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State reconstruction of wave packets moving in time-dependent potentials and the existence of Wronskian pairs

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Abstract. We determine a class of time-dependent potentials that support the state reconstruction of one-dimensional wave packets. For this we extend the projection method (Leonhardt U and Raymer M G 1996 *Phys. Rev. Lett.* **76** 1985) to explicitly time-dependent situations. We require the existence of Wronskian pairs (regular and irregular wavefunctions) and analyse the consequences on the possible potentials.

Quantum-mechanical wave packets travelling in known but otherwise arbitrary potentials possess an interesting property: the motion of the packet reveals the quantum state [1–4]. The spatio-temporal probability distribution $\mathrm{pr}(x, t)$ of the corresponding particles contains sufficient information to retrieve the density matrix ρ_{mn} of the wave packet (denoted in the energy representation). This theoretical concept [1–4] unifies and generalizes several experimental methods of state determination: Optical homodyne tomography [5–7], molecular fluorescence tomography [8, 9], and atomic-beam tomography [10]. Up to now, however, the concept [1–4] has been restricted to stationary potentials‡. State reconstruction of wave packets travelling in time-dependent potentials is interesting, because the motion could increase in complexity (most notably in quantum chaos). Furthermore, the phase retrieval of nonlinear waves [12] is based on an effective time-dependent potential. This problem is particularly relevant [12] for the state determination of travelling Bose–Einstein condensates observed in phase-contrast imaging [13]. Can we extend the ideas developed for stationary potentials [1–4] to the time-dependent case [14]?

What are these ideas? The density matrix ρ_{mn} in the energy representation is reconstructed as the average

$$\rho_{mn} = \left\langle\!\!\left\langle \frac{\partial}{\partial x}\left[\psi_m^*(x, t)\, \varphi_n(x, t)\right] \right\rangle\!\!\right\rangle_{x,t} \tag{1}$$

with respect to the measured positions x at all times t. By $\langle\!\langle F(x, t)\rangle\!\rangle_{x,t}$ we denote the average

$$\langle\!\langle\, F(x, t)\, \rangle\!\rangle_{x,t} \equiv \lim_{T\to\infty} T^{-1} \int_{-T/2}^{+T/2} \int_{-\infty}^{+\infty} \mathrm{pr}(x, t)\; F(x, t)\, \mathrm{d}x\, \mathrm{d}t \tag{2}$$

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‡ After submission of this paper, a letter [11] appeared that describes a hydrodynamical method for state reconstruction of wave packets that travel in potentially time-dependent potentials.

of a function $F(x,t)$ with respect to the spatio-temporal probability distribution $\mathrm{pr}(x,t)$. Here

$$\psi_n(x,t) = u_n(x)\mathrm{e}^{-\mathrm{i}\omega_n t} \qquad \varphi_n(x,t) = v_n(x)\mathrm{e}^{-\mathrm{i}\omega_n t} \tag{3}$$

denote the regular and irregular wavefunctions of the energy eigenstates $|n\rangle$. (For simplicity we assume a discrete spectrum. For the continuous case see [15].) Both the regular and the irregular wavefunctions are solutions of the Schrödinger equation

$$\mathrm{i}\dot{\phi}_n = -\tfrac{1}{2}\phi_n'' + U\phi_n \tag{4}$$

in appropriate units. Regular wavefunctions are normalized to unity, whereas irregular ones obey the Wronskian condition

$$W_n = u_n v_n' - u_n' v_n = 2. \tag{5}$$

The condition implies [3] that irregular wavefunctions must not be normalizable. Analytic examples of irregular wavefunctions are given in [16–18]. The key mathematical property of the spatial derivative $(\psi_m^*\varphi_n)'$ of regular and irregular wavefunction is the fact [1–4] that these objects form an orthonormal system on products of wavefunctions $\psi_\mu\psi_\nu^*$, i.e.

$$D_{\mu\nu}^{mn} \equiv \lim_{T\to\infty} T^{-1}\int_{-T/2}^{+T/2}\int_{-\infty}^{+\infty} \psi_\mu\psi_\nu^*\,(\psi_m^*\varphi_n)'\,\mathrm{d}x\,\mathrm{d}t = \delta_{\mu m}\delta_{\nu n}. \tag{6}$$

Therefore, $(\psi_m^*\varphi_n)'$ projects the density-matrix elements ρ_{mn} out of the spatio-temporal probability distribution

$$\mathrm{pr}(x,t) = \langle x,t\,|\,\hat{\rho}\,|\,x,t\rangle = \sum_{\mu\nu}\rho_{\mu\nu}\psi_\mu(x,t)\,\psi_\nu^*(x,t). \tag{7}$$

State reconstruction of wave packets from $\mathrm{pr}(x,t)$ is a non-trivial property, because some counterexamples are known [19] for multi-dimensional spaces where the mapping between $\mathrm{pr}(x,t)$ and the quantum state is not unique. Therefore, to extend state reconstruction to the case of time-dependent potentials, we seek a similar structure as in the stationary case. There are no stationary states in general, but we might assume that a basis of states $|n\rangle$ exists that have pairs of regular and irregular wavefunctions $\psi_n(x,t)$ and $\varphi_n(x,t)$. What do we mean by that? Let us assume that the functions ψ_n and φ_n are solutions of the Schrödinger equation (4) that form a *Wronskian pair*

$$\psi_n^*\varphi_n' - \psi_n'\varphi_n^* = W_n \qquad W_n' = 0. \tag{8}$$

How to find the wavefunctions ψ_n and φ_n will not concern us at the moment; we will come to this point later. Let us first examine the implications of the sheer existence of Wronskian pairs. Given a function ψ_n, equation (8) formulates a differential equation for φ_n with the solution

$$\varphi_n = W_n\psi_n\int\frac{\mathrm{d}x}{\psi_n^*\psi_n} \tag{9}$$

as is easily verified. The integration in the solution (9) is an undetermined integral with the set of integration constants corresponding to the set of unique solutions of the differential equation (8). Therefore, equation (9) is the general solution of (8). Equation (9) thus describes uniquely the relation between the two functions ψ_n and φ_n that form a Wronskian pair (8).

To proceed, we expand the wavefunctions ψ_n in (real) amplitude and (real) phase functions

$$\psi_n = u_n\mathrm{e}^{\mathrm{i}S_n}. \tag{10}$$

We see from (9) that φ_n has the same phase factor as ψ_n:

$$\varphi_n = v_n\mathrm{e}^{\mathrm{i}S_n} \tag{11}$$

and the amplitude

$$v_n = W_n u_n \int \frac{\mathrm{d}x}{u_n^2}. \tag{12}$$

Let us formulate the Schrödinger equation (4) in terms of amplitude and phase:

$$-\tfrac{1}{2}u_n'' + \big(U + \tfrac{1}{2}S_n'^2 + \dot{S}_n\big)u_n = 0 \tag{13}$$

$$\dot{u}_n + \tfrac{1}{2}S_n''u_n + S_n'u_n' = 0 \tag{14}$$

(and identical equations for v_n). Equation (13) plays the role of the stationary Schrödinger equation in the explicitly time-dependent case. We see that the potential U is modified by the term $\frac{1}{2}S_n'^2+\dot{S}_n$ that contains the spatial structure and the evolution of the phase S_n. Equation (14) is a form of the conservation law for the probability density u_n^2 with the probability flux $S_n'u_n^2$, because from (14) we obtain the result that $\partial(u_n^2)/\partial t + (S_n'u_n^2)'$ vanishes.

We show in appendix A that v_n satisfies the Schrödinger equation (13) automatically, whereas the probability conservation (14) seriously restricts the possible choice of the phase functions S_n

$$S_n'' = -\frac{1}{2}\frac{\dot{W}_n}{W_n}. \tag{15}$$

The phase S_n is a quadratic function in space

$$S_n = a_n(t)\frac{x^2}{2} + b_n(t)x - \Omega_n(t). \tag{16}$$

Given the structure (16) of the phase S_n, we utilize the probability conservation (14) to determine the structure of the amplitudes u_n. We show in appendix B that $u_n(x,t)$ is a scaled function $w_n(\xi)$ such that

$$u_n = \eta^{-1/2}w_n(x/\eta - \zeta) \qquad \eta = \eta(t) \quad \zeta = \zeta(t) \tag{17}$$

$$a_n = \eta^{-1}\dot{\eta} \qquad b_n = \eta\dot{\zeta}. \tag{18}$$

The irregular wavefunctions obey the same scaling.

We have seen that the existence of Wronskian pairs does restrict the wavefunctions. Let us require another property that originates from the normalization

$$D_{mn}^{mn} = 1 \tag{19}$$

of the desired orthogonal system (6) on products of wavefunctions. From (10) and (11) we obtain

$$D_{mn}^{mn} = \lim_{T\to\infty} T^{-1}\int_{-T/2}^{+T/2}\int_{-\infty}^{+\infty} u_m u_n\big[(u_m v_n)' + \mathrm{i}(S_m' - S_n')u_m v_n\big]\,\mathrm{d}x\,\mathrm{d}t. \tag{20}$$

In order to guarantee that D_{mn}^{mn} is real we require that $(S_m' - S_n')$ be zero, i.e.

$$S_n = S(x,t) - \Omega_n(t). \tag{21}$$

From (16) and (18) we obtain

$$S(x,t) = \frac{\dot{\eta}}{\eta}\frac{x^2}{2} + \eta\dot{\zeta}x. \tag{22}$$

This result restricts the class of potentials $U(x,t)$. To see this we define the function

$$F_n \equiv U + \tfrac{1}{2}S'^2 + \dot{S} - \dot{\Omega}_n \tag{23}$$

and show in appendix C that F_n obeys the scaling

$$F_n = \eta^{-2}G_n(x/\eta - \zeta). \tag{24}$$

Therefore we are lead to the requirement that the spatially independent part of F_n scales as

$$\dot{\Omega}_n(t) = \frac{\omega_n}{\eta^2(t)}. \tag{25}$$

The set of constants ω_n play the role of energy eigenvalues and will be determined soon. We obtain for the phases

$$S_n(x,t) = \frac{\dot{\eta}}{\eta}\frac{x^2}{2} + \eta\dot{\zeta}x - \omega_n \int \frac{\mathrm{d}t}{\eta^2}. \tag{26}$$

Furthermore, $F_n + \dot{\Omega}_n$ should scale as

$$F_n + \dot{\Omega}_n = U + \tfrac{1}{2}S'^2 + \dot{S} = \eta^{-2}V(x/\eta - \zeta). \tag{27}$$

We use this scaling property and equation (22) to obtain the class of potentials that support a Wronskian pair (8) with the property (21):

$$U = \eta^{-2}V(x/\eta - \zeta) - \frac{\ddot{\eta}}{\eta}\frac{x^2}{2} - (2\dot{\eta}\dot{\zeta} + \eta\ddot{\zeta})x - \frac{\eta^2\dot{\zeta}^2}{2}. \tag{28}$$

This is the central result of our paper. The existence of Wronskian pairs (8) with the property (21) restricts the class of time-dependent potentials $U(x,t)$. Apart from a quadratic term they are scaled and shifted stationary potentials $V(\xi)$. The explicit time dependence is brought about by the scaling function $\eta(t)$ and the potentially time-dependent shift $\zeta(t)$.

We also employ the scaling property (27) to find the set of wavefunctions and the numbers ω_n. The amplitudes u_n obey (13) and, consequently,

$$-\tfrac{1}{2}u_n'' + \eta^{-2}V(x/\eta - \zeta)u_n = \eta^{-2}\omega_n u_n. \tag{29}$$

We apply the scaling (17) of the wavefunctions and see that the $w_n(\xi)$ are the eigenfunctions of the stationary Schrödinger equation

$$-\frac{1}{2}\frac{\mathrm{d}^2 w_n}{\mathrm{d}\xi^2} + V(\xi)w_n = \omega_n w_n \tag{30}$$

with potential $V(\xi)$ and eigenvalues ω_n. The irregular wavefunction are then given by (12).

So far, we were concerned about the implications of the existence of Wronskian pairs (8) in the case of a time-dependent potential. We determined the class of potentials that support such pairs. Finally, we prove that our mathematical objects are indeed useful for state reconstruction. We consider the overlap (6), utilize the structure (10) and (11) of the wavefunctions and the phases (26) to obtain

$$D_{\mu\nu}^{mn} = \lim_{T\to\infty} T^{-1}\int_{-T/2}^{+T/2}\int_{-\infty}^{+\infty} u_\mu u_\nu\,(u_m v_n)'\,\exp\big[\mathrm{i}(\omega_m - \omega_n - \omega_\mu + \omega_\nu)\theta\big]\,\mathrm{d}x\,\mathrm{d}t \tag{31}$$

with

$$\theta(t) = \int \frac{\mathrm{d}t}{\eta^2}. \tag{32}$$

We see from the scaling of the wavefunctions, equations (17), that the spatial integral in $D_{\mu\nu}^{mn}$ scales as

$$\int_{-\infty}^{+\infty} u_\mu u_\nu\,(u_m v_n)'\,\mathrm{d}x \propto \frac{1}{\eta^2(t)} = \dot{\theta}(t). \tag{33}$$

We employ θ as an integration variable in the temporal integral in (31), which is always possible, because $\dot{\theta} = \eta^{-2} > 0$. We see that $D_{\mu\nu}^{mn}$ vanishes unless

$$\omega_m - \omega_n = \omega_\mu - \omega_\nu. \tag{34}$$

This frequency constraint is one cornerstone of the orthogonality proof for the $(u_m v_n)'$ on the products of wavefunctions $u_\mu u_\nu$. In addition, we note that the amplitudes u_n and v_n are solutions of the Schrödinger equation (13) with the effective potential $U + \frac{1}{2}S'^2 + \dot{S}$ and the eigenfrequencies ω_n. Then we apply the reconstruction theorem [1] of one-dimensional Schrödinger equations to prove that

$$D^{mn}_{\mu\nu} \propto \delta_{\mu m}\delta_{\nu n}. \tag{35}$$

We refer the reader to [3, section 3] for an extensive review of the underlying mathematics.

Finally, we turn to the normalization $D^{mn}_{mn} = 1$. We perform a three-line calculation starting from equations (20) and (21), and, observing $W_n = u_n' v_n - u_n' v_n$ and $W_n' = 0$, obtain

$$\begin{aligned} D^{mn}_{mn} &= \lim_{T\to\infty} T^{-1} \int_{-T/2}^{+T/2} \int_{-\infty}^{+\infty} u_m u_n \, (u_m v_n)' \, \mathrm{d}x \, \mathrm{d}t \\ &= \lim_{T\to\infty} T^{-1} \int_{-T/2}^{+T/2} \int_{-\infty}^{+\infty} \left[W_n u_n^2 + (u_m u_n)' \, u_m v_n \right] \mathrm{d}x \, \mathrm{d}t \\ &= \lim_{T\to\infty} T^{-1} \int_{-T/2}^{+T/2} W_n \, \mathrm{d}t - D^{mn}_{mn}. \end{aligned} \tag{36}$$

We see from (36) that the time average of the Wronskian W_n is twice the overlap integral D^{mn}_{mn}. The normalization $D^{mn}_{mn} = 1$ thus implies that

$$\lim_{T\to\infty} T^{-1} \int_{-T/2}^{+T/2} W_n \, \mathrm{d}t = 2. \tag{37}$$

This generalizes the Wronskian condition (5) to our case of explicitly time-dependent potentials.

In summary, state reconstruction of one-dimensional wave packets moving in time-dependent potentials is possible but restricted to a particular class (28) of potentials, if we require a similar structure (8) as in the time-independent case [1–4]. In essence, the allowed potentials $U(x,t)$ are appropriately scaled and shifted stationary potentials $V(\xi)$ with an additional quadratic term. The time dependence is brought about by an arbitrary scaling $\eta(t)$ and shift $\zeta(t)$. Of course, our result does not prove that otherwise state reconstruction is impossible, but a radically different approach is required. In fact, Johansen [11, 20] has recently found a hydrodynamical method for determining the state of a wave packet that moves in a (potentially) time-dependent potential. Here the density matrix $\langle x + y, t_0 \,|\, \hat{\rho} \,|\, x - y, t_0 \rangle$ in position representation is reconstructed from the assumed knowledge of all temporal derivatives of the probability distribution $\mathrm{pr}(x, t_0)$ at a certain time t_0. This is equivalent to knowledge of the total spatio-temporal evolution $\mathrm{pr}(x,t)$, i.e. to our case, if and only if $\mathrm{pr}(x,t)$ is an analytic function in t on the real axis. Furthermore, Johansen [11] represents the density matrix $\langle x + y, t_0 \,|\, \hat{\rho} \,|\, x - y, t_0 \rangle$ as a power series $\sum_{n=0}^{\infty} f_n(x, t_0)(n!)^{-1}(2\mathrm{i}y)^n$, assuming $\langle x + y, t_0 \,|\, \hat{\rho} \,|\, x - y, t_0 \rangle$ to be analytic in y for all values of x.

We may speculate that quantum chaos might limit quantum-mechanical state reconstructions. Why? Classical state measurements are difficult for a chaotic system. The evolution of the system may show little (or a drastic) influence of the initial conditions. Therefore we would expect problems in quantum state determinations due to quantum signatures of chaos [21]. Expressed in terms of the hydrodynamic approach, chaos may render the probability distribution $\mathrm{pr}(x,t)$ and the density matrix $\langle x + y, t \,|\, \hat{\rho} \,|\, x - y, t \rangle$ less analytic. Note also that our class of allowed potentials correspond to regular motions of wave packets, because the $U(x,t)$ support a complete set of wavefunctions (17) that are scaled energy eigenfunctions of the potential $V(\xi)$. Therefore, to close this paper with a speculation, the onset of quantum chaos may indeed limit our fundamental ability to infer quantum states from moving wave packets.

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Appendix A

In this appendix we determine the structure of the phase factors S_n that is compatible with the existence of a Wronskian pair (8). We will see that the probability conservation (14) imposes a serious constraint. Let us start from the relation (12) between the irregular and regular wavefunctions

$$v_n = W_n u_n \int \frac{\mathrm{d}x}{u_n^2}. \tag{A.1}$$

We take the first and the second spatial derivative, and get

$$v_n' = u_n' W_n \int \frac{\mathrm{d}x}{u_n^2} + \frac{W_n}{u_n} \tag{A.2}$$

$$v_n'' = u_n'' W_n \int \frac{\mathrm{d}x}{u_n^2}. \tag{A.3}$$

Therefore

$$-\tfrac{1}{2} v_n'' + \left(U + \tfrac{1}{2} S_n'^2 + \dot{S}_n\right) v_n = 0 \tag{A.4}$$

is satisfied, because u_n solves the identical equation (13). Let us see what

$$\dot{v}_n + \tfrac{1}{2} S_n'' v_n + S_n' v_n' = 0 \tag{A.5}$$

i.e. the probability conservation for v_n, requires. We differentiate the irregular wavefunction (A.1) with respect to the time t, get

$$\dot{v}_n = \dot{u}_n W_n \int \frac{\mathrm{d}x}{u_n^2} + u_n \frac{\partial}{\partial t} W_n \int \frac{\mathrm{d}x}{u_n^2} \tag{A.6}$$

and therefore

$$\dot{v}_n + \tfrac{1}{2} S_n'' v_n + S_n' v_n' = u_n \left(\frac{\partial}{\partial t} W_n \int \frac{\mathrm{d}x}{u_n^2} + S_n' \frac{W_n}{u_n^2} \right). \tag{A.7}$$

The right-hand side of this equation vanishes if

$$\frac{\partial}{\partial t} W_n \int \frac{\mathrm{d}x}{u_n^2} + S_n' \frac{W_n}{u_n^2} = 0. \tag{A.8}$$

We take the spatial derivative of this equation and use the probability conservation (14) for the regular wavefunctions to obtain

$$
\begin{aligned}
0 &= \frac{\partial}{\partial t}\left(\frac{W_n}{u_n^2}\right) + S_n'' \frac{W_n}{u_n^2} + S_n'\left(\frac{W_n}{u_n^2}\right)' \\
&= \frac{1}{u_n^3}\left(\dot{W}_n u_n - 2W_n \dot{u}_n + S_n'' W_n u_n - 2S_n' W_n u_n'\right) \\
&= \frac{1}{u_n^2}\left(\dot{W}_n + 2S_n'' W_n\right)
\end{aligned}
\tag{A.9}
$$

and, consequently,

$$
S_n'' = -\frac{1}{2}\frac{\dot{W}_n}{W_n} \qquad \text{with} \quad W_n' = 0. \tag{A.10}
$$

The phases S_n are restricted to be quadratic functions in x.

Appendix B

In this appendix we determine the wavefunctions u_n that satisfy

$$
\dot{u}_n + \tfrac{1}{2} a u_n + (ax + b) u_n' = 0. \tag{B.1}
$$

We try the scaling ansatz

$$
u_n = \eta^{-1/2} w_n(\xi) \qquad \xi = x/\eta(t) - \zeta(t) \tag{B.2}
$$

and differentiate

$$
\dot{u}_n = -\frac{1}{2}\frac{\dot{\eta}}{\eta} u_n - \eta^{-1/2}\frac{\mathrm{d}w_n(\xi)}{\mathrm{d}\xi}\left(\frac{\dot{\eta}}{\eta^2} x + \dot{\zeta}\right) \tag{B.3}
$$

$$
u_n' = \eta^{-1/2}\frac{\mathrm{d}w_n(\xi)}{\mathrm{d}\xi}\,\frac{1}{\eta}. \tag{B.4}
$$

The term in (B.1) that is proportional to u_n vanishes if

$$
a = \frac{\dot{\eta}}{\eta}. \tag{B.5}
$$

The term that contains the derivative $\mathrm{d}w_n/\mathrm{d}\xi$ is zero if, in addition,

$$
b = \eta\dot{\zeta}. \tag{B.6}
$$

In this way we have found the general solution of (B.1).

Appendix C

In this appendix we determine the scaling of

$$
F_n = U + \tfrac{1}{2} S'^2 + \dot{S} - \dot{\Omega}_n. \tag{C.1}
$$

In terms of the F_n the Schrödinger equation (13) reads as

$$
u_n'' = 2F_n u_n. \tag{C.2}
$$

Therefore

$$
\dot{u}_n'' = 2(\dot{F}_n u_n + F_n \dot{u}_n) = 2(\dot{F}_n u_n - \tfrac{1}{2} S'' F_n u_n - S' F_n u_n') \tag{C.3}
$$

using the probability conservation (14). On the other hand, we take the second spatial derivative of (14), observe $S''' = 0$, and get

$$\dot{u}_n'' = -\tfrac{5}{2} S'' u_n'' - S' u_n''' = -5 S'' F_n - 2 S' F_n u_n' - 2 S' F_n' u_n. \tag{C.4}$$

We combine equations (C.3) and (C.4) to obtain

$$\dot{F}_n + 2 S'' F_n + S' F_n' = 0 \tag{C.5}$$

or, via the quadratic structure (16) of the phase S,

$$\dot{F}_n + 2a F_n + (ax + b) F_n' = 0. \tag{C.6}$$

We proceed along similar lines as in appendix B and finally obtain

$$F_n = \eta^{-2} G_n(\xi) \qquad \xi = x/\eta(t) - \zeta(t). \tag{C.7}$$

In this way we determined the scaling of the right-hand side of the Schrödinger equation (13), if we impose the existence of Wronskian pairs (8).

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