A new approach to quantum backflow

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Abstract. We derive some rigorous results concerning the backflow operator introduced by Bracken and Melloy. We show that it is linear bounded, self adjoint, and not compact. Thus the question is underlined whether the backflow constant is an eigenvalue of the backflow operator. From the position representation of the backflow operator we obtain a more efficient method to determine the backflow constant. Finally, detailed position probability flow properties of a numerical approximation to the (perhaps improper) wave function of maximal backflow are displayed.

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1. Introduction and summary

Let a 1-dimensional free solution of the Schrödinger equation contain positive momenta only, and let \( P_x(t) \) be this wave function’s probability (at time \( t \)) to detect the particle at any position \( x \). Then \( P_x(t) \) starts out from 0 at time \( t = -\infty \) and tends towards 1 for \( t \to \infty \). Because of \( \dot{P}_x(t) = j(t,x) \), the (position probability) current \( j(t,x) \) is naively expected to be nonnegative for every \((t,x)\). Yet there exist positive momentum wave functions such that the current at, e.g., \( x = 0 \) is negative at certain intermediate times. In this case the half space probability as a function of time, i.e., \( P_0 : \mathbb{R} \to [0,1] \) is not monotonically increasing.

This so called quantum backflow effect seems to have been mentioned first by Allcock in his work on the time of arrival in quantum physics [1], while Bracken and Melloy [2] have given the first detailed account of the phenomenon in 1994. Allcock presented the backflow effect in order to disprove the hypothesis that the current at \( x = 0 \) yields the probability density of arrival times for a free positive momentum wave packet at \( x = 0 \). Recently it has been shown that the backflow effect indicates discrepancies among two other proposals of arrival time densities [3]. More specifically it has been shown in reference [3] that none of the arrival time densities, which obey Kijowski’s axioms [4], coincides with the one of Bohmian mechanics [5]. Furthermore their average arrival times differ if and only if the wave function in question leads to backflow, in which latter case the average Bohmian arrival time precedes that of
Kijowski’s distributions.

Bracken and Melloy posed the question whether the backflow of probability is restricted by a stronger bound than the obvious one given by 1. Though the existence of such a stronger bound was not to be expected, they attempted to numerically compute the smallest upper bound \( \lambda \) for the decrease of \( P \). By converting this backflow constant into the supremum of the spectrum of an integral operator \( K \) in momentum space, surprisingly enough, Bracken and Melloy approximately found its value to be 0.04. Meanwhile the precision of the value of \( \lambda \) has been improved by Eveson, Fewster, and Verch to 0.038452.

In the present work we describe a new approximation method to determine \( \lambda \), which provides independent confirmation of the results of [6]. Such confirmation is in need since a rigorous proof for the conjecture \( \lambda < 1 \) is still missing. The basic idea is to use a decomposition of the integral operator \( K \) into a sum of Fourier transformed multiplication operators. In this way the method of fast Fourier transform becomes applicable and \( \lambda \) can be approximated with less computational effort. We obtain an improved value for \( \lambda \) of 0.0384517. As a byproduct of our numerical computations we approximate the (perhaps improper) wave function of maximal backflow and we exhibit some of its more detailed position probability flow properties.

The primary goal of this work, however, is to provide some exact results concerning the integral operator \( K \) of Bracken and Melloy. From a unitary equivalence it will become obvious that \( K \) is linear bounded and self-adjoint. Then we prove that \( K \) is not compact by showing that \(-1\) belongs to the spectrum of \( K \) yet it is not an eigenvalue. We have not been able to conclusively answer the question whether \( \lambda \) is an eigenvalue of \( K \) in the strict mathematical sense. However we shall provide numerical plausibility that this is indeed the case. A more extensive discussion of some of our results concerning the backflow phenomenon is given in reference [7].

2. The backflow constant

The free Schrödinger evolution \( U_t : L^2(\mathbb{R}) \to L^2(\mathbb{R}) \) from time 0 to time \( t \in \mathbb{R} \) is given in the momentum representation by

\[
(U_t \phi)(k) = \phi_t(k) := \exp \left( -i k^2 t \right) \phi(k).
\]

Here \( t \) denotes the rescaled time variable \( \hbar \hbar_{\text{phys}} / (2m) \). Let \( \psi_t \) denote the inverse \( L^2 \)-Fourier transform of \( \phi_t \), i.e.,

\[
\psi_t(x) := (F^* \phi_t)(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(ikx) \phi_t(k) \, dk.
\]

Let a particle have the momentum space wave function \( \phi \) at time 0. If \( \| \phi \| = 1 \), the probability that a position measurement at time \( t \) yields a position \( x > 0 \) reads

\[
P(\phi_t) := \int_0^\infty |\psi_t(x)|^2 \, dx = \langle \phi_t, F \Pi F^* \phi_t \rangle.
\]

Here \( \Pi : L^2(\mathbb{R}) \to L^2(\mathbb{R}) \) denotes the orthogonal projection with

\[
(\Pi f)(x) = \begin{cases} f(x) & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases}.
\]
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If a unit vector $\phi \in L^2(\mathbb{R})$ has its support contained in $\mathbb{R}_{\geq 0}$, i.e., if $\Pi \phi = \phi$, the probability $P(\phi_t)$, according to Dollard’s lemma \[8\], obeys $P(\phi_t) \to 0$ for $t \to -\infty$ and $P(\phi_t) \to 1$ for $t \to \infty$. However, the mapping $t \mapsto P(\phi_t)$ need not monotonically increase from 0 to 1. Rather it may decrease during several intermediate time intervals.\[2\] Thus there exist momentum space wave functions $\phi \in \mathcal{H}_+ := \Pi \left( L^2(\mathbb{R}) \right)$ such that $P(\phi_s) > P(\phi_t)$ holds for some $s < t$. For such $\phi$ holds
\[
\lambda(\phi) := \sup \{ P(\phi_s) - P(\phi_t) \mid s, t \in \mathbb{R} \text{ with } s < t \} > 0.
\]
Unit vectors $\phi \in \mathcal{H}_+$ without backflow yield $\lambda(\phi) = 0$. We define the backflow constant by
\[
\lambda := \sup \{ \lambda(\phi) \mid \phi \in \mathcal{H}_+ \text{ with } \|\phi\| = 1 \}.
\]

Introducing the orthogonal projection $\tilde{\Pi}_t := U^*_t \mathcal{F} \Pi \mathcal{F}^* U_t$ we obtain for any unit vector $\phi \in L^2(\mathbb{R})$
\[
P(\phi_s) - P(\phi_t) = \left\langle \phi, \left( \tilde{\Pi}_s - \tilde{\Pi}_t \right) \phi \right\rangle.
\]
Because of
\[
\tilde{\Pi}_s - \tilde{\Pi}_t = U^*_t \left( \tilde{\Pi}_{\frac{s+t}{2}} - \tilde{\Pi}_{\frac{s-t}{2}} \right) U_{\frac{s+t}{2}}
\]

it follows that
\[
\lambda = \sup \left\{ \left\langle \phi, U^*_t \left( \tilde{\Pi}_{\tau T} - \tilde{\Pi}_{\tau T} \right) U_{\tau t} \phi \right\rangle \mid \phi \in \mathcal{H}_+, \|\phi\| = 1, \tau \in \mathbb{R}, T \in \mathbb{R}_{>0} \right\}.
\]

Since the unitary $U_t$ stabilizes $\mathcal{H}_+$ we infer
\[
\lambda = \sup \bigcup_{T>0} \sigma \left( \Pi B_T \Pi \right),
\]
where $B_T$ denotes the backflow operator
\[
B_T := \tilde{\Pi}_{\tau T} - \tilde{\Pi}_{\tau T},
\]
and $\sigma (A)$ denotes the spectrum of a linear operator $A$. This follows from theorem 2, section 8, chapter XI of \[9\]. Observe the bounds $-id \leq B_T \leq id$.

Let the one parameter family of unitary dilation operators $V_\mu : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ with $\mu \in \mathbb{R}_{>0}$ be given by $(V_\mu \phi)(k) = \sqrt{\mu} \phi(\mu k)$. The operators $V_\mu$ commute both with $\Pi$ and with $\mathcal{F} \Pi \mathcal{F}^*$ and a brief computation shows that
\[
V_\mu U_t V_\mu^* = U_{\mu 2t}.
\]
From this it follows that
\[
V_\mu \Pi B_T \Pi V_\mu^* = \Pi B_{\mu 2T} \Pi.
\]
Since the spectrum of an operator is invariant under a unitary transformation we have the following result, on which our numerical computation will be based.

**Proposition 1** For any fixed real $T > 0$ holds $\lambda = \sup \sigma \left( \Pi B_T \Pi \right)$.

In view of this result we choose $T = 1$ in what follows. The corresponding operators $U_{T=1}$ and $B_{T=1}$ will be abbreviated by $U$ and $B$. 
3. Equivalence with the treatment of Bracken and Melloy

Now we will prove that our definition of $\lambda$ indeed is equivalent to the one of Bracken and Melloy [2]. These authors heuristically introduce $\lambda$ via time integrals of currents at point $x = 0$ over arbitrary finite intervals. From this they motivate their final definition of $\lambda$ as the supremum of the spectrum of the integral operator

$$K : L^2(\mathbb{R}_>0) \to L^2(\mathbb{R}_>0)$$

with $(K f)(k) = -\frac{1}{\pi} \int_0^\infty \frac{\sin(k^2 - q^2)}{k-q} f(q) \, dq$.

Let $\eta : \mathcal{H}_+ \to L^2(\mathbb{R}_>0)$ denote the unitary operator with $(\eta \phi)(k) = \phi(k)$ for all $k > 0$ and for all $\phi$ in $\mathcal{H}_+$.

**Proposition 2** For all $\phi \in \mathcal{H}_+$ there holds $K \eta \phi = \eta \Pi B \Pi \phi$, i.e., the restriction of $\Pi B \Pi$ to $\mathcal{H}_+$ and $K$ are unitary equivalent.

**Proof.** Since $\Pi B \Pi$ is bounded it is sufficient to show $\eta \Pi B \Pi \phi = K \eta \phi$ for all $\phi$ from a dense subspace $D \subset \mathcal{H}_+$. We shall choose $D = S(\mathbb{R})$, the space of all $C^\infty$ functions from $\mathbb{R}$ to $\mathbb{C}$ with fast decrease and with their support contained in $\mathbb{R}_>0$.

As a prerequisite we first demonstrate a relation between the orthogonal projection $\mathcal{F} \Pi F^*$ and the Hilbert transformation

$$H : L^2(\mathbb{R}) \to L^2(\mathbb{R}), \quad (H f)(k) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{f(q)}{k-q} \, dq.$$  

Here $\mathcal{P}$ indicates that the improper integral is meant as the principal value. For $f \in S(\mathbb{R})$ we obtain by means of Lebesgue’s dominated convergence theorem and by means of Sochozki’s formula [10]

$$(\mathcal{F} \Pi F^* f)(k) = \frac{1}{2\pi} \int_{0}^{\infty} e^{-ikx} \left( \int_{-\infty}^{\infty} e^{ixq} f(q) \, dq \right) \, dx$$

$$= \frac{1}{2\pi} \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} f(q) \left( \int_{0}^{\infty} e^{i(q-k)x-\epsilon x} \, dx \right) \, dq$$

$$= -\frac{1}{2\pi i} \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} f(q) \, dq$$

$$= -\frac{1}{2\pi i} \left\{ \mathcal{P} \int_{-\infty}^{\infty} f(q) \, dq - i\pi f(k) \right\}$$

$$= \frac{1}{2i} (H f)(k) + \frac{f(k)}{2}.$$  

By continuity we infer

$$\mathcal{F} \Pi F^* = \frac{1}{2} (-i H + id).$$  

(2)

From equation (2) it is easy to show that the Hilbert transformation is unitary and that $\sigma(H) = \{i, -i\}$.

From the equations (1) and (2) follows

$$B = \frac{1}{2i} (UHU^* - U^*HU).$$  

(3)
From this we obtain for $k > 0$ and $\phi \in \mathcal{D}$

$$
(\Pi B \Pi \phi) (k) = \frac{e^{-ik^2/2i}}{2i} (HU^* \phi) (k) - \frac{e^{ik^2/2i}}{2i} (HU \phi) (k)
$$

$$
= -\frac{1}{\pi} \int_0^\infty \sin \left(\frac{k^2 - q^2}{k - q}\right) \phi (q) \, dq = (K \phi) (k).
$$

Clearly for $k < 0$ holds $(\Pi B \Pi \phi) (k) = 0$. By continuity we have $\Pi B \Pi \phi = \eta^{-1} K \eta \phi$ for all $\phi \in \mathcal{H}_+$. Thus the restriction of $\Pi B \Pi$ to $\mathcal{H}_+$ is unitary equivalent to $K$.

Therefore the defining relation of $\mathcal{H}$, $\lambda = \sup \sigma(K)$, indeed holds.

4. Noncompactness

**Proposition 3** The backflow operator $\Pi B \Pi$ is not compact.

**Proof.** For $\Pi B \Pi$ holds $-id \leq \Pi B \Pi \leq id$. Therefore $\sigma(\Pi B \Pi) \subset [-1, 1]$. For every unit vector $\phi \in \mathcal{H}_+$, according to Dollard’s lemma \[8\] holds

$$
\lim_{T \to \infty} \langle \phi, \Pi B T \Pi \phi \rangle = -1.
$$

Since the spectrum of $\Pi B T \Pi$ does not vary with $T$ it follows that $-1 \in \sigma(\Pi B \Pi)$. If $\Pi B \Pi$ were compact, then $-1$ were an eigenvalue of $\Pi B \Pi$. Let $\phi \in L^2(\mathbb{R})$ with $\|\phi\| = 1$ denote an eigenvector of $\Pi B \Pi$ with eigenvalue $-1$, i.e., $\Pi B \Pi \phi = -\phi$ holds. Since $\Pi B \Pi \phi \in \mathcal{H}_+$ it holds that $\phi \in \mathcal{H}_+$. Then it follows from the triangle inequality, from the unitarity of the Hilbert transformation $H$, and from equation (3) that

$$
1 = \|\phi\| = \|\Pi B \Pi \phi\| = \|\Pi B \phi\|
$$

$$
\leq \|B \phi\| = \frac{1}{2} \| (U H U^* - U^* H U) \phi \|
$$

$$
\leq \frac{1}{2} (\|U H U^* \phi\| + \|U^* H U \phi\|) = \frac{1}{2} (\|H U^* \phi\| + \|H U \phi\|) = 1
$$

Thus the triangle inequality becomes an equality and we have

$$
\| (U H U^* - U^* H U) \phi\| = \|U H U^* \phi\| + \|U^* H U \phi\|
$$

from which it follows that there exists some $\alpha \in \mathbb{C}$ such that

$$
U H U^* \phi = \alpha U^* H U \phi.
$$

Since $U H U^*$ and $U^* H U$ are unitary it follows that $|\alpha| = 1$. From the above sequence of inequalities it also follows that

$$
\|\Pi B \phi\| = \|B \phi\|.
$$

This is equivalent to $\Pi B \phi = B \phi$. Thus the eigenvector condition $\Pi B \Pi \phi = -\phi$ implies $B \phi = -\phi$, from which by means of equation (3) it follows that

$$
\frac{1}{2i} (\alpha - 1) H U \phi = -U \phi.
$$

Thus $U \phi =: \Phi \in \mathcal{H}_+$ is an eigenvector of $H$. Since $\sigma(H) = \{i, -i\}$ it follows that $\alpha - 1 \in \{2, -2\}$. Because of $|\alpha| = 1$ this implies $\alpha = -1$ and $H \Phi = i \Phi$. Thus it follows that

$$
\mathcal{F} \Pi \mathcal{F}^* \Phi = \frac{1}{2} (-i H + id) \Phi = \Phi.
$$
Thus we have $\Pi F^* \Phi = F^* \Phi$ for some nonzero $\Phi \in \mathcal{H}_+$. Now the following lemma implies the contradiction $\Phi = 0$. Thus $-1$ is not an eigenvalue of the backflow operator. Since every nonzero spectral value of a compact operator is an eigenvalue, the backflow operator necessarily is noncompact. □

**Lemma 1** Let $\Phi \in L^2(\mathbb{R})$ with $\Pi \Phi = \Phi$ and $\Pi F^* \Phi = F^* \Phi$. Then $\Phi = 0$ holds.

**Proof.** Any function from $L^2(\mathbb{R})$ is locally integrable. Therefore the inverse Fourier transform of $\Phi \in \mathcal{H}_+$ is the distributional boundary value of the holomorphic function $\tilde{\Phi}$ on the complex upper half plane defined by

$$
\tilde{\Phi}(z) = \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{iak} e^{-bk} \Phi(k) dk.
$$

If the boundary value obeys $\Pi F^* \Phi = F^* \Phi$, then the distribution $F^* \Phi$ is zero on $\mathbb{R}_{<0}$. From the generalized uniqueness theorem, see theorem B.10 on p. 100 of [12], it follows that $\Phi = 0$. Thus also the boundary value $F^* \Phi$ of $\tilde{\Phi}$ vanishes. Since $F^*$ is unitary we also have $\Phi = 0$. □

5. **Numerical Computation of the backflow constant $\lambda$**

In [2, 6] the integral operator $K$ is approximated by a finite square matrix, whose largest eigenvalue is taken as an approximation of $\lambda$. If, however, we apply the power-method to the expression for $\lambda$, which is given in proposition [11], we immediately approximate the largest eigenvalue without having to compute any matrix. One only needs to apply multiplication operators and fast Fourier transformations to an arbitrary initial vector. The power method works as follows. [11]

Let the matrix $A \in \mathbb{C}^{N \times N}$ be symmetric. Let $a$ be the eigenvalue of $A$ with the largest absolute value. Let $v_0 \in \mathbb{C}^N$ be a nonzero vector with nonzero component within the eigenspace of $A$ corresponding to $a$. Then the sequence $(v_n)_{n \in \mathbb{N}_0}$ is recursively defined by

$$
v_{n+1} = \frac{1}{\|v_n\|} A v_n.
$$

Then holds

$$
a = \lim_{n \to \infty} \frac{v_n^\dagger v_{n+1}}{\|v_n\|}.
$$

Since $\sigma(\Pi B \Pi) \subset [-1, \lambda]$ we apply the power method to the nonnegative, discretized operator $\Pi B \Pi + id$. Its largest eigenvalue then approximates $\lambda + 1$ while $v_n$ tends towards the corresponding eigenvector.

The analysis was started with $N_0 = 10^4$ grid-points covering the interval $[0, q_0]$, where $q_0$ is set to 50. Now the power-method was applied with 1000 iterations to a constant starting vector. Then we repeated the computation for to $N = N_0 h$ grid-points and a larger momentum interval $[0, q]$ with $q = q_0 \sqrt{h}$ for $h = 1, 2, \ldots, 40$. In this way the covered interval grows while the absolute step size $q/N$ gets smaller. The results $\lambda_h$ for different factors of accuracy $h$ then were used to extrapolate to $h \to \infty$ leading to an approximation $\lambda_\infty$ for the backflow-constant. The results of this computation can be seen in figure [11].
In order to check for the possibility that the constant starting vector $v_o$ has vanishing component within the eigenspace of the dominating eigenvalue various other starting vectors have been chosen as well. After only few iterations they all led to the same results. Since it seems extremely unlikely that all chosen starting vectors have vanishing components within the eigenspace of the dominating eigenvalue, our algorithm is likely to approximate the largest spectral value of $\Pi B \Pi + id$.

![Graph](image1.png)

Figure 1: $\lambda$ plotted against $h$ and fit $\lambda_\infty + b/\sqrt{h}$.

![Graph](image2.png)

Figure 2: $\lambda$ plotted against $1/\sqrt{h}$ and polynomial fit of third order.

An even better result for $\lambda_\infty$ is achieved by fitting the graph of figure 2 with a polynomial of third order. The extrapolated value for the backflow-constant can then
be read off from the intersection of the y-axis with the graph. (This corresponds to
the point $1/\sqrt{\hbar} = 0$ on the x-axis and $\hbar \to \infty$ respectively.) This yields

$$\lambda_\infty = 0.0384517$$

which agrees with the value given in [6] by $0.038452$.

By means of the power-method we also get an approximation of the possibly
improper eigenvector associated with the backflow constant. It will be discussed briefly
in the next section.

6. Approximate backflow maximizing vector

Since the operator $K$ of Bracken and Melloy is real, the (improper?) backflow maxi-
mizing eigenvector may be chosen to be real valued in the momentum representation.
From this it follows that the position representation at time 0 has even real part and
and odd imaginary part. More generally, the time dependent wave function is invari-
ant under the combined parity and time reversal operation.

We take as an approximate backflow maximizing vector the vector $v_n$ obtained
from the power method, where we choose $N = 10^4$, $q = 50$ and we make $n = 1000$
itations. The starting vector $v_0$ is – as before – simply the constant function. This
leads – as one can read off from figure 2 – to quite a bad approximation of $\lambda$ by about
0.0297, but a further increase of the accuracy leaves the appearance of the approxi-
mate eigenvector $v_n$ as displayed in figure 5 totally unchanged.

![Figure 3: $v_n$ in momentum and configuration space (below, real part
—all, imaginary part ——).](image)

The position probability density of $v_n$ subject to the free time evolution is dis-
played in figures 4, 5. These figures by themselves do not provide unquestionable
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evidence for the appearance of backflow.

Figure 4: Position probability density of \((v_n)_t\) for \(-20 < x < +20\) at times \(t \in \{-3, -2, \ldots, +3\}\).

Figure 5: Position probability density of \((v_n)_t\) for \(-20 < x < +20\) and \(-3 < t < +3\).

In order to strikingly illustrate the backflow we compute for the approximate
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backflow maximizing vector $v_n$, the current $j(t, x)$ at position $x = 0$ as a function of time. The result is shown in figure 6 where the backflow-domain $| -1, 1]$ is plainly identifiable. This interval seems to be the only one in which $v_n$ leads to a backflow through $x = 0$. The area below it, as required, approximately sums up to the backflow constant. The corresponding half space probability as a function of time is also shown in figure 6. Further evidence for the backflow phenomenon of $v_n$ is provided by figure 7. This figure shows some integral curves of the space time vector field $(1, j/\rho)$, the flow lines of the Bohmian velocity field, within the backflow-domain. All the integral curves which pass the line $x = 0$ at a time $t$ with $-1 < t < 1$ pass it in the negative direction.

![Image of figure 6](image)

Figure 6: $j(t, 0)$ (——) of $v_n$ and the corresponding half space probability (– – –) as functions of time.

The question which remains open is this: Is there really a backflow-eigenvalue – in the strict mathematical sense – to which $\lambda_\infty$ is an approximation? From the approximate eigenvector $v_n$ evidence can be found that there is indeed one. To this end we compute the contribution of the interval $[0, q]$ to the norm-square of $v_n$ and compare it to $\int_0^q |f(k)|^2 dk$ with $f(k) = N \cdot \sin(k^2)/k$ where $N$ is a normalization constant. Note that $f \in L^2(\mathbb{R})$. The results are shown in figure 8. The two graphs are very similar and the norm of the $v_n$ seems to converge even faster than that of $f$. Thus it seems plausible that $\lambda$ is indeed an eigenvalue of the backflow operator.

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Figure 7: Flow lines of the velocity field $j/\rho$ of $v_n$. The flow lines between -- -- - pass through $x = 0$ in the negative direction. Two consecutive flow lines are separated by a probability of approximately $2.4 \cdot 10^{-3}$.

Figure 8: Norm-squares of $v_n$ (——), and $\sin(k^2)/k$ (– – –).

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