Relation between quantum dwell times and flux-flux correlations

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We examine the connection between the dwell time of a quantum particle in a region of space and flux-flux correlations at the boundaries. It is shown that the first and second moments of a flux-flux correlation function which generalizes a previous proposal by Pollak and Miller [Phys. Rev. Lett. **53**, 115 (1984)], agree with the corresponding moments of the dwell-time distribution, whereas the third and higher moments do not. We also discuss operational approaches and approximations to measure the flux-flux correlation function and thus the second moment of the dwell time, which is shown to be characteristically quantum and larger than the corresponding classical moment even for freely moving particles.

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I. INTRODUCTION

Time observables, i.e., times measured as random variables after a microscopic system is prepared, in particular according to a given wave function, are very common in the laboratories. Examples are the lifetimes of excited species, or the arrival times of ions, atoms, or molecules at a scintillation detector, a microchannel plate, or a laser-illuminated region. Nevertheless, incorporating time observables into quantum mechanics is a problematic task [1], and it has even been discouraged by many physicists influenced by Pauli's theorem and the extended notion that "time is only a parameter" within the quantum realm. Time observables are characterized experimentally, for a given preparation of the initial state, by a distribution or by their statistical moments, and useful information may be extracted from them. The spectacular progress in quantum state manipulation with laser and magnetic cooling techniques emphasizes the need to treat atomic motion quantally rather than classically [2,3], and the timeliness of a quantum approach to time quantities. Much work has been carried out in the last two decades trying to formulate time observables theoretically and also to connect the abstract proposals with actual or idealized experiments. Central to these investigations have been the tunneling time, the arrival time, and the dwell time [1].

The dwell time of a particle in a region of space and its close relative, the delay time [4], are in particular rather fundamental quantities that characterize the duration of collision processes, the lifetime of unstable systems [5], the response to perturbations [6], ac conductance in mesoscopic conductors [7], or the properties of chaotic scattering [8]. In addition, the importance of dwell and delay times is underlined by their relation to the density of states, and to the virial expansion in statistical mechanics [9].

The theory of the quantum dwell time is quite peculiar and subtle in several respects [10,11]. To begin with, unlike other time quantities, there has been a broad consensus on its operator representation [5,6],

$$\hat{T}_D = \int_{-\infty}^{\infty} dt \hat{\chi}_{\mathcal{R}}(t), \tag{1}$$

where $\hat{\chi}_{\mathcal{R}}(t)$ is the (Heisenberg) projector onto a region of space, which we shall limit here to one dimension for simplicity, $\mathcal{R}=\{x: x_1 \leq x \leq x_2\}$,

$$\hat{\chi}_{\mathcal{R}}(t) = e^{i\hat{H}t/\hbar}\int_{x_1}^{x_2} dx|x\rangle\langle x|e^{-i\hat{H}t/\hbar}. \tag{2}$$

We shall also assume that the Hamiltonian holds a purely continuous spectrum with degenerate (delta-normalized) scattering eigenfunctions $|\phi_{\pm k}\rangle$ corresponding to incident plane waves $|\pm k\rangle$, with energy $E_k = k^2\hbar^2/(2m)$.

The operator $\hat{T}_D$ is positive definite and essentially self-adjoint. Moreover, being a "time duration" rather than a time instant, $\hat{T}_D$ commutes with the Hamiltonian without conflict with Pauli's theorem, and therefore it can be diagonalized in the eigenspace of $\hat{H}$. This simplifies the derivation of the corresponding quantum dwell-time distribution which, for a state $|\psi\rangle = |\psi(t=0)\rangle$, is formally given by[1]

$$\Pi(\tau) = \langle\psi|\delta(\hat{T}_D - \tau)|\psi\rangle. \tag{3}$$

Following the same manipulation done for the S operator in one-dimensional scattering theory [12], it is convenient to define an on-the-energy-shell 2×2 dwell-time matrix T, by factoring out an energy delta,

$$\langle\phi_k|\hat{T}_D|\phi'_k\rangle = \delta(E_k - E_{k'})\frac{|k|\hbar^2}{m}\mathsf{T}_{kk'}, \tag{4}$$

where $\langle\phi_k|\phi_{k'}\rangle = \delta(k-k')$ and

[1]We shall leave aside in this work other sources of fluctuations such as mixed states or ensembles of Hamiltonians. For these two cases one could consider distributions of *average* dwell times, whereas here we shall be interested in the distribution of the dwell time itself for pure states and a single Hamiltonian.

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$$\mathsf{T}_{kk'} = \langle \phi_k | \hat{\chi}_{\mathcal{R}} | \phi_{k'} \rangle \frac{hm}{|k|\hbar^2}, \quad E_k = E_{k'}. \tag{5}$$

In particular, T_{kk} is the average dwell time for a finite space region defined by Büttiker in the stationary regime [13],

$$\mathsf{T}_{kk} = \frac{1}{j(k)} \int_{x_1}^{x_2} dx |\phi_k(x)|^2, \tag{6}$$

where $j(k)$ is the incoming flux associated with $|\phi_k\rangle$.

Diagonalization of T leads generically to an interesting quantum peculiarity [14]: the existence of two different dwell-time eigenvalues. For free motion $t_{\pm}(k) = mL[1 \pm \sin(kL)/kL]/\hbar k$, $L = x_2 - x_1$, in clear contrast to the classical time $t_{\rm class} = mL/\hbar k$. As a consequence, the quantum dwell-time distribution will have a broader spread (variance) than the one for a corresponding ensemble of classical particles.

In spite of the nice properties of $\hat{T}_D$, a direct and sufficiently noninvasive measurement of the dwell time of a quantum particle in a region of space, so that the statistical moments are produced by averaging over individual dwell-time values, is yet to be discovered. If the particle is detected (and thus localized) at the entrance of the region of interest, its wave function is severely modified ("collapsed"), so that the times elapsed until a further detection when it leaves the region do not reproduce the ideal dwell-time operator distribution, and depend on the details of the localization method. Proposals for operational, i.e., measurement-based approaches to traversal times based on model detectors which study the effect of localization have been discussed by Palao *et al.* [15] and by Ruschhaupt [16]. All operational approaches to the quantum dwell time known so far provide in fact, and only indirectly, just the average, by deducing it from its theoretical relation to some other observable with measurable average. It is obtained, for example, by a "Larmor clock," using a weak homogeneous magnetic field in the region $\mathcal{R}$ and the amount of spin rotations of an incident spin-$\frac{1}{2}$ particle [13,17,18]. An optical analog is provided by the "Rabi clock" [19]. It can also be deduced from average passage times at the region boundaries [12], as well as by measuring the total absorption if a weak complex absorbing potential acts in the region [20–22]. This setup could be implemented with cold atoms and lasers as described in [14,23].

The expression for the average of the dwell time for time-dependent scattering processes in terms of the probability densities corresponds (in sharp contrast to its second moment, as shown below) to the classical expression for an ensemble of classical particles and it reads [24,25]

$$\langle \psi | \hat{T}_D | \psi \rangle = \int_{-\infty}^{\infty} dt \int_{x_1}^{x_2} dx |\psi(x,t)|^2 = \int_0^{\infty} dk |\langle k | \psi^{in} \rangle|^2 \mathsf{T}_{kk}, \tag{7}$$

where $\psi(x,t) = \int_0^\infty dk \langle \phi_k | \psi \rangle \exp(-i\hbar k^2 t/2m) \phi_k(x)$ is the time-dependent wave packet and we assume, here and in the rest of the paper, incident wave packets with positive momentum components. To write Eq. (7) use has been made of the standard scattering relation $\langle \phi_k | \psi \rangle = \langle k | \psi^{in} \rangle$, where $\langle x | k \rangle = (2\pi)^{-1/2} \exp(ikx)$, and ψ^{in} is the freely moving asymptotic incoming state of ψ. Integrals of the form (7) had been used to define time delays by comparing the free motion to that with a scattering center and taking the limit of infinite volume [26].

For a sample of further theoretical studies on the quantum dwell time see [9,14,27–35]. A recurrent topic has been its role and decomposition in tunneling collisions. Instead, we shall focus here on a different, so far overlooked, but rather fundamental aspect, namely, the measurability and physical implications of its second moment.

We shall generalize the approach by Pollak and Miller [36], who showed that the average stationary dwell time agrees with the first moment of a microcanonical flux-flux correlation function (FFCF). We shall demonstrate that this relation holds also for the second moment, and extend their analysis to the time-dependent (wave packet) case. The relation fails for third and higher moments and thus the FFCF contains only part of the information of the dwell-time distribution, although it is certainly the most relevant. We shall also discuss a possible scheme to measure FFCFs, thus paving the road toward experimental access to quantum features of the dwell-time distribution.

II. STATIONARY FLUX-FLUX CORRELATION FUNCTION

A connection between the average stationary dwell time and the first moment of a FFCF has been shown by Pollak and Miller [36]. They define a quantum microcanonical FFCF $C_{PM}(\tau,k) = \mathrm{Tr}\{\mathrm{Re}\, \hat{C}_{PM}(\tau,k)\}$ by means of the operator

$$\hat{C}_{PM}(\tau,k) = 2\pi\hbar[\hat{J}(x_2,\tau)\hat{J}(x_1,0) + \hat{J}(x_1,\tau)\hat{J}(x_2,0) - \hat{J}(x_1,\tau)\hat{J}(x_1,0) - \hat{J}(x_2,\tau)\hat{J}(x_2,0)]\delta(E_k - \hat{H}), \tag{8}$$

where $\hat{J}(x,t) = e^{i\hat{H}t/\hbar} \frac{1}{2m}[\hat{p}\delta(\hat{x}-x) + \delta(\hat{x}-x)\hat{p}] e^{-i\hat{H}t/\hbar}$ is the quantum-mechanical flux operator in the Heisenberg picture, and $\hat{p}$ and $\hat{x}$ are the momentum and position operators.

The motivation for this definition stems from classical mechanics and can be understood intuitively: Eq. (8) counts flux correlations of particles entering $\mathcal{R}$ through x_1 (x_2) and leaving it through x_2 (x_1) a time τ later. Moreover, particles may be reflected and may leave the region $\mathcal{R}$ through its entrance point. This is described by the last two terms, where the minus sign compensates for the change of sign of a back-moving flux. Note that these negative terms lead to a self-correlation contribution that diverges for $\tau \to 0$.

We review in the following the derivation of the average correlation time and show afterward that a similar relation for the second moment holds. As in the rest of the paper, we shall only consider positive incident momenta, so that we shall actually deal with $\hat{C}_{PM}^{+}$, substituting $\delta(E_k - \hat{H})$ by $\delta^{+}(E_k - \hat{H}) \coloneqq \delta(E_k - \hat{H})\Lambda_{+}$, where Λ_{+} is the projector onto the subspace of eigenstates of H with positive momentum incidence. First of all, we note that, by means of the continuity equation,

$$-\frac{d}{dx}\hat{J}(x,t)=\frac{d}{dt}\hat{\rho}(x,t), \tag{9}$$

where $\hat{\rho}(x,t)=e^{i\hat{H}t/\hbar}\delta(\hat{x}-x)e^{-i\hat{H}t/\hbar}$ is the (Heisenberg) density operator, $\hat{C}^{+}_{PM}(\tau,k)$ can be written as

$$\hat{C}^{+}_{PM}(\tau,k)=-2\pi\hbar\left(\frac{d}{d\tau}\hat{\chi}_{\mathcal{R}}(\tau)\right)\left(\frac{d}{dt}\hat{\chi}_{\mathcal{R}}(t)\right)_{t=0}\delta^{+}(E_k-\hat{H}). \tag{10}$$

By a partial integration and using the Heisenberg equation of motion the first moment of the Pollak-Miller correlation function is given by

$$\mathrm{Tr}\left\{\int_0^\infty d\tau\,\tau\hat{C}^{+}_{PM}(\tau,k)\right\} = \mathrm{Tr}\left\{2\pi\hbar\int_0^\infty d\tau\hat{\chi}_{\mathcal{R}}(\tau)\frac{1}{i\hbar}[\hat{\chi}_{\mathcal{R}}(0),\hat{H}]\delta^{+}(E_k-\hat{H})\right\}.$$

Boundary terms of the form $\lim_{\tau\to\infty}\tau^{\gamma}\hat{\chi}_{\mathcal{R}}(\tau)$, $\gamma=0,1,2$, are omitted here and in the following. This omission can be justified by recalling that physical states must be time-dependent and square-integrable so that the contribution of these terms should vanish when an integration over stationary wave functions is performed to account for the wave-packet dynamics. (In the next section we shall discuss explicitly a time-dependent version of the correlation function.) For potential scattering the probability density decays generically as τ^{-3}, which assures a finite dwell-time average, but for free motion it decays as τ^{-1} [37], making τ_D infinite, unless the momentum wave function vanishes at $k=0$ sufficiently fast as k tends to zero [14].

Writing the commutator explicitly and using the cyclic property of the trace gives

$$\mathrm{Tr}\left\{\int_0^\infty d\tau\,\tau\hat{C}^{+}_{PM}(\tau,k)\right\} = \mathrm{Tr}\left\{2\pi\hbar\int_0^\infty d\tau\left(-\frac{d}{d\tau}\hat{\chi}_{\mathcal{R}}(\tau)\right)\hat{\chi}_{\mathcal{R}}(0)\delta^{+}(E_k-\hat{H})\right\},$$

and integration over τ yields the final result of Pollak and Miller,

$$\mathrm{Tr}\left\{\int_0^\infty d\tau\,\tau\hat{C}^{+}_{PM}(\tau,k)\right\}=2\pi\hbar\,\mathrm{Tr}\{\hat{\chi}_{\mathcal{R}}(0)\delta^{+}(E_k-\hat{H})\}=\mathsf{T}_{kk}. \tag{11}$$

Expressing the trace in the basis $|\phi_k\rangle$ gives back the stationary dwell time of Eq. (6), i.e., the diagonal element of the on-the-energy-shell dwell-time operator, T_{kk}.

The calculation of the average in [36] is different in some respects. (a) The coordinates x_1 and x_2 are taken to minus and plus infinity, but it can be carried out for finite values modifying Eq. (8) of [36] accordingly. (b) Formally there are no explicit boundary terms at infinity but a regularization is required in Eq. (16) of [36], which is justified for wave packets. (c) $\delta(E_k-\hat{H})$ is used instead of $\delta^{+}(E_k-\hat{H})$. That simply provides an additional contribution for negative momenta parallel to the one obtained here for positive momenta. (d) In our derivation the average correlation time is found to be real directly, in spite of the fact that $\hat{C}^{+}_{PM}(\tau,k)$ is not self-adjoint, whereas in [36] the real part is taken. [The discussion of the imaginary time average in [36] is based on a modified version of Eq. (8).]

Next, we will show that the second moment of the Pollak-Miller FFCF equals the second moment of T. This was not observed in Ref. [36]. Proceeding in a similar way as above, see the Appendix,

$$\mathrm{Tr}\left\{\mathrm{Re}\int_0^\infty d\tau\tau^2\hat{C}^{+}_{PM}(\tau,k)\right\} = \frac{4\pi^2m^2}{\hbar^2k^2}\left[\left(\int_{x_1}^{x_2}dx|\phi_k(x)|^2\right)^2+\left|\int_{x_1}^{x_2}dx\phi_k^{*}(x)\phi_{-k}(x)\right|^2\right] = (\mathsf{T}^2)_{kk}. \tag{12}$$

This shows that the relation between dwell times and flux-flux correlation functions goes beyond average values and that $C^{+}_{PM}(\tau,k)$ includes quantum features of the dwell time: note that the first summand in $[\cdots]$, Eq. (12), is nothing but $(\mathsf{T}_{kk})^2$, whereas the second summand is positive, which allows for a nonzero on-the-energy-shell dwell-time variance $(\mathsf{T}^2)_{kk}-(\mathsf{T}_{kk})^2$. We insist that the stationary state considered has positive momentum, $\phi_k(x)$, $k>0$, but this second term implies the degenerate partner $\phi_{-k}(x)$ as well, and is generically nonzero.

The question arises if these connections hold for the other moments of $C^{+}_{PM}(\tau,k)$. The answer is no, as we will show in the next section with a more general approach.

III. TIME-DEPENDENT FLUX-FLUX CORRELATION FUNCTION

In the following we present a time-dependent version of the above flux-flux correlation function and show its relation to dwell times. So far, FFCFs have been mostly considered in chemical physics to define reaction rates for microcanonical or canonical ensembles [38]. However, a physically intuitive time-dependent version can be defined in terms of the operator

$$\hat{C}(\tau)=\int_{-\infty}^{\infty}dt[\hat{J}(x_2,t+\tau)\hat{J}(x_1,t)+\hat{J}(x_1,t+\tau)\hat{J}(x_2,t) - \hat{J}(x_1,t+\tau)\hat{J}(x_1,t)-\hat{J}(x_2,t+\tau)\hat{J}(x_2,t)], \tag{13}$$

which leads to the flux-flux correlation function

$$C(\tau)=\langle\mathrm{Re}\,\hat{C}(\tau)\rangle_{\psi}, \tag{14}$$

where the real part is taken to symmetrize the non-self-adjoint operator $\hat{C}(\tau)$ as before.

As in the stationary case, Eq. (14) counts flux correlations of particles entering $\mathcal{R}$ through x_1 or x_2 at a time t and leaving it either through x_1 or x_2 a time τ later. Moreover, one has to integrate over the entrance time t. It is easy to show that the first moment of the classical version of Eq.

(13), where $\hat{J}$ is replaced by the classical dynamical variable of the flux, gives the average of the classical dwell time.

As in Eq. (10), we may rewrite $\hat{C}(\tau)$ in the form

$$\hat{C}(\tau) = -\int_{-\infty}^{\infty} dt \frac{d}{d\tau}\hat{\chi}_{\mathcal{R}}(\hat{x},t+\tau)\frac{d}{dt}\hat{\chi}_{\mathcal{R}}(\hat{x},t). \quad (15)$$

First of all we note that the FFCF $C(\tau)$ is not normalized; in fact its negative contributions exactly cancel the positive ones,

$$\int_0^{\infty} d\tau \hat{C}(\tau) = \int_{-\infty}^{\infty} dt \hat{\chi}_{\mathcal{R}}(t)\frac{d}{dt}\hat{\chi}_{\mathcal{R}}(t) = 0. \quad (16)$$

Next we derive the average of the time-dependent correlation function. With a partial integration one finds

$$\int_0^{\infty} d\tau\, \tau \hat{C}(\tau) = \int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \hat{\chi}_{\mathcal{R}}(\hat{x},t+\tau)\frac{d}{dt}\hat{\chi}_{\mathcal{R}}(\hat{x},t).$$

A second partial integration with respect to t, replacing d/dt by $d/d\tau$ and integrating over τ gives

$$\int_0^{\infty} d\tau\, \tau \hat{C}(\tau) = \int_{-\infty}^{\infty} dt \hat{\chi}^2_{\mathcal{R}}(\hat{x},t) = \int_{-\infty}^{\infty} dt \hat{\chi}_{\mathcal{R}}(\hat{x},t) = \hat{T}_D, \quad (17)$$

where the projector property of $\hat{\chi}_{\mathcal{R}}$ has been used. Equation (17) generalizes the result of Pollak and Miller to time-dependent dwell times.

A similar calculation can be performed for the second moment of $C(\tau)$. After three partial integrations with vanishing boundary contributions to get rid of the factor τ^2 one obtains

$$\int_0^{\infty} d\tau\, \tau^2 \hat{C}(\tau) = 2\int_{-\infty}^{\infty} dt \int_0^{\infty} d\tau \hat{\chi}_{\mathcal{R}}(\hat{x},t+\tau)\hat{\chi}_{\mathcal{R}}(\hat{x},t).$$

We evaluate the real part of this expression. Making the substitutions $t+\tau \to t$ and $\tau \to -\tau$ in the complex conjugated term, we find

$$\mathrm{Re}\int_0^{\infty} d\tau\, \tau^2 \hat{C}(\tau) = \hat{T}_D^2. \quad (18)$$

IV. EXAMPLE: FREE MOTION

In this section we study the simple case of free motion to show the relations between dwell times and FFCF. For a stationary flux of particles with energy E_k, $k>0$, described by $\phi_k(x) = \langle x|k\rangle = (2\pi)^{-1/2}e^{ikx}$, the first three moments of the ideal dwell-time distribution on the energy shell are given by

$$\mathsf{T}_{kk} = \frac{mL}{\hbar k}, \quad (19)$$

$$(\mathsf{T}^2)_{kk} = \frac{m^2L^2}{\hbar^2k^2}\left(1 + \frac{\sin^2(kL)}{k^2L^2}\right), \quad (20)$$

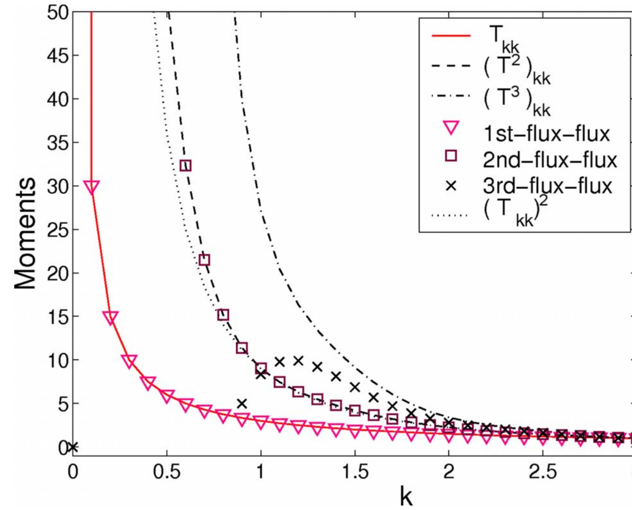

FIG. 1. (Color online) Comparison of the first three moments: T_{kk}, $(\mathsf{T}^2)_{kk}$, and $(\mathsf{T}^3)_{kk}$ (dotted-dashed line) with the corresponding moments of the flux-flux correlation function, for a free-motion stationary state with fixed k. $(\mathsf{T}_{kk})^2$ is also shown (dotted line). $\hbar = m = 1$ and $L=3$.

$$(\mathsf{T}^3)_{kk} = \frac{m^3L^3}{\hbar^3k^3}\left(1 + 3\frac{\sin^2(kL)}{k^2L^2}\right). \quad (21)$$

As proved above, the first two moments agree with the corresponding moments of the Pollak-Miller FFCF, but for the third moment we obtain

$$\mathrm{Tr}\left\{\mathrm{Re}\int_0^{\infty} d\tau\, \tau^3 \hat{C}^+_{PM}(\tau,k)\right\} = \frac{m^3L^3}{\hbar^3k^3}\left[1 - \frac{3[1+\cos^2(kL)]}{k^2L^2} + \frac{3\sin(2kL)}{L^3k^3}\right]. \quad (22)$$

In Fig. 1 the first three moments are compared. The agreement between $(\mathsf{T}^3)_{kk}$ and Eq. (22) is very good for large values of k, but they clearly differ for small k.

However, the agreement of the first two moments suggests a similar behavior of $\Pi(\tau)$ and $C(\tau)$. To calculate $\Pi(\tau)$ for a wave function $\tilde{\psi}(k) \coloneqq \langle k|\psi\rangle$ with only positive momentum components we use the wave-number representation taking into account the bimodality of the dwell time, $t_{\pm}(k) = mL[1 \pm \sin(kL)/kL]/\hbar k$,[2]

$$\Pi(\tau) = \frac{1}{2}\sum_j \sum_{\gamma=\pm} \frac{|\tilde{\psi}(k_j^{\gamma}(\tau))|^2}{|F'_{\gamma}(k_j^{\gamma}(\tau))|}, \quad (23)$$

where the j sum is over the solutions $k_j^{\gamma}(\tau)$ of the equation $F_{\gamma}(k) \equiv t_{\gamma}(k) - \tau = 0$ and the derivative is with respect to k. In particular, we use the following wave function for the calculation [12]:

[2] The corresponding eigenstates are $|t_{\pm}(k)\rangle = \{|k\rangle \pm \exp[ik(x_1+x_2)]|-k\rangle\}/\sqrt{2}$.

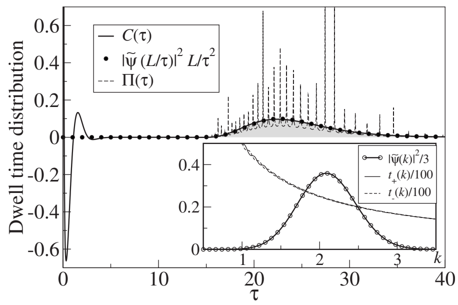

FIG. 2. Comparison of dwell-time distribution $\Pi(\tau)$ (dashed line) and flux-flux correlation function $C(\tau)$ (solid line) for the freely moving wave packet (24). Furthermore, the alternative free-motion dwell-time distribution $\pi(\tau)$, Eq. (28), is plotted (circles). The inset shows the momentum distribution and the eigenvalues $t_{\pm}(k)$. We set $\hbar=m=1$ and $|x_0|$ large enough to avoid overlap of the initial state with the space region $\mathcal{R}=[0,50]$. $k_0=2$, $\Delta k=0.4$, and $\alpha=0.5$.

$$\tilde{\psi}(k)=N(1-e^{-\alpha k^2})e^{-(k-k_0)^2/[4(\Delta k)^2]}e^{-ikx_0}\Theta(k), \tag{24}$$

where N is the normalization constant and $\Theta(k)$ the step function. For the free flux-flux correlation function we write

$$C(\tau)=\mathrm{Re}\int_0^\infty dk\int_0^\infty dk'\,\tilde{\psi}^*(k)\tilde{\psi}(k')\langle k|\hat{C}(\tau)|k'\rangle, \tag{25}$$

and $C_{kk'}(\tau)=\langle k|\hat{C}(\tau)|k'\rangle$ in the free case is given by

$$C_{kk'}(\tau)=\frac{m}{2\pi\hbar k}\delta(k-k')\frac{d^2}{d\tau^2}[2f(\hbar k\tau/m) - f(\hbar k\tau/m-L)-f(\hbar k\tau/m+L)], \tag{26}$$

where

$$f(x)=-2e^{imx^2/(2\hbar\tau)}\left(\frac{i\pi\hbar\tau}{2m}\right)^{1/2}+i\pi x\,\mathrm{erfi}\left(\sqrt{\frac{im}{2\hbar\tau}}x\right). \tag{27}$$

The result is shown in Fig. 2. The FFCF shows a hump around the mean dwell time, as expected (the area under this hump is 0.9993), but it strongly oscillates for small τ and diverges for $\tau\to 0$. As discussed above, this is due to the self-correlation contribution of wave packets which are at x_1 or x_2 at the times t and $t+\tau$ *without* changing the direction of motion in between. A similar feature has been observed in a traversal-time distribution derived by means of a path integral approach [39].

In contrast, $\Pi(\tau)$ behaves regularly for $\tau\to 0$, but shows peaks in the region of the hump. This is because the denominator of Eq. (23) becomes zero if the slope of the eigenvalues $t_{\pm}(k)$ is zero, which occurs at every crossing point of $t_+(k)$ and $t_-(k)$.

Another dwell-time distribution for free motion can be defined based on the operator $\hat{t}_D=mL/|\hat{p}|$, obtained heuristically from quantization of the classical dwell time. The eigenfunctions of this operator are momentum eigenfunctions, $|\pm k\rangle$, $k>0$, and the corresponding eigenvalues are twofold degenerate and equal to the classical time, $mL/\hbar|k|$. The distribution of dwell times for this operator, as always for positive-momentum states, is given by

$$\pi(\tau)=\frac{mL}{\hbar\tau^2}\left|\tilde{\psi}\left(\frac{mL}{\hbar\tau}\right)\right|^2. \tag{28}$$

The distribution $\pi(\tau)$ agrees with $C(\tau)$ in the region near the average dwell time and tends to zero for $\tau\to 0$. However, it does not show the resonance peaks of $\Pi(\tau)$. The on-the-energy-shell version of $\hat{t}_D$, t, is also worth examining. By factoring out an energy delta function as in Eq. (4) we get for a plane wave $|k\rangle$ the average $\mathsf{t}_{kk}=mL/(\hbar k)$, which is equal to T_{kk}, but the second moment differs, $(\mathsf{t}^2)_{kk}=(\mathsf{t}_{kk})^2=(\mathsf{T}_{kk})^2\leqslant(\mathsf{T}^2)_{kk}$, see Fig. 1; in other words, the variance on the energy shell is zero since only one eigenvalue is possible for t. Contrast this with the extra term in Eq. (20), which again emphasizes the nonclassicality of the dwell-time operator $\hat{T}_D$ and its quantum fluctuation.

Could both $\hat{T}_D$ and $\hat{t}_D$ be physically significant? In the absence of a direct dwell-time measurement, this depends on their relation to other observables. The present results indicate that the second moment of the flux-flux correlation function is related to the former and not to the latter, providing indirect support for the physical relevance of the dwell-time resonance peaks, but other observables could behave differently.

V. DISCUSSION

We have demonstrated that the relationship found by Pollak and Miller [36] between the first moment of a distribution FFCF and the average stationary dwell time is also valid for the second moment and for flux-flux correlations of wave packets. On the other hand, this relationship is not valid for the third moment. While this brings dwell-time information closer to experimental realization, the difficulty is translated onto the measurement of the FFCF, which is not necessarily an easy task. The simplest approximation is to substitute in C the expectation of the product of two flux operators by the product of their expectation values (the product of the current densities). Using the wave packet of Eq. (24), we have compared the second moment calculated with the full expression (14), $\langle\hat{T}_D^2\rangle_C$, and with this approximation, $\langle\hat{T}_D^2\rangle_{C_0}$, in Fig. 3. The two results approach as $\Delta_k\to 0$. Other factors that make the approximation better are the increase of L and/or of k_0.

The exact result can in fact be approached systematically, still making use of ordinary current densities, as follows: First we decompose $\hat{J}(x_i,t+\tau)\hat{J}(x_j,t)$ by means of the resolution of the identity

$$\hat{1}=\hat{P}+\hat{Q}, \tag{29}$$

$$\hat{P}=|\psi\rangle\langle\psi|, \tag{30}$$

so that

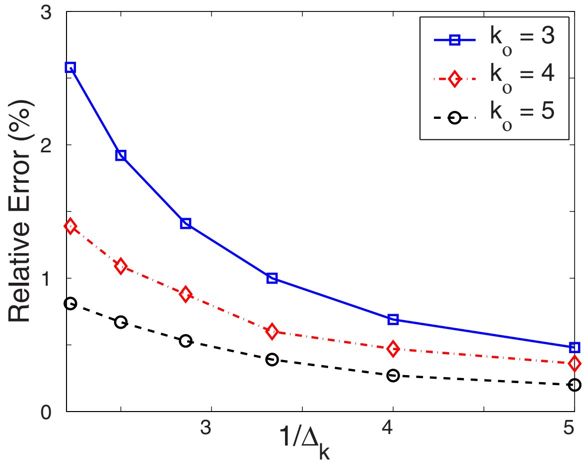

FIG. 3. (Color online) Comparison of the relative error of the second moment using the approximation $C_0(\tau)$ instead of $C(\tau)$ for the freely moving wave packet of Eq. (24), $\alpha=0.5$, $\hbar=m=1$, and $L=100$.

$$\hat{J}(x_i,t+\tau)\hat{J}(x_j,t) = \hat{J}(x_i,t+\tau)(|\psi\rangle\langle\psi| + \hat{Q})\hat{J}(x_j,t). \quad (31)$$

It is useful to decompose $\hat{Q}$ further in terms of a basis of states orthogonal to $|\psi\rangle$ and to each other, $\{|\psi_j^Q\rangle\}$,

$$\hat{Q} = \sum_j |\psi_j^Q\rangle\langle\psi_j^Q|, \quad (32)$$

that could be generated systematically, e.g., by means of a Gram-Schmidt orthogonalization. Now we can split Eq. (13),

$$\hat{C}(\tau) = \hat{C}_0(\tau) + \hat{C}_1(\tau), \quad (33)$$

where

$$\hat{C}_0(\tau) = \int_{-\infty}^{\infty} dt[\hat{J}(x_2,t+\tau)|\psi\rangle\langle\psi|\hat{J}(x_1,t) + \hat{J}(x_1,t+\tau)|\psi\rangle \times\langle\psi|\hat{J}(x_2,t) - \hat{J}(x_1,t+\tau)|\psi\rangle\langle\psi|\hat{J}(x_1,t) - \hat{J}(x_2,t+\tau)|\psi\rangle\langle\psi|\hat{J}(x_2,t)], \quad (34)$$

$$\hat{C}_1(\tau) = \sum_j \int_{-\infty}^{\infty} dt[\hat{J}(x_2,t+\tau)|\psi_j^Q\rangle\langle\psi_j^Q|\hat{J}(x_1,t) + \hat{J}(x_1,t+\tau)|\psi_j^Q\rangle \times\langle\psi_j^Q|\hat{J}(x_2,t) - \hat{J}(x_1,t+\tau)|\psi_j^Q\rangle\langle\psi_j^Q|\hat{J}(x_1,t) - \hat{J}(x_2,t+\tau)|\psi_j^Q\rangle\langle\psi_j^Q|\hat{J}(x_2,t)]. \quad (35)$$

Similarly, we define $C(\tau)=C_0(\tau)+C_1(\tau)$ by taking the real part of $\langle\psi|\hat{C}_0(\tau)+\hat{C}_1(\tau)|\psi\rangle$. C_0 is the zeroth order approximation discussed before and only involves ordinary, measurable current densities [3]. The nondiagonal terms from C_1, $\langle\psi|\hat{J}(x_i,t)|\psi_j^Q\rangle\langle\psi_j^Q|\hat{J}(x_j,t+\tau)|\psi\rangle$ can also be related to ordinary fluxes (diagonal elements of $\hat{J}$) by means of the auxiliary states

$$|\psi_1\rangle = |\psi\rangle + |\psi_j^Q\rangle,$$

$$|\psi_2\rangle = |\psi\rangle + i|\psi_j^Q\rangle,$$

$$|\psi_3\rangle = |\psi\rangle - i|\psi_j^Q\rangle, \quad (36)$$

since one easily finds that

$$\langle\psi|\hat{J}(x,t)|\psi_j^Q\rangle = \frac{1}{2}\langle\psi_1|\hat{J}(x,t)|\psi_1\rangle - \frac{1}{4}\langle\psi_2|\hat{J}(x,t)|\psi_2\rangle - \frac{1}{4}\langle\psi_3|\hat{J}(x,t)|\psi_3\rangle + \frac{i}{4}\langle\psi_3|\hat{J}(x,t)|\psi_3\rangle - \frac{i}{4}\langle\psi_2|\hat{J}(x,t)|\psi_2\rangle. \quad (37)$$

To summarize, the present paper provides a route of access to the second moment of the quantum dwell time through flux-flux correlation functions. This is interesting because the second moment is characteristically quantum and, unlike the first moment, it differs structurally from (and is larger than) the corresponding classical quantity: On the energy shell the dwell time shows a quantum fluctuation (nonzero variance) which vanishes classically. While the analysis of the quantum dwell time has been mostly limited to its average in the existing studies, the present results motivate further research on the role played by the (pure-state, single Hamiltonian) second moment of the dwell time in fields such as lifetime fluctuations, chaotic systems, conductivity,[3] or time-frequency metrology. Many fundamental and applied questions can be posed from here. For example, is the second moment affecting the quality factor of ultracold atomic clocks? The time spent by the atom in a spatial region determines their stability, which increases in principle for slower atoms, but quantum motion effects have been shown to become more and more relevant as the atomic velocity decreases [40,41]. This and other intriguing questions on the quantum dwell time are left for separate studies.

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APPENDIX: DERIVATION OF EQ. (12)

The starting point is

$$\mathcal{I} = \mathrm{Tr}\left\{\int_0^{\infty} d\tau\, \tau^2 \hat{C}_{PM}^{+}(\tau,k)\right\}. \quad (A1)$$

Integrating by parts, neglecting the term at infinity, and using Heisenberg's equation of motion, it takes the form

[3]The second moment of the dwell time determines in particular the charge relaxation resistance and thus the ac conductivity in nanostructured mesoscopic capacitors [7].

$$\mathcal{I} = \frac{4\pi m}{i\hbar^2 k} \int_0^\infty d\tau\, \tau \langle \phi_k | \hat{\chi}_R(\tau) [\hat{\chi}_R(0), \hat{H}] | \phi_k \rangle. \tag{A2}$$

Making use of the fact that ϕ_k is an eigenstate of $\hat{H}$, and reordering,

$$\mathcal{I} = \frac{4\pi m}{i\hbar^2 k} \int_0^\infty d\tau\, \tau \langle \phi_k | [\hat{H}, \hat{\chi}_R(\tau)] \hat{\chi}_R(0) | \phi_k \rangle. \tag{A3}$$

Integrating by parts again and using Heisenberg's equation once more,

$$\mathcal{I} = \frac{4\pi m}{\hbar k} \int_0^\infty d\tau \langle \phi_k | \hat{\chi}_R(\tau) \hat{\chi}_R(0) | \phi_k \rangle. \tag{A4}$$

Now the real part is taken,

$$\mathrm{Re}(\mathcal{I}) = \frac{\mathcal{I} + \mathcal{I}^*}{2} = \frac{2\pi m}{\hbar k} \int_0^\infty d\tau \langle \phi_k | [\hat{\chi}_R(\tau)\hat{\chi}_R(0) + \hat{\chi}_R(0)\hat{\chi}_R(\tau)] \times | \phi_k \rangle, \tag{A5}$$

and resolutions of the identity are introduced,

$$\mathrm{Re}(\mathcal{I}) = \left\{ \frac{2\pi m}{\hbar k} \int_0^\infty d\tau \int_{-\infty}^\infty dk' \int_{x_1}^{x_2} dx \int_{x_1}^{x_2} dx'\, e^{i(E_k - E_{k'})\tau/\hbar} \times \phi_k^*(x)\phi_{k'}(x)\phi_{k'}^*(x')\phi_k(x') \right\} + \text{c.c.}, \tag{A6}$$

where c.c. means complex conjugate. Making the changes $\tau \to -\tau$ and $x, x' \to x', x$ in the c.c. term, it takes the same form as the first one, but with the time integral from $-\infty$ to 0. Adding the two terms, the τ integral provides an energy delta function that can be separated into two deltas which select $k' = \pm k$ to arrive at Eq. (12).

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