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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 non-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) wavefunction of maximal backflow are displayed.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction and summary

Let a one-dimensional free solution of the Schrödinger equation contain positive momenta only, and let $P_x(t)$ be this wavefunction'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 non-negative for every (t, x). Yet there exist positive momentum wavefunctions such that the current at, for example, $x = 0$ 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 [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 wavefunction in question leads to a backflow, in which case the average Bohmian arrival time precedes that of Kijowski's distributions.

Bracken and Melloy [2] posed the question whether the backflow of probability is restricted by a stronger bound than the obvious one given by 1. Though a stronger bound would come as a surprise, they attempted to numerically compute the smallest upper bound λ for the decrease of P. By converting this backflow constant λ 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 λ has been improved by Eveson, Fewster and Verch [6] to 0.038 452.

In the present work, we describe a new approximation method to determine λ, which provides independent confirmation of the results of [6]. Such a 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 λ can be approximated with less computational effort. We obtain an improved value of 0.038 4517 for λ. As a by-product of our numerical computations, we approximate the (perhaps improper) wavefunction 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 λ 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 [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

$$(U_t\phi)(k) = \phi_t(k) := \exp(-\mathrm{i}k^2 t)\phi(k).$$

Here t denotes the rescaled time variable $\hbar t_{\mathrm{phys}}/(2m)$. Let ψ_t denote the inverse L^2-Fourier transform of ϕ_t, i.e.

$$\psi_t(x) := (\mathcal{F}^*\phi_t)(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(\mathrm{i}kx)\phi_t(k)\,\mathrm{d}k.$$

Let a particle have the momentum space wavefunction ϕ at time 0. If $\|\phi\| = 1$, the probability that a position measurement at time t yields a position $x > 0$ reads

$$P(\phi_t) := \int_0^{\infty} |\psi_t(x)|^2\,\mathrm{d}x = \langle \phi_t, \mathcal{F}\Pi\mathcal{F}^*\phi_t \rangle.$$

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

$$(\Pi f)(x) = \begin{cases} f(x) & \text{for} \quad x > 0 \\ 0 & \text{for} \quad x < 0. \end{cases}$$

If a unit vector $\phi \in L^2(\mathbb{R})$ has its support contained in $\mathbb{R}_{\geqslant 0}$, 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 wavefunctions $\phi \in \mathcal{H}_+ := \Pi(L^2(\mathbb{R}))$ such that $P(\phi_s) > P(\phi_t)$ holds for some $s < t$. For such ϕ 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 $\widetilde{\Pi}_t := U_t^* \mathcal{F}\Pi\mathcal{F}^* U_t$ we obtain for any unit vector $\phi \in L^2(\mathbb{R})$

$$P(\phi_s) - P(\phi_t) = \langle \phi, (\widetilde{\Pi}_s - \widetilde{\Pi}_t)\phi\rangle.$$

Because of

$$\widetilde{\Pi}_s - \widetilde{\Pi}_t = U^*_{\frac{t+s}{2}}\big(\widetilde{\Pi}_{\frac{s-t}{2}} - \widetilde{\Pi}_{\frac{t-s}{2}}\big)U_{\frac{t+s}{2}},$$

it follows that

$$\lambda = \sup\{\langle \phi, U_\tau^*(\widetilde{\Pi}_{-T} - \widetilde{\Pi}_T)U_\tau\phi\rangle \mid \phi \in \mathcal{H}_+, \|\phi\| = 1, \tau \in \mathbb{R}, T \in \mathbb{R}_{>0}\}.$$

Since the unitary U_τ stabilizes $\mathcal{H}_+$ we infer

$$\lambda = \sup \bigcup_{T>0} \sigma(\Pi B_T \Pi),$$

where B_T denotes the backflow operator

$$B_T := \widetilde{\Pi}_{-T} - \widetilde{\Pi}_T \tag{1}$$

and $\sigma(A)$ denotes the spectrum of a linear operator A. This follows from theorem 2, section 8 and chapter XI of [9]. Observe the bounds $-id \leqslant B_T \leqslant id$.

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_μ commute both with Π and $\mathcal{F}\Pi\mathcal{F}^*$ and a brief computation shows that

$$V_\mu U_t V_\mu^* = U_{\mu^2 t}.$$

From this it follows that

$$V_\mu \Pi B_T \Pi V_\mu^* = \Pi B_{\mu^2 T}\Pi.$$

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* $\lambda = \sup\sigma(\Pi B_T \Pi)$.

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 to U and B.

3. Equivalence with the treatment of Bracken and Melloy

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

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

with

$$(Kf)(k) = -\frac{1}{\pi}\int_0^\infty \frac{\sin(k^2 - q^2)}{k - q} f(q)\,\mathrm{d}q.$$

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 ϕ 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 $\mathcal{H}_+$ is unitary equivalent to K.*

Proof. Since $\Pi B\Pi$ is bounded it is sufficient to show $\eta\Pi B\Pi\phi = K\eta\phi$ for all ϕ from a dense subspace $\mathcal{D} \subset \mathcal{H}_+$. We shall choose $\mathcal{D} = \mathcal{S}_+(\mathbb{R})$, the space of all $\mathcal{C}^\infty$ 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 $\mathcal{F}\Pi\mathcal{F}^*$ and the Hilbert transformation

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

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

$$\begin{aligned}
(\mathcal{F}\Pi\mathcal{F}^* f)(k) &= \frac{1}{2\pi}\int_0^\infty \mathrm{e}^{-\mathrm{i}kx}\left(\int_{-\infty}^\infty \mathrm{e}^{\mathrm{i}xq} f(q)\,\mathrm{d}q\right)\mathrm{d}x \\
&= \frac{1}{2\pi}\lim_{\varepsilon\searrow 0}\int_{-\infty}^\infty f(q)\left(\int_0^\infty \mathrm{e}^{\mathrm{i}(q-k)x-\varepsilon x}\,\mathrm{d}x\right)\mathrm{d}q \\
&= -\frac{1}{2\pi\mathrm{i}}\lim_{\varepsilon\searrow 0}\int_{-\infty}^\infty \frac{f(q)}{q - k + \mathrm{i}\varepsilon}\,\mathrm{d}q \\
&= -\frac{1}{2\pi\mathrm{i}}\left\{\mathcal{P}\int_{-\infty}^\infty \frac{f(q)}{q-k}\,\mathrm{d}q - \mathrm{i}\pi f(k)\right\} \\
&= \frac{1}{2\mathrm{i}}(Hf)(k) + \frac{f(k)}{2}.
\end{aligned}$$

By continuity we infer

$$\mathcal{F}\Pi\mathcal{F}^* = \tfrac{1}{2}(-\mathrm{i}H + \mathrm{i}d). \tag{2}$$

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

From equations (1) and (2) it follows

$$B = \frac{1}{2\mathrm{i}}(UHU^* - U^*HU). \tag{3}$$

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

$$(\Pi B \Pi \phi)(k) = \frac{e^{-ik^2}}{2i}(HU^*\phi)(k) - \frac{e^{ik^2}}{2i}(HU\phi)(k)$$
$$= -\frac{1}{\pi}\int_0^\infty \frac{\sin(k^2 - q^2)}{k - q}\phi(q)\,dq = (K\phi)(k).$$

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 [2], $\lambda = \sup \sigma(K)$, indeed holds.

4. Noncompactness

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

Proof. For $\Pi B \Pi$ holds $-id \leqslant \Pi B \Pi \leqslant id$. 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 would be 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

$$1 = \|\phi\| = \|\Pi B \Pi \phi\| = \|\Pi B \phi\|$$
$$\leqslant \|B\phi\| = \tfrac{1}{2}\|(UHU^* - U^*HU)\phi\|$$
$$\leqslant \tfrac{1}{2}(\|UHU^*\phi\| + \|U^*HU\phi\|) = \tfrac{1}{2}(\|HU^*\phi\| + \|HU\phi\|) = 1.$$

Thus the triangle inequality becomes an equality and we have

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

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

$$UHU^*\phi = \alpha U^*HU\phi.$$

Since UHU^* and U^*HU 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

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

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

$$\mathcal{F}\Pi\mathcal{F}^*\Phi = \tfrac{1}{2}(-iH + id)\Phi = \Phi.$$

Thus we have $\Pi\mathcal{F}^*\Phi = \mathcal{F}^*\Phi$ 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 non-compact. □

Lemma 1. *Let* $\Phi \in L^2(\mathbb{R})$ *with* $\Pi\Phi = \Phi$ *and* $\Pi\mathcal{F}^*\Phi = \mathcal{F}^*\Phi$. *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 $\widetilde{\Phi}$ on the complex upper half-plane defined by

$$\widetilde{\Phi} : \{z \in \mathbb{C} \mid \Im z > 0\}, \qquad a + \mathrm{i}b \mapsto \frac{1}{\sqrt{2\pi}} \int_0^\infty \mathrm{e}^{\mathrm{i}ak}\,\mathrm{e}^{-bk}\,\Phi(k)\,\mathrm{d}k.$$

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

5. Numerical computation of the backflow constant λ

In [2, 6] the integral operator K is approximated by a finite square matrix, whose largest eigenvalue is taken as an approximation of λ. If, however, we apply the power method to the expression for λ, which is given in proposition 1, 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 $v_o \in \mathbb{C}^N$ 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

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

Since $\sigma(\Pi B\Pi) \subset [-1, \lambda]$ we apply the power method to the non-negative, 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 up 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 λ_h for different factors of accuracy h then were used to extrapolate to $h \to \infty$ leading to an approximation λ_∞ for the backflow constant. The results of this computation can be seen in figure 1.

In order to check for the possibility that the constant starting vector v_o has a 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 $\Pi B\Pi + id$.

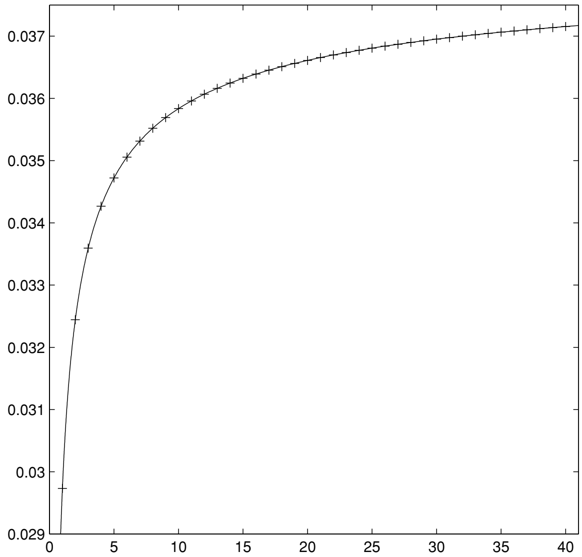

Figure 1. λ plotted against h and fit $\lambda_\infty + b/\sqrt{h}$.

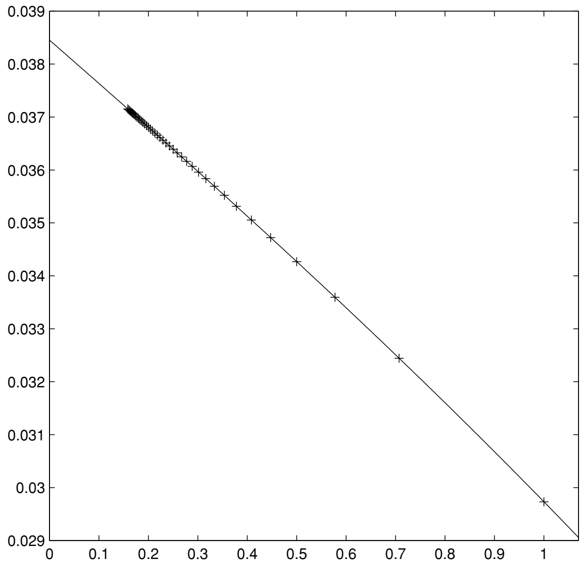

Figure 2. λ plotted against $1/\sqrt{h}$ and polynomial fit of third order.

An even better result for λ_∞ 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 $1/\sqrt{h} = 0$ on the x-axis and $h \to \infty$, respectively.) This yields

$$\lambda_\infty = 0.038\,4517$$

which agrees with the value given in [6] by 0.038 452.

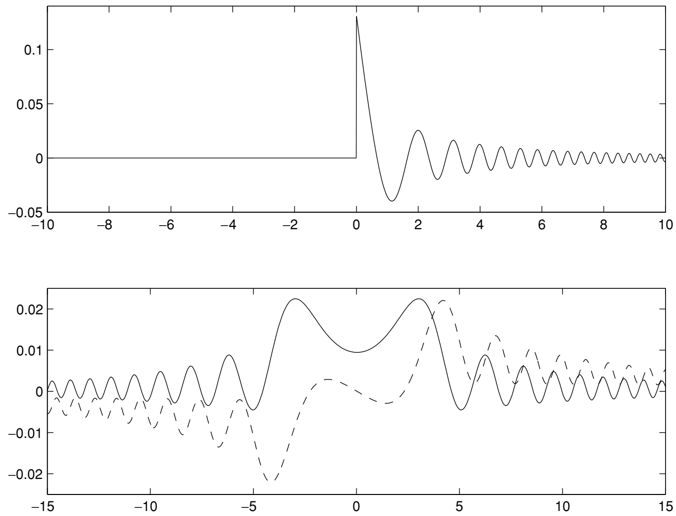

Figure 3. v_n in momentum and configuration space (below, real part ——, imaginary part – – –).

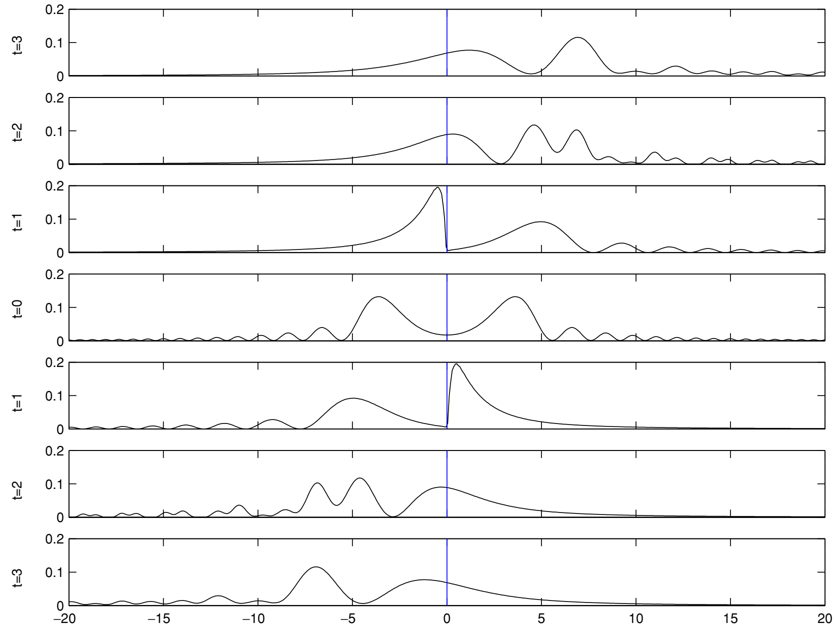

Figure 4. Position probability density of $(v_n)_t$ for $-20 < x < +20$ at times $t \in \{-3, -2, \ldots, +3\}$.

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 maximizing eigenvector may be chosen to be real-valued in the momentum representation. From this it

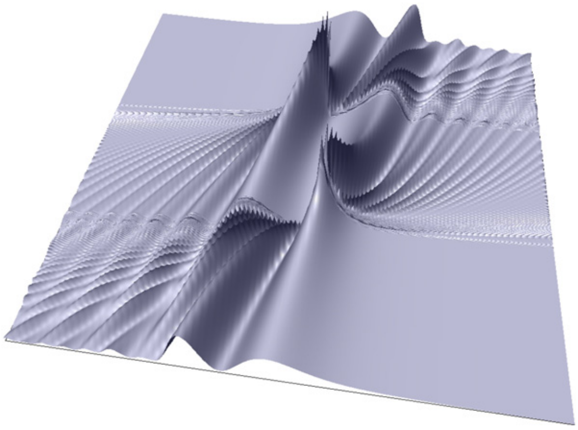

Figure 5. Position probability density of $(v_n)_t$ for $-20 < x < +20$ and $-3 < t < 3$.

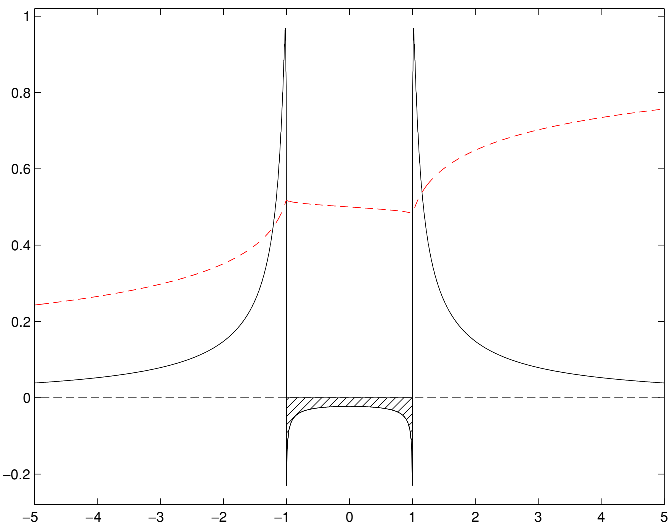

Figure 6. $j(t, 0)$ (——) of v_n and the corresponding half-space probability (– – –) as functions of time.

follows that the position representation at time 0 has an even real part and an odd imaginary part. More generally, the time-dependent wavefunction is invariant 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 $n = 1000$ iterations. 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 λ by about 0.0297, but a further increase of the accuracy leaves the visual appearance of the eigenvector v_n, as displayed in figure 3, unchanged.

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

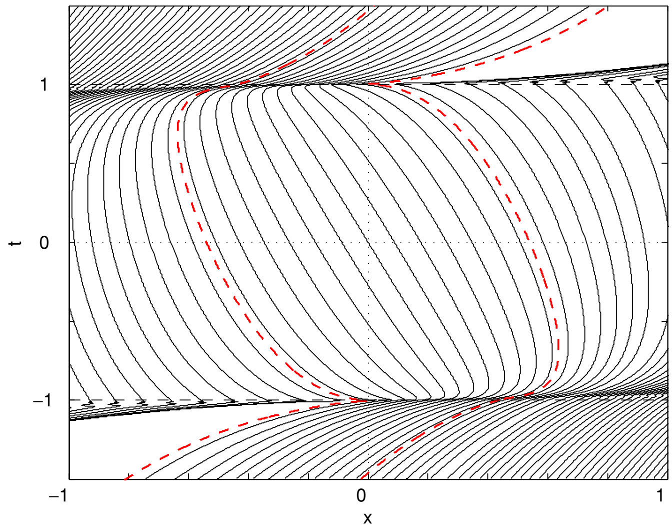

Figure 7. Flow lines of the velocity field j/ρ of v_n. The flow lines between – – – pass through $x = 0$ in the negative direction. Two consecutive flow lines are separated by a probability of approximately 2.4×10^{-3}.

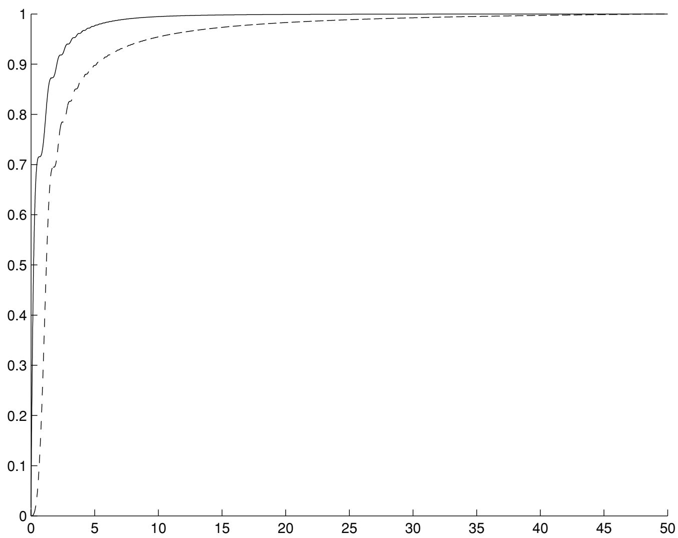

Figure 8. Norm-squares of v_n (——), and $\sin(k^2)/k$ (– – –).

In order to strikingly illustrate the backflow, we compute for the approximate 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 spacetime 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.

The question which remains open is this. Is there really a backflow eigenvalue—in the strict mathematical sense—to which λ_∞ 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 $\int_0^q |f(k)|^2\, \mathrm{d}k$ with $f(k) = \mathcal{N} \sin(k^2)/k$ where $\mathcal{N}$ 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 v_n seems to converge even faster than that of f. Thus it seems plausible that λ is indeed an eigenvalue of the backflow operator.

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