Supplementary material for "Coherent Backscattering in Fock Space: a Signature of Quantum Many-Body Interference in Interacting Bosonic Systems"

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The semiclassical propagator cannot be directly obtained in Fock state representation, since the Fock states form a discrete basis rather than a continuous one as required by the path integral formalism. To solve this problem, we first derive a semiclassical propagator in quadrature representation and then project the result on Fock states.

The quadrature eigenstates $|\mathbf{q}\rangle \equiv |q_1, \ldots, q_L\rangle$ and $|\mathbf{p}\rangle \equiv |p_1, \ldots, p_L\rangle$ are defined as the eigenstates of linear hermitian combinations of the creation and annihilation operators associated with the single-particle orbitals χ_α ($\alpha = 1, \ldots, L$), *i.e.*,

$$b\left(\hat{a}_\alpha + \hat{a}_\alpha^\dagger\right)|\mathbf{q}\rangle = q_\alpha |\mathbf{q}\rangle \tag{1}$$

$$-\mathrm{i}b\left(\hat{a}_\alpha - \hat{a}_\alpha^\dagger\right)|\mathbf{p}\rangle = p_\alpha |\mathbf{p}\rangle, \tag{2}$$

with an arbitrary but fixed scale b. These quadrature eigenstates obey the resolutions of unity

$$\int \mathrm{d}^L q\, |\mathbf{q}\rangle\langle\mathbf{q}| = \hat{1} = \int \mathrm{d}^L p\, |\mathbf{p}\rangle\langle\mathbf{p}| \tag{3}$$

and their overlap matrix elements are given by

$$\langle\mathbf{q}|\mathbf{q}'\rangle = \delta\left(\mathbf{q} - \mathbf{q}'\right), \tag{4}$$

$$\langle\mathbf{p}|\mathbf{p}'\rangle = \delta\left(\mathbf{p} - \mathbf{p}'\right), \tag{5}$$

$$\langle\mathbf{q}|\mathbf{p}\rangle = \frac{1}{2b\sqrt{\pi}} \exp\left(\frac{\mathrm{i}\mathbf{p}\cdot\mathbf{q}}{2b^2}\right). \tag{6}$$

Following the usual steps to derive the Feynman propagator (*i.e.,* splitting up the exponential into a product of N exponentials, inserting unity operators in terms of $\hat{\mathbf{q}}$ and $\hat{\mathbf{p}}$ between each pair of exponentials, and taking the limit $N \to \infty$), we find for the Hamiltonian

$$\hat{H} = \sum_{\alpha\beta} h_{\alpha\beta} \hat{a}_\alpha^\dagger \hat{a}_\beta + \frac{1}{2} \sum_{\alpha\beta\mu\sigma} V_{\alpha\beta\mu\sigma} \hat{a}_\alpha^\dagger \hat{a}_\beta \hat{a}_\mu^\dagger \hat{a}_\sigma \tag{7}$$

[see Eq. (2) in the Letter] a path integral representation of the propagator in quadrature representation as

$$K\left(\mathbf{q}^{(\mathrm{f})}, \mathbf{q}^{(\mathrm{i})}, t\right) = \lim_{N\to\infty} \int \mathrm{d}\mathbf{q}^{(1)} \cdots \int \mathrm{d}\mathbf{q}^{(N-1)} \int \frac{\mathrm{d}\mathbf{p}^{(1)}}{4\pi b^2} \cdots \int \frac{\mathrm{d}\mathbf{p}^{(N)}}{4\pi b^2} \prod_{k=1}^{N} \exp\left[\frac{\mathrm{i}}{2b^2}\mathbf{p}^{(k)}\cdot\left(\mathbf{q}^{(k)} - \mathbf{q}^{(k-1)}\right)\right.$$
$$\left. - \frac{\mathrm{i}\tau}{\hbar} \sum_{\alpha,\beta=1}^{L} h_{\alpha\beta} (\psi_\alpha^{(k)})^* \psi_\beta^{(k)} - \frac{\mathrm{i}\tau}{2\hbar} \sum_{\alpha,\beta\mu,\sigma=1}^{L} V_{\alpha\beta\mu\sigma} (\psi_\alpha^{(k)})^* (\psi_\mu^{(k)})^* \psi_\beta^{(k)} \psi_\sigma^{(k)}\right], \tag{8}$$

with $2b\boldsymbol{\psi}^{(k)} \equiv \mathbf{q}^{(k-1)} + \mathrm{i}\mathbf{p}^{(k)}$, $2b(\boldsymbol{\psi}^{(k)})^* \equiv \mathbf{q}^{(k-1)} - \mathrm{i}\mathbf{p}^{(k)}$, and $\tau \equiv t/N$. Calculating the integrals in stationary phase approximation and finally taking the limit $N \to \infty$ yields the van-Vleck-Gutzwiller propagator

$$K\left(\mathbf{q}^{(\mathrm{f})}, \mathbf{q}^{(\mathrm{i})}, t\right) = \frac{1}{(-2\pi\mathrm{i}\hbar)^{L/2}} \times \sum_\gamma \sqrt{\det \frac{\partial^2 R_\gamma}{\partial\mathbf{q}^{(\mathrm{i})}\partial\mathbf{q}^{(\mathrm{f})}}}\, \mathrm{e}^{\mathrm{i}R_\gamma/\hbar} \tag{9}$$

where the sum runs over all possible classical trajectories defined by the equation of motion

$$\mathrm{i}\hbar \frac{\partial\psi_\alpha(s)}{\partial s} = \sum_{\beta=1}^{L} h_{\alpha\beta}\psi_\beta(s) + \sum_{\beta,\mu,\sigma=1}^{L} V_{\alpha\beta\mu\sigma}\psi_\mu^*(s)\psi_\beta(s)\psi_\sigma(s) \tag{10}$$

and the boundary conditions $2b\mathrm{Re}[\boldsymbol{\psi}(0)] = \mathbf{q}^{(\mathrm{i})}$ and $2b\mathrm{Re}[\boldsymbol{\psi}(t)] = \mathbf{q}^{(\mathrm{f})}$. R_γ is the classical action given by

$$R_\gamma\left(\mathbf{q}^{(\mathrm{f})},\mathbf{q}^{(\mathrm{i})},t\right)=\int_0^t \mathrm{d}s\left\{\frac{\hbar}{2b^2}\mathbf{p}(s)\cdot\dot{\mathbf{q}}(s)-\sum_{\alpha,\beta=1}^{L}h_{\alpha\beta}\psi_\alpha^*(s)\psi_\beta(s)-\frac{1}{2}\sum_{\alpha,\beta,\mu,\sigma=1}^{L}V_{\alpha\beta\mu\sigma}\psi_\alpha^*(s)\psi_\beta(s)\psi_\mu^*(s)\psi_\sigma(s)\right\} \quad (11)$$

with $\mathbf{q}(s)\equiv 2b\mathrm{Re}[\boldsymbol{\psi}(s)]$ and $\mathbf{p}(s)\equiv 2b\mathrm{Im}[\boldsymbol{\psi}(s)]$ evaluated along the trajectory γ.

We now want to project the result onto Fock states. To this end, we need the overlap

$$\langle n|q\rangle=\frac{1}{\sqrt{2^n n!\sqrt{2\pi}b}}\exp\left(-\frac{q^2}{4b^2}\right)H_n\left(\frac{q}{\sqrt{2}b}\right) \quad (12)$$

of a quadrature eigenstate $|q\rangle$ with a Fock state $|n\rangle$ associated with an individual single-particle orbital. For large n, we can employ the WKB approximation for the Hermite polynomials H_n, which yields

$$\langle n|q\rangle\simeq\frac{\sqrt{2/\pi}}{(4b^2n-q^2)^{1/4}} \times\cos\left[\frac{q}{4b^2}\sqrt{4b^2\left(n+1/2\right)-q^2}\right] \quad (13)$$

within the oscillatory region $|q|\leq 2b\sqrt{n}$. Since $\langle n|q\rangle$ decreases exponentially for larger values of $|q|$, we can restrict the integration necessary for the projection onto Fock states to the oscillatory region $|q|\leq 2b\sqrt{n}$.

With this restriction, we substitute $q_\alpha^{(\mathrm{i/f})}\mapsto\theta_\alpha^{(\mathrm{i/f})}$ ($\alpha\in\{1,\ldots,L\}$) with $\theta_\alpha^{(\mathrm{i/f})}\in[-\pi,\pi]$ defined through

$$q_1^{(\mathrm{i})}\equiv 2b\sqrt{n_1^{(\mathrm{i})}+1/2}\cos\left(\theta_1^{(\mathrm{i})}\right), \quad (14)$$

$$q_1^{(\mathrm{f})}\equiv 2b\sqrt{n_1^{(\mathrm{f})}+1/2}\cos\left(\theta_1^{(\mathrm{f})}+\theta_1^{(\mathrm{i})}\right), \quad (15)$$

as well as

$$q_\alpha^{(\mathrm{i/f})}\equiv 2b\sqrt{n_\alpha^{(\mathrm{i/f})}+1/2}\cos\left(\theta_\alpha^{(\mathrm{i/f})}+\theta_1^{(\mathrm{i})}\right) \quad (16)$$

for $\alpha=2,\ldots,L$. The integrations over $\theta_1^{(\mathrm{f})},\ldots,\theta_L^{(\mathrm{f})},\theta_2^{(\mathrm{i})},\ldots,\theta_L^{(\mathrm{i})}$ can now be performed in stationary phase approximation. This selects trajectories that satisfy

$$\psi_1(t)=\sqrt{n_1^{(\mathrm{f})}+1/2}\exp\left\{\mathrm{i}\left(\theta_1^{(\mathrm{f})}+\theta_1^{(\mathrm{i})}\right)\right\}, \quad (17)$$

as well as

$$\psi_\alpha(0)=\sqrt{n_\alpha^{(\mathrm{i})}+1/2}\exp\left\{\mathrm{i}\left(\theta_\alpha^{(\mathrm{f})}+\theta_1^{(\mathrm{i})}\right)\right\} \quad (18)$$

$$\psi_\alpha(t)=\sqrt{n_\alpha^{(\mathrm{f})}+1/2}\exp\left\{\mathrm{i}\left(\theta_\alpha^{(\mathrm{f})}+\theta_1^{(\mathrm{i})}\right)\right\} \quad (19)$$

for $\alpha=2,\ldots,L$. Since the classical equations of motion preserve $|\psi_1(t)|^2+\ldots+|\psi_L(t)|^2$, these stationary phase conditions already imply $|\psi_1(0)|^2=n_1^{(\mathrm{i})}+1/2$ provided the final state $\left|\mathbf{n}^{(\mathrm{f})}\right\rangle$ contains as many particles as the initial state $\left|\mathbf{n}^{(\mathrm{i})}\right\rangle$. Due to the $U(1)$ gauge symmetry, a variation of the global phase $\theta_1^{(\mathrm{i})}$ will trivially give rise to another solution $\boldsymbol{\psi}'=\boldsymbol{\psi}\exp(\theta_1^{(\mathrm{i})})$ that exhibits the same initial and final populations as $\boldsymbol{\psi}$. Therefore, one cannot solve the integral over $\theta_1^{(\mathrm{i})}$ in stationary phase approximation, but needs to do it exactly, which yields an additional factor 2π.

The propagator in Fock space then finally reads

$$K\left(\mathbf{n}^{(\mathrm{f})},\mathbf{n}^{(\mathrm{i})},t\right)=\frac{1}{(-2\pi\mathrm{i}\hbar)^{(L-1)/2}} \times\sum_\gamma\sqrt{\det{}'\frac{\partial^2 R_\gamma}{\partial\mathbf{n}^{(\mathrm{i})}\partial\mathbf{n}^{(\mathrm{f})}}}\mathrm{e}^{\mathrm{i}R_\gamma/\hbar}, \quad (20)$$

where γ indexes all classical trajectories that satisfy the boundary conditions $|\psi_\alpha(0)|^2=n_\alpha^{(\mathrm{i})}+1/2$ and $|\psi_\alpha(t)|^2=n_\alpha^{(\mathrm{f})}+1/2$ for $\alpha=1,\ldots,L$ with the global phase $\theta_1^{(\mathrm{i})}$ being fixed through the choice $\psi_1(0)=[n_1^{(\mathrm{i})}+1/2]^{1/2}$. The prime at the determinant

$$\det{}'\frac{\partial^2 R_\gamma}{\partial\mathbf{n}^{(\mathrm{i})}\partial\mathbf{n}^{(\mathrm{f})}}\equiv\det\left(\frac{\partial^2 R_\gamma}{\partial n_\alpha^{(\mathrm{i})}\partial n_\beta^{(\mathrm{f})}}\right)_{\alpha,\beta=2,\ldots,L} \quad (21)$$

indicates that it is taken with respect to the matrix obtained by skipping the derivatives with respect to the first components.

The transition probability between Fock states at time t is then given by

$$P(\mathbf{n}^{(\mathrm{f})},\mathbf{n}^{(\mathrm{i})},t)=\sum_{\gamma\gamma'}A^{(\gamma)}A^{(\gamma')}\mathrm{e}^{\,i(R^{(\gamma)}-R^{(\gamma')})} \quad (22)$$

with

$$A^{(\gamma)}(\mathbf{n}^{(\mathrm{f})},\mathbf{n}^{(\mathrm{i})},t)=\sqrt{\left|\det{}'\frac{1}{2\pi}\frac{\partial^2 R^{(\gamma)}(\mathbf{n}^{(\mathrm{f})},\mathbf{n}^{(\mathrm{i})},t)}{\partial\mathbf{n}^{(\mathrm{f})}\partial\mathbf{n}^{(\mathrm{i})}}\right|}. \quad (23)$$

A disorder average then suppresses quasi-random contributions from pairs of longer, unrelated paths $\gamma\neq\gamma'$ in the double sum in Eq. (22) and promotes contributions from those pairs of classical solutions that exhibit action degeneracies: $R^{(\gamma)}=R^{(\gamma')}$. For $\mathbf{n}^{(\mathrm{f})}\neq\mathbf{n}^{(\mathrm{i})}$, the dominating contribution to the average transition probability is given by the incoherent ($\gamma=\gamma'$) part of the double sum,

$$\bar{P}^{\mathrm{cl}}(\mathbf{n}^{(\mathrm{f})},\mathbf{n}^{(\mathrm{i})},t)=\sum_\gamma\overline{|A^{(\gamma)}|^2}\,. \quad (24)$$

This result is also expected for the case of backscattering, $\mathbf{n}^{(\mathrm{f})}=\mathbf{n}^{(\mathrm{i})}$, if the dynamics of the system is not invariant under time reversal.

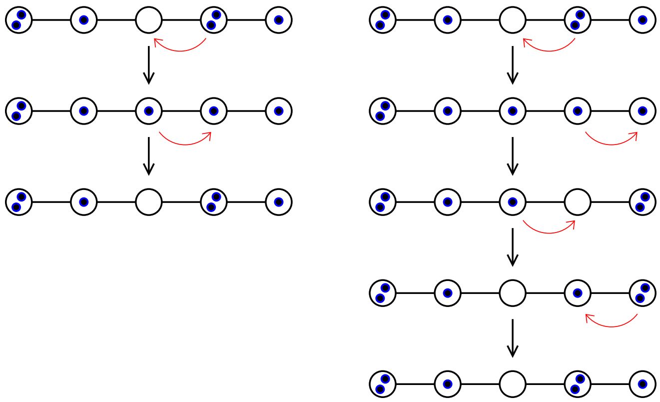

FIG. 1. (Color online) Sketch of a self-retracing (left column) and a non-self-retracing (right column) backscattered trajectiy in population space, for a Bose-Hubbard chain of five sites (marked by open black circles) containing altogether six particles (marked by filled blue circles). The curved (red) arrows indicate the imminent hopping event along the chain, while the vertical (black) arrows indicate the time evolution. The self-retracing trajectory shown in the left column involves two hopping events, with one particle hopping to an adjacent site and back. A non-self-retracing backscattered trajectory within the chain, on the other hand, requires at least four hopping events. In the example shown on the right column, two atoms undergo hoppings to adjacent sites and back in an alternating order.

In the presence of time-reversal invariance, the backscattering probability $P(\mathbf{n}^{(\mathrm{i})}, \mathbf{n}^{(\mathrm{i})}, t)$ contains additional contributions from pairs of backscattered trajectories γ, γ' where $\gamma' = \mathcal{T}\gamma$ is the time reversal of γ. Obviously, this requires that $\gamma \neq \mathcal{T}\gamma$, *i.e.*, that γ is a non-self-retracing trajectory. In the limit of long evolution times t, self-retracing trajectories $\gamma = \mathcal{T}\gamma$ generally represent a negligible minority among the set of all backscattered trajectories. Then we can safely assume that all backscattered trajectories are *non-self-retracing*, which yields the semiclassical prediction

$$\bar{P}(\mathbf{n}^{(\mathrm{i})}, \mathbf{n}^{(\mathrm{i})}, t) = 2\bar{P}^{\mathrm{cl}}(\mathbf{n}^{(\mathrm{i})}, \mathbf{n}^{(\mathrm{i})}, t) = 2\sum_{\gamma} \overline{|A^{(\gamma)}|^2} \quad (25)$$

for the average quantum backscattering probability. The right column of Fig. 1 shows an example of such a non-self-retracing backscattered trajectory within the on-site population space, for the specific case of a Bose-Hubbard chain containing five sites. It involves four inter-site hoppings of particles along the chain.

For very short evolution times, on the contrary, the average quantum backscattering probability within such a Bose-Hubbard chain is obviously dominated by contributions from *self-retracing* trajectories, namely those trajectories in which one particle hops to an adjacent site and back, as shown in the left column of Fig. 1. Hence, for very short times t we obtain

$$\bar{P}(\mathbf{n}^{(\mathrm{i})}, \mathbf{n}^{(\mathrm{i})}, t) = \bar{P}^{\mathrm{cl}}(\mathbf{n}^{(\mathrm{i})}, \mathbf{n}^{(\mathrm{i})}, t) = \sum_{\gamma} \overline{|A^{(\gamma)}|^2}\,, \quad (26)$$

i.e., the classical and quantum backscattering probabilities are expected to agree with each other.

The crossover between the short-time behaviour given by Eq. (26) and the long-time behaviour given by Eq. (25) can generally be expressed as

$$\bar{P}(\mathbf{n}^{(\mathrm{i})}, \mathbf{n}^{(\mathrm{i})}, t) = [1 + \eta(t)]\bar{P}^{\mathrm{cl}}(\mathbf{n}^{(\mathrm{i})}, \mathbf{n}^{(\mathrm{i})}, t) \quad (27)$$

where $\eta(t)$ represents the relative frequency of non-self-retracing trajectories among the set of all backscattered trajectories at the evolution time t. This relative frequency depends on system-specific parameters, such as the relative interaction and disorder strengths U/J and W/J, respectively, in our disordered Bose-Hubbard system. It can be quantitatively determined by means of the computation of classical trajectories within the Bose-Hubbard system under consideration, if a quantitative prediction of $\bar{P}(\mathbf{n}^{(\mathrm{i})}, \mathbf{n}^{(\mathrm{i})}, t)$ is required in this crossover regime.

To provide an estimate for the relevant *time scale* that characterizes this crossover in the case of our Bose-Hubbard chain or ring systems, it is useful to note that at least four inter-site hoppings are required in order to accomplish a backscattered classical trajectory that is not identical to its time-reversed counterpart. Indeed, backscattered trajectories involving only two inter-site hoppings are necessarily self-retracing in population space, as the first hopping event has to be undone by the second hopping event in order to recover the initial distribution of populations, and a trajectory with exactly three inter-site hoppings cannot recover the initial distribution of populations at the end (except for a the special case of a three-site Bose-Hubbard ring) as those hoppings arise between adjacent sites only. Denoting by $\tau = \hbar/J$ the inverse Rabi frequency characterizing inter-site hoppings within the (non-interacting and disorder-free) Bose-Hubbard system, we can therefore roughly estimate this crossover time scale as 4τ, *i.e.*, Eqs. (26) and (25) are predicted to be valid for $t \ll 4\tau$ and $t \gg 4\tau$, respectively. This prediction is found to be in good agreement with our numerical findings, as shown in Fig. 2 of the Letter.