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ORIGINAL PAPER

Sudden excitations of harmonic normal modes

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Abstract
The N-harmonium boson system, i.e., a completely integrable model of N particles where both the external confinement and the two-particle interaction are harmonic, is investigated under the action of sudden time-dependent perturbation. This quench-like external perturbation of confinement has a quadrupolar space-character. The time-independent transition probabilities, which characterize the impact of quench as average occupation numbers, form a complete distribution in the sense of probability theory. The quench-generated energy shift ΔE in the correlated many-body system, and a purity-type Rényi entropy $S_{\alpha=2}$ are calculated. Challenging reinterpretations of such an energy change in terms of variables of a classical thermodynamical system of $N(N-1)/2$ pairs are given as well. As in the case of the ground-state correlated system, an entropy could characterize a global link to energetically optimized independent-particle models.

Keywords Correlation · Entropy · Excitations

1 Survey of the unperturbed model system

Advances in optical trapping of cold atoms have allowed for an unprecedented manipulation over the size of these quantum systems such that the number N of atoms being trapped can be [1] precisely specified. In general, operating on quantum many-body systems provides a way to understanding [2–5]. In particular, for precisely specified interacting quantum systems, time-dependent tuning (quench) of external harmonic

This study on analogies between many-body systems is dedicated to the memory of János Pipek.

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confinement seems to be an easily realizable experimental tool to generate dynamics. Remarkably, this external control can be a continuous one, in contrast to the discrete manipulation of many-body (target) systems with external projectile-impact. Motivated by the feasibility of experimental access to averages of driven many-body systems, here we apply a well-analyzed model system to an energetic study. Such a study on a model system can be considered as a clinical attempt to important energetic and statistical details, which might generate further efforts.

Following earlier works [6,7], here we take a prototype one-dimensional system of N identical particles, bosons, with mass m and scalar coordinates x_i, where $i = 1, 2, ...N$. The Hamiltonian, introduced by Heisenberg as the simplest many-body form to his studies

$$H_N = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + \frac{1}{2} m\, \omega_0^2\, x_i^2 \right) - \frac{1}{2} \Lambda\, m\, \omega_0^2 \sum_{1 \leq i \leq j \leq N} (x_i - x_j)^2, \tag{1}$$

is separable (at $\Lambda \neq 0$) and this fact results in independent normal modes. Thus the basic expectation value in quantum mechanics, the ground-state energy, becomes additive

$$E = \frac{1}{2}\omega_1 + \frac{(N-1)}{2}\omega_2 \tag{2}$$

where, without loss of generality, we take units defined by $m = 1$ and $\hbar = 1$. The frequencies of harmonic normal modes are [6,7] given by $\omega_1 = \omega_0$ and $\omega_2 = \omega_0\sqrt{1 - N\Lambda}$. Notice that the stability, for repulsive interparticle interaction ($\Lambda > 0$), is marked by the $N\Lambda < 1$ condition. There is no such constraint for the attractive, like in nuclear physics, case.

In the energetically-optimal (e), independent-particle modeling one gets for the energy

$$E_e = \frac{N}{2}\omega_e = \frac{N}{2}\omega_0\sqrt{1 - (N-1)\Lambda}, \tag{3}$$

which is based on the additive structure of Eq. (1) without $x_i x_j$ product-terms. For $\Lambda > 0$ the frequency-ordering becomes $\omega_2 < \omega_e < \omega_0$, and for $\Lambda < 0$ the ordering is $\omega_2 > \omega_e > \omega_0$, The difference $E_c = (E - E_e)$ is, according to Wigner [8] pioneering definition, the correlation energy. It is instructive (c.f., next paragraph) to investigate the small-coupling ($\Lambda \to 0$) limit of the correlation energy. By straightforward expansion one arrives at, in our units

$$E_c(\Lambda << 1) = -\frac{N(N-1)}{2}\frac{\Lambda^2}{8}\omega_0. \tag{4}$$

The second derivative, in coupling, of the difference of two variational quantity is negative. This observation on sign is in accord with general statements in quantum chemistry [9].

In the second part of this survey, we derive a challenging correspondence for $E_c(\Lambda << 1)$ by using precise result on the one-particle reduced density matrix [6,7] of the interacting boson system, and its well-known [10,11] *formal equivalence* with the statistical density matrix of an ideal system of N oscillators with frequency $\bar{\omega}(\omega_0, \Lambda, N)$ in thermal equilibrium at temperature $T(\omega_0, \Lambda, N)$. These oscillators do not interact with each other, but only with the heat bath. We note that in field-theoretic attempts to black-hole physics [10,11], the usual association is based on photons. There, the tracing out of high-energy degrees of freedom yields a low-energy effective field theory with an accompanying statistical measure of black-body-like entropy which may be considered as an information loss.

For the equivalent thermodynamical system one has $E = F + T\,S_N$, where F is Helmholtz's free energy, and there is a heat-like product of the temperature T and the von Neumann entropy S_N. These are the variables in the path based on an ideal canonical-ensemble to thermodynamics [12]. Employing precise [6] mappings between the formally equivalent one-matrices, we derive to a direct comparison at weak coupling

$$T\,S_N \equiv T(\omega_0, \Lambda, N)\, S_N(\omega_0, \Lambda, N) = \omega_0 \left[\frac{N(N-1)}{2} \frac{\Lambda^2}{8} \right], \tag{5}$$

where *common* logarithmic factors cancel out in the lhs product. Thus, based on formal equivalence of two density matrices, we get as partial correspondence $T S_N = -E_c$.

Notice that at $N|\Lambda| << 1$ in the quantum-mechanical case, i.e., at $(T/\omega_0) << 1$ in the thermal case, the thermal part of the Helmholtz free energy, i.e., the part beyond its zero-point energy $(1/2)N\bar{\omega}$, is exponentially small. To our best knowledge, the above-derived formal correspondence is *novel* on a prototype many-body system. Besides, the quadratic-in-Λ and the linear-in-number-of-pair characters for the entropy-based part of the ordered-product in Eq. (5) suggests that the correspondence found might hold independently of the statistics in weakly correlated systems. We stress that a proportionality between $-E_c$ and von Neumann entropy S_N is known in quantum chemistry as conjecture [13].

2 Time-dependent perturbation of the model system

The selected details of the previous Section signal that the complete orthonormal sets for independent normal modes are oscillator wave functions

$$\phi_n(\omega, u) = \left(\frac{\omega}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}\, e^{-\frac{1}{2}\omega u^2}\, H_n(\sqrt{\omega} u). \tag{6}$$

As Eq. (2) shows, there is one mode with $\omega_1 = \omega_0$, and $(N-1)$ mode with ω_2. In the ideal, i.e., noninteracting $(\Lambda = 0)$ case all (N) modes are equivalent $(\omega_1 = \omega_2 = \omega_0)$, and that system has zero information-theoretic entropy since its one-matrix is idempotent. Notice here, that below we will use, to simplify mathematics, a common notation ω for these frequencies where this is possible and return to ω_1 and ω_2 channel-notation where it is needed to physics.

The main goal below is to consider the energetic-impact of time-dependent, passing, perturbations with quadratic space-character in normal coordinates. In fact, the $N = 2$ case, with such a perturbation of different sign, was already investigated recently in order to shed light on the sign-dependence of energy shift, a well-known problem in swift proton and antiproton close-impact on inert helium atom [14]. Besides, that study addressed few alarming problems inherent in the time-dependent density-functional method [15] where one works with auxiliary (density-optimal) orbitals instead of precise independent modes.

In short, with perturbations of finite duration one can calculate the energy shift by using Dirac's variation of constant method instead of following in time the evolving wave functions, since we know the Hamiltonian at the beginning and at the end of a passing perturbation. Therefore, the energy shift can be calculated in this case by considering the excitation probabilities as occupation numbers which characterize the transitions from a given (in our case: ground) state to other elements of the orthonormal complete sets. The sum of these probabilistic occupation numbers satisfy the normalization condition, as it should be. They weight the mode-energies in summation over quantum number n to get the total energy change. For a passing (vanishing at $t \to \pm\infty$) perturbation the expectation value of the Hamiltonian with evolving states results in the same [14] time-independent energy change.

Which still remains to our enumeration of tools, is the concretization of the above-outlined occupation numbers. But an insightful method to that concretization is, fortunately, also well-documented due to established works [16,17]. In fact, a complete Chapter [18] written by experts is devoted to similar problems. Briefly, that insightful method rests on an asymptotic analysis via a clever variable-change to map time-dependence into a stationary scattering problem. In our comparative study we employ the expressions, deduced for a single oscillator [16–18], to our case with independent modes. We stress, however, that we consider N-mode systems with precise and energetically-optimized modes. In other words, we investigate the interplay of inherent correlation and external perturbation of quench-character. We believe that the such-obtained results could contribute to understanding.

The required statistical weights to energy averaging, i.e., the occupation (transition) probabilities $W_{2n,0}$ are given by [16–18] the following expression

$$W_{2n,0}(R) = \frac{(2n)!}{2^{2n}(n!)^2}\sqrt{1-R}\,(R)^n = \frac{1}{\sqrt{\pi}}\frac{\Gamma(n+1/2)}{\Gamma(n+1)}\sqrt{1-R}\,(R)^n, \qquad (7)$$

which reflects the selection rule for allowed (upward) transition with a quadratic perturbation. This complete distribution function is normalized since in general

$$\frac{1}{(1-x)^{\eta}} = \sum_{n=0}^{\infty} \frac{\Gamma(n+\eta)}{n!\,\Gamma(\eta)}\, x^n.$$

The reflection coefficient R of the mentioned (auxiliary) scattering problem (see, above) can be calculated in the knowledge of time-details on a quadrupolar perturbation [14,16].

In our work on a confined boson system we restrict ourselves to the quench-like situation. In this abrupt case at $t = 0$, where $\omega^2 \Rightarrow \omega_f^2 = (\omega^2 + \lambda\omega_0^2)$, one gets [17] for the reflection

$$R(\omega, \lambda) = \left[\frac{\omega - \omega_f}{\omega + \omega_f}\right]^2$$

in terms of initial (ω) and final (ω_f) frequencies which characterize the normal modes before and after the quench, respectively. It should be noted that the occupation numbers in Eq. (7) are now simply the squares of expansion coefficients obtained by expanding a given stationary ground-state $\phi_0(\omega, u)$ in terms of a complete set of stationary orthonormal $\phi_n(\omega_f, u)$ functions. The selection rule mentioned is based on parity-consideration in expansion.

Thus, for one mode we have $\omega = \omega_1$ and for the other $(N - 1)$ modes we have $\omega = \omega_2$. The parameter λ measures the strength of a sudden-change in external confinement. It can have both sign, within the stability range $[\omega^2 > -|\lambda|\,\omega_0^2]$ of the system. Furthermore, in the stability range, there is a *duality* in $R(\lambda)$ under the mathematical constraint of $\omega_1\omega_2 = \omega_f^2$. Under such a special constraint, the magnitude of reflection R can not distinguish between physical cases with corresponding $\lambda > 0$ or $\lambda < 0$, i.e., up- or down-tuning.

This duality clearly signals, similarly to earlier observations [19,20] with eigenvalues of one-matrices of the unperturbed system, that simple probabilistic measures alone can not characterize completely the physics. We add here based on Eq. (7) (mode i, with R_i, where $i = 1, 2, e$) the so-called purity $\Pi(R)$, a frequently [19] applied information measure

$$\Pi(R) = \sum_{n=0}^{\infty}[W_{2n,0}(R)]^2 = (1 - R)\,\frac{2}{\pi}\,K(R^2) \leq 1, \tag{8}$$

where $K(x)$ is the complete elliptic integral of the first kind. An other measure, the so-called Rényi's min-entropy [21], is given by $S_{\alpha=\infty}(R) = \ln[1/(1 - R)]$. His $S_{\alpha=2}(R)$ is related to a purity via $\Pi = \exp(-S_2)$ in mode i. Such a connection was considered earlier [22] as a promising path to S_2 via an experimental estimation for Π. In Rényi's classification S_α is a measure of order α of the amount of information. We consider [23] such mathematical measures as potentially useful ones even to not-scale-less problems, and return to physics.

Despite the above-mentioned duality in occupation numbers (statistical weights), the total final energy (E_f) of the system after quench, and thus the $\Delta E = (E_f - E)$ total energy shift, reflect the informations (energy scales) encoded in the Hamiltonian. Keeping in mind the remark at Eq. (6) on simplification in notations, we continue with the determination of channel-contributions, denoted by ΔE_i where $i = 1, 2$. To

$\Delta E = (\Delta E_1 + \Delta E_2)$ we obtain

$$\Delta E_1(\omega_1, R_1) = \omega_1 \sum_{n=0}^{\infty} (2n)\, W_{2n,0}(R_1) = \frac{1}{2}\,\omega_1\, \frac{2R_1}{1-R_i}, \tag{9}$$

$$\Delta E_2(\omega_2, R_2) = (N-1)\,\omega_2 \sum_{n=0}^{\infty} (2n)\, W_{2n,0}(R_2) = \frac{(N-1)}{2}\omega_2\, \frac{2R_2}{1-R_2}. \tag{10}$$

In the knowledge of this precise result, we add the one, denoted by ΔE_e, which is based on an energetically (e) pre-optimized independent-particle modeling outlined in Section I, under the impact of the same change ($\sim \lambda\omega_0^2$) in external confinement. We arrive at

$$\Delta E_e(\omega_e, R_e) = N\,\omega_e \sum_{n=0}^{\infty} (2n)\, W_{2n,0}(R_e) = \frac{N}{2}\omega_e\, \frac{2R_e}{1-R_e}. \tag{11}$$

Motivated by Wigner's definition of correlation energy $E_c(\Lambda) = [E(\Lambda) - E_e(\Lambda)]$ in the ground-state situation, we are tempted to introduce a quench-related term defined as

$$\Delta E_c(\Lambda, \lambda) = [\Delta E(\Lambda, \lambda) - \Delta E_e(\Lambda, \lambda)]$$

which also reflects the difference between exact and energetically pre-optimized independent-particle descriptions. Now we take the perturbative limit where $\lambda \to 0$ at fixed N, ω_0 and (small) Λ, thus all $R_i << 1$. To a useful comparison with Eq. (4) we obtain

$$\Delta E_c(\Lambda, \lambda) = +\,\frac{N(N-1)}{2}\,\frac{\Lambda^2\,\lambda^2}{64}\omega_0 \tag{12}$$

The positivity is expected on physical grounds since the quench acts as an external agent which tries to diminish rigid individual behaviors (i.e., difference in modes) reflected in Eq. (4) into the direction of a common behavior (i.e., similar, energetically optimized modes). Precisely, it is this observation which suggests us to make finally a somewhat cavalier conjecture via $\Delta E_c(\Lambda, \lambda) = \Delta[T S_N]$. By such a conjecture, which is motivated by the first law of macroscopic thermodynamics as well, we are tempted to view ΔE_c as the result of certain heat-transfer (ΔQ) to a classical system of pairs.

3 Summary, remarks and outlook

In this work the N-harmonium boson system, i.e., a completely integrable model of N particles where both the external confinement and the two-particle interaction are harmonic, is investigated under the action of a quench-like-in-time perturbation. This external perturbation of confinement has a quadrupolar space-character. The time-independent transition probabilities, which characterize the impact of quench as average occupation numbers, are used to calculate analytically the energy shift ΔE in the many-body system, and the purity-related Rényi's entropy $S_{\alpha=2}$. Challenging reinterpretations, Eqs. (4) and (12), of characteristic energy differences, in terms of variables of a classical thermodynamical system of $N(N-1)/2$ pairs, are given as well for both the ground- and exited-state situations.

We stress, as first remark, that our controllable quench is in the external [14] confinement and not in the particle-particle interaction. Their coupling ($\sim \Lambda$) is not changed. However, controllable quench in that coupling could also be interesting to a general, detailed understanding. Indeed, such a change is in the focus of efforts in [2–5] at fixed confinement. Our previous experience [23] with such a quench in the simpler two-particle ($N = 2$) harmonic model suggests that a similar connection as the one in Eq. (12) for the important difference of stationary energies, i.e., quantum mechanical expectation values, can be found as well. Details due to different quenches, and their possible interplay, require a dedicated study.

We add for completeness, that the time-dependence (after sudden quenches at $t = 0$) of the evolving wave functions and associated time-dependent one-matrices [23] contain, via their time-dependent eigenvalues, useful probabilistic information on inherent dynamics in isolated interacting systems. Comparison of the such-obtained time-dependent entropic measures, say a time-dependent system purity [23], with stationary quantities characterized in this study based on independent modes, could allow important [14] conclusions on observable quantities. As a final remark, we note that it would be interesting to extend the present approach with abrupt confinement-tuning, to cases with other particle-particle interaction. Say, for the contact interaction which seems to be realistic and externally tunable (via Feshbach resonances) in Bose systems of harmonically confined atoms [24,25].

As an outlook we turn to a really theoretical challenge. According to earlier insights on the black-hole aspect of matter [26], there one also has a large number of unobservable internal configurations which may reflect, via an entropy, the end of certain processes. Our quench-mediated changes, generated in a given closed entangled system, in its energy and an associated entropy, already suggest that one may identify realistic processes, and their modulating role, in that fascinating field as well. For instance, a process in which there is a suddenly captured cloud of matter which changes the internal energy of a black-hole. In our modeling this would correspond to situation with total (t) energy $E^{(t)}(\omega_0, \Lambda, N_1 + N_2) \equiv [E_1(\omega_0, \Lambda, N_1) + E_2(\omega_0, \Lambda, N_2)] \equiv F^{(t)} + T^{(t)} S_N^{(t)}$. A future analysis of this situation, along the second law of thermodynamics, is desirable. Indeed, the "thermalization process" from subsystem's T_1 and T_2 to a common T is quite challenging.

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