Energy-time representation for quantum systems

Gabino Torres-Vega*
Physics Department, CINVESTAV, Apartado postal 14-740, 07000 Mexico, Distrito Federal, Mexico
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We introduce a picture of quantum dynamics in which the representation basis vectors are the quantities that evolve, instead of state vectors or operators. These vectors allow us to pick the parts of a probability density that correspond to some values of energy or time, providing us with energy and time representations. The properties of these representations are analyzed and an application to the free particle is presented.

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I. INTRODUCTION

Even though time appears explicitly in the equation of motion for quantum systems, its determination from wave packets has shown to be quite difficult, but that is also the case for classical probability densities. For quantum systems, and when valid [1,2], Pauli’s theorem prevents the existence of a time operator conjugate to the Hamiltonian [1–5], but there is some criticism to his statement [1,2] and there are several examples in which a time operator conjugate to the Hamiltonian has been built [1,6–9].

Some authors have quantized the classical expressions for time in terms of $p$ and $q$, with the usual inherent difficulties like symmetrization of nonlinear functions, the appearance of non-Hermitian operators with divergencies, etc. [6,10–12]. These difficulties have caused the abandonment of the hermiticity requirement for a quantum observable and a move to the use of positive operator-valued measures [11–17] or to the use of Hamiltonians with CPT (charge, position, and time) symmetry [18].

Other authors have put aside the time variable that appears in the equations of motion and have taken a part of the system as the clock. Since those clocks might not be linearly related to usual clocks, only in limiting cases one can recover the usual equations of motion [19–22].

There is also the procedure in which the Hamiltonian itself, for a free particle, is modified in order to admit a self-adjoint conjugate operator [23–25]. The time eigenstate that is obtained, the Kijowski state [23], also appears in other situations, even if the time problem is treated including an external system coupled to the one of interest in order to model an experimental arrangement [26].

Besides the cited developments in quantum theory, what is needed is a way to extract the time information from wave functions. It is possible to explicitly handle the time variable for a single classical particle by realizing a canonical transformation to an energy-time description of the dynamics [15,16,27,28]. In a previous paper [29], an energy-time representation for classical densities has been introduced and in this paper we introduce time-dependent representation vectors, which will provide us with a quantum energy and time representations. This approach is inspired in the results for determining the arrival time in quantum systems [23,29–32] and it does not need quantization of the particular and explicit expressions of time in terms of coordinate and position, nor of the modification of the Hamiltonian operator, nor of the lifting of the requirement of self-adjointness of observable operators, and nor of internal or external clocks.

We make use of a picture of quantum mechanics in which the representation vectors are the ones that evolve and state vectors and operators are static. We use the relationship between the clock and a given system in order to define probe functions, which will sample a wave packet at different energies or times. In this way, energy and time no longer are a parameter but they become part of the description of quantum densities.

We start with Sec. II in which we make some comments regarding the relationship between time, clocks, and equations of motion. The basic concept behind probe functions was introduced in Ref. [29] for a classical system. Based on that, a picture for the study of the time properties of the dynamics of quantum wave packets is presented in Sec. III. There is also a simple application to the free particle. At the end there are some concluding remarks.

II. TIME CONCEPT

We can think of time as a measure of how much a system has changed, and a clock is a reference system that is used for the measurement of time or change. However, these two systems do not interact between themselves but they become interlaced at the moment we use a clock as the reference for measuring the amount of change of some quantities of the system of interest, as is seen, for instance, in Schrödinger’s equation of motion

\[
\frac{i\hbar}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle. \tag{1}
\]

This equation might take a different explicit form depending upon the reference system for time that we chose. Once the equation of motion is written down, a way of extracting the time information from wave packets is needed and is the subject of the remaining of this manuscript.

III. QUANTUM SYSTEMS

A. Time superoperator

There were some earlier indications that the derivative with respect to energy can be considered as a time operator [33]. Let us introduce a time superoperator

*Electronic address: gabino@fis.cinvestav.mx
\[ i = \hbar \frac{d}{dH}. \]  

(2)

With \( d/d\hat{H} \) we mean a “differentiation” of powers of the Hamiltonian, i.e., \( (d/d\hat{H})\hat{H}^n = n\hat{H}^{n-1} \). We can achieve this effect, for instance, with the help of an operator that has a constant commutator with \( \hat{H} \). Recall that if two operators \( \hat{A} \) and \( \hat{B} \) are such that \( [\hat{A}, \hat{B}] = \text{const} \) then \( [\hat{A}, \hat{B}^n] = n[\hat{A}, \hat{B}]\hat{B}^{n-1} \). The time operator has units of time and has the propagator as \( e^{-i\hat{H}t} \).

A Hermitian operator \( \hat{A} \) depends on \( \hat{H} \), i.e., the time-dependent Schrödinger equation, is always an eigenfunction of the time superoperator. This superoperator is not linear when applied to wave packets because when applied to a linear combination of two wave packets \( a|\psi(t)\rangle + b|\phi(t)\rangle \), we will get only the evolution time \( t \) times the same linear combination.

We have here a different situation than the one considered in Ref. [2]. In that paper, it was shown that if we have two Hermitian operators \( \hat{A} \) and \( \hat{B} \) and \( |\phi\rangle \) is an eigenfunction of \( \hat{A} \), then the commutator action on \( |\phi\rangle \) results in an state orthogonal to \( |\phi\rangle \). Therefore, \( \hat{A}, \hat{B}, \) and \( [\hat{A}, \hat{B}] \) have different domains and the validity of Pauli’s theorem about the nonexistence of a time operator might be questionable. However, here we are taking as the time operator the superoperator \( \hbar d/d\hat{H} \), and the action of the commutator between \( \hat{H} \) and \( \hat{i} \) on a time-dependent state \( |\psi(t)\rangle \) is

\[
[\hat{i}, \hat{H}]|\psi(t)\rangle = \dot{\hat{H}}|\psi(t)\rangle - \hat{H}\dot{|\psi(t)\rangle} = i\hbar|\phi(t)\rangle + \hat{H}\dot{i}|\psi(t)\rangle - i\hat{H}|\phi(t)\rangle = i\hbar|\phi(t)\rangle, \]

i.e., the resulting vector is in the same space as \( |\phi(t)\rangle \) and the relationship between operator and superoperator

\[
\left[ i\hbar \frac{d}{d\hat{H}}, \hat{H} \right] = i\hbar \hat{I} \]

is valid in the evolution space.

Now, the above relationship [Eq. (5)] is just another way of writing the evolution equation since, when applied to a time-dependent state \( |\psi(t)\rangle \), we obtain the usual time-dependent Schrödinger equation.

Since \( [\hat{i}, \hat{H}] = \hbar i \hat{I} \), we find that \( [\hat{i}, \hat{H}^n] = n\hbar i \hat{I} \hat{H}^{n-1} \), and then

\[
[\hat{i}, e^{-i\hat{H}t}] = \tau e^{-i\hat{H}t}, \]

(6)

where \( \tau \) is a real constant. This is another way of saying that \( e^{-i\hat{H}t} \) is the evolution operator and that \( |\psi(t)\rangle \) is an eigenfunction of \( \hat{i} \) since if we apply Eq. (6) to a wave packet at time \( t \), \( |\psi(t)\rangle \), we find that \( \hat{i}\hat{i}^{\dagger} |\psi(t+\tau)\rangle = (t+\tau) |\psi(t+\tau)\rangle \).

If we multiply Eq. (6) by \( e^{i\hat{H}t} \) we get

\[
e^{i\hat{H}t}e^{-i\hat{H}t} = \hat{i} + \tau. \]

(7)

Also, since \( [\hat{\tau}, \hat{H}] = n\hbar \hat{I} \hat{H}^{n-1} \), we have that

\[
\left[ e^{i\hat{\tau}t}, \hat{H} \right] = \epsilon e^{i\hat{\tau}t}, \]

(8)

where \( \epsilon \) is a real constant. If we apply this equality to \( |\psi(t)\rangle \), we find that \( e^{i\hat{\tau}t} |\psi(t)\rangle \) is a solution for a system to which a constant potential has been added, i.e.,

\[
\hbar \frac{d}{dt} e^{i\hat{\tau}t} |\psi(t)\rangle = (\hat{H} + \epsilon) e^{i\hat{\tau}t} |\psi(t)\rangle. \]

(9)

After the application of \( e^{-i\hat{\tau}t} \) from the left to the equality (8) we find that

\[
e^{-i\hat{\tau}t} \hat{H} e^{i\hat{\tau}t} = \hat{H} - \epsilon. \]

(10)

B. Probe states

We can also generate a “time grid” for quantum systems with a state such as \( \nu_0(p; T=0; X) = e^{-ip\hat{X}t}, \) in momentum space, and propagating it backwards and forwards in time. This wave packet gives a constant density in momentum space with a narrow width in coordinate space around \( q=X \). These characteristics are desirable for the probe states that we need; they have the same characteristics as the classical probe states [29]. Backwards and forwards propagation will result in a collection of densities, which can be used to sample a given wave packet and determine its distribution in energy or time, for instance. The probe function \( \nu_0(p; T=0; X) \), before any propagation, can be assigned with the time front \( T=0 \). The time grid can change dramatically for different \( X \). A good choice for \( X \) is in the middle of the wave packet, but it can take any real value that lies inside the system.

For classical systems we were able to use probe functions, which are punctual in phase space, moving along the trajectories of the system. But for quantum systems the most we can do is to use the whole line \( q=X \).

Note that these probe states have been in use since the early times of quantum mechanics. The relationship between coordinate and momentum representations of a wave packet \( |\psi\rangle \) are

\[
\psi(q; t) = \int_{-\infty}^{\infty} dp e^{ip\hat{q}t} |\psi(p; t)\rangle
= \int_{-\infty}^{\infty} dp \left[ \phi(p) e^{-ip\hat{q}t} \right] = \langle \nu_0(t; q) | \phi \rangle. \]

(11)
\[ \psi(p; t) = \int_{-\infty}^{\infty} dq e^{-i\phi \hbar} \psi(q; t) = \langle \nu_p(t; p) | \psi \rangle, \]  
(12)

where \( |\nu_p(t; q)\rangle = e^{i\phi \hbar} |q\rangle \) and \( |\nu_p(t; p)\rangle = e^{i\phi \hbar} |p\rangle \). Then, the coordinate representation of quantum mechanics can be seen as the sampling of the initial wave function \( |\psi\rangle \) for arrival at \( q \) at time \( t \) and the momentum representation as the sampling of the initial wave function for having momentum \( p \) at time \( t \). Contrary to Schrödinger, Heisenberg, or interaction pictures of quantum mechanics, here the representation vectors are the time-dependent quantities and wave packets and operators are static. This is a picture of quantum mechanics that has not been recognized as such before. The only difference with the probe states that we use is that we will sample for only a specific point \( q = X \). Our probe functions are nothing more than the evolution of the representation vectors \( |q\rangle \) for a particular point \( q = X \). These states were used in a previous paper concerning marginal probe functions suited for arrival time distributions [32].

For our purposes, we will consider only the first type of probe functions and we will separate into negative and positive momentum parts. In quantum mechanics, the distinction between right and left movers is necessarily an approximated concept, because the requirement \( q = X \) is not exactly compatible with the requirement \( p > 0 \) (or \( p < 0 \)), but it is necessary to make a classification like that. Let us rewrite \( \langle X | \psi(T) \rangle \) as

\[ \langle X | \psi(T) \rangle = \langle X | e^{-i\hat{H} \hat{T} \hbar} | \psi \rangle \]
\[ = \int_{-\infty}^{0} dp \langle X | p \rangle \langle p | e^{-i\hat{H} \hat{T} \hbar} | \psi \rangle \]
\[ + \int_{0}^{\infty} dp \langle X | p \rangle \langle p | e^{-i\hat{H} \hat{T} \hbar} | \psi \rangle \]
\[ = \int_{Sp(\hat{H})} dE e^{-i\hat{E} \hat{T} \hbar} \left[ \int_{-\infty}^{0} dp \langle X | p \rangle \langle p | E | \psi \rangle \right] \]
\[ + \int_{0}^{\infty} dp \langle X | p \rangle \langle p | E | \psi \rangle \].
\[ = \int_{Sp(\hat{H})} dE e^{-i\hat{E} \hat{T} \hbar} \left[ \int_{-\infty}^{0} dp \langle X | p \rangle \langle p | E | \psi \rangle \right] \]
\[ + \int_{0}^{\infty} dp \langle X | p \rangle \langle p | E | \psi \rangle \].
\[ (13) \]

Thus, probe states for energy are defined as

\[ |\nu^{-}(E; X)\rangle = \int_{-\infty}^{0} dp |E|p\rangle \langle p | X \rangle, \]
\[ (14) \]

\[ |\nu^{+}(E; X)\rangle = \int_{0}^{\infty} dp |E|p\rangle \langle p | X \rangle. \]
\[ (15) \]

From here after, we will use the notation \( \int_{0}^{\infty} dp \langle p | X \rangle \langle x | p \rangle \) for the integrals \( \int_{-\infty}^{0} dp \langle p | X \rangle \langle x | p \rangle \) and \( \int_{0}^{\infty} dp \langle p | X \rangle \langle x | p \rangle \). But we should keep in mind that the point \( p = 0 \) is not included in the integral over negative momentum. In what follows we will also use the operators \( \hat{T} = e^{-i\hat{H} \hat{T} \hbar} \), \( \hat{S}_x = \hat{X} \langle X | \rangle \), \( \hat{S}_y = \hat{E} \langle E | \rangle \), and \( \hat{S}_z = |E\rangle \langle E | \). The sum of the above states is an eigenfunction of the Hamiltonian

\[ |\nu(E; X)\rangle = |\nu^{-}(E; X)\rangle + |\nu^{+}(E; X)\rangle = |E\rangle \langle E | X \rangle, \]
\[ (16) \]

with eigenvalue \( E(X) \). For a time representation we can use

\[ |\nu^{\pm}(T; X)\rangle = \int_{0}^{\infty} dp e^{i\hat{E} \hat{T} \hbar} \langle \pm p | X \rangle = e^{i\hat{E} \hat{T} \hbar} \hat{P}_X |X\rangle. \]
\[ (17) \]

Since the time probe states have a small width in \( q \), we have replaced \( t \) with \( T \), the relative time. The sum of the above states is the backwards propagation of the line \( q = X \),

\[ |\nu(T; X)\rangle = |\nu^{-}(T; X)\rangle + |\nu^{+}(T; X)\rangle = \hat{T} |X\rangle. \]
\[ (18) \]

This sum is an eigenstate of the time superoperator with eigenvalue \(-\hat{T}\).

The energy and time probe states are related through Fourier-type transforms

\[ \int_{Sp(\hat{H})} dE e^{i\hat{E} \hat{T} \hbar} \langle \nu^{-}(E; X) \rangle = |\nu^{\pm}(T; X)\rangle, \]
\[ (19) \]
\[ \int_{Sp(\hat{H})} dE e^{i\hat{E} \hat{T} \hbar} \langle \nu^{+}(E; X) \rangle = |\nu^{-}(T; X)\rangle, \]
\[ (20) \]
\[ \int_{-\infty}^{\infty} dT e^{-i\hat{E} \hat{T} \hbar} |\nu^{\pm}(T; X)\rangle = |\nu^{\pm}(E; X)\rangle, \]
\[ (21) \]

and

\[ \int_{-\infty}^{\infty} dT e^{-i\hat{E} \hat{T} \hbar} |\nu^{\pm}(T; X)\rangle = |\nu^{\pm}(E; X)\rangle. \]
\[ (22) \]

We see that we can transform from one representation to the other in a familiar way. Then, it is not necessary to recur to additional procedures such as the expansion in terms of Laguerre polynomials of the energy wave packet [34], or to the holomorphic Fourier transform [35]. A drawback of those proposals is that they do not consider separately the left and right movers.

\[ \text{C. Orthogonality} \]

Some inner products between time probe functions are

\[ \langle \nu(T'; X') | \nu(T; X) \rangle = \langle X' | e^{i(T'-T)\hat{H} \hbar} | X \rangle, \]
\[ (23) \]
\[ \langle \nu^{\pm}(T'; X') | \nu^{\pm}(T; X) \rangle = \int_{Sp(\hat{H})} dE e^{i(T'-T)\hat{E} \hbar} \langle \nu^{\pm}(E; X') | \nu^{\pm}(E; X) \rangle, \]
\[ (24) \]
\[ \langle \nu^{\pm}(T'; X') | \nu^{\pm}(T; X) \rangle = \langle X' | \hat{S}_x | X \rangle, \]
\[ (25) \]
\[ \langle \nu^{-}(T'; X') | \nu^{-}(T; X) \rangle + \langle \nu^{+}(T'; X') | \nu^{+}(T; X) \rangle = \delta(X' - X), \]
\[ (26) \]
\[ \int_{-\infty}^{\infty} dX \langle \nu^2(T';X)|\nu^2(T;X) \rangle = \int_{0}^{\infty} dp \langle e^{i(T-T')\hat{H}}|p \rangle, \]

(27)

\[ \int_{-\infty}^{\infty} dX \left[ \langle \nu^2(T';X)|\nu^2(T;X) \rangle + \langle \nu^*(T';X)|\nu^*(T;X) \rangle \right] = \text{Tr} \left[ e^{i(T-T')\hat{H}} \right], \]

(28)

Then, these vectors are orthogonal and any wave packet can be written in terms of them.

### D. Moments

Some expectation values are

\[ \langle \nu(E';X')|\hat{H}^{n}|\nu(E;X) \rangle = E^n \delta(E' - E)(X'|\hat{F}_E|X), \]

(43)

\[ \int_{S_p(i\hbar)} dE \langle \nu(E;X')|\hat{H}^{n}|\nu(E;X) \rangle = \text{Tr}[(X'|\hat{F}_E^n|X)], \]

(44)

\[ \int_{-\infty}^{\infty} dX \langle \nu(E';X')|\hat{H}^{n}|\nu(E;X) \rangle = \delta(E' - E)E^n, \]

(45)

\[ \langle \nu(E;X)|\hat{H}^{n}|\nu(E;X) \rangle = E^n\langle X|E \rangle^2, \]

(46)

\[ \int_{S_p(i\hbar)} dE \langle \nu(E;X)|\hat{H}^{n}|\nu(E;X) \rangle = E^n \delta(0), \]

(47)

\[ \langle \nu^2(E';X')|\hat{H}^{n}|\nu^2(E;X) \rangle = E^n \delta(E' - E)(X'|\hat{F}_E|X)^2, \]

(48)

\[ \langle \nu^2(E;X')|\hat{H}^{n}|\nu^2(E;X) \rangle = E^n\langle X'|\hat{F}_E^n|X \rangle^2, \]

(49)

\[ \int_{-\infty}^{\infty} dX \langle \nu^2(E';X')|\hat{H}^{n}|\nu^2(E;X) \rangle = E^n \delta(E' - E)(E|\hat{F}_E^n|E), \]

(50)

\[ \int_{-\infty}^{\infty} dX \langle \nu^2(E';X')|\hat{H}^{n}|\nu^2(E;X) \rangle = E^n\langle X'|\hat{F}_E^n|X \rangle, \]

(51)

\[ \int_{-\infty}^{\infty} dX \left[ \langle \nu^2(E';X')|\nu^2(E;X) \rangle + \langle \nu^*(E';X')|\nu^*(E;X) \rangle \right] = E^n \delta(E' - E), \]

(52)

\[ \int_{S_p(i\hbar)} dE \langle \nu^2(E;X')|\hat{H}^{n}|\nu^2(E;X) \rangle = E^n\langle X'|\hat{F}_E^n|X \rangle, \]

(53)

\[ \int_{-\infty}^{\infty} dX \left[ \langle \nu^2(E';X')|\nu^2(E;X) \rangle + \langle \nu^*(E';X')|\nu^*(E;X) \rangle \right] = E^n. \]

(54)

The time moments are

\[ \int_{-\infty}^{\infty} dX \langle \nu(T';X') \left( i\hbar \frac{d}{d\hat{H}} \right)^n \nu(T;X) \rangle = (-T)^n \langle X'|e^{i(T-T')\hat{H}}|X \rangle, \]

(55)
\[
\left\langle \nu^\dagger(T,X) \left( \frac{ih}{dH} \right)^n \nu^\dagger(T,X) \right\rangle = (-T)^n \langle X| \hat{T}_p^n e^{i(T-T')\hat{H}} \hat{T}_p^n |X \rangle.
\]

(56)

The energy width for the full probe state is then given by
\[
\Delta \hat{H}_p = \sqrt{\langle \nu(E|X) \hat{H}^2 \nu(E|X) \rangle - \langle \nu(E|X) \hat{H} \nu(E|X) \rangle^2} = E|X|E| \sqrt{1 - (X|E|^2},
\]
and the time width is
\[
\Delta \hat{T}_p = \sqrt{\langle \nu(T|X) \hat{T}^2 \nu(T|X) \rangle - \langle \nu(T|X) \hat{T} \nu(T|X) \rangle^2} = T \sqrt{X|X| (1 - (X|X)}.
\]

(58)

\section*{E. Projectors}

Some operators formed with the probe vectors are
\[
|\nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)| = \langle X| \hat{T}_p^n |X \rangle^\dagger \hat{I}_E,
\]

(59)

\[
\int_{-\infty}^{\infty} dX |\nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)| = (E| \hat{T}_p^n |E \rangle \hat{I}_E,
\]

(60)

\[
\int_{-\infty}^{\infty} dX [\nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)| + \langle \nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)|] = \hat{I}_E,
\]

(61)

\[
|\nu(E|X)\rangle \langle \nu(E|X)| = \hat{I}_E \hat{I}_X \hat{I}_E,
\]

(62)

\[
\int_{-\infty}^{\infty} dX |\nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)| = 0,
\]

(63)

\[
\langle \nu(E|X)\rangle \langle \nu(E|X)| = \hat{I}_E \hat{I}_X \hat{I}_E,
\]

(64)

\[
\int_{-\infty}^{\infty} dX |\nu(E|X)\rangle \langle \nu(E|X)| = \hat{I}_E.
\]

(65)

The \( n \)th power of the above operators are
\[
(|\nu(E|X)\rangle \langle \nu(E|X)|)^n = (X|E|^{2(n-1)} |\nu(E|X)\rangle \langle \nu(E|X)| ,
\]

(66)

\[
(|\nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)|)^n = (X| \hat{T}_p^n |E \rangle^{2(n-1)} \times |\nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)| ,
\]

(67)

\[
\left( \int_{-\infty}^{\infty} dX |\nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)| \right)^n = (E| \hat{T}_p^n |E \rangle^{2(n-1)} \hat{I}_E,
\]

(68)

\[
\left( \int_{-\infty}^{\infty} dX [\nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)| + \langle \nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)|] \right)^n = \hat{I}_E
\]

(69)

\[
(|\nu^\dagger(E|X)\rangle \langle \nu^\dagger(E|X)|)^n = (E| \hat{T}_p^n |X \rangle \langle X| \hat{T}_p^n |E \rangle \hat{I}_E
\]

(70)

\[
(|\nu(E|X)\rangle \langle \nu(E|X)|)^n = (X|E|^2) \hat{I}_E
\]

(71)

\[
\left( \int_{-\infty}^{\infty} dX |\nu(E|X)\rangle \langle \nu(E|X)| \right)^n = \hat{I}_E
\]

(72)

For the time probe vectors we find that
\[
|\nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)| = \hat{U}^\dagger(T) \hat{T}_p^n \hat{T}_p \hat{U}(T),
\]

(73)

\[
\int_{-\infty}^{\infty} dX |\nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)| = 0,
\]

(74)

where \( \hat{T}_p(T) = \hat{U}^\dagger(T) \hat{T}_p \hat{U}(T) \).

\[
|\nu(T|X)\rangle \langle \nu(T|X)| = \hat{U}^\dagger(T) \hat{T}_X \hat{U}(T),
\]

(75)

\[
\langle \nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)| = (X| \hat{T}_p^n |X \rangle^{n-1} |\nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)| ,
\]

(76)

\[
\left( \int_{-\infty}^{\infty} dX |\nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)| \right)^n = \hat{T}_p^n,
\]

(77)

\[
(|\nu(T|X)\rangle \langle \nu(T|X)|)^n = (X|X|^{n-1} |\nu(T|X)\rangle \langle \nu(T|X)| ,
\]

(78)

\[
\left( \int_{-\infty}^{\infty} dX |\nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)| \right)^n = \hat{T}_p^n(T),
\]

(79)

\[
(|\nu(T|X)\rangle \langle \nu(T|X)|)^n = (X|X|^{n-1} |\nu(T|X)\rangle \langle \nu(T|X)| ,
\]

(80)

So some of these operators are semi and full quasiorthogonal projectors (not normalizable).

\section*{F. Closure relationships}

There are semi and full closure relationships for probe vectors. For the time probe vectors we can write
\[
\int_{-\infty}^{\infty} dX |\nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)| = \hat{T}_p(T).
\]

(81)

But, when we sum up the above equalities we complete the closure relationship
\[
\int_{-\infty}^{\infty} dX [\nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)| + \langle \nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)|] = \hat{I}.
\]

(82)

Also,
\[
\left( \int_{-\infty}^{\infty} dX |\nu^\dagger(T|X)\rangle \langle \nu^\dagger(T|X)| \right)^n = \hat{I}.
\]

(83)
The spectral decomposition of the Hamiltonian is

$$\hat{\mathbf{H}}^n = \int_{-\infty}^{\infty} dX \int_{Sp(H)} dE \mathbf{E}^n [\nu(E;X)] \langle \nu(E;X) |$$

$$= \int_{-\infty}^{\infty} dX \int_{Sp(H)} dE \mathbf{E}^n [\nu^r(E;X)] \langle \nu^r(E;X) |$$

$$+ \nu^s(E;X) \langle \nu^s(E;X) |$$

$$= \int_{-\infty}^{\infty} dX \left( -i \hbar \frac{d}{dT} \right)^n [\nu(T;X)] \langle \nu(T;X) |.$$

The spectral decomposition of \( \hat{Q}^n(T) \) is

$$\int_{-\infty}^{\infty} dXX^n [\nu(T;X)] \langle \nu(T;X) | = \hat{Q}^n(T).$$

Since the probe vectors are orthogonal with respect to \( X \), we can use them in order to give a spectral decomposition of the position operator in terms of time and of energy. Let us form the self-adjoint operator

$$\int_{-\infty}^{\infty} dXX^n [\nu^r(T;X)] \langle \nu^r(T;X) | + \nu^s(T;X) \langle \nu^s(T;X) |$$

$$= \hat{U}^r(T) \hat{\mathbf{J}}_p \hat{Q}^r(T) + \hat{\mathbf{J}}_p \hat{Q}^r(T) \hat{U}^r(T).$$

The result is the left and right movers decomposition of \( \hat{Q}^n(T) \) in the Heisenberg picture. We can also form the operator

$$\int_{-\infty}^{\infty} dXX^n [\nu^r(T;X)] \langle \nu^r(T;X) | + \nu^s(T;X) \langle \nu^s(T;X) |$$

$$= \hat{I}_p \hat{\mathbf{J}}_p \hat{Q}^r(T) + \hat{\mathbf{J}}_p \hat{Q}^r(T) \hat{I}_p.$$
\[ \langle \psi | \hat{H}^n | \psi \rangle = \int_{S_p(h)} dE \int_{-\infty}^{\infty} dX \langle \psi | \nu^2(T;X) \rangle \langle \nu^2(T;X) | \hat{H}^n | \psi \rangle, \]  
\[ (101) \]

\[ \langle \psi | \hat{H}^n | \psi \rangle = \int_{S_p(h)} dE \int_{-\infty}^{\infty} dX \langle \psi | \nu^2(T;X) \rangle \langle \nu^2(T;X) \rangle \hat{H}^n | \psi \rangle \]
\[ + \langle \psi | \nu^2(T;X) \rangle \langle \nu^2(T;X) | \hat{H}^n | \psi \rangle, \]  
\[ (102) \]

Then, the energy widths, for a system in the state \( |\psi\rangle \), are
\[ \Delta H_\pm(X) = \sqrt{\langle \hat{H}_\pm^2(X) \rangle - \langle \hat{H}_\pm \rangle^2(X).} \]  
\[ (104) \]

\[ \Delta H(X) = \sqrt{\langle \hat{H}^2(X) \rangle - \langle \hat{H} \rangle^2(X).} \]  
\[ (105) \]

where
\[ \langle \hat{H}_z(X) \rangle = \int_{S_p(h)} dEE^n |\psi^2(E;X) \rangle ^2; \]  
\[ (106) \]

\[ \langle \hat{H}^n \rangle(X) = \int_{S_p(h)} dEE^n |\psi(E;X) \rangle ^2. \]  
\[ (107) \]

Other ones are
\[ \int dZ \int_{-\infty}^{\infty} dX dT^n[|\psi^2(T;X)|^2] = \int Z dT \langle \psi(T) | \hat{T}^n \left( \frac{i \hbar}{d\hat{H}} \right) | \psi(T) \rangle, \]  
\[ (108) \]

and
\[ \int dZ \int_{-\infty}^{\infty} dX dT^n[|\psi^2(T;X)|^2] \]
\[ = \int Z dT \int_{-\infty}^{\infty} dX dT^n[|\psi(T;X)|^2] = \int Z dT \langle \psi(T) | \left( \frac{i \hbar}{d\hat{H}} \right) | \psi(T) \rangle, \]  
\[ (109) \]

where \( Z \) is an interval of time, around \( T=0 \), which encloses \( |\psi\rangle \) only once. An \( X \) component is likely to not diverge since it is related to the arrival-time density.

The widths in \( T \) can be defined as
\[ \Delta T_\pm(X) = \sqrt{\langle T_\pm^2(X) \rangle - \langle T_\pm \rangle^2(X),} \]  
\[ (110) \]

\[ \Delta T(X) = \sqrt{\langle T^2(X) \rangle - \langle T \rangle^2(X),} \]  
\[ (111) \]

where
\[ \langle T_\pm^2 \rangle(X) = \int Z dT \int_{-\infty}^{\infty} dX dT^n[|\psi^2(T;X)|^2]; \]  
\[ (112) \]

\[ \langle T^n \rangle(X) = \int Z dT \int_{-\infty}^{\infty} dX dT^n[|\psi(T;X)|^2]. \]  
\[ (113) \]

K. Change of representation functions

The change of representation functions are
\[ \langle q \mid \nu^2(E;X) \rangle = \psi_E(q) \int_0^\infty dp \frac{e^{-ip\nu(X)\hbar}}{\sqrt{2\pi\hbar}} \psi_E^* (\pm p), \]  
\[ (114) \]

\[ \langle p \mid \nu^2(E;X) \rangle = \Theta(\pm p) \psi_E(p) \int_0^\infty dp' \frac{e^{-ip'\nu(X)\hbar}}{\sqrt{2\pi\hbar}} \psi_E^* (\pm p'), \]  
\[ (115) \]

\[ \langle q \mid \nu^2(T;X) \rangle = \int_0^\infty dp \frac{e^{-ip\nu(T)\hbar}}{\sqrt{2\pi\hbar}} e^{i\hbar\langle T \rangle} \delta(q - X), \]  
\[ (116) \]

\[ \langle p \mid \nu^2(T;X) \rangle = \Theta(\pm p) e^{i\hbar\langle T \rangle} \delta(q - X), \]  
\[ (117) \]

L. Evolution in time and energy spaces

One of the components of the time representation of the wave function at time \( t \) is
\[ \langle \nu(T;X) \mid \psi(t) \rangle = \langle X \mid e^{-i\hbar\hat{H}} \mid \psi(t) \rangle \]
\[ = \langle X \mid e^{-i\hbar\hat{H}} e^{-i\hbar\langle T \rangle} \mid \psi \rangle = \langle X \mid e^{-i\hbar(T + \hat{H})} \mid \psi \rangle \]
\[ = \langle \nu(T + t;X) \mid \psi \rangle. \]  
\[ (122) \]

Then we just shift the wave packet in time space in order to evolve it.

Evolution in energy space is realized by a phase factor
\[ \langle \nu(E;X) \mid \psi(t) \rangle = \langle X \mid E \rangle \langle E \mid e^{-i\hbar\hat{H}} \mid \psi \rangle \]
\[ = e^{-i\hbar\langle E \rangle} \langle \nu(E;X) \mid \psi \rangle. \]  
\[ (123) \]

The squared magnitude of this function will lose the phase factor and then it will not change with time.

M. Time-slice operators

There are two types of time operators using the probe states. A set of operators is
\[ \hat{\nu} \mid \psi(t) \rangle = |\nu(X;T)\rangle \langle \nu(X;T) \mid \left( \frac{i \hbar}{d\hat{H}} \right) \mid \psi(t) \rangle \]  
\[ (124) \]

and
\[ \hat{H}\psi(t) = \nu(T;X)\langle \nu(T;X) \rangle \left( i\hbar \frac{d}{d\hat{H}} \right) \psi(t). \tag{125} \]

With this set of operators, when applied to a wave packet \(|\psi(t)\rangle\), we will obtain the wave-packet time \(t\) (the evolution time) times the slice at relative time \(T\) times the amount of probability coming from the support of the slice.

A second set is

\[ \hat{T}\psi(t) = \langle \nu^*(T;X)|\psi(t)\rangle \left( i\hbar \frac{d}{d\hat{H}} \right) \nu^*(T;X) \tag{126} \]

and

\[ \hat{\hat{T}}\psi(t) = \langle \nu(T;X)|\psi(t)\rangle \left( i\hbar \frac{d}{d\hat{H}} \right) \nu(T;X). \tag{127} \]

These operators return the relative time \(-T\) of the slice, times the slice, and times the probability coming from the support of the slice.

For instance, \(\hat{H}\) and \(i\) do not commute

\[ \int_{-\infty}^{\infty} dX \hat{H} = \int_{-\infty}^{\infty} dX \hat{H} \nu(T;X) \langle \nu(T;X) \rangle \left( i\hbar \frac{d}{d\hat{H}} \right) \]

\[ = \int_{-\infty}^{\infty} dX \hbar e^{i\hat{H}t}|X\rangle\langle X|e^{-i\hat{H}t} \left( i\hbar \frac{d}{d\hat{H}} \right) \]

\[ = \hat{\hat{H}} \left( i\hbar \frac{d}{d\hat{H}} \right) = -i\hbar + \left( i\hbar \frac{d}{d\hat{H}} \right) \hat{H} \]

\[ = -i\hbar + \int_{-\infty}^{\infty} dX \hbar \hat{H}, \tag{128} \]

and there are similar results for the rest of the time operators. Another one is

\[ \hat{\hat{H}}\psi(t) = \hat{\hat{H}} \nu(T;X)|\psi(t)\rangle \left( i\hbar \frac{d}{d\hat{H}} \right) \nu(T;X) \]

\[ = \langle \nu(T;X)|\psi(t)\rangle \left( -i\hbar + i\hbar \frac{d}{d\hat{H}} \right) \nu(T;X). \tag{129} \]

\[ \langle q|\nu^2(E;X)\rangle = \frac{e^{q(T+\sigma E;X)/\hbar}}{\sqrt{2\pi\hbar}}, \tag{130} \]

which are plane waves with momentum \(\pm\sqrt{2mE}\) and centered at \(q=X\). For going to the momentum representation we need the following functions:

\[ \langle p|\nu^2(E;X)\rangle = \delta(p-\sqrt{2mE}) \frac{e^{qT\pm\sigma X}/\hbar}}{\sqrt{2\pi\hbar}}. \tag{131} \]

These functions are the previous plane waves but are now in momentum space. The transformation functions between time and coordinate representations are

\[ \langle q|\nu^2(T;X)\rangle = \int_{-\infty}^{\infty} dp e^{ip(T+\sigma E;X)/\hbar} e^{iT\pm\sigma X}/\hbar} \]. \tag{132} \]

These functions are similar to Kijowski’s states [23] in coordinate space but without the \(\sqrt{\mu/m\hbar}\) factor, i.e., they are “presence” probe functions. The momentum version of these functions are

\[ \langle p|\nu^2(T;X)\rangle = \Theta(p) e^{iT\pm\sigma X}/\hbar} \frac{e^{ipX}/\hbar}}{\sqrt{2\pi\hbar}}. \tag{133} \]

\[ \text{FIG. 1. Squared magnitude of the time components } \langle \nu(T;X)|\psi \rangle \text{ and } \langle \nu^*(T;X)|\psi \rangle \text{ for the Gaussian wave packet (136) under free evolution. For this calculation } p_0=1 \text{ and } \sigma=1. (a) All, (b) left, and (c) right movers. The vertical scale is different for each figure and we use dimensionless units.} \]
presentations. If we know the wave function in the coordinate representation, the energy wave function can be found as
\[
\langle \psi^E | (E;X) \rangle = \frac{e^{-iX \sqrt{2mE} \hbar}}{\sqrt{2\pi \hbar}} \psi(p = \pm \sqrt{2mE}),
\]
and the time representation would be given as
\[
\langle \psi^T | (T;X) \rangle = \int_{-\infty}^{\infty} dp \frac{e^{ipX\hbar}}{\sqrt{2\pi \hbar}} \psi(\pm p;T).
\]
These quantities are easily recognizable and some of them have been used in the determination of the presence distribution for a free particle.

For instance, a plot of the squared magnitude of the time components \( \langle \psi^T | (T;X) \rangle \) of the Gaussian wave packet in \( p \),
\[
\psi(p) = \frac{1}{\sqrt{\sigma \sqrt{2\pi}}} \exp \left\{ - \frac{(p-p_0)^2}{4\sigma^2} \right\},
\]
is shown in Fig. 1 and the energy components are shown in Fig. 2.

In Fig. 1 we observe something similar to what is known as “diffraction in time” [36–38]. Diffraction in time is a transient effect, a temporal oscillation, which appears when matter waves are released from a shutter or a confinement region. Here, they appear as a consequence of truncation of the wave function, a discontinuity in momentum space.

When the \( E \)-\( X \) wave function is Gaussian,
\[
\langle \psi^E | (E;X) \rangle = \frac{1}{\sqrt{\sigma \sqrt{2\pi}}} e^{-iX \sqrt{2mE} \hbar},
\]
the \( q \) representation becomes
\[
\langle \psi^q | (q;X) \rangle = \frac{1}{\sqrt{\sigma \sqrt{2\pi}}} e^{-iX \sqrt{2mE} \hbar}.
\]

In Fig. 3 we observe something similar to what is known as “diffraction in time” [36–38]. Diffraction in time is a transient effect, a temporal oscillation, which appears when matter waves are released from a shutter or a confinement region. Here, they appear as a consequence of truncation of the wave function, a discontinuity in momentum space.

When the \( E \)-\( X \) wave function is Gaussian,
\[
\langle \psi^E | (E;X) \rangle = \frac{1}{\sqrt{\sigma \sqrt{2\pi}}} e^{-iX \sqrt{2mE} \hbar},
\]
the \( q \) representation becomes
\[
\langle \psi^q | (q;X) \rangle = \frac{1}{\sqrt{\sigma \sqrt{2\pi}}} e^{-iX \sqrt{2mE} \hbar}.
\]