

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

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We predict a generic manifestation of quantum interference in many-body bosonic systems resulting in a coherent enhancement of the average return probability in Fock space. This enhancement is both robust with respect to variations of external parameters and genuinely quantum insofar as it cannot be described within mean-field approaches. As a direct manifestation of the superposition principle in Fock space, it arises when many-body equilibration due to interactions sets in. Using a semiclassical approach based on interfering paths in Fock space, we calculate the magnitude of the backscattering peak and its dependence on gauge fields that break time-reversal invariance. We confirm our predictions by comparing them to exact quantum evolution probabilities in Bose-Hubbard models, and discuss the relevance of our findings in the context of many-body thermalization.

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The existence of a superposition principle for quantum states is a cornerstone in our picture of the physical world, with observable implications in the form of coherent phenomena that have been experimentally demonstrated with impressive precision during the last century [1–3]. Within the context of linear wave equations, quantum superposition effects represent particular cases of the general phenomenon of wave coherence. For quantum systems described by the single-particle Schrödinger equation, this analogy between quantum and classical waves was exploited to demonstrate coherent quantum effects, such as Anderson localization in disordered metals [4] or coherent backscattering (CBS) [5], by using classical (in particular electromagnetic) wave analogues [6–8].

In the quantum description of many-body systems, such an analogy between quantum dynamics and classical wave phenomena does not hold. Within a first-quantized approach, the quantum mechanical description of a system of N interacting particles in D dimensions requires us to extend the space in which the Schrödinger field $\psi(\vec{r}_1, \dots, \vec{r}_N, t)$ is defined to ND dimensions. We can still identify the quantum superposition principle with the linearity of the many-body Schrödinger equation, but the latter does no longer describe a classical wave in real D -dimensional space: Many-body quantum interference is a high-dimensional phenomenon.

This observation remains true even if we adopt a real-space description in terms of the *quantum* field $\hat{\psi}(\vec{r}, t)$. Indeed, $\hat{\psi}(\vec{r}, t)$ is an operator instead of a complex amplitude and does not represent a quantum state. Nevertheless, quantum fields are a suitable starting point to implement approximations to the full many-body problem in terms of classical wave equations for single particles, which effectively amounts to the substitution $\hat{\psi}(\vec{r}, t) \rightarrow \psi(\vec{r}, t)$ at the level of the Heisenberg equations of motion for $\hat{\psi}(\vec{r}, t)$. This approach leads to the mean-field Gross-Pitaevskii equation (GPE) [9] and also to the Truncated Wigner method [10–13] with its quan-

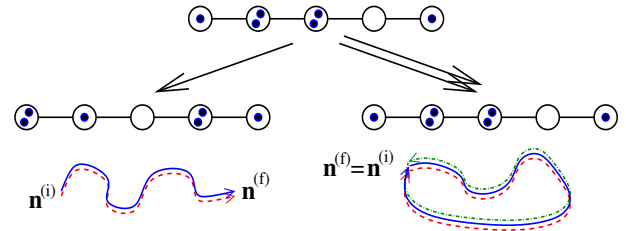


FIG. 1. (Color online) Illustration of Coherent Backscattering in Fock space. A many-body system, represented here by a Bose-Hubbard chain with $L = 5$ sites and $N = 6$ particles, is prepared in a well-defined initial Fock state $\mathbf{n}^{(i)} = (n_1^{(i)}, \dots, n_L^{(i)})$ (upper part). After a given evolution time t , the final populations are found to be $\mathbf{n}^{(f)}$ (lower parts). A solution γ of the Gross-Pitaevskii equation joining $\mathbf{n}^{(i)}$ with $\mathbf{n}^{(f)}$ contributes with an amplitude $K_\gamma \simeq A_\gamma e^{iR_\gamma}$ to this process, where R_γ is a classical action. Under averaging, only pairs of identical Fock space trajectories yield a systematically nonvanishing contribution to the probability $P = |\sum_\gamma K_\gamma|^2$ when $\mathbf{n}^{(f)} \neq \mathbf{n}^{(i)}$ (left column). For $\mathbf{n}^{(f)} = \mathbf{n}^{(i)}$ (right column), however, constructive interference additionally arises if trajectories are paired with their time-reversed counterparts (dotted green line). This gives rise to a coherent enhancement of the probability to detect the system in the initial Fock state after the evolution, as compared to other states with comparable distributions of the population.

tum (Wigner-Moyal) corrections [14]. Since the GPE is a classical field equation, its nonlinearity does not pose a conflict with the linearity of quantum evolution. For the same reasons, however, the $\psi(\vec{r}, t)$ field cannot represent a quantum state and its physical meaning requires further interpretation as a condensate fraction or order parameter. In particular, interference effects resulting from the (weakly nonlinear) GPE are *not* a consequence of many-body interference; they are *classical wave* effects proper of a classical field equation and are generically suppressed already for small interactions [15–18].

In this paper we report a semiclassical description

of the quantum mechanism responsible for many-body interference phenomena in interacting bosonic systems, which is schematically illustrated in Fig. 1. Our approach is based on coherent sums over *multiple solutions* of the GPE in occupation number space. It predicts quantum coherence effects which are in quantitative agreement with numerical simulations of Bose-Hubbard models describing cold atoms in optical lattices.

Since many-body interference is most visible in genuine many-body observables (*i.e.*, which cannot be written as sums of expectation values of single-particle operators), we will study, as a representative example, the microscopic evolution probability from one many-body state to another one. Following standard techniques [19], we introduce a discrete and orthogonal but otherwise arbitrary set of L single-particle states ("orbitals") χ_1, \dots, χ_L . The associated set of commuting bosonic occupation number operators \hat{n}_α has common (Fock) eigenstates $|\mathbf{n}\rangle = |n_1, \dots, n_L\rangle$ and integer eigenvalues n_α denoting the number of particles in each single-particle orbital χ_α . The transition probability between Fock states at time t reads then

$$P(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) = |\langle \mathbf{n}^{(f)} | \hat{U}(t) | \mathbf{n}^{(i)} \rangle|^2, \quad (1)$$

with $\hat{U}(t) \equiv \exp(-i\hat{H}t/\hbar)$ and the general many-body Hamiltonian exhibiting two-body interaction

$$\hat{H} = \sum_{\alpha\beta} h_{\alpha\beta} \hat{a}_\alpha^\dagger \hat{a}_\beta + \frac{1}{2} \sum_{\alpha\beta\eta\sigma} V_{\alpha\beta\eta\sigma} \hat{a}_\alpha^\dagger \hat{a}_\beta \hat{a}_\eta^\dagger \hat{a}_\sigma, \quad (2)$$

which is expressed in terms of the ladder operators \hat{a}_α (\hat{a}_α^\dagger) that annihilate (create) a particle in the orbital χ_α (with $\hat{n}_\alpha = \hat{a}_\alpha^\dagger \hat{a}_\alpha$). We shall later on refer to the more specific case of a Bose-Hubbard (BH) model describing, *e.g.*, cold atoms in optical lattices, which corresponds to the choice

$$\begin{aligned} \hat{H}_{\text{BH}} &= \sum_{\alpha} \epsilon_{\alpha} \hat{n}_{\alpha} - J \sum_{\alpha} (e^{i\phi} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha+1} + e^{-i\phi} \hat{a}_{\alpha+1}^{\dagger} \hat{a}_{\alpha}) \\ &+ \frac{U}{2} \sum_{\alpha} \hat{n}_{\alpha} (\hat{n}_{\alpha} - 1). \end{aligned} \quad (3)$$

Our calculation (see [20] for details) is based on an asymptotic expansion of the many-body propagator,

$$K^{\text{sc}}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) \simeq \langle \mathbf{n}^{(f)} | \hat{U}(t) | \mathbf{n}^{(i)} \rangle, \quad (4)$$

which is formally valid for $n_{\alpha}^{(i,f)} \gg 1$. To this end, we have to consider all solutions (indexed by γ)

$$\psi^{(\gamma)}(s) \equiv \psi^{(\gamma)}(s; \mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) \equiv [\psi_1^{(\gamma)}(s), \dots, \psi_L^{(\gamma)}(s)] \quad (5)$$

of the mean-field Gross-Pitaevskii equation (GPE)

$$i\hbar \frac{\partial}{\partial s} \psi_{\alpha} = \sum_{\beta} h_{\alpha\beta} \psi_{\beta} + \sum_{\beta\eta\sigma} V_{\alpha\beta\eta\sigma} \psi_{\beta} \psi_{\eta}^* \psi_{\sigma} \quad (6)$$

that instead of initial conditions satisfy the bilateral boundary (or shooting) conditions $|\psi_{\alpha}(0)|^2 = n_{\alpha}^{(i)} + 1/2$ and $|\psi_{\alpha}(t)|^2 = n_{\alpha}^{(f)} + 1/2$ and have $\arg \psi_{\alpha=1}(0) = 0$ [20]. In terms of those solutions $\psi^{(\gamma)}(s)$, the semiclassical propagator is then expressed as

$$K^{\text{sc}}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) = \sum_{\gamma} A^{(\gamma)} \exp[iR^{(\gamma)} + i\pi\Phi^{(\gamma)}/4] \quad (7)$$

where, for each solution, the semiclassical amplitude

$$A^{(\gamma)}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) = \sqrt{\left| \det' \frac{1}{2\pi} \frac{\partial^2 R^{(\gamma)}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t)}{\partial \mathbf{n}^{(f)} \partial \mathbf{n}^{(i)}} \right|}, \quad (8)$$

is given by the (dimensionless) classical action

$$\begin{aligned} R^{(\gamma)}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) &= \\ &\int_0^t \left(\sum_{\alpha} \theta_{\alpha}^{(\gamma)}(s) \dot{I}_{\alpha}^{(\gamma)}(s) - H[\psi^{(\gamma)}(s)]/\hbar \right) ds \end{aligned} \quad (9)$$

with $\psi_{\alpha}^{(\gamma)}(s) \equiv \sqrt{I_{\alpha}^{(\gamma)}(s)} \exp[i\theta_{\alpha}^{(\gamma)}(s)]$ and

$$H(\psi) = \sum_{\alpha\beta} h_{\alpha\beta} \psi_{\alpha}^* \psi_{\beta} + \frac{1}{2} \sum_{\alpha\beta\eta\sigma} V_{\alpha\beta\eta\sigma} \psi_{\alpha}^* \psi_{\eta}^* \psi_{\beta} \psi_{\sigma} \quad (10)$$

the classical (mean-field) Hamiltonian. The Morse index $\Phi^{(\gamma)}$ counts the number of conjugate points along the trajectory γ . As indicated by \det' , the derivatives in Eq. (8) are to be taken with respect to $n_2^{(i/f)}, \dots, n_L^{(i/f)}$ with $n_1^{(i/f)}$ being fixed by the total number of particles [20].

The heuristic use of $H(\psi)$ as the classical limit in bosonic systems has a long history [21] and lies behind most studies of the quantum-classical correspondence in Bose-Hubbard models [12–14, 22]. However, a rigorous approach in which a semiclassical propagator is constructed by a stationary phase analysis of the *exact* path-integral representation of $\hat{U}(t)$ in the spirit of the van Vleck-Gutzwiller approach for first-quantized systems [23] was missing in previous studies. Importantly, our propagator K^{sc} is valid also if the classical limit is non-integrable, thus going beyond the successful WKB method of Refs. [24, 25] for $L = 2$ and the EBK approach of Ref. [22] for $L = 3$. Contrary to previous classical and quasiclassical approaches (including the standard implementations of the Truncated Wigner method [10–13]), the classical information appears in Eq. (7) in terms of a boundary value problem generally exhibiting many solutions, instead of an initial value problem with a unique solution.

Substituting Eqs. (4) and (7) into Eq. (1) yields

$$P(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) = \sum_{\gamma\gamma'} A^{(\gamma)} A^{(\gamma')} e^{i(R^{(\gamma)} - R^{(\gamma')})}. \quad (11)$$

From the typical scaling $R^{(\gamma)} - R^{(\gamma')} \propto N$ of the action differences, the contributions to the double sum in

Eq. (11) contain a large number of highly oscillatory terms that tend to cancel each other. Averaging, e.g., over a disorder potential that is contained in the matrix elements $h_{\alpha\beta}$ then selects contributions from those pairs of classical solutions that generically exhibit action quasi-degeneracies: $R^{(\gamma)} - R^{(\gamma')} \sim 0$. The first non-vanishing contribution to the average transition probability (which is denoted by a horizontal bar, as any other averaged expression) is then given by the incoherent ($\gamma = \gamma'$) part of the double sum,

$$\bar{P}^{\text{cl}}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) = \sum_{\gamma} \overline{|A^{(\gamma)}|^2} \quad (12)$$

$$= \int_0^{2\pi} \frac{d\theta_2}{2\pi} \dots \int_0^{2\pi} \frac{d\theta_L}{2\pi} \overline{\prod_{\alpha=2}^L \delta[n_{\alpha}^{(f)} - |\psi_{\alpha}(\mathbf{n}^{(i)}, \boldsymbol{\theta}, t)|^2]}$$

where $\psi(\mathbf{n}^{(i)}, \boldsymbol{\theta}, t)$ is the unique solution of the GPE (6) with initial conditions satisfying $|\psi_{\alpha}^{(i)}|^2 = n_{\alpha}^{(i)} + 1/2$ and $\arg \psi_{\alpha}^{(i)} = \theta_{\alpha}$ with $\theta_{\alpha=1} = 0$ [26]. Eq. (12) is the averaged transition probability obtained using the classical Truncated Wigner method [27].

Having identified \bar{P}^{cl} as the classical probability, any other robust contribution to \bar{P} is necessarily a signature of many-body quantum interference. As shown schematically in Fig. 1, having exact and generic action degeneracies for $\gamma \neq \gamma'$ requires the presence of *time-reversal invariance* (TRI), which means that for each solution $\psi^{(\gamma)}(s)$ of the GPE one can find suitable phases ω_{α} such that its time-reversal partner $\psi^{(\mathcal{T}\gamma)}(s)$, with

$$\psi_{\alpha}^{(\mathcal{T}\gamma)}(s; \mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) \equiv e^{i\omega_{\alpha}} [\psi_{\alpha}^{(\gamma)}(t-s; \mathbf{n}^{(i)}, \mathbf{n}^{(f)}, t)]^*, \quad (13)$$

is also a solution of the GPE but with the initial and final conditions interchanged. In that case, it follows from Eq. (9) that γ and $\mathcal{T}\gamma$ have the same classical actions and semiclassical amplitudes. Obviously, as the trajectories γ, γ' in the double sum (11) refer to a specific $\mathbf{n}^{(i)}$ and a specific $\mathbf{n}^{(f)}$, a pairing $\gamma' = \mathcal{T}\gamma$ is only possible if $\mathbf{n}^{(f)} = \mathbf{n}^{(i)}$ [28]. Finally, as long as generically $\gamma \neq \mathcal{T}\gamma$, we obtain as our main result

$$\bar{P}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) \simeq (1 + \delta_{\mathbf{n}^{(f)}, \mathbf{n}^{(i)}} \delta_{\text{TRI}}) \bar{P}^{\text{cl}}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t) \quad (14)$$

with $\delta_{\text{TRI}} \equiv 1$ in the presence of TRI and 0 otherwise. This reflects *coherent backscattering (CBS) in Fock space*, *i.e.*, a coherent enhancement of the averaged quantum probability of return in Fock space over the classical value due to quantum many-body interference. Resulting from phase cancellations among oscillatory functions, this enhancement is a non-perturbative effect in the effective Planck constant $\hbar_{\text{eff}} \sim N^{-1}$.

To confirm our result, Eq. (14), we performed extensive numerical calculations for the BH model defined in Eq. (3) for chain and ring topologies. We defined our ensemble average through independent variations of the on-site energies ϵ_{α} , which are randomly selected from the

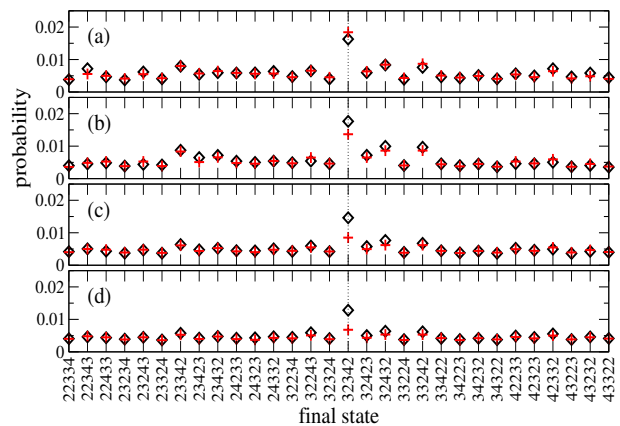


FIG. 2. (Color online) Average quantum (black diamonds) and classical (red crosses) evolution probabilities in Fock space for a Bose-Hubbard chain ($L = 5, N = 14$), at different evolution times (a) $t = 1.5\tau$, (b) $t = 2.5\tau$, (c) $t = 5\tau$, (d) $t = 10\tau$, with $\tau \equiv \hbar/J$. The average was performed over an ensemble of 10^3 realizations of on-site energies $\epsilon_{\alpha} \in [0, 10J]$, with interaction strength $U = 4J$. The probabilities are displayed for the set of Fock states $\mathbf{n}^{(f)}$ having the same total interaction energy as $\mathbf{n}^{(i)} = (3, 2, 3, 2, 4)$ (marked by the vertical dashed line). Although for $t \gtrsim 5\tau$ equilibration in Fock space generally sets in, the quantum backscattering probability to $\mathbf{n}^{(f)} = \mathbf{n}^{(i)}$ is, in accordance with Eq. (14), systematically enhanced by about a factor two as compared to other final states $\mathbf{n}^{(f)} \neq \mathbf{n}^{(i)}$ and to its classical prediction.

interval $0 < \epsilon_{\alpha} < W$. Taking advantage of the literature concerned with classical equilibration and chaos for this kind of Hamiltonians [29–31], we fixed the numerical values of the free parameters U/J and W/J such that the classical phase space has a dominant chaotic component. The time t is measured in units of the inverse Rabi frequency, $\tau \equiv \hbar/J$, between neighbouring sites. The quantum transition probability $\bar{P}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t)$ is then computed with a Runge-Kutta solver, using the exact quantum propagation of the initial state in full Fock space, followed by the disorder average over the on-site energies. The classical probability $\bar{P}^{\text{cl}}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t)$, on the other hand, is directly computed from Eq. (12) where, for a given random choice of the on-site energies, $\psi(\mathbf{n}^{(i)}, \boldsymbol{\theta}, t)$ is determined by the numerical solution of the L -dimensional GPE.

In Fig. 2 we show the time dependence of \bar{P} and \bar{P}^{cl} as a function of $\mathbf{n}^{(f)}$ for the BH model (3) with $L = 5$, $N = 14$ and a chain topology (*i.e.* the site 1 is not connected to the site L by a single hopping matrix element) starting from a generically chosen initial state $\mathbf{n}^{(i)} = (3, 2, 3, 2, 4)$. After a transient time regime in which quantum and classical results resemble each other, for $t \gtrsim 5\tau$, a CBS peak at the initial state $\mathbf{n}^{(i)}$ on top of a roughly constant background, in quantitative agreement with Eq. (14). This peak is not reproduced by the classical probabilities ruling out short-time effects or self-

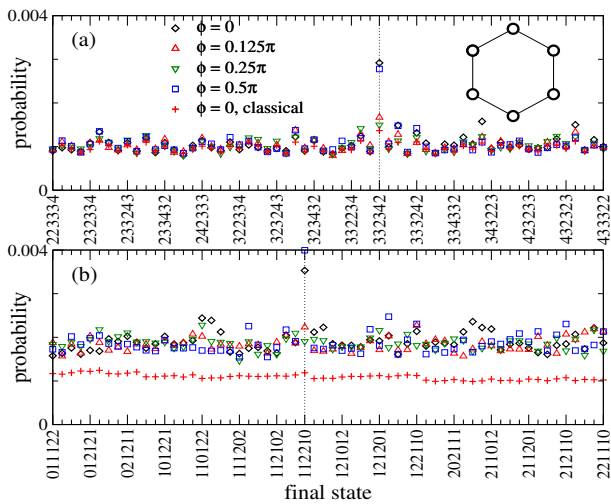


FIG. 3. (Color online) Evolution probability $\bar{P}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t)$ in Fock space averaged over random on-site energies $\epsilon_\alpha \in [0, W]$ for a Bose-Hubbard ring of $L = 6$ sites (see inset). We show results for evolution times $t = 10\tau$, hopping phases $\phi = 0, \pi/8, \pi/4, \pi/2$ (black diamonds, red upper triangles, green lower triangles, blue squares) and initial states $\mathbf{n}^{(i)}$ indicated by a vertical line. In (a) we have $N = 17$ particles, with interaction strength $U = 4J$ and $W = 10J$. The lower (more “quantum”) panel (b) has $N = 7$, $U = J$ and $W = 2J$. In both cases, the breaking of time-reversal invariance for $\phi = \pi/8, \pi/4$ destroys the coherent enhancement of the backscattering probability to the initial state. In the semiclassical regime (a) the evolution probabilities globally agree with the classical prediction for $\phi = 0$ (red crosses), while they significantly exceed the latter in the quantum regime (b).

trapping due to rare realizations of the random on-site energies as possible alternative origins of the enhancement.

Fig. 3 shows the CBS peak at $t = 10\tau$ for a BH ring (see inset) with $L = 6$ sites (in which a hopping matrix element connects the site 1 to the site L) in the presence of nonvanishing hopping phases ϕ [see Eq. (3)] which break TRI. We clearly see the suppression of the CBS peak in the absence of TRI at $\phi = \pi/8$ and $\pi/4$. For $\phi = \pi/2$, on the other hand, TRI is again established using $\omega_\alpha = \alpha\pi$ in Eq. (13) and the CBS peak re-appears.

From the experimental point of view, CBS in many-body space could possibly be observed with ultracold bosonic atoms. The specific ring geometry of Fig. 3 could be realized in hexagonal (graphene) optical lattices [32]. By means of a red-detuned laser beam which is tightly focused perpendicular to the graphene lattice, an individual hexagon could be isolated from the lattice. Displacing the focus of the laser beam with respect to the geometric center of this hexagon would allow one to load this ring in a non-uniform manner, *i.e.* such that the atomic populations differ from site to site. While the ring is initially to be loaded in the deep Mott insulator regime, in which inter-site hopping along the ring is neg-

ligibly small, a sudden increase of the hopping strength at time $t = 0$ will make the atoms propagate along the ring. At a given final propagation time, the system would have to be quenched back to the Mott regime and the atomic populations on the individual sites would have to be measured using, e.g., high-resolution imaging techniques [33]. In order to obtain the final probability distribution in Fock space with good statistical accuracy, optical disorder [34] can be used to randomly vary the on-site energies in a controlled manner, and an artificial gauge field [35] could be induced in order to break TRI. The lower panel of Fig. 3 displays the numerically computed Fock state probabilities on such a ring for the initial state $\mathbf{n}^{(i)} = (1, 1, 2, 2, 1, 0)$ [36]. It clearly displays the CBS enhancement despite the fact that this initial state is far from semiclassical ($N/L \simeq 1$).

Our results represent a further step in the active field of thermalization in closed many-body systems [29, 37–40]. Indeed, Eq. (14) shows that in equilibrium, even in the semiclassical limit and when the classical system displays full ergodicity, many-body quantum interference generically inhibits *quantum* ergodicity in equilibrium, *i.e.*

$$\bar{P}(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t \gg t_{\text{eq}}) \neq 1/\mathcal{N}_{\text{acc}} \quad (15)$$

where $\mathcal{N}_{\text{acc}} \equiv \mathcal{N}_{\text{acc}}(\mathbf{n}^{(i)})$ is the number of final Fock states that are energetically accessible to $\mathbf{n}^{(i)}$. This result, however, is not in conflict with signatures of many-body thermalization at the level of single-particle observables, like the equilibration towards uniform occupation numbers reported in Ref. [40]. As a matter of fact, Eq. (14) has an extremely small effect on such single-particle observables, as can be easily seen by calculating the averaged values $\bar{n}_\alpha(t)$, which gives the expected uniform behaviour

$$\bar{n}_\alpha(t, \mathbf{n}^{(i)}) = (N/L) + \mathcal{O}(1/\mathcal{N}_{\text{acc}}) \quad (16)$$

in the regime of classical ergodicity. However, for a genuine many-body observable like the inverse participation ratio $\text{IPR}(t) \propto \sum_{\mathbf{n}} P(\mathbf{n}, \mathbf{n}, t)$, one may obtain a strong quantum correction, $\overline{\text{IPR}}(t) = 2 \overline{\text{IPR}}^{\text{cl}}(t)$, in the presence of TRI.

To summarize, we presented a semiclassical approach in the van Vleck-Gutzwiller spirit, using sums over interfering paths that solve a classical mean field equation, which successfully captures genuine quantum interference in interacting bosonic systems. We used this approach to predict a clear-cut quantum (and genuinely many-body) effect, namely the coherent enhancement of the return probability in Fock space. Our predictions are fully confirmed by extensive simulations of Bose-Hubbard models with different topologies, even in the deep quantum regime where experimental observation using ultracold atoms is possible.

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

$$b(\hat{a}_\alpha + \hat{a}_\alpha^\dagger)|\mathbf{q}\rangle = q_\alpha|\mathbf{q}\rangle \quad (17)$$

$$-ib(\hat{a}_\alpha - \hat{a}_\alpha^\dagger)|\mathbf{p}\rangle = p_\alpha|\mathbf{p}\rangle, \quad (18)$$

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

$$\int d^L q |\mathbf{q}\rangle\langle\mathbf{q}| = \hat{1} = \int d^L p |\mathbf{p}\rangle\langle\mathbf{p}| \quad (19)$$

and their overlap matrix elements are given by

$$\langle\mathbf{q}|\mathbf{q}'\rangle = \delta(\mathbf{q} - \mathbf{q}'), \quad (20)$$

$$\langle\mathbf{p}|\mathbf{p}'\rangle = \delta(\mathbf{p} - \mathbf{p}'), \quad (21)$$

$$\langle\mathbf{q}|\mathbf{p}\rangle = \frac{1}{2b\sqrt{\pi}} \exp\left(\frac{i\mathbf{p} \cdot \mathbf{q}}{2b^2}\right). \quad (22)$$

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 $N \rightarrow \infty$), we find for the Hamiltonian

$$\hat{H} = \sum_{\alpha\beta} h_{\alpha\beta} \hat{a}_\alpha^\dagger \hat{a}_\beta + \frac{1}{2} \sum_{\alpha\beta\mu\sigma} V_{\alpha\beta\mu\sigma} \hat{a}_\alpha^\dagger \hat{a}_\beta \hat{a}_\mu^\dagger \hat{a}_\sigma \quad (23)$$

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

$$K(\mathbf{q}^{(f)}, \mathbf{q}^{(i)}, t) = \lim_{N \rightarrow \infty} \int d\mathbf{q}^{(1)} \dots \int d\mathbf{q}^{(N-1)} \int \frac{d\mathbf{p}^{(1)}}{4\pi b^2} \dots \int \frac{d\mathbf{p}^{(N)}}{4\pi b^2} \prod_{k=1}^N \exp\left[\frac{i}{2b^2} \mathbf{p}^{(k)} \cdot (\mathbf{q}^{(k)} - \mathbf{q}^{(k-1)}) - \frac{i\tau}{\hbar} \sum_{\alpha,\beta=1}^L h_{\alpha\beta} (\psi_\alpha^{(k)})^* \psi_\beta^{(k)} - \frac{i\tau}{2\hbar} \sum_{\alpha,\beta,\mu,\sigma=1}^L V_{\alpha\beta\mu\sigma} (\psi_\alpha^{(k)})^* (\psi_\mu^{(k)})^* \psi_\beta^{(k)} \psi_\sigma^{(k)}\right], \quad (24)$$

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

$$K(\mathbf{q}^{(f)}, \mathbf{q}^{(i)}, t) = \frac{1}{(-2\pi i \hbar)^{L/2}} \times \sum_\gamma \sqrt{\det \frac{\partial^2 R_\gamma}{\partial \mathbf{q}^{(i)} \partial \mathbf{q}^{(f)}}} e^{iR_\gamma/\hbar} \quad (25)$$

where the sum runs over all possible classical trajectories

defined by the equation of motion

$$i\hbar \frac{\partial \psi_\alpha(s)}{\partial s} = \sum_{\beta=1}^L h_{\alpha\beta} \psi_\beta(s) + \sum_{\beta,\mu,\sigma=1}^L V_{\alpha\beta\mu\sigma} \psi_\mu^*(s) \psi_\beta(s) \psi_\sigma(s) \quad (26)$$

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

$$R_\gamma(\mathbf{q}^{(f)}, \mathbf{q}^{(i)}, t) = \int_0^t ds \left\{ \frac{\hbar}{2b^2} \mathbf{p}(s) \cdot \dot{\mathbf{q}}(s) - \sum_{\alpha,\beta=1}^L h_{\alpha\beta} \psi_\alpha^*(s) \psi_\beta(s) - \frac{1}{2} \sum_{\alpha,\beta,\mu,\sigma=1}^L V_{\alpha\beta\mu\sigma} \psi_\alpha^*(s) \psi_\beta(s) \psi_\mu^*(s) \psi_\sigma(s) \right\} \quad (27)$$

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

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

$$\langle n|q\rangle = \frac{1}{\sqrt{2^n n! \sqrt{2\pi b}}} \exp\left(-\frac{q^2}{4b^2}\right) H_n\left(\frac{q}{\sqrt{2b}}\right) \quad (28)$$

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

$$\begin{aligned} \langle n|q\rangle &\simeq \frac{\sqrt{2/\pi}}{(4b^2 n - q^2)^{1/4}} \\ &\times \cos\left[\frac{q}{4b^2} \sqrt{4b^2(n+1/2) - q^2}\right] \end{aligned} \quad (29)$$

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 $q_\alpha^{(i/f)} \mapsto \theta_\alpha^{(i/f)}$ ($\alpha \in \{1, \dots, L\}$) with $\theta_\alpha^{(i/f)} \in [-\pi, \pi]$ defined through

$$q_1^{(i)} \equiv 2b\sqrt{n_1^{(i)} + 1/2} \cos\left(\theta_1^{(i)}\right), \quad (30)$$

$$q_1^{(f)} \equiv 2b\sqrt{n_1^{(f)} + 1/2} \cos\left(\theta_1^{(f)} + \theta_1^{(i)}\right), \quad (31)$$

as well as

$$q_\alpha^{(i/f)} \equiv 2b\sqrt{n_\alpha^{(i/f)} + 1/2} \cos\left(\theta_\alpha^{(i/f)} + \theta_1^{(i)}\right) \quad (32)$$

for $\alpha = 2, \dots, L$. The integrations over $\theta_1^{(f)}, \dots, \theta_L^{(f)}, \theta_2^{(i)}, \dots, \theta_L^{(i)}$ can now be performed in

stationary phase approximation. This selects trajectories that satisfy

$$\psi_1(t) = \sqrt{n_1^{(f)} + 1/2} \exp\left\{i\left(\theta_1^{(f)} + \theta_1^{(i)}\right)\right\}, \quad (33)$$

as well as

$$\psi_\alpha(0) = \sqrt{n_\alpha^{(i)} + 1/2} \exp\left\{i\left(\theta_\alpha^{(f)} + \theta_1^{(i)}\right)\right\} \quad (34)$$

$$\psi_\alpha(t) = \sqrt{n_\alpha^{(f)} + 1/2} \exp\left\{i\left(\theta_\alpha^{(f)} + \theta_1^{(i)}\right)\right\} \quad (35)$$

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

The propagator in Fock space then finally reads

$$\begin{aligned} K\left(\mathbf{n}^{(f)}, \mathbf{n}^{(i)}, t\right) &= \frac{1}{(-2\pi i \hbar)^{(L-1)/2}} \\ &\times \sum_\gamma \sqrt{\det' \frac{\partial^2 R_\gamma}{\partial \mathbf{n}^{(i)} \partial \mathbf{n}^{(f)}}} e^{iR_\gamma/\hbar}, \end{aligned} \quad (36)$$

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

$$\det' \frac{\partial^2 R_\gamma}{\partial \mathbf{n}^{(i)} \partial \mathbf{n}^{(f)}} \equiv \det \left(\frac{\partial^2 R_\gamma}{\partial n_\alpha^{(i)} \partial n_\beta^{(f)}} \right)_{\alpha, \beta=2, \dots, L} \quad (37)$$

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