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Negative Probability Current in a Freely Falling Quantum Particle

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A quantum particle (represented by a Gaussian wave packet) under uniform gravity, projected upward (the conventional positive direction) along the vertical degree of freedom *x*, may have a negative probability current on a set of points *q*. This imposes the condition that the position and momentum observables of the state are negatively correlated. We calculate the effect of the negative correlation on the individual contributions to the probability current by the positive and negative momentum amplitudes of the state using an integral representation of the probability current. Negative position-momentum correlation causes a transient attenuation of all contributions to the probability flow, and wave packet spreading is temporarily mitigated.

Keywords: ballistic particle, position-momentum correlation, probability current, quantum mechanics

INTRODUCTION

Consider a quantum particle of mass m in a uniform gravitational field g (with potential V(x) = mgx) localized in the classically allowed region. Using a Gaussian state with a positive group velocity (the upward direction), we derive an inequality among the wave packet parameters that determine a time-dependent region of negative probability current. This unusual situation depends on the position-momentum covariance (Bohm 1951; Levy-Leblond 1986; Campos 1998):

$$\Delta(\mathrm{xp})_t = \frac{1}{2}\langle \hat{\mathrm{x}}\hat{\mathrm{p}} + \hat{\mathrm{p}}\hat{\mathrm{x}}\rangle - \langle \hat{\mathrm{x}}\rangle\langle \hat{\mathrm{p}}\rangle \tag{1}$$

The position and momentum observables *x* and *p*, respectively, are said to be anti-correlated at time *t* if $\Delta(xp)_t < 0$. We show that if a Gaussian state in free fall has a negative probability current on a point *q*, the state must necessarily be initially anti-correlated in *x* and *p*, and we determine the durations of the negative probability current and the anti-correlation regimes, which do not coincide.

We also derive an integral representation of the probability current *J* at the point *q*, and we use it to identify the contributions to the probability current by the positive and negative amplitudes of the momentum wave function:

$$\mathrm{J} = \mathrm{J}^+ + \mathrm{J}^- + \mathrm{J}^\mathrm{I} \tag{2}$$

where the J^+ term is entirely due to the positive momentum amplitude of the state, while the J^- term of Equation 2 similarly arises from the negative momentum amplitude. The third term J^I is an interference term from both momenta. If the state is initially anti-correlated, we show the current contributions J^+, J^- and J^I may be temporarily attenuated.

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This paper extends the previous work on negative probability currents of free particle states (Villanueva 2018, 2020). We show that a ballistic quantum particle can exhibit the same property that the probability of particle detection can flow in the opposite direction of the wave packet's group velocity. Since atomic fountains have been realized experimentally, our theoretical predictions can be tested with particle detection statistics.

METHODS

The Gaussian Wave Packet

For our purposes, a time-dependent quantity A is denoted by A_t, and its value at the initial time $t = 0$ is A_0. We represent the freely falling particle, with a vertical degree of freedom x, as the Gaussian wave packet (Heller 1975):

$$\psi(x,t) = \exp\left(\frac{\iota}{\hbar}\left(\alpha_t(x-x_t)^2 + p_t(x-x_t) + \gamma_t\right)\right) \tag{3}$$

described by four parameters: two are real (p_t and x_t) and two are complex (α_t and γ_t). The quantities p_t and x_t are the expectation values for momentum and position, respectively, given by the classical expressions of a freely falling particle of mass m:

$$x_t = -\frac{1}{2}gt^2 + \frac{p_0}{m}t + x_0 \tag{4}$$

$$p_t = p_0 - mgt \tag{5}$$

The complex parameter α_t describes the time evolution of the Gaussian state, and we obtain an explicit expression for α_t by substituting Equation 3 into the time-dependent Schrodinger equation with potential $V(x) = mgx$ to obtain a first-order differential equation for α_t. Solving this differential equation gives us:

$$(\alpha_R)_t = \left((\alpha_R)_0 + \frac{2t|\alpha_0|^2}{m}\right)\frac{1}{D_t} \tag{6}$$

$$(\alpha_I)_t = \frac{(\alpha_I)_0}{D_t} \tag{7}$$

$$D_t = 1 + \frac{4t(\alpha_R)_0}{m} + \frac{4t^2|\alpha_0|^2}{m^2} \tag{8}$$

where $(\alpha_R)_t$ and $(\alpha_I)_t$ are the real and imaginary parts of α_t, respectively. If we similarly define $(\gamma_R)_t$ and $(\gamma_I)_t$ for γ_t and impose the normalization condition on the Gaussian state, we obtain a constraint between $(\alpha_I)_t$ and $(\gamma_I)_t$ such that $(\alpha_I)_t > 0$. The parameter $(\alpha_R)_t$ is a physically irrelevant global phase factor, while $(\gamma_I)_t$ is not independent of $(\alpha_I)_t$. Thus $(\alpha_I)_t$ (together with p_t and x_t) is sufficient to describe the system. For example, the position uncertainty of the free fall Gaussian wave packet is:

$$(\Delta x)_t = \frac{1}{2}\sqrt{\frac{\hbar}{(\alpha_I)_t}} \tag{9}$$

The Negative Probability Current Region

Assume that the free fall Gaussian wave packet has a positive (*i.e.* upward) initial group velocity p_0/m, and it is initially well localized in the classically allowed region $x < x_{TP}$, where $x_{TP} = p_0^2 / 2mg^2$ is the classical turning point. The expectation value or centroid x_t, which corresponds to the peak of the position density function $|\psi(x,t)|^2$, satisfies the classical equation of motion (Equation 4) according to Ehrenfest's theorem. This implies that the peak of the position density function increases until it reaches the classical turning point, with the width of the position density function given by the position uncertainty (Equation 9).

Let q be the point along the x-axis where we calculate the probability current of the Gaussian wave packet. We consider only the case $x_t < q$ when the centroid x_t of the Gaussian wave packet is approaching point q from below. Let $A_t = p_t / 2(x_t - q)$ so that $A_t < 0$, since $p_t > 0$ and $q > x_t$. Using the well-known expression for the probability current at q:

$$J(q,t) = \frac{\iota\hbar}{2m}\left(\psi\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial\psi}{\partial x}\right)\Big|_{x=q} \tag{10}$$

where the asterisk represents complex conjugation; the probability current of the free fall Gaussian state at the point q is:

$$J(q,t) = \frac{1}{m}(p_t + 2(q - x_t)(\alpha_R)_t)\, P(q,t) \tag{11}$$

$$P(q,t) = |\psi(q,t)|^2 = \sqrt{\frac{2(\alpha_I)_t}{\pi\hbar}}\left(-\frac{2(\alpha_I)_t}{\hbar}\,(q - x_t)^2\right) \tag{12}$$

where $P(q,t)$ is the probability density at q. If the probability current is to be negative at q, we must have $(\alpha_R)_t < A_t < 0$. This negative probability current is temporary and vanishes at time $t = \tau_J$ determined by $p_\tau + 2(q - x_\tau)\,(\alpha_R)_\tau = 0$.

The time-dependent probability of detecting the particle in the region $x > q$ is:

$$\Pi^q(t) = \int_q^\infty |\psi(x,t)|^2\, dx \tag{13}$$

In this context, the equation of continuity satisfied by J (because probability in a closed system is conserved) is equivalent to:

$$\Delta\Pi^q = \Pi^q(t_2) - \Pi^q(t_1) = \int_{t_1}^{t_2} J(q,t)\, dt \tag{14}$$

Hence, the rate of change of Π^q is determined by the current J at q. If $J < 0$ at q, we have an unusual quantum effect: the probability Π^q of detecting the particle in the region $x > q$ decreases as the wave packet enters the region $x > q$.

For a given set of parameters p_t, x_t, and $(\alpha_R)_t$, we can interpret the inequality $(\alpha_R)_t < A_t$ as the condition a set of points q must satisfy such that $J(q, t) < 0$. This region of negative probability current is determined by the inequality:

$$q > x_t - \frac{p_t}{2(\alpha_R)_t} \tag{15}$$

In other words, the probability current is negative if evaluated at any point q within the region specified by the inequality (Expression 15).

Position-Momentum Anti-correlation

The physical content of $(\alpha_R)_t < 0$ is expressible in terms of the position-momentum covariance, given by Equation 1. For the free fall Gaussian wave packet, we have:

$$\Delta(xp)_t = \frac{\hbar}{2}\frac{(\alpha_R)_t}{(\alpha_I)_t} \tag{16}$$

The observables x and p are anti-correlated at time t if $\Delta(xp)_t$ is negative, *i.e.* $(\alpha_R)_t < 0$ since $(\alpha_I)_t$ is positive from Equation 9. Hence a free fall Gaussian wave packet with a negative probability current at time t must necessarily be anti-correlated in x and p at the same time. From Equations 6–8, the position-momentum covariance is linearly increasing over time:

$$\Delta(xp)_t = \Delta(xp)_0 + \frac{\hbar t}{m}\frac{|\alpha_0|^2}{(\alpha_I)_0} \tag{17}$$

If the free fall Gaussian state is initially anti-correlated in x and p, *i.e.* $\Delta(xp)_0 < 0$, the position-momentum covariance becomes zero at time:

$$\tau_A = -\frac{m}{2}\frac{(\alpha_R)_0}{|\alpha_0|^2} \tag{18}$$

The duration of the x-p anti-correlation does not coincide with that of the negative probability current. If we consider $q = 0$, since $(\alpha_R)_t = 0$ at time $t = \tau_A$, from Equation 9, the probability current at the origin $J(0, \tau_A)$ is already positive.

The position-momentum covariance manifests in the position expectation value of the Gaussian wave packet, Equation 3, expressed as (Villanueva 2018):

$$\Delta x_t^{\,2} = \Delta x_0^{\,2} + \Delta(xp)_0\frac{2t}{m} + \Delta p_0^{\,2}\frac{t^2}{m^2}$$

where the term linear in t allows a decrease in the position uncertainty if the initial position-momentum covariance is negative. In this case, the position density is temporarily "contracted" in a smaller neighborhood about its position expectation value, and the particle is more localized.

Integral Representation of the Probability Current

Using the current operator (Boykin 2000):

$$\hat{J}_q = \frac{1}{2m}\left(\hat{p}\,|q\rangle\langle q| + |q\rangle\langle q|\,\hat{p}\right) \tag{19}$$

where $|q>$ is the position eigenket at the point q; the probability current at q of a state ψ is the expectation value of J_q with respect to ψ. The current operator appears in discussions of the backflow effect (Yearsley *et al.* 2012; Halliwell *et al.* 2013), arrival-time distributions (Delgado and Muga 1997; Delgado 1998), probability currents in discrete models (Boykin *et al.* 2010), and semi-classical dynamics (Mason *et al.* 2013). Evaluating Equation 19 in momentum space obtains the integral representation of the probability current at q, given by:

$$\langle\hat{J}_q\rangle = \frac{1}{4\pi\hbar m}\int dp'\exp\left(-\frac{\iota}{\hbar}qp'\right)\phi^*(p',t)\int dp\,(p+p')\exp\left(\frac{\iota}{\hbar}qp\right)\phi(p,t) \tag{20}$$

where ϕ is the momentum wave function, and the integrals of p and p' range over the entire real line. If we consider integrals of the form:

$$I^+ = \int_0^\infty dp\;\exp\left(\frac{\iota}{\hbar}qp\right)\phi(p,t) \tag{21}$$

$$I^- = \int_{-\infty}^0 dp\;\exp\left(\frac{\iota}{\hbar}qp\right)\phi(p,t) \tag{22}$$

we can decompose the probability current, given by Equation 20 in the form of Equation 2, where:

$$J^+ = \frac{1}{4\pi\iota m}\left((I^+)^*\frac{\partial I^+}{\partial q} - (I^+)\frac{\partial (I^+)^*}{\partial q}\right) \tag{23}$$

$$J^- = \frac{1}{4\pi\iota m}\left((I^-)^*\frac{\partial I^-}{\partial q} - (I^-)\frac{\partial (I^-)^*}{\partial q}\right) \tag{24}$$

$$J^{I} = J^{A} + J^{B} \tag{25}$$

$$J^{A} = \frac{1}{4\pi\iota m}\left((I^{+})^{*}\frac{\partial I^{-}}{\partial q} - (I^{-})\frac{\partial (I^{+})^{*}}{\partial q}\right) \tag{26}$$

$$J^{B} = \frac{1}{4\pi\iota m}\left((I^{-})^{*}\frac{\partial I^{+}}{\partial q} - (I^{+})\frac{\partial (I^{-})^{*}}{\partial q}\right) \tag{27}$$

To obtain I^{+} for the free fall Gaussian state, we calculate the Fourier transform of Equation 3:

$$\phi(p,t) = \sqrt{\frac{\iota}{2\alpha_t}}\exp\left(\frac{\iota}{\hbar}(\gamma_t - px_t)\right)\exp\left(-\frac{\iota}{4\hbar\alpha_t}(p-p_t)^2\right) \tag{28}$$

We evaluate Equation 21 using the standard integral (Equation 3.322.2 of Gradshteyn and Ryzhik 2007):

$$\int_0^{\infty} du\ \exp(-a^2u^2 - 2bu) = \sqrt{\frac{\pi}{4a^2}}\exp\left(\frac{b^2}{a^2}\right)\operatorname{erfc}\left(\frac{b}{a}\right) \tag{29}$$

provided $Re(a^2) > 0$, where $erfc(u)$ is the complementary error function and:

$$a^2 = \frac{\iota}{4\hbar\alpha_t} \tag{30}$$

$$b = -a^2\big(p_t + 2\alpha_t(q - x_t)\big) \tag{31}$$

$$u_t = \frac{b}{a} = -a\big(p_t + 2\alpha_t(q - x_t)\big) \tag{32}$$

Hence, we obtain:

$$I^{+} = \sqrt{\frac{\pi\hbar}{2}}\ \psi(q,t)\ \operatorname{erfc}(u_t) \tag{33}$$

where $\psi(q, t)$ is the position amplitude at the point q. The I^{-} term is similarly computed, and from Equations 23–27, the current contributions are:

$$J^{+} = \frac{\iota\hbar}{8m}\left(f\frac{\partial f^{*}}{\partial q} - f^{*}\frac{\partial f}{\partial q}\right) \tag{34}$$

$$J^{-} = \frac{\iota\hbar}{8m}\left(g\frac{\partial g^{*}}{\partial q} - g^{*}\frac{\partial g}{\partial q}\right) \tag{35}$$

$$J^{A} = \frac{\iota\hbar}{8m}\left(g\frac{\partial f^{*}}{\partial q} - f^{*}\frac{\partial g}{\partial q}\right) \tag{36}$$

$$J^{B} = \frac{\iota\hbar}{8m}\left(f\frac{\partial g^{*}}{\partial q} - g^{*}\frac{\partial f}{\partial q}\right) \tag{37}$$

where $f = \psi(q, t)\ erfc(u_t)$ and $g = \psi(q, t)\ erfc(-u_t)$.

RESULTS AND DISCUSSION

As an example, consider a particle with mass $m = 2.9 \times 10^6$, initial mean momentum $p_0 = 0.00020$, initial mean position $x_0 = 0$, and parameter $(\alpha_I)_0 = 0.00152$ (all values in this paper are in atomic units where $\hbar = 1$). These parameters represent a freefall ultra-cold cesium atom moving towards the turning point $x_{TP} = 21.7$ *a.u.* at 0.15 μm/s, such that $|x_0 - x_{TP}|$ has the same order of magnitude as $(\Delta x)_0 = 21.4$ *a.u.*, the initial position uncertainty. The initial region of negative current is $q > 0.058$ *a.u.* Figure 1 illustrates the current $J(q, t)$ evaluated at three different points: $q_1 = 0.04$ *a.u.*, $q_2 = 0.08$ *a.u.*, and $q_3 = 0.12$ *a.u.* The point q_1 is outside the region $q > 0.058$ *a.u.*, hence the initial probability current $J(q_1, 0)$ is positive. In contrast, the points q_2 and q_3 are inside the region, thus the initial probability currents $J(q_2, 0)$ *and* $J(q_3, 0)$ are negative.

Figure 2b depicts the initial position density (dash), and the region of negative current $q > 0.058$ *a.u.* is the right "tail' of the free fall Gaussian position density; note that the position density at time $t = 1.5\tau_A$ has a smaller width. This contractive wave packet behavior is induced by an initial *x-p* anti-correlation. In contrast, in Figure 2a we have a typical wave packet with a vanishing initial *x-p* correlation, accompanied by the customary wave packet spreading.

The decrease in the wave packet width in Figure 2b can be explained. In the time interval $0 < t < \tau_A$, we have from Equation 9 the inequality $(\Delta x)_t < (\Delta x)_0$, implying that the position uncertainty is decreasing, attaining its minimum possible value at time τ_A. For $t > \tau_A$, the wave packet spreads indefinitely and regains the initial position uncertainty $(\Delta x)_0$ at time $2\tau_A$. The spreading of the wave packet is temporarily mitigated in this time scale, which has important consequences in quantum metrology (Caves *et al.* 1980; Braginsky and Khalili 1992; Yuen 1983; Giovannetti *et al.* 2004).

Using Equation 4, and the expressions $p_t = p_0 - mgt$ and $x_t = -gt^2/2 + p_0t/m + x_0$, we solve for the duration τ_J from the condition $p_\tau + 2(q - x_\tau)(\alpha_R)_\tau = 0$, and we obtain two positive solutions for τ_J: – namely, 4.735×10^8 *a.u.* and *6.32*

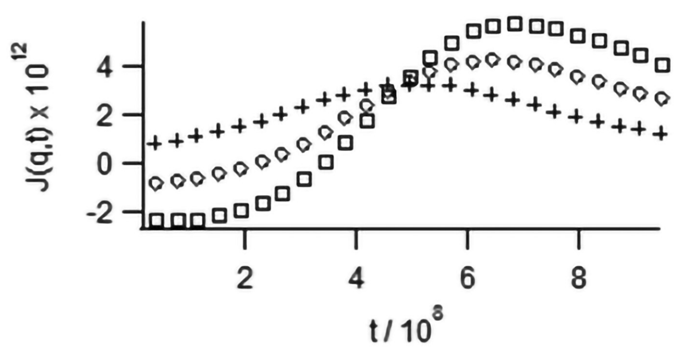

Figure 1. Probability current $J(q,t)$ *vs.* time t at different points: $q_1 = 0.04$ (cross), $q_2 = 0.08$ (circle), and $q_3 = 0.12$ (box). The time interval is $0 \leq t \leq 2\tau_A$, where $\tau_A = 4.7 \times 10^8$ (all values are in atomic units).

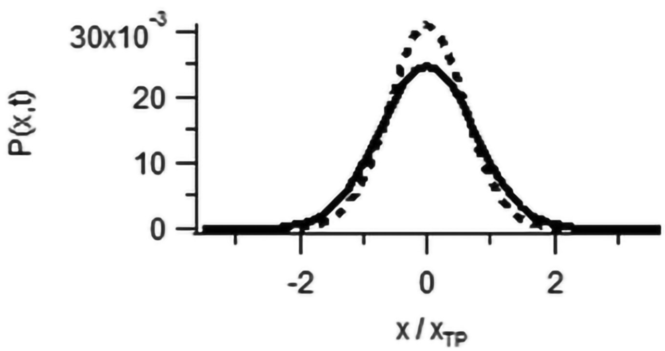

Figure 2a. Position density $P(x,t)$ *vs.* x / x_{TP} for $(\alpha_R)_0 = 0$ at different times: $t = 0$ (dash), and $t = 1.5\,\tau_A$ (solid), where $\tau_A = 4.7 \times 10^8$ (all values are in atomic units).

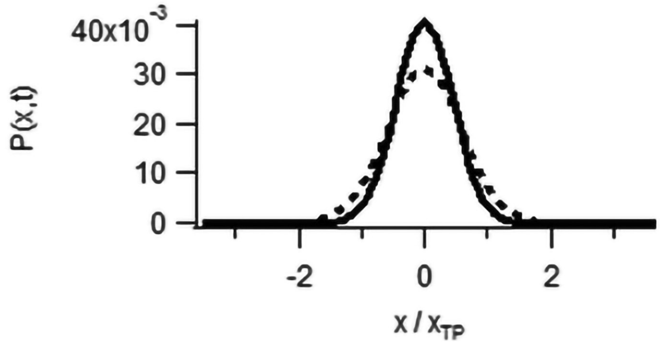

Figure 2b. Position density $P(x,t)$ *vs.* x / x_{TP} for $(\alpha_R)_0 = -0.00172$ at different times: $t = 0$ (dash) and $t = 1.5\ \tau_A$ (solid), where $\tau_A = 4.7 \times 10^8$ (all values are in atomic units).

$\times\ 10^{11}$ *a.u.*, where $t_{TP} = 6.32 \times 10^{11}$ *a.u.* is the arrival time of the centroid x_t at the turning point. The first solution is slightly smaller than $\tau_A = 4.741 \times 10^8$. However, in the scale of the figures in this paper, $\tau_J \approx \tau_A$.

The current decomposition, given by Equation 2, can be discussed in terms of the probability current ratios:

$$R_t = \frac{J(x_{TP}, t)}{|J(x_{TP}, 0)|} \tag{38}$$

$$R^+{}_t = \frac{J^+(x_{TP}, t)}{|J(x_{TP}, 0)|} \tag{39}$$

$$R^-{}_t = \frac{J^-(x_{TP}, t)}{|J(x_{TP}, 0)|} \tag{40}$$

$$R^I{}_t = \frac{J^I(x_{TP}, t)}{|J(x_{TP}, 0)|} \tag{41}$$

with the point q set at the turning point. Using the parameter set in Figure 1 (mass m, initial mean momentum p_0, and initial mean position x_0), we illustrate in Figure 3a the current ratios for the typical, initially uncorrelated state with $(\alpha_R)_0 = 0$. The effect of x-p anti-correlation is shown in Figure 3b where $(\alpha_R)_0 = -0.00344$, where the rate of increase of J_t is slower for the anti-correlated case, and all current contributions are negligible in a time scale of order τ_A.

In Figures 3a and b in the manuscript, we compared the probability currents (normalized to their initial values) at the turning point of two Gaussian wave packets with identical wave packet parameters, with the sole exception that the wave packet in Figure 3b has a negative correlation between its position and momentum.

The Gaussian wave packet in Figure 3a is a typical minimum-uncertainty wave packet at the initial time $t = 0$. Both wave packets are ascending towards the classical turning point and are continually being scattered by the potential. Nevertheless, only the wave packet in Figure 3b has a negative probability current.

Therefore, the linear potential will not produce a negative probability current if the wave packet is a typical minimum-uncertainty wave packet at the initial time $t = 0$, as long as the expectation value of the Gaussian wave packet is approaching the turning point from below, which is the situation assumed in this paper. Therefore, it is the negative correlation of the position and momentum observables that causes the negative probability current.

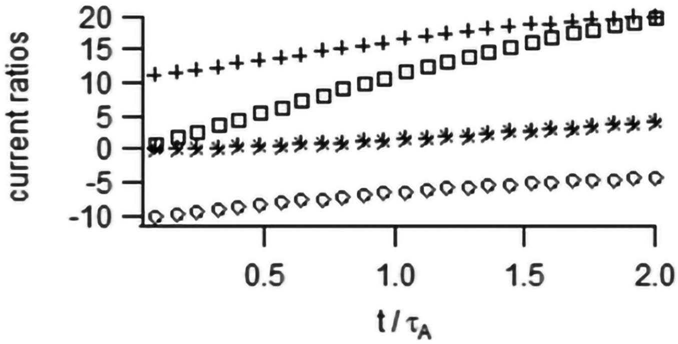

Figure 3a. Current ratios R_t (box), $R^+{}_t$ (cross), $R^-{}_t$ (circle), and $R^I{}_t$ (asterisk) *vs.* time t for $(\alpha_R)_0 = 0$. The time interval is $0 \leq t \leq 2\tau_A$, where $\tau_A = 3.5 \times 10^8$ (atomic units).

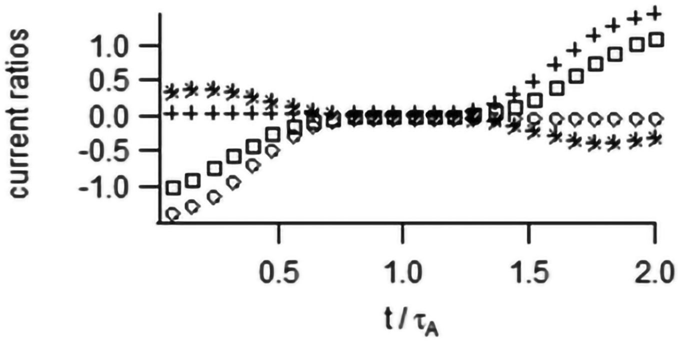

Figure 3b. Current ratios R_t (box), $R^+{}_t$ (cross), $R^-{}_t$ (circle), and $R^I{}_t$ (asterisk) *vs.* time t for $(\alpha_R)_0 = -0.00344$. The time interval is $0 \leq t \leq 2\tau_A$, where $\tau_A = 3.5 \times 10^8$ (atomic units).

CONCLUSION

We determined the set of points where a free fall Gaussian wave packet with a positive group velocity may have a negative probability current, expressed by the inequality (Expression 15). This negative probability current implies an initial *x*-*p* anti-correlation. Using its integral representation, the probability current is decomposed into several terms depending on the sign of the momentum amplitude. The current contributions of the free fall Gaussian wave packet were explicitly determined, and the effect of *x*-*p* anti-correlation is a temporary attenuation of the probability flow. Wave packet spreading is temporarily halted, and this has implications for precision measurements in quantum metrology.

Our conclusions also raise a question of interest within the context of arrival times of ballistic particles (Villanueva 2016). What is the effect of a negative probability current on the arrival-time distribution of a ballistic particle? If we restrict the time scale to the order of τ_A, during which a contraction of the position wave packet width accompanies position-momentum anti-correlation; we can imagine (as a preliminary conjecture or hypothesis) a similar sharpening effect on the arrival-time distribution. This, and other possible issues between position-momentum anti-correlation and arrival-time distributions, will be pursued elsewhere.

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