Sudden quench in a model Hamiltonian with interactions: The time-dependent components of Wigner's correlation

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Based on the correlated ground-state wave function of an exactly solvable interacting one-dimensional two-electron model Hamiltonian we address the switch-off of the external confining interaction in order to calculate the exact time-evolving wave function from a correlated initial state. The Hartree-Fock approximation for the initial state of the model system is considered as well. By taking the differences of kinetic and potential energy terms obtained with these treatments, the time-dependent components of Wigner's correlation energy are determined.

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I. INTRODUCTION AND MOTIVATION

It is now standard textbook knowledge [1] that the simple one-dimensional, two-fermion Hamiltonian

$$\hat{H} = -\frac{1}{2}\left(\frac{d^2}{dx_1^2}+\frac{d^2}{dx_2^2}\right)+\frac{1}{2}\lambda\left(x_1^2+x_2^2\right)+\frac{1}{2}\Lambda(x_1-x_2)^2 \tag{1}$$

has analytic solutions [2] in the exact and Hartree-Fock (HF) treatments for its singlet ground state. These solutions can be used to define Wigner's correlation energy, an important measure of inseparable entanglement in a stationary state [3]. The correlation energy is a basic quantity in many fields. In the present paper we investigate its time-dependent extension to the stationary case defined on the time domain in analogy to Ref. [4].

Actually, governed by the time-dependent density-functional method (TD-DFT), there is a large effort [4–11] involving the application of one-dimensional, two-particle models to the time domain numerically. This effort motivates us to perform a detailed analytical study on the time-dependent components of Wigner's correlation energy. Traditionally, this energy is defined by using wave functions of the Schrödinger equation. The DFT and TD-DFT methods are derived also from the many-particle Schrödinger equation but are expressed finally entirely in terms of the density. An effective single-particle formulation of these methods is of considerable practical interest and could contribute to our understanding [12]. Thus, the analysis of details about the link between the traditional and density-based treatments is an important theoretical issue relevant to the development of reliable density-based tools.

The exact stationary solution is based on the $x_+ = (x_1+x_2)/\sqrt{2}$ and $x_- = (x_1-x_2)/\sqrt{2}$ canonical transformations introduced to rewrite the Hamiltonian $\hat{H}$ as follows:

$$\hat{H} = -\frac{1}{2}\left[\frac{d^2}{dx_+^2}-\lambda x_+^2\right]-\frac{1}{2}\left[\frac{d^2}{dx_-^2}-(\lambda+2\Lambda)x_-^2\right]. \tag{2}$$

Due to this separated form, its ground-state wave function $\psi(x_+,x_-)$ becomes a product,

$$\psi(x_+,x_-) = \left(\frac{\sqrt{\lambda}}{\pi}\right)^{1/4}\exp\left[-\frac{1}{2}\sqrt{\lambda}\,x_+^2\right]\left(\frac{\sqrt{\lambda+2\Lambda}}{\pi}\right)^{1/4} \times \exp\left[-\frac{1}{2}\sqrt{\lambda+\Lambda}\,x_-^2\right]. \tag{3}$$

The $\psi(x_1,x_2)$ function has a pointwise [13] decomposition in terms of natural [14] orbitals,

$$\psi(x_1,x_2) = \sum_{n=0}^{\infty}[(1-z^2)^{1/2}\,z^n]\left[\left(\frac{\bar{\omega}}{\pi}\right)^{1/4}\frac{1}{\sqrt{2^n\,n!}}\right]^2 \times e^{-\frac{1}{2}\bar{\omega}(x_1^2+x_2^2)}\,H_n(\sqrt{\bar{\omega}}x_1)H_n(\sqrt{\bar{\omega}}x_2), \tag{4}$$

where $z = [(\lambda+2\Lambda)^{1/4}-\lambda^{1/4}]/[(\lambda+2\Lambda)^{1/4}+\lambda^{1/4}]$ and $\bar{\omega} = [\lambda(\lambda+2\Lambda)]^{1/4}$. The occupation numbers in the associated single-particle reduced density matrix [15,16] are $P_n = (1-z^2)z^{2n}$, and the uncertainty product takes [17] the following informative form:

$$(\Delta x)^2(\Delta p)^2 = \frac{1}{4}\left[1+\frac{\Lambda^2}{\lambda(\lambda+2\Lambda)}\right]. \tag{5}$$

The exact ground-state energy is the sum of kinetic and potential terms. With the $\psi(x_1,x_2)$ function from Eq. (3) to the original Hamiltonian in Eq. (1), this energy becomes

$$E(\lambda,\Lambda) = \frac{1}{4}(\sqrt{\lambda}+\sqrt{\lambda+2\Lambda})+\frac{\lambda}{4}\left(\frac{1}{\sqrt{\lambda}}+\frac{1}{\sqrt{\lambda+2\Lambda}}\right) + \frac{1}{2}\frac{\Lambda}{\sqrt{\lambda+2\Lambda}} \tag{6}$$

and reduces to $E(\lambda,\Lambda) = (1/2)(\sqrt{\lambda}+\sqrt{\lambda+2\Lambda})$, as the separable form in Eq. (2) dictates.

By solving the HF integro-differential equation, one gets [1] for the space wave function

$$\psi_{HF}(x_1,x_2) = \left(\frac{\alpha}{\pi}\right)^{1/4}\exp\left[-\frac{1}{2}\alpha x_1^2\right]\left(\frac{\alpha}{\pi}\right)^{1/4}\exp\left[-\frac{1}{2}\alpha x_2^2\right], \tag{7}$$

where $\alpha_{HF} = \sqrt{\lambda+\Lambda}$ is the resulting value. Notice that during the evaluation of the HF equation for two interacting

fermions the exchange term drops out. Alternatively, applying for the HF wave function its conveniently (see Sec. II) rewritten form

$$\psi_{HF}(x_+,x_-) = \left(\frac{\alpha}{\pi}\right)^{1/4} \exp\left[-\frac{1}{2}\alpha x_+^2\right] \left(\frac{\alpha}{\pi}\right)^{1/4} \times \exp\left[-\frac{1}{2}\alpha x_-^2\right] \tag{8}$$

and a variational calculation for the ground-state energy with the reordered Hamiltonian

$$\hat{H} = -\frac{1}{2}\left[\frac{d^2}{dx_+^2} - (\lambda+\Lambda)x_+^2\right] - \frac{1}{2}\left[\frac{d^2}{dx_-^2} - (\lambda+\Lambda)x_-^2\right] + \frac{1}{2}\Lambda(x_-^2 - x_+^2), \tag{9}$$

we arrive at the HF result for α since the last term vanishes upon integration and

$$E(\alpha,\lambda,\Lambda) = \frac{1}{2}\left(\alpha + \frac{\lambda+\Lambda}{\alpha}\right). \tag{10}$$

One can see why the HF wave functions are called total-energy optimal ones [12].

In terms of the precise $[E(\alpha_{HF},\lambda,\Lambda) \equiv E_{HF}(\lambda,\Lambda)]$ stationary ground-state energies, Wigner's correlation (c) energy is defined (for $t \leqslant 0$ in our case) as a difference,

$$E_c(\lambda,\Lambda) = E(\lambda,\Lambda) - E_{HF}(\lambda,\Lambda), \tag{11}$$

which results in $E_c(t=0^-,\Lambda\to 0) \simeq -(\sqrt{\lambda}/8)(\Lambda/\lambda)^2$ at small coupling. Since the kinetic and potential energy terms of Eqs. (6) and (10) satisfy the virial theorem, the correlation energy consists of two equal parts. The simple product form in Eqs. (7) and (8), with a properly chosen α_e parameter, could serve as a ground-state wave function to an effective (e) single-particle approximation based on the noninteracting picture.

We note at this point that in the case of a repulsive interparticle coupling in $\hat{H}$, we have a strong restriction, $-0.5\,\lambda \leqslant \Lambda \leqslant 0$, on its value. This is more stringent than the lower limit allowed by the Hartree-Fock approximation, in which $-\lambda \leqslant \Lambda \leqslant 0$. Considering the sign of the interparticle coupling, the occupation numbers P_n and also the uncertainty product have a dual property [16] which was further emphasized recently for an extended model [18] with three particles. Thus, entropic measures cannot resolve the sign of Λ. We restrict ourselves in this theoretical study to the attractive case.

The rest of this paper is organized as follows. Section II is devoted to the analytical result derived for the time-dependent correlation energy by switching off suddenly, at $t = 0$, the external confining field characterized by λ in the original Hamiltonian. Section III contains a short summary and our comments.

II. RESULTS

We apply a sudden [10,19] complete quench at $t = 0$ for the external ($\sim\lambda$) confinement in the Hamiltonian, Eqs. (2) and (9), and write the new (n) Hamiltonian as follows:

$$\hat{H}_n = -\frac{1}{2}\frac{d^2}{dx_+^2} - \frac{1}{2}\left[\frac{d^2}{dx_-^2} - 2\Lambda x_-^2\right]. \tag{12}$$

We solve two separated, time-dependent single-particle Schrödinger equations using the propagator method for the two independent (normalized) initial states in the product form of Eq. (3) and in $\psi_{HF}(x_+,x_-) \equiv \phi_{HF}(x_+)\phi_{HF}(x_-)$ of Eq. (8). The single-particle Green's function, with an attractive harmonic potential $(1/2)\omega^2\,\xi^2$ [instead of $(1/2)2\Lambda\,\xi^2$] in $\hat{H}_n$ to a time-dependent, one-dimensional single-particle Schrödinger equation, is given by

$$G(\xi,\xi',\omega,t) = \left(\frac{\omega}{2\pi\, i \sin\omega t}\right)^{1/2} \times \exp\left\{\frac{i\omega}{2\sin\omega t}\left[(\xi^2+\xi'^2)\cos\omega t - 2\xi\xi'\right]\right\}, \tag{13}$$

which reproduces the well-known free case [20] when $\omega \to 0$. Then we use this propagator with a model (m) initial state $\phi_m(\xi) = (\omega_m/\pi)^{1/4}\exp[-(1/2)\omega_m\xi^2]$ in

$$\Phi_m(\xi,t) = \int_{-\infty}^{\infty} d\xi'\, G(\xi,\xi',\omega,t)\,\phi_m(\xi'). \tag{14}$$

The resulting time-dependent wave function $\Phi_m(\xi,t)$ has the following form:

$$\Phi_m(\xi,t) = \left(\frac{\omega_m}{\pi}\right)^{1/4} \sqrt{A_m}\, \exp\left[-\frac{1}{2}\xi^2 B_m(1 - i\,C_m)\right], \tag{15}$$

where the new coefficients, $A_m(\omega_m,\omega,t)$, $B_m(\omega_m,\omega,t)$, and $C_m(\omega_m,\omega,t)$, are given by

$$A_m = \frac{\omega}{\omega\cos\omega t + i\omega_m \sin\omega t},$$
$$B_m = \frac{\omega_m\,\omega^2}{\omega^2\cos^2\omega t + \omega_m^2\sin^2\omega t},$$
$$C_m = \frac{1}{2}\,\frac{\omega_m^2 - \omega^2}{\omega_m\omega}\,\sin(2\omega t).$$

When $\omega_m = \omega$, one recovers the Schrödinger state function for an attractive harmonic oscillator in its ground state since $\sqrt{A_m} = \exp(-i\omega t/2)$, $B_m = \omega$, and $C_m = 0$ in that case. Furthermore, there is a remarkable relation between the time-dependent coefficients,

$$B_m(t)[1 - iC_M(t)] = i\,\frac{\dot{A}_m(t)}{A_m(t)},$$

in complete formal agreement with the evaluation [21] based on different $A(t)$ inputs.

Based on the above details and using the relevant (see below) substitutions for ξ, ω_m, and ω in Eqs. (13) and (15) as dictated by Eqs. (11), (3), and (8), we write the product forms of the time-dependent exact and Hartree-Fock solutions as

$$\Psi(x_+,x_-,t) = \Phi(x_+,t)\Phi(x_-,t),$$
$$\Psi_{HF}(x_+,x_-,t) = \Phi_{HF}(x_+,t)\Phi_{HF}(x_-,t).$$

In order to facilitate the evaluation and reading, in Table I we summarize the relevant correspondences between the parameters applied. The attractive case, $\Lambda \geqslant 0$, is analyzed.

TABLE I. Correspondence between parameters applied. The $\Lambda \geqslant 0$ case is used.

	Exact		Hartree-Fock	
ξ	ω_m^2	ω^2	ω_m^2	ω^2
x_+	λ	0	$\lambda+\Lambda$	0
x_-	$\lambda+2\Lambda$	2Λ	$\lambda+\Lambda$	2Λ

First, we discuss the total energies obtained after the sudden quench at $t=0$ of the external confining field. Since the field behind the interparticle interaction is conservative, we obtain the constant total energies from Eqs. (6) and (10), respectively,

$$E(t>0)=\frac{1}{4}\sqrt{\lambda}+\left(\frac{1}{4}\sqrt{\lambda+2\Lambda}+\frac{1}{2}\frac{\Lambda}{\sqrt{\lambda+2\Lambda}}\right), \quad (16)$$

$$E_{HF}(t>0)=\frac{1}{4}\sqrt{\lambda+\Lambda}+\left(\frac{1}{4}\sqrt{\lambda+\Lambda}+\frac{1}{2}\frac{\Lambda}{\sqrt{\lambda+\Lambda}}\right). \quad (17)$$

For small coupling one has $E_c(t>0,\Lambda\to 0)\simeq -5\sqrt{\lambda}(\Lambda/\lambda)^2/16$, which is $(5/2)\times E_c(\Lambda\to 0)$. The ratio $R_c(\Lambda/\lambda)=E_c(t>0)/E_c$ tends to unity asymptotically for high values of (Λ/λ), as expected. At a moderate value of $\Lambda=\lambda/4$ in Eq. (1), this ratio is $R_c\simeq 2.2$.

The separated kinetic and potential components of the last sums in Eqs. (16) and (17) are, as we will show below, time dependent. It is this behavior of the separated components which could make an effective single-particle approximation via only the sum of these components difficult. The quantum-mechanical definitions of the time-dependent kinetic- and potential-energy terms in the exact and Hartree-Fock treatments are given by using simple extension of the definition of energies of a stationary system [22]. Therefore, we calculate these energy terms with states $\Psi(x_+,x_-)$, $\Psi_{HF}(x_+,x_-)$ and Eq. (12) for $\hat{H}_n$. Equipped with Table I, first, we give the expectation value of the model potential term, denoted as $V_m^-(t>0)$, calculated by the last term of the Hamiltonian $\hat{H}_n$ in Eq. (12):

$$V_m^-(t>0)=\tfrac{1}{2}(\Lambda/B_m^-), \quad (18)$$

where the extra superscripts signal that it is determined by the (x_-)-dependent component of a product state, with relevant parameters from the second line of Table I. The kinetic energies $K_m(t)$ have two ($j=+$ and $j=-$) contributions, and they are calculated from

$$K_m^j(t>0)=\frac{1}{2}\int_{-\infty}^{\infty}d\xi'\int_{-\infty}^{\infty}d\xi\left|\frac{\partial}{\partial\xi}\Psi_m(\xi,\xi',t)\right|^2 =\frac{1}{4}B_m^j(t)\left\{1+\left[C_m^j(t)\right]^2\right\}, \quad (19)$$

which shows the role of the phase of a complex quantum-mechanical description.

The total (constant) energy takes the following form in our notations:

$$E_m(t>0)=K_m^+ +[K_m^-(t>0)+V_m^-(t>0)]. \quad (20)$$

The first components of the kinetic energies K_m^+ are obviously time independent and are given by $\sqrt{\lambda}/4$ and $\sqrt{\lambda+\Lambda}/4$. The sums in Eq. (20) are time independent as well. They are given by $[K_m^-(t>0)+V_m^-(t>0)]=(\omega_m^2+\omega^2)/4\omega_m$. For attractive interparticle interaction, the periodic time dependences of Wigner's kinetic (k) and potential (p) correlation energies are encoded in the differences of the corresponding, exact and HF, second and third terms of Eq. (20). We add for illustrative purposes

$$E_c^k(t>0)=\frac{1}{4}\left[\frac{\sqrt{\lambda+2\Lambda}}{f_1(t)}-\frac{\sqrt{\lambda+\Lambda}}{f_2(t)}\right]+\frac{\sin^2(2\sqrt{2\Lambda}t)}{32\Lambda} \times\left[\frac{\lambda^2}{\sqrt{\lambda+2\Lambda}f_1(t)}-\frac{(\lambda-\Lambda)^2}{\sqrt{\lambda+\Lambda}f_2(t)}\right],$$

$$E_c^p(t>0)=\frac{\Lambda}{2}\left[\frac{f_1(t)}{\sqrt{\lambda+2\Lambda}}-\frac{f_2(t)}{\sqrt{\lambda+\Lambda}}\right],$$

where $f_1(t)=1+(\lambda/2\Lambda)\sin^2(\sqrt{2\Lambda}t)$ and $f_2(t)=1+[(\lambda-\Lambda)/2\Lambda]\sin^2(\sqrt{2\Lambda}t)$. The time periodicity occurs in units of $T=\pi/(4\sqrt{2\Lambda})$, which increases when Λ decreases.

As we mentioned at Eq. (11), one can define an effective single-particle picture using, for instance, $\alpha_e\equiv 2\sqrt{\lambda}\sqrt{\lambda+2\Lambda}/(\sqrt{\lambda}+\sqrt{\lambda+2\Lambda})$ in Eq. (8), which, before the sudden quench, reproduces the exact single-particle probability density $n(x)$, the basic variable of DFT. The associated effective (Kohn-Sham) potential, with a certain prescription for the constant term in it, was determined earlier [23]. We can [24] also define, besides the density-optimal [12] choice, a wave-function-optimal single-particle approximation via an overlap maximization between the exact $\psi(x_1,x_2)$ and the right-hand side of Eq. (7). This constraint results in $\alpha_e=\bar{\omega}$, to which $\bar{\omega}$ is given at Eq. (4). Thus, we could name this last, well-motivated choice the wave-function-optimal one [14] in effective approximations.

In the time domain, by taking an α_e via $\omega_m\equiv\alpha_e$ in Table I, one could easily perform an investigation similar to the Hartree-Fock case above, where we followed the changes in the true (and not in an effective) Schrödinger Hamiltonian at the wave-function level by using precise propagators. But in the motivating efforts [22] in TD-DFT one attempts to determine a single-particle potential energy for an effective Hamiltonian which, in the corresponding time-dependent Schrödinger equation, results in the exact time-dependent probability density $n(x,t)$ via its auxiliary time-dependent orbital. We finish our paper with a brief discussion of this case.

An effective potential energy, denoted by $V_e^d(x,t)$ for a noninteracting Hamiltonian, can be constructed via the following [22] textbook equation:

$$V_e^d(x,t)=\frac{1}{4}(\ln n_e)''+\frac{1}{8}[(\ln n_e)']^2-\frac{1}{2}(k_e')^2-\frac{\partial k_e}{\partial t}, \quad (21)$$

where primes indicate differentiations with respect to x. This $V_e^d(x,t)$ follows from the real part of a complex equation obtained after substitution of $\Phi_e(x,t)=\sqrt{n_e(x,t)}\exp[ik_e(x,t)]$ into the single-particle time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\Phi_e(x,t)=\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+V_e^d(x,t)\right]\Phi_e(x,t). \quad (22)$$

The probability current [1] with the above $\Phi_e(x,t)$ is simply

$$j_e(x,t) = n_e(x,t)\,\frac{\partial k_e(x,t)}{\partial x}, \tag{23}$$

and the continuity equation of Schrödinger's wave mechanics,

$$\frac{\partial}{\partial t}\,n_e(x,t) + \frac{\partial}{\partial x}\,j_e(x,t) = 0,$$

is satisfied, of course, with these real quantities, independent of the real potential. From the imaginary part of the above-mentioned resulting complex equation one gets

$$n_e \nabla\cdot\nabla k_e + \nabla k_e\cdot\nabla n_e + \partial_t n_e = 0. \tag{24}$$

In our one-dimensional problem, this constraint is equivalent to the continuity equation. Clearly, the circle in the above single-particle modeling of possible practical importance might be closed simply by specifying the real $n_e(x,t)$ and $j_e(x,t)$ quantities of $\Phi_e(x,t)$.

In light of this practically desirable but hard [19,25] mapping problem and with the knowledge of our exact propagating function $\Psi(x_1,x_2,t)$, we calculate the normalized probability density $n(x,t)$ and the probability current $j(x,t)$ as follows:

$$n(x,t) = \int_{-\infty}^{\infty} |\Psi(x,x',t)|^2\,dx',$$

$$j(x,t) = Re\int_{-\infty}^{\infty} \Psi^*(x,x',t)\,\frac{\partial}{i\,\partial x}\,\Psi(x,x',t)\,dx'.$$

After straightforward calculation, the basic quantity of TD-DFT becomes

$$n(x,t) = \sqrt{\frac{\Omega(t)}{\pi}}\,e^{-\Omega(t)\,x^2}, \tag{25}$$

where a new frequency, $\Omega(t)$, is introduced via the definition of

$$\Omega(t) \equiv \frac{2\,B_m^+(t)\,B_m^-(t)}{B_m^+(t) + B_m^-(t)}.$$

In terms of the already known quantities the exact current is given by

$$j(x,t) \;=\; \Omega(t)\,x\,n(x,t)\left[\frac{C_m^+(t) + C_m^-(t)}{2}\right], \tag{26}$$

where the two separate phases from Eq. (15) appear in an arithmetic-mean form. Needless to say, these exact results satisfy the fundamental continuity equation.

With the exact $n(x,t)$ and $j(x,t)$ the circle may be closed, similar to recent efforts with one-dimensional two-particle models [4–7,22], by putting them into Eq. (23) in order to find an effective phase $k_e(x,t)$, but only up to a purely time-dependent function, i.e., one has $k_e(x,t) \Rightarrow K_e(x,t) = [k_e(x,t) + f(t)]$. Due to the $f(t)$ function, $K_e(x,t)$ can modulate the effective potential via the last term in Eq. (21). Thus, since $f(t)$ does not modify the kinetic energy contribution, only the expectation value of the potential energy is subject to it. Clearly, we arrive at the dynamical version of the freedom considered earlier in time-independent energetics [23] to fix a constant there. We postpone therefore the presentation of our mapping results for the potentials and energies, corresponding to different (and not only sudden) quenches in the correlated model system, to a dedicated future presentation. There, in particular, the capability of the adiabatic $[K_e(x,t) = 0]$ and dynamic approximations will be investigated in detail within the TD-DFT framework.

III. SUMMARY

There is a general expectation that, in principle, the time-dependent density-functional theory is an exact formulation of the time evolution of an interacting system. Motivated by this challenge of considerable practical interest, in this study we have investigated the time-dependent extension of Wigner's correlation by using an interacting one-dimensional model system. We applied a sudden quench in the external confinement behind the singlet ground-state state in order to propagate the wave functions from their initial forms in the exact and Hartree-Fock treatments. We have derived, and discussed briefly, the exact time-dependent probability density and probability current density, which can be the inputs in constructing an effective single-particle potential according to the motivating recent efforts. We pointed out, however, a freedom in such a construction which resides in a purely time-dependent phase component to an auxiliary complex wave function on which the presently applied mapping of exact probabilistic information onto a single-particle model is based.

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