Conjugate states to the energy eigenstates: 
The continuous energy spectrum case

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Abstract. The usual method for obtaining the eigenstates of an operator is to solve the corresponding eigenvalue equation. This procedure cannot be applied when the operator of interest is not known at all. We develop a method which generates the eigenstates of an operator, an the operator itself, which will be conjugate to a given known operator. This is particularly useful for the case of the time operator in Quantum Mechanics. We illustrate the method by obtaining time eigenstates for the free particle.

1. Introduction

The purpose of this talk is to propose a way to handle the time variable in Classical and Quantum Mechanics. Our point of view would be that of considering time as the coordinate which is conjugate to the energy variable. The usual set of conjugate coordinates is position-momentum and time-energy could be an alternative symplectic set of coordinates with which we can describe the dynamics of a classical or quantum system.

Quantum time functions usually are found by quantizing the classical expression for the time of a particle, leading to many inherent difficulties like arriving to quantities which are not well defined, and facing the problem of symmetrization of products of functions. Consequently, only in few cases this can be done explicitly. For instance, for a free particle, the classical expression for time is

$$t = t_0 + \frac{m q}{p},$$

a quantity which is not defined at $p = 0$, and with many possible quantum versions of it [1]. Time eigenstates for other systems are hard, if not impossible, to find with this method.

There is also a method of time propagation of the coordinate eigenstate $\delta(q)$ multiplied by $\sqrt{p/m}$, generating that way the required time states [2]. This method is appropriate for the free particle and it was suggested to use it also for any potential function [3–6].

One of the proposed methods for finding of time operators is solving of the differential equation that results from the conjugate condition $[\hat{T}, \hat{H}] = i\hbar \hat{I}$. This method requires the solution of complicated differential equations [7].

Another proposal for time operators and Lyapunov functions makes use of the sum of terms of the form $|E'\rangle\langle E|/(E - E')$. One limitation of this proposal is that the domain of the resulting operators is a subset of the Hilbert space [7–11].
2. The method
In this section, we define and find the properties of the conjugate states to the energy eigenstates. We expect that the resulting states, and the operators that can be obtained from them, be related to the time operator and to its eigenstates.

The conjugate states that will be generated can be used as another coordinate, as an alternative representation for quantum states and operators, and, in particular, they can be used to construct a quantum time operator.

We will illustrate the use of the generated states with the free particle model, for quantum systems and with a nonlinear oscillator model for classical systems.

2.1. Classical systems. The normal direction to the energy shells
Let us consider first the case of Classical systems. This will make more understandable the quantum case.

From the euclidean geometry point of view, the vanishing of the Poisson bracket for the same function, in this case the Hamiltonian of the system,

$$\{ H(p, q), H(p, q) \} = \nabla H \cdot X_H = 0$$

defines a vector field $X_{\perp H} := \nabla H$ which is normal to the energy shells. We can take advantage of this vector field to generate a conjugate variable to the energy variable. The main characteristic of the new variable is that it crosses all of the energy shells. Thus one of the variables is well defined but the corresponding conjugate variable is not, just what is needed for a coordinate system.

Thus, the method is to take any of the normal shells to the energy shells as a zero-time shell and, by means of time propagation of them, generate a conjugate, or symplectic orthogonal, time variable. This process will generate a coordinate set in which the description of the system is the most simple possible because the set of variables needed to follow the evolution of a given system is reduced, from $(q, p, t)$ to only $(t, E)$, i.e. we are replacing a parametric description of the system with a non parametric one.

2.2. Motion along the normal direction to the constant energy shells
To generate the curves which are normal to the constant energy shells, in the euclidean sense, we define a dynamical system for the phase space point $z_{\perp H}$ with the vector field $X_{\perp H}$ and parameter $\epsilon$,

$$\frac{dz_{\perp H}}{d\epsilon} = X_{\perp H}, \quad \text{i.e.} \quad \frac{dq_{\perp H}}{d\epsilon} = \frac{\partial H}{\partial q}, \quad \frac{dp_{\perp H}}{d\epsilon} = \frac{\partial H}{\partial p}$$

To illustrate how these curves look like, let us consider a particular system: a nonlinear oscillator with Hamiltonian

$$H(z) = \frac{p^2}{2} + \frac{k}{2} \left( \sqrt{a^2 + q^2} - \ell \right)^2,$$  \hspace{1cm} (1)

where $k, a, \ell \in (0, \infty)$ are the parameters of the model. The normal curves to the constant energy shells for this system are shown in Fig. 1.

The curves generated with the vector field $X_{\perp}$ are normal to the constant energy curves in the Euclidean geometry sense. However, the time curves should be normal to the constant energy shells in the symplectic geometry sense. These normal curves have the nice property that they cross all of the constant energy shells, thus they are very useful for generating the time curves.
2.3. Generating a time coordinate

Taking advantage of the fact that the origin of time is arbitrary, we proceed to generate a time coordinate by time evolving any of normal curves to the constant energy shells. The simplest curves are the ones that cross the location of the extremal points of the potential function, or the curve of zero momentum. Those curves are just straight lines passing through the fixed points.

For instance, for the nonlinear oscillator, we can take as the zero-time curve the constant coordinate curve that crosses the extremal point of the potential function with positive coordinate. After time evolution of that curve, we obtain the time coordinate system shown in Fig. 2.

Since now we have a time coordinate, we can assign a time-energy set of values to each point in the phase space. The time values so obtained are shown in Fig. 3, the surface of time values. The domain of the time function is not the whole of the phase space with the separatrix removing the regions which do not belong to the domain of $t(p,q)$.

2.4. Unfolding the degeneracy of the energy values and classical distributions in energy-time

One of the advantages of having a time-energy coordinate system is that we can unfold the degeneracy of the energy values; to each value of energy correspond two values of the momentum of a particle. What we can do to unfold the energy values degeneracy is to extend the values of the energy to the negative side of the real axes, with the sign of the energy values corresponding to the sign of the momentum values.

We illustrate this procedure by considering a Gaussian probability density in phase space centered at $(q,p) = (0,-1)$,

$$
\rho(q,p) = \frac{1}{2\pi} e^{-(q-q_0)^2/2\sigma^2 - \sigma(p-p_0)^2/2}.
$$

(2)

This density has a part with negative momentum. So, in the time-energy coordinates, with $\epsilon = \text{sign}(p)E$, the phase-space Gaussian looks like the one shown in Fig. 4.
Figure 3. Time values for the nonlinear oscillator when the zero-time curve is the $q = q_0$ line, where $q_0$ is the location of the minimum of the potential function located at the positive part of the real axes. Here, $\ell = 2$, $k = 9.8$ and $a = 1$. Dimensionless units.

Figure 4. Classical time-energy representation of a phase-space Gaussian density centered at $(q, p) = (0, -1)$, for the nonlinear oscillator with $a = 1$, $\ell = 2$, $k = 9.8$, and $\sigma = .8$. Dimensionless units.

3. Quantum systems
We will now consider the quantum analogue of the procedure just outlined for classical systems. We will assume that energy spectrum $\{E\}^\infty_0$ of the given quantum system is continuous and that the minimum value that the energy can take is zero.

3.1. Unfolding of the energy degeneracy
Let us start the quantum treatment by rewriting a given time dependent wave function in terms of energy and momentum eigenstates as

$$|\psi(t)\rangle := e^{-it\hat{H}/\hbar} |\psi\rangle = \int_{-\infty}^{0} dp \int_{0}^{\infty} dE \ e^{-itE/\hbar} |E\rangle \langle E| p \rangle (p|\psi\rangle + \int_{0}^{\infty} dp \int_{0}^{\infty} dE \ e^{-itE/\hbar} |E\rangle \langle E| p \rangle (p|\psi\rangle.$$

After the replacements $\epsilon = \text{sign}(p) E$, we get

$$|\psi(t)\rangle := - \int_{-\infty}^{0} dp \int_{0}^{\infty} d\epsilon \ e^{i\epsilon t/\hbar} |\epsilon\rangle \langle -\epsilon| p \rangle (p|\psi\rangle + \int_{0}^{\infty} dp \int_{0}^{\infty} d\epsilon \ e^{-i\epsilon t/\hbar} |\epsilon\rangle \langle \epsilon| p \rangle (p|\psi\rangle$$

$$= \int_{-\infty}^{0} d\epsilon \ e^{-i(-t)\epsilon/\hbar} \langle \epsilon| \psi\rangle - |\epsilon\rangle + \int_{0}^{\infty} d\epsilon \ e^{-it\epsilon/\hbar} \langle \epsilon| \psi\rangle + |\epsilon\rangle,$$

where $| - E\rangle := |E\rangle$, and

$$\langle \epsilon| \psi\rangle_+ = \int_{-\infty}^{0} dp \langle \epsilon| p \rangle (p|\psi\rangle \text{ and } \langle \epsilon| \psi\rangle_- := \int_{0}^{\infty} dp \langle \epsilon| p \rangle (p|\psi\rangle.$$
3.2. A spectral decomposition of the identity operator

Let us introduce a spectral decomposition of the identity operator in terms of the energy eigenstates, and let us rewrite it as

\[ \hat{I} = \int_0^\infty dE |E\rangle \langle E| = \int_0^\infty dE' dE \delta(E - E') |E'\rangle \langle E| \]

\[ = \int_0^\infty dE' dE \frac{1}{2\pi \hbar} \int_{-\infty}^\infty dt \ e^{it(E - E')/\hbar} |E'\rangle \langle E| \]

\[ = \int_{-\infty}^\infty dt \int_0^\infty dE' dE \frac{e^{-itE'/\hbar}}{\sqrt{2\pi \hbar}} |E'\rangle \langle E| \frac{e^{itE/\hbar}}{\sqrt{2\pi \hbar}} := \int_{-\infty}^\infty dt \ |t\rangle \langle t| \] (3)

where we have defined the kets \(|t\rangle\) as

\[ |t\rangle := \int_0^\infty dE \frac{e^{-itE/\hbar}}{\sqrt{2\pi \hbar}} |E\rangle. \] (4)

These are the kets that will be taken as time eigenkets in what follows. It contains all of the energy eigenkets, it is conjugate to them, and they are the time shifting of the zero-time ket \(|t = 0\rangle = \frac{1}{\sqrt{2\pi \hbar}} \int_0^\infty dE |E\rangle\). (5)

They are a good candidate for a conjugate coordinate to the energy eigenstates in Quantum Mechanics.

Recall that the commutator between \(\hat{I}\) and \(\hat{H}\) vanishes.

3.3. A time operator

Now, let us consider the operator

\[ \hat{T} := \int_{-\infty}^\infty dt \ t |t\rangle \langle t| = \int_0^\infty dE' dE \frac{1}{2\pi \hbar} \int_{-\infty}^\infty dt \ e^{it(E - E')/\hbar} \]

\[ = \int_0^\infty dE' dE \frac{e^{-itE'/\hbar}}{\sqrt{2\pi \hbar}} |E'\rangle \langle E| \frac{e^{itE/\hbar}}{\sqrt{2\pi \hbar}} := \int_0^\infty dE' dE |E'\rangle \langle E| \delta'(E - E'). \] (6)

The commutator between \(\hat{T}\) and the Hamiltonian is

\[ [\hat{T}, \hat{H}] = \int_0^\infty dE' dE \frac{1}{2\pi \hbar} \int_{-\infty}^\infty dt \ e^{it(E - E')/\hbar} \left[ |E'\rangle \langle E|, \hat{H} \right] \]

\[ = \int_0^\infty dE' dE \left( -\frac{i\hbar}{\partial E} \right) \delta(E - E') \]

\[ = \int_0^\infty dE' dE \left( \frac{i\hbar}{\partial E} \right) (E - E') |E'\rangle \langle E| \]

\[ - i\hbar \int_0^\infty dE' (E - E') |E'\rangle \langle E| \delta(E - E') \]

\[ = i\hbar \int_0^\infty dE' dE \delta(E - E') |E'\rangle \langle E| = i\hbar \hat{I}. \] (7)

where we have made use of the integration by parts. This is the result expected for the commutator between a time operator and the Hamiltonian.

Note that the time operator \(\hat{T}\) is symmetric and its domain is the Hilbert space; the envelope of the energy eigenstates \(|E\rangle\) is infinite.
4. States which are conjugate to the energy eigenstates

Based on the above results, we define a time eigenstate as

\[ |t\rangle := \int_{-\infty}^{\infty} d\epsilon \frac{e^{-i\epsilon t/\hbar}}{\sqrt{2\pi \hbar}} |\epsilon\rangle = \int_{0}^{\infty} dE e^{-iE t/\hbar} \hat{P}_- |E\rangle + \int_{0}^{\infty} dE e^{iE t/\hbar} \hat{P}_+ |E\rangle. \]

where \( \epsilon \in \mathbb{R}, E = |\epsilon|, |\epsilon\rangle = |E\rangle \), and

\[ \hat{P}_- = \int_{-\infty}^{0} dp |p\rangle \langle p|, \quad \text{and} \quad \hat{P}_+ = \int_{0}^{\infty} dp |p\rangle \langle p|. \quad (8) \]

This a state with a part evolving forward and another part evolving backwards in time. This definition unfolds the energy degeneracy due to that for a given value of the energy there correspond two values of the momentum.

4.1. Evolution equations for the transformation functions

The transformation function between the time and energy representations is,

\[ \langle t|E \rangle := \frac{e^{iEt/\hbar}}{\sqrt{2\pi \hbar}}. \quad (9) \]

This function is an eigenfunction of the time operator in the energy representation

\[ -i\hbar \frac{\partial}{\partial E} \langle E|t \rangle = -i\hbar \frac{\partial}{\partial E} e^{-iEt/\hbar} = -t \langle E|t \rangle, \quad (10) \]

and it is also an eigenfunction of the energy operator in the time representation

\[ i\hbar \frac{\partial}{\partial t} \langle t|E \rangle = i\hbar \frac{\partial}{\partial t} e^{iEt/\hbar} = -E \langle t|E \rangle. \quad (11) \]

The negative signs on the right hand sides of these equations are due to that we are dealing with the basis states and not with wave functions.

5. The free particle

We will consider the free particle model, a simple system with a continuous energy spectrum. We will illustrate how the time eigenstates defined in previous section look like for this system.

5.1. Energy eigenstates

A set of eigenfunctions of the one-dimensional free-particle Hamiltonian operator

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dq^2}, \quad (12) \]

is

\[ \langle q|E \rangle_{\pm} = \frac{e^{\pm i\sqrt{2mE} q/\hbar}}{\sqrt{2\pi \hbar}}. \quad (13) \]

An alternative set of eigenfunctions is given by

\[ \langle q|E \rangle_o = \frac{1}{\sqrt{2\pi \hbar}} \sin \left( \sqrt{2mE} \frac{q}{\hbar} \right) \quad \text{and} \quad \langle q|E \rangle_e = \frac{1}{\sqrt{2\pi \hbar}} \cos \left( \sqrt{2mE} \frac{q}{\hbar} \right). \quad (14) \]
We combine pairs of solutions into one written in terms of the variable $\epsilon \in \mathbb{R}$, $E = |\epsilon|$, 

$$\langle q|\epsilon\rangle_e = \cos \left( \frac{\sqrt{2m|\epsilon|}}{\hbar} q \right), \quad \langle q|\epsilon\rangle_o = \text{sgn}(\epsilon) \sin \left( \frac{\sqrt{2m|\epsilon|}}{\hbar} q \right),$$  

(15)

$$\langle q|\epsilon\rangle_\pm = \frac{e^{\pm \text{sgn}(\epsilon) \sqrt{2m|\epsilon|}} q/\hbar}{\sqrt{2\pi\hbar}},$$  

(16)

where

$$\hat{H}|\epsilon\rangle = E |\epsilon\rangle.$$  

(17)

5.2. Time eigenstates

Different time eigenstates for the free particle are then defined as

$$\langle q|t\rangle_e = \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} e^{-it'\epsilon'/\hbar} \cos \left( \text{sgn}(\epsilon') \sqrt{2m|\epsilon'|} q \right),$$  

(18)

$$\langle q|t\rangle_o = \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} e^{-it'\epsilon'/\hbar} \sin \left( \text{sgn}(\epsilon') \sqrt{2m|\epsilon'|} q \right),$$  

(19)

and

$$\langle q|t\rangle_\pm = \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} e^{-it'\epsilon'/\hbar} e^{\pm \text{sgn}(\epsilon') \sqrt{2m|\epsilon'|} q/\hbar}.$$  

(20)

5.3. Orthogonality of conjugate states

It is easy to see that the conjugate states are orthogonal indeed

$$\langle t'|t\rangle_e = \int_{-\infty}^{\infty} dq \langle t'|q\rangle \langle q|t\rangle_e = \delta(t - t') + \delta(t + t'),$$  

(22)

$$-\langle t'|t\rangle_o = \int_{-\infty}^{\infty} dq -\langle t'|q\rangle \langle q|t\rangle_o = \delta(t - t'),$$  

(23)

$$+\langle t'|t\rangle_+ = \int_{-\infty}^{\infty} dq +\langle t'|q\rangle \langle q|t\rangle_+ = \delta(t - t').$$  

(24)
Figure 5. Time evolution of some time eigenstates for the free particle. Approximated expressions for $\mathcal{E} = 10$. Dimensionless units.

6. Evolution of time eigenstates

In order to have an idea of how these states look like, we consider the approximation obtained by calculating the integrals with finite limits

$$\langle q|t\rangle_e = \lim_{\mathcal{E} \to \infty} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\mathcal{E}}^{\mathcal{E}} d\varepsilon \ e^{i\varepsilon t/\hbar} \cos \left( \text{sign}(\varepsilon) \sqrt{2m|\varepsilon|} \frac{q}{\hbar} \right)$$

$$\langle q|t\rangle_o = \lim_{\mathcal{E} \to \infty} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\mathcal{E}}^{\mathcal{E}} d\varepsilon \ e^{i\varepsilon t/\hbar} \sin \left( \text{sign}(\varepsilon) \sqrt{2m|\varepsilon|} \frac{q}{\hbar} \right), \quad (25)$$

and

$$\langle q|t\rangle_{\pm} = \lim_{\mathcal{E} \to \infty} \frac{1}{\sqrt{2\pi\hbar}} \int_{-\mathcal{E}}^{\mathcal{E}} d\varepsilon \frac{e^{i\varepsilon t/\hbar}}{\sqrt{2\pi\hbar}} e^{\pm\text{sign}(\varepsilon)i\sqrt{2m|\varepsilon|} q/\hbar}.$$  

(26)

Plot of some of these functions are shown in Fig. 5. These functions are initially highly concentrated around the origin and, as time goes by, they depart from the origin and spread.

The time operator can be approximated in the same way and it is shown in Fig. 6

7. Conclusion

We have found symmetric operators with domain the envelope of the energy eigenstates $\{|E\}\to\infty$, i.e. the whole of the Hilbert space, and with orthogonal eigenstates which are conjugate to the
energy eigenstates. Thus, they are good candidates for being time operators because they comply with the requirements for such operators.

As we have seen, in fact there are several time operators which can be used in different situations. There are time operators which differentiate between the sign of the momentum, and there are other time operators that include both signs of the momentum into them.

We are optimistic about the operators introduced in this paper to be good candidates for time operators.

References

[1] Aharonov Y and Bohm D 1961 Phys. Rev. 122 1649
[2] Kijowski J 1974 Rep. Math. Phys. 6 361
[3] Baute A D, Sala-Mayato R, Palao J P, Muga J G and Egusquiza I L 2000 Phys. Rev. A 61 022118
[4] Baute A D, Egusquiza I L and Muga J G 2001 Phys. Rev. A. 64 012501
[5] Torres-Vega G and García-Jiménez M N 2013 Entropy 15 2415
[6] Torres-Vega G 2013 Entropy 15 4105
[7] Sombillo D L B and Galapon E A 2012 J. Math. Phys. 53 043702
[8] Hall M J W 2008 Comment on “An Arrow of Time Operator for Standard Quantum Mechanics” (a sign of the time!) (Preprint quant-ph 0802.2682)
[9] Hegerfeldt G C, Muga J G and Muñoz J 2010 Phys. Rev. A 82 012113
[10] Arai A and Matsuzawa Y 2008 Rev Math Phys 20 951
[11] Arai A 2009 Lett. Math. Phys. 87 67