We introduce a self-adjoint operator that indicates the direction of time within the framework of standard quantum mechanics. That is, as a function of time its expectation value decreases monotonically for any initial state. This operator can be defined for any system governed by a Hamiltonian with a uniformly finitely degenerate, absolutely continuous and semibounded spectrum. We study some of the operator’s properties and illustrate them for a large equivalence class of scattering problems. We also discuss some previous attempts to construct such an operator, and show that the no-go theorems developed in this context are not applicable to our construction.

The emergence of irreversible phenomena in systems governed by reversible dynamical laws is a fundamental problem for both classical and quantum physics. In this context, the construction of a quantity indicating the direction of time is one of the central goals. As a functional of the state of the system, such a quantity must vary monotonically in time. A quantity having this property is often termed a Lyapunov functional. The need for a Lyapunov functional arises in different quantum mechanical problems such as the decay of a metastable state, resonant processes, and other irreversible phenomena. The main result of this paper is the explicit construction of a Lyapunov operator – an operator whose expectation value decreases monotonically independently of the initial state – within the framework of standard quantum mechanics.

The question of whether a Lyapunov functional can be defined for classical and quantum Hamiltonian dynamical systems on phase space and Hilbert space, respectively, has been investigated by various authors. An early and fundamental theorem by Poincaré states that no "local" function on phase space can give rise to a quantity with the characteristics of nonequilibrium entropy, i.e. a Lyapunov functional. Close to a century later, in the late 70’s, it was demonstrated by Misra that if this restriction on the phase space functions is lifted, a Lyapunov functional can be constructed. Soon after, in an attempt to generalize this result, Misra, Prigogine, and Courbage (MPC) published a paper containing a proof which was taken by many to imply that standard quantum mechanics does not allow for a Lyapunov operator. This proof is based on a number of assumptions, one of which – as we shall see – for the sole purpose of constructing a Lyapunov operator is not essential.

Of course, a most natural candidate for a Lyapunov operator is a time operator $T$ canonically conjugate to the Hamiltonian $H$, such that $T$ and $H$ form an imprimitivity system (implying that each generates a translation on the spectrum of the other). Yet, a well known theorem of Pauli appears to tell us that this is impossible. Recently, Galapon has attempted to bypass Pauli’s arguments and find pairs of $T$ and $H$ satisfying the canonical commutation relations (CCR), but which are not in the class of imprimitivity systems. Nevertheless, it can be shown that the $T$ operator that has been obtained in this way does not have the Lyapunov property. By contrast, other authors have given up on the conjugacy of $T$ and $H$. In this context, Unruh and Wald’s (UW) proof that a "monotonically perfect clock" does not exist should be noted. However, while there is no widespread agreement on the definition of a time operator, most agree that it should have the Lyapunov property. In this paper it is our purpose to present a Lyapunov operator rather than a time operator, and it is precisely for this reason – that beyond the Lyapunov property we do not impose any further requirements on our operator – that the various no-go theorems previously mentioned do not apply to our construction.

We begin by presenting our arrow of time operator and proving that it has the required Lyapunov property. We do not attempt to derive or motivate its form, for which, see [8, 9]. Following this, we obtain its spectrum and eigenfunctions. Next, we address the two seemingly relevant no-go theorems by MPC and UW previously referred to, and show that they do not apply to our construction. We then go on to present the results of simulations illustrating the Lyapunov property for a large equivalence class of one dimensional potentials for which Møller wave-operators exist. We end by discussing open questions and directions for future research.

Let us consider a Hamiltonian with finite uniform degeneracy and a continuous spectrum $E \in [0, \infty)$. We claim that the operator

$$H = \sum_{n=1}^{\infty} \frac{1}{n^2} \psi_n \langle \psi_n | \psi_n \rangle \frac{\partial}{\partial x} \psi_n + \sum_{n=1}^{\infty} \frac{1}{n} \psi_n \langle \psi_n | \psi_n \rangle \frac{\partial}{\partial y} \psi_n$$

where $\psi_n$ are orthonormal eigenfunctions of $H$ with eigenvalues $E_n = n^2/4$.
\[ M_F = -\frac{1}{2\pi i} \sum_j \int_0^\infty dE \int_0^\infty dE' \frac{\langle E', j \rangle \langle E', j \rangle}{E - E' + i0^+}, \]  

(1)

where \( E \) denotes the energy and \( j \) the degeneracy, is an ever decreasing Lyapunov operator \[1\]. (Note the use of natural units \( \hbar = c = 1 \).) To see this let us write down the expectation value of \( M_F \) at time \( t \geq 0 \) with respect to some arbitrary initial state \( |\psi\rangle \in \mathcal{H} \)

\[ \langle M_F(t) \rangle_{\psi} = \langle \psi | e^{i\hat{H}t} M_F e^{-i\hat{H}t} | \psi \rangle = -\frac{1}{2\pi i} \sum_j \int_0^\infty dE \int_0^\infty dE' \frac{e^{i(E-E')t}\psi_j^*(E)\psi_j(E')}{E - E' + i0^+}. \]  

(2)

Using contour integration it is easy to verify that eq. (2) may be reexpressed as

\[ \langle M_F(t) \rangle_{\psi} = -\frac{1}{4\pi^2} \sum_j \int_0^\infty dE \int_0^\infty dE' \int_{-\infty}^\infty d\sigma \frac{e^{i(E-\sigma)t}\psi_j^*(E)\psi_j(E')}{(E - \sigma + i0^+) (E' - \sigma - i0^+)} \]

\[ = -\frac{1}{2\pi i} \sum_j \int_0^\infty dE \psi_j^*(E) e^{iEt} \int_{-\infty}^\infty d\sigma \frac{e^{-i\sigma t} \tilde{f}_j(\sigma)}{E - \sigma + i0^+}, \]  

(3)

with \( \tilde{f}_j(\sigma) = \frac{1}{2\pi} \int_0^\infty \frac{dE' \psi_j(E')}{\sigma - E' + i\sigma} \) (implying that \( \tilde{f}_j(\sigma) \in L^2(\mathbb{R}) \)). Then according to the Paley-Wiener theorem \[10\] \( \tilde{f}_j(\sigma) \) is the Fourier transform of a function \( f_j(\tau) \in L^2(\mathbb{R}^-) \), that is

\[ \tilde{f}_j(\sigma) = \int_{-\infty}^0 d\tau e^{-i\sigma \tau} f_j(\tau). \]  

(4)

Substituting back into eq. (3) we get

\[ \langle M_F(t) \rangle_{\psi} = -\frac{1}{2\pi i} \sum_j \int_0^\infty dE \psi_j^*(E) e^{iEt} \int_{-\infty}^\infty d\sigma \frac{e^{-i\sigma t}}{E - \sigma + i0^+} \int_{-\infty}^0 d\tau e^{-i\sigma \tau} f_j(\tau), \]

\[ = \sum_j \int_0^\infty dE \psi_j^*(E) e^{iEt} \int_{-\infty}^0 d\tau \Theta(-t - \tau) e^{-iE(t+\tau)} f_j(\tau) \]

\[ = \sum_j \int_{-\infty}^{-t} d\tau \int_0^\infty dE \psi_j^*(E) e^{-iE\tau} f_j(\tau), \]  

(5)

where \( \Theta(x) \) is the Heavyside function. From the definition of \( \tilde{f}_j(\sigma) \) and eq. (4) we have that

\[ f_j(\tau) = \frac{i}{4\pi^2} \int_{-\infty}^\infty d\sigma e^{i\sigma \tau} \int_0^\infty \frac{dE' \psi_j(E')}{\sigma - E' + i0^+} \]

\[ = \frac{1}{2\pi} \Theta(-\tau) \int_0^\infty dE' e^{iE'\tau} \psi_j(E'). \]  

(6)

Eq. (6) now assumes the form

\[ \langle M_F(t) \rangle_{\psi} = 2\pi \int_{-\infty}^{-t} d\tau \left| \sum_j f_j(\tau) \right|^2. \]  

(7)

The expectation value of \( M_F \) is thus seen to be nonnegative and monotonically decreasing with time, irrespectively of the initial state, tending to zero in the limit that \( t \) goes to infinity.

To obtain the full spectrum of \( M_F \), i.e. find its upper bound, we introduce the operator

\[ M_B = \frac{1}{2\pi i} \sum_j \int_0^\infty dE \int_0^\infty dE' \frac{\langle E', j \rangle \langle E', j \rangle}{E - E' - i0^+}. \]  

(8)

Similarly, \( M_B \) can be shown to be an ever increasing nonnegative operator. In particular, as \( t \) tends to minus infinity the expectation value of \( M_B \) tends to zero. Now

\[ M_F + M_B = 1, \]  

(9)

and since \( M_B \) is nonnegative as well, it follows that \( M_F \) is bounded from above by one.

The eigenstates of \( M_F \) are found by solving the eigenvalue equation \( M_F |m, j\rangle = m|m, j\rangle \), \( m \in [0, 1] \), with \( j \) indicating the degeneracy. In the energy representation
the eigenvalue equation takes on the form

\[ -\frac{1}{2\pi i} \int_0^\infty dE' \frac{g_m^{(j)}(E')}{z - E'} = mg_m^{(j)}(z), \quad \text{Imz} \neq 0. \]

Here \( g_m^{(j)}(E) \doteq \langle E, j|m, j \rangle \); the kernel’s independence of \( j \) allowing us to set \( \langle E, j|m, k \rangle = 0 \). We assume the existence of analytical functions \( g_m^{(j)}(z) \), which in the limit that \( z \to E + i0^+ \) equal \( g_m^{(j)}(E) \). This allows us to analytically continue eq. (10) into the complex plane

\[ -\frac{1}{2\pi i} \int_0^\infty dE' \frac{g_m^{(j)}(E')}{z - E'} = mg_m^{(j)}(z), \quad \text{Imz} \neq 0. \]  

Taking the difference between the limits from above and below the real axis we get

\[ \int_0^\infty dE' \left( \frac{1}{E - E' + i0^+} - \frac{1}{E - E' - i0^+} \right) g_m^{(j)}(E') = -2\pi im \left( g_m^{(j)}(E + i0^+) - g_m^{(j)}(E - i0^+) \right), \]

and hence

\[ g_m^{(j)}(E) = m \left( g_m^{(j)}(E + i0^+) - g_m^{(j)}(E - i0^+) \right). \]

\( g_m^{(j)}(z) \) can now be continued to a second Riemann sheet by making use of the branch cut along \( [0, \infty) \) in eq. (11). The eigenvalue equation reduces to

\[ g_m^{(j)}(e^{2\pi iz}) = -\left( \frac{1 - m}{m} \right) g_m^{(j)}(z). \]

The rotation on the left-hand side can be written using the dilation group defined via \( D_\alpha f(z) = f(e^{\alpha z}) \). It is easy to check that the generator of this group is \( \frac{d}{dz} \), i.e. \( e^{\alpha z} \frac{d}{dz} f(z) = f(e^{\alpha z}) \). Taking \( \alpha = 2\pi i \), eq. (14) can be reexpressed as

\[ e^{2\pi iz} \frac{d}{dz} g_m^{(j)}(z) = -\left( \frac{1 - m}{m} \right) g_m^{(j)}(z), \]

admitting solutions of the form \( g_m^{(j)}(z) = N_m z^\beta \) with \( \beta = (k + \frac{1}{2}) - \frac{i}{2\pi} \ln \left( \frac{1 - m}{1 + m} \right) \), \( k \in \mathbb{Z} \), and \( N_m \) a normalization factor dependent on \( m \). Setting \( k = -1 \) and \( N_m = \frac{1}{2\pi \sqrt{m} \ln(1 - m)} \), the solutions are orthogonal, i.e. satisfy \( \int_0^\infty dE g_m^{(j)*}(E) g_m^{(j')}(E) = \delta(m - m') \). The full set of (delta-function normalized) eigenfunctions is therefore given by

\[ g_m^{(j)}(E) = \frac{E - \frac{\pi}{2} \ln \left( \frac{1 - m}{1 + m} \right) - i}{2\pi \sqrt{m} \ln(1 - m)}. \]

Let us now address MPC’s and UW’s no-go theorems. Without going into details, MPC claimed that within standard quantum mechanics a nonequilibrium entropy operator cannot be defined. What is important for our purpose is that by a nonequilibrium entropy operator MPC mean a Lyapunov operator \( \ell \) such that \( [H, \ell] = D \geq 0 \). Their proof rests on the assumption that the measurement of \( \ell \) and its rate of change \( D \) should be mutually compatible, i.e. \([\ell, D]\) = 0. While one can debate whether this assumption is reasonable or not, it is easy to show that it is not satisfied by \( M_F \). Hence, there is no conflict with MPC’s no-go theorem.

UW proved that a monotonically perfect clock cannot be defined within the framework of standard quantum mechanics. By such a clock UW mean an ever increasing Lyapunov operator \( \ell \) with the additional property that it has a vanishing probability of “running backwards”. Thus, if we break up the spectrum of \( \ell \) into an infinite succession of finite sized nonoverlapping intervals, and let \( \ell_n \) denote an eigenstate of the projection operator onto the nth interval centered about \( \ell_n \), then for \( t > 0 \)

\[ \langle \ell_m < \ell_n | e^{-iHt} | \ell_n \rangle = 0. \]

However, as is readily verified, \( M_F \) does not share this extra property \[12\], and so no conflict arises with UW’s no-go theorem as well.

Next, we present the results of simulations illustrating the Lyapunov property. We consider the propagation from \( x = -\infty \) to \( x = \infty \) of a one dimensional free Gaussian wave-packet with \( p_0 = 6.4\mu \) and \( \xi_0 = 3\mu \) describing the propagation of a free particle of mass \( \mu \). \( t \) is given in units of \( [\mu]^{-1} \).

FIG. 1: Monotonic decrease of \( \langle M_F \rangle \). The figure depicts the monotonic decrease in time of \( \langle M_F \rangle \) for a free Gaussian wave-packet with \( p_0 = 6.4\mu \) and \( \xi_0 = 3\mu \) describing the propagation of a free Gaussian wave-packet with \( p_0 = 6.4\mu \) and \( \xi_0 = 3\mu \) describing the propagation of a free particle of mass \( \mu \). \( t \) is given in units of \( [\mu]^{-1} \).

\[ \psi(x, t) \]

\[ = \left( \frac{\mu^2 \xi_0^2}{\pi (\mu + i\xi_0^2 t)^2} \right)^{1/4} \exp \left( -\frac{\mu^2 \xi_0^2 x^2 + ip_0 (p_0 t - 2\mu x)}{2 (\mu + i\xi_0^2 t)} \right), \]

where \( p_0 \) and \( \xi_0 \) are the location and width of the wave-packet at \( t = 0 \) in momentum space. \( M_F \) is given by

\[ M_F = -\frac{1}{i\pi \mu} \sum_{j = \pm} \int_0^\infty dp \int_0^\infty dp' |p, j \rangle \langle p', j| \]

\[ = \frac{1}{i\pi \mu} \int \int dp dp' \frac{|\langle p, j | \langle p', j| \rangle|}{p^2 - p'^2 + i0^+}, \]
with \(|p, \pm\rangle\) denoting a plane wave state with a momentum \(\pm p\), respectively, and \(\mu\) the mass. Fig. (1) shows \(\langle M_F \rangle\) as a function of time. If we now expand \(\psi(x, t)\) in terms of the eigenfunctions of \(M_F\), \(\psi_\pm(m, t) = \langle m, \pm |\psi(t)\rangle\), then as time progresses the bulk of the state’s support must shift from eigenfunctions having a higher value of \(m\) to zero. See Fig. (2).

![Graphs showing time evolution of \(|\psi(x, t)|^2\) and \(|\psi(m, t)|^2\).

FIG. 2: Time frames of \(|\psi(x, t)|^2\) and \(|\psi(m, t)|^2\), \(\psi(m, t) = \langle m, + |\psi(t)\rangle + \langle m, - |\psi(t)\rangle\), \(t = -0.3, -0.05, 0, 0.05, 0.3 [\mu]^{-1}\), as computed for the Gaussian wave-packet of Fig. 1. \(x\) is measured in units of \([\mu]^{-1}\). The dotted line gives the value of \(\langle M_F \rangle\).

The behavior of the Lyapunov operator we have computed for the free particle evolution is precisely the same for a large equivalence class of Hamiltonians related to the free particle Hamiltonian, \(H_0\), via the intertwining property of the Møller wave-operators \(\Omega_\pm\). To see this let \(H_I\) be any Hamiltonian of this class, then \(H_I = \Omega_+ H_0 \Omega_+^\dagger\). In particular, \(|E_I = E, \pm\rangle = \Omega_+ |E_0 = E, \pm\rangle\), implying that \(M_F(t) = \Omega_+ M_F(0) \Omega_+^\dagger\), with the zero index serving to denote the free system [13]. If in the limit that \(t \to -\infty \) \(|\psi_0(t)|^2\) \(\to 1\), i.e. both systems share the same asymptotic initial state, then \(|\psi_I(t)\rangle = \Omega_+ |\psi_0(t)\rangle\). It follows that \(\langle \psi_I(t) | M_F(t) | \psi_I(t) \rangle = \langle \psi_0(t) | M_F(0) | \psi_0(t) \rangle\) and \(\langle m_I = m, \pm |\psi_I(t)\rangle = \langle m_0 = m, \pm |\psi_0(t)\rangle\) [14].

To conclude, we have presented an arrow of time operator within the framework of standard quantum mechanics. This operator can be defined for any system governed by a Hamiltonian with a uniformly finitely degenerate, absolutely continuous and semibounded spectrum [15]. An immediate question that arises is whether our result can be generalized to Hamiltonians with different spectral properties. It is interesting that by discretizing \(M_F = 2M_F - I\) we obtain Galapon’s \(T\) operator [4], which can be shown not to have the Lyapunov property, yet unlike our operator satisfies CCR with the Hamiltonian.

In a forthcoming paper we will see how the existence of an arrow of time operator naturally leads to the existence of a new representation of the dynamics, in which the direction of time is manifestly exhibited. This ”irreversible representation” is characterized by the property that the time evolution is a semigroup, and is particularly convenient for the description of processes such as the decay of unstable states, resonance phenomena, and other irreversible phenomena.

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[11] Whether $M_F$ is trivially generalized in the case of infinite degeneracy, or whether its form is different, is the subject of ongoing work.

[12] To be more precise, $M_F$ does not share this property in that even though its expectation value is monotonically decreasing in time, a single measurement may increase its expectation value.

[13] Here it is implicitly implied that the wave-operators do not mix degenerate eigenstates. However, this assumption is not necessary, and the discrete indices on the two sides may just as well refer to different bases.

[14] Note that this holds even if the spectrum of $H_I$ contains bound states, since the continuum maps only onto the continuum.

[15] The generalization to the bounded spectrum case is straightforward, and will be presented in a forthcoming publication.