J Math Chem (2015) 53:1274–1279
DOI 10.1007/s10910-015-0487-5

ORIGINAL PAPER

Information-theoretic aspects of friction in the quantum mechanics of an interacting two-electron harmonic atom

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Received: 22 November 2014 / Accepted: 28 February 2015 / Published online: 8 March 2015

Abstract In the standard prescriptions (Albrecht in Phys Lett 56B:127, 1975; Hasse in J Math Phys 16:2005, 1975), nonlinear potentials were proposed to introduce a Hermitian potential operator into a Hamiltonian in order to consider quantized friction at the Schrödinger wave-function level. However, this route to understanding quantized friction is not unique. Thus, motivated by important sub-questions put forward by Albrecht and Hasse in the works cited above on the proper choice of parameters introduced in the proposed potentials, we investigate here the information-theoretic aspect of friction using an exact stationary solution for a two-particle interacting one-dimensional oscillator model atom. Specifically, we calculate the *change* in the diagonal entropy with respect to the well-documented frictionless case, and analyze its parameter-dependence.

Keywords Quantum friction · Entropy · Harmonic atom model

1 Motivation

Interest in the fundamentals of dissipative systems at the quantum level has remained high since the early days of quantum mechanics. Quantum dynamics with dissipation are clearly relevant to many processes in physics, chemistry, and biology. However,

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the question of how to modify the classical Lagrangian and Hamiltonian formalisms and the corresponding quantization methods in order to include these aspects has not been answered in a unique way. There are different approaches, which seem to be [1] incompatible with each other. The main approaches are (i) the system-plus-reservoir model, (ii) models based on explicitly time-dependent Hamiltonians, and (iii) nonlinear Schrödinger equations.

For instance, recent theoretical attempts within time-dependent density-functional theory (TD-DFT) provide explicit prescriptions for the mean-field potentials describing quantum dissipation via a Caldeira–Leggett bath of harmonic oscillators [2], or via a potential term in the auxiliary time-dependent Schrödinger equation of TD-DFT, which breaks time-reversal invariance so as to cool the sub-system [3]. While in the bath-approach the time-derivative of the center-of-mass coordinate of the many-body system plays a decisive role, in the other approaches this role is played by the time-derivative of the probability density.

As we mentioned in item (iii) above, a standard [1,4,5] way to circumvent the problem of finding classical Hamiltonians for dissipative systems, that can be canonically [6,7] quantized, is to add a Hermitian friction operator *directly* to the Hamilton operator. The construction of such a term requires a nonlinear potential, parametrized [4,5] and dicussed for the single-particle, or single mode, case. Remarkably, even with nonlinear potentials in the Schrödinger equation one can get [5] stationary solutions for the wave function in a few realistic problems. One such example is the ground-state solution [5] for a harmonic oscillator. There, according to Hasse, one gets in the *single-mode* (j) case

$$\psi_j(x_j, \gamma, c) = \left(\frac{\widetilde{\omega}}{\pi}\right)^{1/4} e^{i\,\widetilde{\omega}\,t/2}\; e^{-(\widetilde{\omega}+i\,c\,\gamma)\,x_j^2/2} \tag{1}$$

where Hartree atomic units, $\hbar = m_e = 1$, are employed. In this equation γ characterizes the *strength* of the nonlinear Hermitian potential [4,5] operator in the Schrödinger equation, the damped frequency is $\widetilde{\omega} = \omega\sqrt{1-(c\gamma/\omega)^2}$ instead of the unperturbed value ω, and the crucial parameter c may be [4] a real constant, or a real function of time. For instance, with $c = 1/2$ one gets the same [5] damped quantum frequency as in the classical treatment.

Precisely, it is the explicit form of Eq. (1) for a single-degree of freedom, denoted there by x_j, which motivates our study of an information-theoretic measure in an exactly solvable two-electron model atom with inter-particle interaction. Since that model is (see, below) separable into independent normal modes by using normal coordinates, it provides a remarkable possibility for further investigation into the parameter-set behind such nonlinear extensions to Schrödinger equations. In such a way we extend the earlier analysis of [4,5] for a single mode to the interacting, correlated case. Atomic units will be used in the rest of the paper, as in Eq. (1) above.

2 Characterization of the entropy

We start with the exact ground-state solution to the time-independent Schrödinger equation for the following [8,9] Hamiltonian

$$\hat{H}_0 == -\frac{1}{2}\left(\frac{d^2}{dx_1^2}+\frac{d^2}{dx_2^2}\right)+\frac{1}{2}\omega^2(x_1^2+x_2^2)-\frac{1}{2}\Lambda\omega^2(x_1-x_2)^2. \qquad (2)$$

Using the canonical transformation, $x_+ = (x_1 + x_2)/\sqrt{2}$ and $x_- = (x_1 - x_2)/\sqrt{2}$, one gets

$$\hat{H}_0 = \left[-\frac{1}{2}\frac{d^2}{dx_+^2}+\frac{1}{2}\omega_1^2 x_+^2\right]+\left[-\frac{1}{2}\frac{d^2}{dx_-^2}+\frac{1}{2}\omega_2^2 x_-^2\right], \qquad (3)$$

where $\omega_1 = \omega$ and $\omega_2 = \omega\sqrt{1-2\Lambda}$. While $\Lambda \in [0, 0.5]$ corresponds to repulsive inter-particle interaction, in the attractive case one has $\Lambda < 0$. Due to the separation in Eq. (3), the exact ground-state wave function $\Psi(x_1, x_2)$ becomes a product in canonical variables

$$\begin{aligned}\Psi_0(x_+, x_-) &= \psi_0(x_+)\,\psi_0(x_-)\\ &= \left(\frac{\omega_1}{\pi}\right)^{1/4}\exp\left(-\frac{1}{2}\omega_1 x_+^2\right)\left(\frac{\omega_2}{\pi}\right)^{1/4}\exp\left(-\frac{1}{2}\omega_2 x_-^2\right). \qquad (4)\end{aligned}$$

We proceed [10,11] by calculating the reduced one-particle density matrix via the above solution and from its diagonal elements the one-particle probability density. Using Mehler's decomposition [12] as well, this density is given by

$$n_0(x,\omega_1,\omega_2) = \sum_{m=0}^{\infty} P_m^{(0)}\left[\left(\frac{\bar{\omega}_0}{\pi}\right)^{1/4}\frac{1}{\sqrt{2^m m!}}\right]^2\left[e^{-\frac{1}{2}\bar{\omega}_0 x^2}\,H_m(\sqrt{\bar{\omega}_0}x)\right]^2. \qquad (5)$$

Here $\bar{\omega}_0 = \sqrt{\omega_1\omega_2}$, the frequency in Löwdin's natural orbitals, and $P_m(\xi_0) = (1-\xi_0)(\xi_0)^m$, with $\xi_0(\Lambda) = \left[(\sqrt{\omega_1}-\sqrt{\omega_2})/(\sqrt{\omega_1}+\sqrt{\omega_2})\right]^2$, are occupation numbers.

Based on the exact representation in Eq. (5), the diagonal [13,14] von Neumann entropy, denoted in this case by $S(\xi_0)$, and used below as a useful reference, is given by

$$S(\xi_0) = -\ln(1-\xi_0) - \frac{\xi_0}{1-\xi_0}\ln\xi_0. \qquad (6)$$

One can see that this entropy is zero (as always in an auxiliary, independent-particle treatment) only for a non-interacting system where $\Lambda = 0$. Besides, for correlated systems ($\Lambda \neq 0$), this measure of inseparable correlation is independent of the sign of the inter-particle coupling, There is an interesting *duality* [10] encoded in the quadratic dependence of ξ_0 on $\sqrt{\omega_1}$ and $\sqrt{\omega_2}$. This duality means that to any allowed repulsive coupling there exists a corresponding attractive one for which the calculated entropies are equal. How such duality could change by going to the new situation, where $c\gamma \neq 0$, is a challenging question.

Now, we consider both of our canonical variables x_+ and x_-, behind the independent *normal modes*. Notice that only the center-of-mass coordinate is considered, via its time-derivative, in the framework of an independent-particle TD-DFT [2] model. However, in order to consider the interplay of entanglement and the parameter set (c, γ) characterizing nonlinear potential constructions [4,5], we will allow *similar*

changes in both normal modes. So, we will apply the same c and γ to normal modes since they are tied, physically, to the original particle-coordinates x_1 and x_2. Thus, we apply the stationary *form* given above in Eq. (1) to extend our $\psi_0(x_j)$ terms ($j = \pm$) of Eq. (4) to $\psi_0(x_j, \gamma, c)$.

Then we follow the straightforward algebraic path detailed in Eqs. (4–5) in order to return to the original coordinates and arrive at the new probability density $n_0(x, \widetilde{\omega}_1, \widetilde{\omega}_2)$, where $\widetilde{\omega}_k \equiv \omega_k\sqrt{1-(c\gamma/\omega_k)^2}$ and $k = 1, 2$. We stress that the Schrödinger Hamiltonian is not separable in the original coordinates. This fact is reflected in finite values of an entropy calculated from occupation numbers of natural orbitals. The occupation number is unity only if the system is noninteracting $\Lambda = 0$, or the ground-state function is approximated via an independent-particle model, i.e., by products of states in the x_1 and x_2 variables.

At the end of the algebraic path we obtain the corresponding new probability density with new occupation numbers $P_m(\xi) = (1-\xi)\xi^m$. The effect of γ, which characterizes the strength of the nonlinear [4,5] Hermitian potential operator, is encoded in

$$\xi(\Lambda, \gamma) = \left[\frac{\sqrt{\widetilde{\omega}_1} - \sqrt{\widetilde{\omega}_2}}{\sqrt{\widetilde{\omega}_1} + \sqrt{\widetilde{\omega}_2}}\right]^2. \tag{7}$$

The deviation of $\xi(\Lambda, \gamma)$ from $\xi_0(\Lambda)$, as a function of γ, is responsible for the entropy-change at finite coupling $\Lambda \neq 0$. The new entropy $S(\xi)$, to be compared with Eq. (6), becomes

$$S(\Lambda, \gamma) = -\ln(1-\xi) - \frac{\xi}{1-\xi}\ln\xi. \tag{8}$$

Motivated by the distinguished [2] role of the center-of-mass coordinate in the mean-field TD-DFT, first we analyze the case of $\widetilde{\omega}_2 = \omega_2$. This means that we neglect any change in that normal mode which depends on the relative coordinate. In this *restricted* situation ξ can vanish for repulsive coupling, where $\Lambda \in [0, 0.5]$, if $2\Lambda = (c\gamma/\omega_1)^2$. This would result in $S(\xi) = 0$. In the attractive case, where $\Lambda < 0$, no such condition exists. The possibility of duality, which appears [10,11] at unique pairs of attractive and repulsive couplings, disappears when $c\gamma \neq 0$. The ξ parameter may tend to unity at $\Lambda \to 0.5$, or at $(c\gamma/\omega_1) \to 1$, i.e., at the critical limits (separately) for coupling or damping. In these (separate) situations the entropy $S(\xi)$ would tend to infinity logarithmically. Since $(\xi/\xi_0) \leq 1$, independently of the sign of Λ, one may be tempted to conclude that an information-theoretic measure $S(\xi)$ of a repulsively interacting two-particle subsystem could be non-monotonic, at fixed and allowed interparticle coupling Λ, as a function of $c\gamma$.

After the above analysis on the restricted situation, we turn to the case without restriction in Eq. (7), i.e., we allow changes in *both* normal modes. In this case, without loss of generality we consider weak damping, i.e., we take $c\gamma$ small enough. Taylor's expansion results in

$$\xi(\Lambda, \gamma) = \xi_0(\Lambda)\left[1 + \frac{1}{\omega_1\,\omega_2}\,\frac{\omega_1+\omega_2}{\sqrt{\omega_1\,\omega_2}}\,(c\,\gamma)^2\right]. \tag{9}$$

Since $\xi(\Lambda, \gamma) \geq \xi_0(\Lambda)$ for arbitrary (allowed) values of the repulsive or attractive interparticle coupling if $c\gamma \neq 0$, the corresponding entropic measures show that $S(\xi) \geq S(\xi_0)$. This is an expected behavior considering the influence of damping on top of a correlated initial state. If this character turns out to be in harmony with further physical arguments, then one may conclude that consideration of all normal modes is required. Clearly, such a conclusion may put constraints on a restricted (see, above) model, where only the center-of-mass coordinate is considered. Without *a priori* reasons one cannot neglect the relative coordinate.

Finally, we discuss briefly the motivaton for the choice of a parameter c needed in nonlinear potential constructions [4,5]. As was pointed out by Hasse for a single-mode, with $c = 1/2$ one gets the same damped quantum frequency as in the classical limit. Our present result, summarized in Eq. (9), is not in contradiction even with a finite $c(t)$ value suggested by Albrecht, since the *change* in entropy it causes seems to be physically realistic. No such clear conclusion can be obtained, however, with a model restricted by the neglect of an equally important degree of freedom.

3 Summary and outlook

In this work we have analyzed an information-theoretic measure, the von Neumann entropy, of an interacting two-particle quantum system with quantum friction. The analysis has been performed in a parameter-space which appears to characterize the construction [4,5] of a non-linear Hermitian potential term to be added to a basic model Hamiltonian which constitutes a cornerstone in a large variety of fields in physics. Considering the fact that even the classical mechanics of nonconservative systems requires generalizing standard tools, such as Hamilton's stationary action principle [15], further efforts are needed in the more complex field of quantized friction in open quantum systems. The results obtained in this note on the interplay of interaction and damping may have relevance in the promising field of dissipative state-preparation [16], where the main goal is the preparation of a desired stationary state by engineering the coupling of a sub-system to its environment.

We finish this short note by commenting on the possibility of a mapping via which our present analysis could find an immediate *application*. It has been suggested recently [17] that under certain restrictions a quadratic Hamiltonian, such as the one in Eq. (3), could replace another one with a different inter-particle interaction. For instance, we can use a prescribed equivalence of ground-state energies of the present and of another well-known model [18], also with harmonic external confinement, by applying the mapping

$$\frac{\lambda}{(x_1 - x_2)^2} \longmapsto \frac{\Lambda\omega_0^2}{2}(x_1 - x_2)^2. \tag{10}$$

From the energy-equivalence condition $(\omega_0/2)(1 + \sqrt{1 - 2\Lambda}) = (\omega_0/2)(1 + \sqrt{1 - 4\lambda})$ we get $\lambda = \Lambda/2$. This interrelation can be used, at least from an information-theoretic [19] point of view, to analyze that entangled system which maps onto our

quadratic Hamiltonian. With $\Lambda = 0.5$, we get $\lambda = 1/4$ for its critical value, consistent with what is already known [20].

Acknowledgments The authors thank Professor P. M. Echenique for warm hospitality at the DIPC. One of us (I.N.) acknowledges useful conversations with Professor I. V. Tokatly. This work has been supported in part by the Basque Departamento de Educación, Universidades e Investigación, the University of the Basque Country UPV/EHU (Grant No. IT-366-07).

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