drives a wave packet into a mixed state that is well approximated by the time average of the initial state over one oscillation period.

1. Introduction

Wave packets in anharmonic potentials follow the orbit of the corresponding classical particle in the initial stage of the time evolution, but later on peculiar quantum effects, revivals and partial revivals [1–4] occur. In a closed anharmonic quantum system partial revivals are related to the periodic formation of highly nonclassical Schrödinger-cat states, which, in this context, are coherent superpositions of two spatially separated, well localized wave packets [5].

However, in an open system nonclassical states are expected to be particularly sensitive to the environment induced decoherence. In this paper we analyze the mixed states resulting from the decoherence of wave packets and spontaneously formed Schrödinger-cat states in the Morse potential [6].

2. Description of the Model

The Morse oscillator is an anharmonic linear system, which is often used to describe a vibrating diatomic molecule. The corresponding Hamiltonian [7] can be written in the following dimensionless form

$$H = P^2 + (s + 1/2)^2[\exp(-2X) - 2\exp(-X)], \qquad (1)$$

where the parameter s determines the shape of the potential, see e.g. [4]. The Hamiltonian (1) sustains $[s]+1$ normalizable eigenstates (bound states) denoted by $|\phi_n\rangle$, and the eigenvalues are $E_m(s) = -(s-m)^2$, $m = 0, 1, \ldots [s]$, where $[s]$ denotes the largest integer that is smaller than s. Positive energies correspond to the continuous part of the spectrum of H. In this paper we consider a Morse potential with 55 bound states, which is a realistic number for a model molecule.

Our initial wave packets will be Morse coherent states [8], $|x_0, p_0\rangle$, which are localized in the phase space around the point (x_0, p_0).

The environment (E) is represented by a set of harmonic oscillators, and the interaction is written in the rotating wave approximation

$$H_E = \sum_k \hbar\omega_k(a_k^\dagger a_k + 1/2), \qquad V = \hbar\hat{\mu}^\dagger \sum_k g_k a_k + \hbar\hat{\mu}\sum_k g_k a_k^\dagger, \qquad (2)$$

where $\hat{\mu}$ transforms each eigenstate of H into a superposition of different eigenstates corresponding to *lower* energy values. Considering the example of a vibrating diatomic molecule in the environment of the free electromagnetic field, $\hat{\mu}$ is the upper triangular part (in the basis $\{|\phi_n\rangle\}$) of the molecular dipole moment operator, and g_k characterizes the coupling to the kth mode of the radiation field. The operator $\hat{\mu}$ is considered to be proportional to X. We assume that the environment is in thermal equilibrium at a given temperature T, and the environmental oscillators have continuous distribution with frequency dependent density of states, $D(\omega)$. Keeping in mind the example of a diatomic molecule, we set $D(\omega) \propto \omega^2$, and $g(\omega) \propto \sqrt{\omega}$.

Standard techniques [9] lead to the following Markovian master equation in the Schrödinger picture

$$\frac{d}{dt}\rho = -\frac{i}{\hbar}[H, \rho] - \left(\hat{\mu}^\dagger\hat{\mu}_e\rho + \hat{\mu}\hat{\mu}_a^\dagger\rho - \hat{\mu}_a^\dagger\rho\hat{\mu} - \hat{\mu}_e\rho\hat{\mu}^\dagger + \text{h.c.}\right), \qquad (3)$$

where ρ denotes the reduced density operator of the anharmonic oscillator and

$$\langle\phi_m|\hat{\mu}_a|\phi_n\rangle = \pi\langle\phi_m|\hat{\mu}|\phi_n\rangle \; D(\omega_{nm})g^2(\omega_{nm})\overline{n}(\omega_{nm}). \qquad (4)$$

Here $\omega_{nm} = |E_m - E_n|/\hbar$, and $\overline{n}(\omega) = [\exp(\hbar\omega/kT) - 1]^{-1}$ denotes the average number of quanta in the corresponding mode of the environment. The matrix elements of $\hat{\mu}_e$ can be obtained from that of $\hat{\mu}_a$ by replacing $\overline{n}(\omega_{nm})$ by $\overline{n}(\omega_{nm}) + 1$. The subscripts e and a refer to emission and absorption, respectively.

As we can see, the matrix elements of the operators that induce the transitions depend on the Bohr frequency of the involved transition, which is a genuine anharmonic feature. In the case of the harmonic oscillator (HO) $\hat{\mu}$ can be identified with the usual annihilation operator a, and both $\hat{\mu}_a$ and $\hat{\mu}_e$ are proportional to $\hat{\mu} \equiv a$, thus Eq. (3) reduces to the amplitude damping master equation [10, 11].

3. The Direction of the Decoherence

The master equation (3) has been investigated in Ref. [12] and it was found that the scheme of the decoherence is similar to the process of the phase relaxation [10]

of the HO. That is, at the decoherence time t_d the density operator $\rho_{\text{dec}} = \rho(t = t_d)$ can be described by a mixture of states localized along the phase space orbit of the corresponding classical particle. Figure 1.A visualizes a typical result, the Wigner function W [13] of the initial state $|x_0 = 0.5, p_0 = 0\rangle$ is shown together with that of the corresponding ρ_{dec}, see the contour lines. As it can be seen, the phase information, which is related to the position of the center of the wave packet along a certain classical trajectory, is completely destroyed.
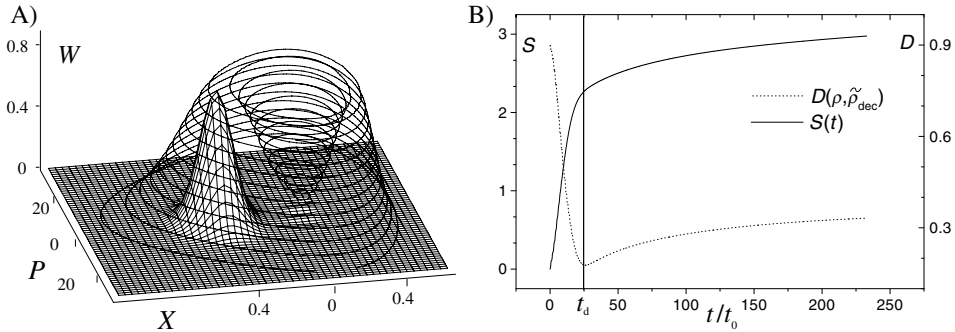
Fig. 1. A) The Wigner function of the initial Morse coherent state $|x_0 = 0.5, p_0 = 0\rangle$ and of the corresponding ρ_{dec}, the latter (shown by the contour lines) is magnified by 15. B) The entropy $S = -\text{Tr}(\rho \ln \rho)$ and the distance between $\rho(t)$ and $\tilde{\rho}_{\text{dec}}$ as a function of time divided by the period of small oscillations, t_0. The strength of the system-environment coupling has been set so that the rate of the $E_0 \rightarrow E_1$ transition is 10^4 times smaller than $1/t_0$. The decoherence time t_d is emphasized by the vertical line. All the plotted quantities are dimensionless

Considering the process of phase relaxation [10] in the harmonic case with an initial HO coherent state $|\beta\rangle$, we obtain $\rho_{\text{dec}}^{\text{HO}} = \int P(\alpha)|\alpha\rangle\langle\alpha|d^2\alpha$ with $P(\alpha = re^{i\varphi}) = \delta(r - R)/2\pi$, where $R = |\beta|$. The density operator $\rho_{\text{dec}}^{\text{HO}}$ can be interpreted as the mixture (in fact, integral) of states $|\alpha = Re^{i\varphi}\rangle$, $\varphi \in [0, 2\pi)$, and $R = |\beta|$ fixed. It can be proven by evaluating the matrix elements that $\rho_{\text{dec}}^{\text{HO}} = \sum_n p_n|n\rangle\langle n|$ also holds, where $\{|n\rangle\}$ are HO energy eigenstates and $p_n = |\langle n|\beta\rangle|^2$. Alternatively, $\rho_{\text{dec}}^{\text{HO}}$ can also be viewed as the time average of the state $|\beta(t)\rangle\langle\beta(t)|$ over an oscillation period in the harmonic potential.

These three interpretations are equivalent, but their analogs in the anharmonic case mean different density operators. Detailed investigation of the result of the decoherence in the Morse potential shows that the best approximation is the time average of the initial wave packet over an oscillation period, $\tilde{\rho}_{\text{dec}} = N \int \rho(t)dt$, where N provides normalization and t ranges from 0 to the end of the first oscillation period. The Wigner function corresponding to $\tilde{\rho}_{\text{dec}}$ obtained in this way reflects all the important properties of the exact W. Additionally, the distance $D(\rho(t), \tilde{\rho}_{\text{dec}}) = \sqrt{\text{Tr}[(\rho(t) - \tilde{\rho}_{\text{dec}})^2]}$ reaches its minimal value at the decoherence time t_d, when

decoherence dominated dynamics turns into dissipation dominated time evolution, see Fig. 1.B and Ref. [14]. As some energy has already been transferred from the environment to the system till t_d, we cannot expect D to become exactly zero.

4. Conclusions

We investigated the mixed states that are results of the decoherence in the Morse potential. The origin of the decoherence in our model was the same as in the case of a damped harmonic oscillator, but we have demonstrated that anharmonicity qualitatively changes the dynamics: Decoherence drives the state of the Morse system into a mixture that can be well approximated by the time average of the initial localized wave packet over one oscillation period.

Acknowledgements

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