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Engineering active motion in quantum matter

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We introduce a framework for engineering active quantum matter that involves mimicking the role of self-propulsion through an external trapping potential that is moving along imposed trajectories traced by classical active dynamics. This approach in the presence of dissipation not only recovers essential dynamical behavior of classical activity, including the ballistic to diffusive crossover of its mean-square displacement, but also reveals additional features of activity that are of quantum origin. These quantum-active features are revealed in nondissipative systems, and manifest as novel exponents of the mean-square displacement at short timescales.

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I. INTRODUCTION

Over the past two decades, nonequilibrium physics has been shaped by two remarkable developments: the rise of active matter, which has unveiled a plethora of out-of-equilibrium self-organization phenomena, and the advancement of methods enabling the precise control and manipulation of individual inherently quantum objects.

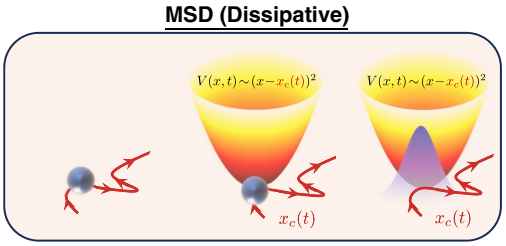
The first development, active matter, concerns the description of agents that are capable of using energy from their environment to propel themselves [1–3], either autonomously [4–6] or through the actuation with time-dependent external fields [7–10]. Such agents, called active particles, were first realized at the micron scale about two decades ago [4], and induce a spectacular plethora of nonequilibrium phenomena. For a single particle, this includes the emergence of a mean-squared displacement (MSD) beyond the generic Stokes-Einstein relation and characteristic ballistic motion that enables the usage of active particles as efficient micromotors for targeted drug delivery. At the many-body level, the local driving of active systems opens up a world of spectacular phenomena. This includes the spontaneous emergence of a center-of-mass motion induced by nonreciprocal interactions of isotropic particles [11–17], and the emergence of novel types of phase transitions that lead to so-called flocks where particles align over large distances and move collectively in a spontaneously chosen direction. These flocks exploit nonequilibrium fluctuations to bypass the Mermin-Wagner theorem and exhibit true long-range order in two dimensions [18,19], showing giant number fluctuations that violate the central limit theorem, making it impossible to measure (predict) the density in a finite domain [20]. Other phenomena specific to active matter include motility-induced phase separation where an ensemble of purely repulsively interacting particles spontaneously phase separate into a coexisting gaslike and a liquidlike phase [21], as well as living clusters that dynamically form, break up, and reform recursively [22–25]. Many of these phenomena have been shown in the past decade to occur at a broad range of scales, ranging from macroscopic robots, birds, and drones [26–29], down to the microscale and larger nanoscale, i.e., 10 nm–1 μm, where bacteria, molecular motors, and synthetic colloidal microswimmers thrive [30–35].

The second development revolves around the evolution of cold-atom physics, that was invigorated by the observation of Bose-Einstein condensation in dilute atomic gases [36,37]. Ever since, much progress has been achieved regarding the developments of techniques for cooling, trapping, and the controlled manipulation of quantum objects both at the single [38,39] and the many-particle level [40,41], even in nonequilibrium situations [42–45].

This codiscovery of new phenomena in active matter and novel methods for controlling atoms in the deep quantum regime begs the question of whether novel active nonequilibrium phase transitions and pattern formation could also be realized at a scale where quantum effects must be considered. In particular, one may wonder if there is a quantum analog to active phenomena like motility-induced phase separation, dynamic clustering, or giant density fluctuations. However, progress in understanding this interplay has been limited thus far since it is yet unknown how a self-propelled particle could be realized in the quantum regime. Accordingly, existing attempts to investigate active systems at the quantum scale are limited to a relatively small number of pioneering works either in identifying and exploring original formal analogies between descriptions of quantum systems and classical active behavior [46–52], or examining innovative models involving classical swimmers embedded in quantum media such as fermionic liquids [53], Bose-Einstein condensates [54], and superfluid He^4 [55–57]. In all these semiclassical approaches, the driven agent remains a classical object. Recently, the role

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Setup / Timescales	Classical Self-propelled Particle	Mimicking Classical Self-propulsion	Mimicking Quantum Self-propulsion
very short	t	t	t
short	t	t^4	t^6
intermediate	t^2	t^2	t^2
long	t	t	t

FIG. 1. *Schematics and dynamics of dissipative quantum and classical overdamped active systems.* (Left) Classical self-propelled particle (blue) with trajectory (red) and corresponding characteristic scaling of the MSD of an ensemble of self-propelled particles. (Center) Displacing a passive classical particle with a moving harmonic trapping potential (red to yellow paraboloid) mimics self-propulsion. (Right) Replacing the trapped classical particle by a quantum particle (wave function in blue) enables mimicking of quantum self-propulsion.

of activity [58,59] in the form of hopping terms across lattice sites, has also been considered in quantum many-body systems with non-Hermitian Hamiltonians [60,61]. These highly original approaches allow exploration of activated dynamics on a lattice, which does however restrict them from exploring generic active matter phenomena in continuum space.

In this work, we present a framework that is orthogonal to these existing approaches. This allows us to *bypass the challenge of realizing intrinsically self-propelled quantum particles*. The central idea is to *mimic self-propulsion* by guiding quantum particles with a moving external trapping potential along the path of an active particle (Fig. 1). We show that this driven quantum particle, despite not self-propelling autonomously, recovers all desirable properties of an active quantum particle (Fig. 1). That is, our approach leads to a fully quantized Hamiltonian that describes a quantum particle that

(1) breaks local detailed balance,

(2) moves in continuum space,

(3) leads to a MSD that is quadratic at intermediate timescales in the presence of dissipation [5],

(4) leads to a MSD that is linear at long timescales (active diffusion [5]).

In particular, this approach is beyond semiclassical and lattice-based realizations of active matter and leads to new active quantum effects even at the single-particle level that are accentuated in the absence of dissipation.

While the focus of this work is on introducing a minimal framework of active quantum particles and, accordingly, exploration of collective phenomena is beyond its scope, we emphasize that this approach allows for an almost direct realization of single and collective active matter phenomena with quantum particles. Our approach can be realized using ultracold atoms in time-dependent optical traps [62–66], in which the positions of the potential minimum can be externally programed almost at will and at very high speeds [67–71]. Our work thus opens a door to a new class of materials, namely, that of active quantum matter.

II. MIMICKING QUANTUM PROPULSION

We now consider a quantum particle trapped in a time-dependent potential which is uniquely parametrized by its minimum position $x_c(t)$. This position is externally programed to follow random paths drawn from an ensemble of trajectories generated by classical active dynamics [5,72–74]. Specifically, we consider active Ornstein-Uhlenbeck particles (AOUP), where the velocities follow a classical stochastic process with both a random diffusive component controlled by the diffusion constant D and persistent motion governed by the persistence time τ [75], given by the equation of motion

$$\tau\ddot{x}_c = -\dot{x}_c + \sqrt{2D}\eta(t), \tag{1}$$

where $\eta(t)$ is a zero-mean delta-correlated white noise. We now write the time-dependent Hamiltonian as

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x}, t), \tag{2}$$

where $\hat{V}(\hat{x}, t)$ is the potential energy operator associated with a classical trapping potential $V(x, t)$, $\hat{p} = -i\hbar\partial_x$ is the momentum operator, and m, ω, $\hat{x}$ are the particle mass, harmonic trap frequency, and position operator, respectively. In the following, we consider two cases, dissipative and nondissipative. In the *dissipative* case, we assume that the quantum particle is weakly coupled to its environment such that the dynamics of its density matrix $\hat{\rho}(t)$ is governed by the Lindblad equation [76]

$$\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H}(t), \hat{\rho}] + \hat{\mathcal{D}}(\hat{\rho}, t) \tag{3}$$

and the (Markovian) dissipator is given by

$$\begin{aligned}\hat{\mathcal{D}}(\hat{\rho}, t) = \nu_+\big(\hat{a}^\dagger\hat{\rho}\hat{a} - \tfrac{1}{2}\{\hat{a}\hat{a}^\dagger, \hat{\rho}\}\big) \\ + \nu_-\big(\hat{a}\hat{\rho}\hat{a}^\dagger - \tfrac{1}{2}\{\hat{a}^\dagger\hat{a}, \hat{\rho}\}\big),\end{aligned} \tag{4}$$

where $\hat{a}$ ($\hat{a}^\dagger$) is the annihilation (creation) operator, while ν^+ and ν^- are the gain and loss rates for the excitations of the quantum particle in the trap, respectively, and correspond to an equilibrium temperature (T) of the thermal bath through $\nu_+/\nu_- = e^{-\hbar\omega/k_BT}$ where k_B is the Boltzmann constant and $\hbar$ is the reduced Planck constant [77]. In the *nondissipative* (or Hamiltonian) case, the dissipator in Eq. (3) vanishes, $\hat{\mathcal{D}} \equiv 0$. We note that the used form of the Lindblad equation is one specific choice to model the coupling to a thermal bath. In a future work, we will examine how the predicted quantum-active effects depend on the specific choice of the bath-coupling model [78]. However, we will show further below that quantum-active effects in terms of unusual dynamic exponents in the MSD exist even in the complete absence of dissipation.

We define the quantum MSD, or the spread of the time-dependent wave function $|\psi_t\rangle$, as the expectation value

$$\begin{aligned}\mathrm{MSD} &\equiv \overline{\langle\psi_t|\hat{x}^2|\psi_t\rangle} - \langle\psi_{t=0}|\hat{x}^2|\psi_{t=0}\rangle \\ &= \overline{\mathrm{Tr}[\hat{\rho}(t)\hat{x}^2]} - \mathrm{Tr}[\hat{\rho}(0)\hat{x}^2].\end{aligned} \tag{5}$$

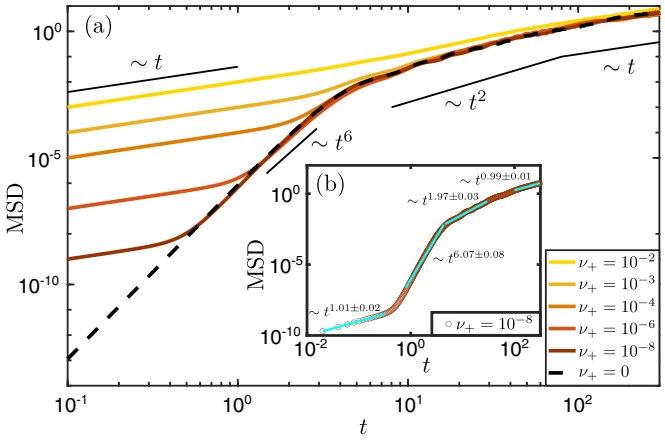


FIG. 2. *MSD of a dissipative quantum-active particle*. (a) MSD at various timescales for $D = 0.01$, $\tau = 10$, and $\nu_- = 10^{-2}$. (b) Fits of the MSD (cyan solid lines) for $\nu_+ = 10^{-8}$ indicating the scaling behavior presented in Fig. 1 for a quantum-active particle. Uncertainties represent the standard deviation across 500 simulations and do not account for possible systematic numerical uncertainties.

Here, $\overline{\cdots}$ denotes the average over prescribed stochastic trajectories, that we will specify below. In what follows, we analyze Eq. (3) both analytically and numerically, starting from the ground state $|\psi_{t=0}\rangle$, which is the quantum analog of initialization in the potential minimum in the classical case. Further details of our analysis and methods provided in the Supplemental Material (SM) [79]. We choose $\sqrt{\hbar/m\omega}$ and ω^{-1} as units of length and time, respectively.

III. DISSIPATIVE CASE

Here, we consider a harmonic trapping potential

$$V(x,t) = \tfrac{1}{2}m\omega^2[x - x_c(t)]^2, \tag{6}$$

where $x_c(t)$ is a stochastic path, that is individually generated for each initial condition by solving Eq. (1). Figure 1 illustrates the scenarios that we discuss in the following: a classical self-propelled particle (left), a passive particle in the potential $V(x,t)$ (center), and a quantum particle with a corresponding potential energy operator $\hat{V}(\hat{x},t)$ (right). Numerical results for the quantum MSD scaling are shown in Fig. 2, while the analytical calculation of the dynamical exponents in both classical cases is provided in the SM.

At very short timescales ($t \ll \tau$, first row in Fig. 1), the quantum MSD scales diffusively (MSD $\sim t$), reflecting the behavior observed in both classical cases. In Fig. 2, we identify this diffusive regime for any nonzero temperature (i.e., $\nu_+ \neq 0$), which is also confirmed analytically in the SM, Sec. II B. However, while classical active particle demonstrate this diffusive behavior also for short timescales ($t \ll \tau$, second row in Fig. 1), displacing a particle by a moving trapping potential leads to a distinct regime for both classical and quantum particles mimicking self-propulsion. This regime is characterized by a rapid growth of the MSD, scaling as t^6 in the quantum-active case [Fig. 2(a)] and as t^4 in its classical counterpart. We note that this quantum t^6 scaling is also not observed in the underdamped classical case [80]. The duration of this regime for the quantum particle increases as the temperature T decreases (i.e., for lower ν_+), due to a progressive shortening of the initial diffusive regime. This suggests that the anomalous regime has a quantum origin, as quantum effects arising from the Hamiltonian dynamics become more pronounced at lower temperatures. In fact, importantly, at zero temperature (i.e., $\nu_+ = 0$), the initial diffusive regime of the MSD disappears entirely [black dashed line in Fig. 2(a)]. At intermediate timescales ($t \sim \tau$, third row in Fig. 1), the quantum-active dynamics exhibits a ballistic regime (MSD $\sim t^2$), before eventually entering a diffusive regime (MSD $\sim t$) at much longer times ($t \gg \tau$, fourth row in Fig. 1). Both these regimes are observed in corresponding classical cases. Power-law fits of the MSD in various dynamical regimes for $\nu_+ = 10^{-8}$ [Fig. 2(b)] clearly reveal all the regimes listed in Fig. 1. Thus, a quantum particle in a harmonic trapping potential that moves along predetermined stochastic trajectories exhibits all the characteristic properties of classical activity (i–iv in the Introduction), and additionally points to quantum-active effect occurring at short times.

MSD (Nondissipative)

Setup / *Timescales*	Mimicking Classical Self-propulsion	Mimicking Quantum Self-propulsion		
short	$t^{2(q+1)}$	$q<2$: t^4	$q=2$: t^6	$q>2$: $-t^4$
intermediate	t^2	Cross-over		
long	t	t		

FIG. 3. *MSD of nondissipative quantum and classical active systems*. (Left) MSD of a classical Hamiltonian particle in a moving trapping potential $V(x,t)$ (7); this case is akin to the center column in Fig. 1 but without dissipation [80]. (Right) MSD of a Hamiltonian quantum particle in a moving trapping potential $V(x,t)$; this case is akin to the right column in Fig. 1 but without bath coupling.

IV. NONDISSIPATIVE CASE

To further explore the significance of quantum-active effects, without partially masking it with contributions from the thermal bath, we now focus solely on the nondissipative (Hamiltonian) case. We consider a family of power-law trapping potentials $V(x,t)$, defined as

$$V(x,t) = V_0|x - x_c(t)|^q, \quad q > 0, \tag{7}$$

with the prefactor $V_0 = \frac{1}{2}\hbar^{1-\frac{q}{2}}m^{\frac{q}{2}}\omega^{\frac{q}{2}+1}$.

The regimes emerging for classical and quantum particles mimicking self-propulsion are summarized in Fig. 3. Without dissipation, the diffusive regime at very short times is absent in both classical and quantum cases. We now determine the short-time ($t \ll \tau$) behavior of the MSD for a quantum particle using time-dependent perturbation theory (see the SM, Sec. I B) to obtain

$$\text{MSD} = A_q \int_0^t \int_0^t dt' dt'' \overline{x_c(t')x_c(t'')}. \tag{8}$$

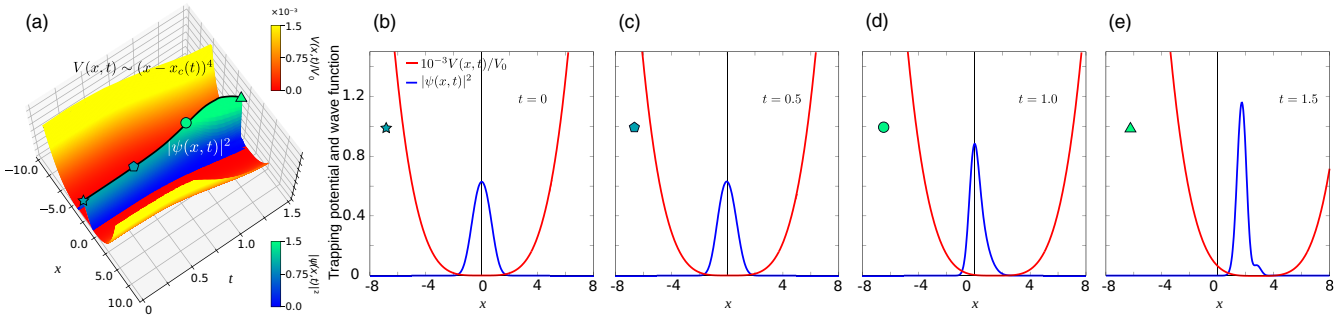


FIG. 4. *Transient localization of the wave function*. (a) Time evolution of the confining potential $V(x,t)$ and the wave-function profile $\langle\psi_t|\psi_t\rangle \equiv |\psi(x,t)|^2$, shown using red-yellow and blue-green color maps, respectively, for $D = 1$, $\tau = 1$, $q = 4$. In the final state, the peak of the profile (shown with the black line) increases in height compared to the initial state, indicating stronger localization. (b)–(e) Potential (red) and wave-function profiles (blue) at different time instants $t = 0$, 0.5, 1.0, and 1.5, respectively. The time instants marked by different symbols in (a) correspond to those in (b)–(e).

This result has the following physical interpretation: the leading-order contribution to the MSD at short times is fully determined by the prescribed stochastic trajectory, i.e., by the active driving protocol of the Ornstein-Uhlenbeck process (1). In contrast, in the classical case, the scaling of the MSD is given by a Green-Kubo relation that involves velocity autocorrelations (see the SM):

$$\mathrm{MSD} = \int_0^t \int_0^t dt' dt'' \overline{\dot{x}(t')\dot{x}(t'')}. \tag{9}$$

We note that, in the quantum case, the trapping potential exponent q in Eq. (7) enters the prefactor A_q of Eq. (8), which is entirely quantum in origin. This prefactor determines whether short-time localization is stronger (negative A_q) or weaker (positive A_q). We remark that the emergence of a negative MSD is possible by virtue of its definition (5), and its initial ground-state condition. A negative MSD indicates that the wave function initially becomes narrower than its ground-state configuration, as is demonstrated in Fig. 4(a). The mechanism is illustrated through time-sequential snapshots in Figs. 4(b)–4(e): on one side of the maximum of the wave function (or, more precisely, of $\langle\psi_t|\psi_t\rangle$), the moving potential localizes the wave function, essentially by pushing it, whereas on the other side, delocalization is negligible due to the low wave-function amplitude on that side. Such negative MSD cannot occur for a classical stochastic particle with a sharp initial position. Even when the classical system is initiated with a nonzero temperature equilibrium configuration which has a nonzero initial MSD, the MSD increases with a t^2 scaling (see the SM, Sec. III D). Thus, the occurrence of a negative MSD at short times is a pure quantum effect.

For a harmonic potential ($q = 2$) the prefactor A_q vanishes ($A_q = 0$), with the leading correction scaling as t^6 arising from second-order perturbation theory (see the SM, Sec. I E). For $q \neq 2$ (and thus $A_q \neq 0$), the leading-order contribution to the MSD (8) is t^4 (see the SM, Sec. I C). In contrast, for the classical case, the potential exponent q directly enters the dynamical exponent, resulting in a $t^{2(q+1)}$ scaling (see the SM, Sec. III).

To test our analytical predictions, we now examine numerically in Fig. 5 how the shape of the trapping potential $V(x,t)$ influences the MSD for $q = 1.5$, 2, and 4. In Figs. 5(a) and 5(b), we see that for $q \neq 2$, the short-time quantum-active scaling of the MSD is indeed $\sim t^4$. For $q = 4$, the MSD is initially negative, indicating that the quantum-active particle is transiently more localized than its ground state. Conversely, the MSD for $q = 1.5$ scales positively as $\sim t^4$, rather than $\sim t^6$ as for the harmonic potential. At longer timescales ($t \gg \tau$), as expected, the MSD is fully determined by the trap motion, and the nondissipative quantum particle enters the diffusive regime regardless of q [see Figs. 5(c) and 5(d)]. Quantum-active effects become apparent when comparing the MSD to its classical counterpart, as the behavior differs at both shorter and longer timescales [Figs. 5(a) and 5(c)]. Specifi-

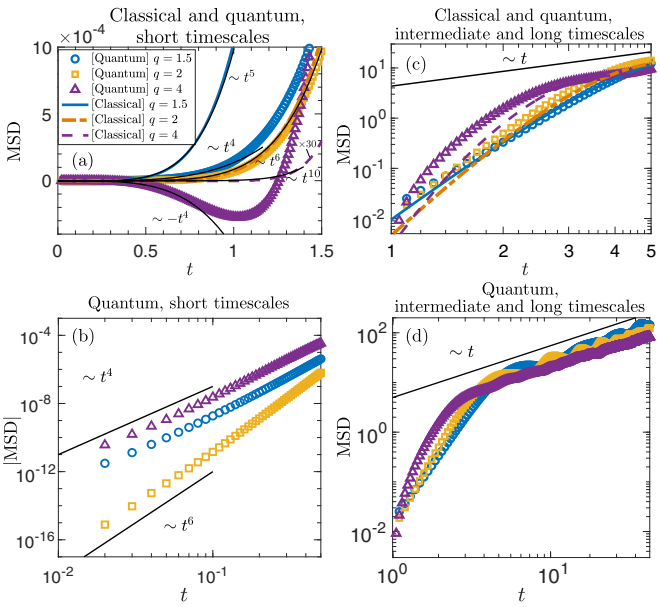


FIG. 5. *MSD of a nondissipative quantum-active particle*. (a) MSD at short timescales for $D = 1$ and $\tau = 10$ reveals quantum-active scaling being in general different from classical. (b) Log-log plot of the absolute values of MSD indicates $\sim t^4$ scaling for $q \neq 2$ and $\sim t^6$ for $q = 2$. (c), (d) Crossover to the diffusive regime at long timescales for $D = 1$ and $\tau = 1$. (a), (c) Comparison of quantum and classical active MSD. In all panels, an average is taken over 500 stochastic trajectories for each q considered.

cally, Fig. 5(a) highlights the characteristic $t^{2(q+1)}$ scaling of the classical particle. Thus, the t dependence of the MSD between classical and active quantum particles is in general qualitatively different.

V. CONCLUSION AND DISCUSSIONS

In this work, we introduced a generic approach for exploring quantum-active matter in continuum space. This approach involves mimicking the role of propulsion in active particles through imposing a trapping potential that is moving along imposed trajectories governed by classical active stochastic dynamics. We show that this framework for a single quantum degree of freedom captures essential dynamical features of classical self-propelled active particles in the presence of any dissipation. These features include a mean-squared displacement (MSD) that scales diffusively ($\sim t$) at short times, ballistically ($\sim t^2$) at intermediate times, and again diffusively ($\sim t$) at times much longer than the persistence time τ of the active dynamics. Notably, this approach also reveals quantum-active dynamical features with no classical equivalent and that are most pronounced in the absence of dissipation. These features manifest as anomalous dynamical exponents of the MSD at short timescales. Most notably, the quantum-active t^6 scaling shown in Fig. 2 is clearly observed in the range up to 10^{-3}–10^{-2}, corresponding to typical particle displacements of 0.03–0.1 in the oscillator length units. In the ultracold-atom setup, where the oscillator length is typically $\sqrt{\hbar/m\omega} \sim 1$ μmu, this translates to a physical displacement of about 30–100 nm. Recent advances in quantum gas microscopy have enabled spatial resolutions down to 45 nm [81], placing this quantum-active t^6 regime within the potential experimental observation. Remarkably, the MSD can even transiently acquire negative values for sharp trap geometries, representing an increased localization of the wave function with time transiently. This phenomenon cannot emerge classically, and is counterintuitive given that active systems are typically superdiffusive at intermediate timescales.

We stress that this work focuses on establishing a conceptually new and generic approach to study quantum-active matter that is meant to inspire future simulations and experiments. This approach is generalizable, and can be combined with or extended to interacting forms of classical active matter. This may include alternate forms of microscopic activity including run-and-tumble or active Brownian dynamics [82–84]. While the generalization to the many-body regime is beyond the scope of this work, we would like to remark that (i) experimental setups are now available to individually control more than 10^3 quantum particles [64], which could be adapted in the future to mimic quantum active matter at the many-body level. (ii) In principle, a random but temporally and spatially correlated potential (a specific type of colored spatiotemporal noise) can be utilized to mimic quantum-active motion at the many-body level at low to moderate densities and to predict a viable path toward realizing, e.g., flocking and motility-induced phase separation. On the other hand, the effect of quantum phenomena such as exchange symmetry of indistinguishable quantum particles (e.g., fermions or bosons) [85–88], or collective behavior of exotic quantum many-body ground-states (e.g., Bose-Einstein condensates) [89], on the dynamics of an externally activated process could also be interesting avenues to explore within the current context presented. Importantly, our theoretical predictions can be tested using state-of-the-art experimental techniques in ultracold atoms confined to optical traps where the trap minimum can be programed on prescribed stochastic trajectories. As such, our framework of active quantum matter could provide a paradigm for uncovering phenomenology involving the nontrivial coupling of quantum fluctuations with nonequilibrium features of activity.

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