

Heat-to-motion conversion for quantum active matterAlexander-Georg Penner^{1,*}, Ludmila Viotti^{2,*}, Rosario Fazio^{2,3}, Liliana Arrachea⁴, and Felix von Oppen¹¹*Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany*²*The Abdus Salam International Center for Theoretical Physics, 34151 Trieste, Italy*³*Dipartimento di Fisica, Università di Napoli “Federico II,” I-80126 Napoli, Italy*⁴*Centro Atómico Bariloche and Instituto de Nanociencia y Nanotecnología CONICET-CNEA (8400), San Carlos de Bariloche, Argentina*

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We introduce a model of an active quantum particle and discuss its properties. The particle has a set of internal states that mediate exchanges of heat with external reservoirs. Heat is then converted into motion by means of a spin-orbit term that couples internal and translational degrees of freedom. The quantum features of the active particle manifest both in the motion and in the heat-to-motion conversion. Furthermore, the stochastic nature of heat exchanges impacts the motion of the active particle and fluctuations can be orders of magnitude larger than the average values. The combination of spin-orbit interaction under nonequilibrium driving may bring active matter into the realm of cold atomic gases where our proposal can be implemented.

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Introduction. Active particles, of natural origin or artificially fabricated, propel themselves by converting environmental energy through nonequilibrium processes. The field of active matter, bridging between biology, chemistry, and physics, has grown enormously over the years, leading to the discovery of a multitude of novel phenomena at the single- and many-particle levels. This body of work has been extensively described in several reviews and books (see, e.g., [1–5]).

While this effort has been overwhelmingly devoted to classical particles, it is natural to wonder whether active motion can also be realized in the quantum regime. Several new questions arise in this context. It would be important to understand necessary ingredients, identify suitable (possibly artificial) systems, and explore regimes realizing active quantum particles. One would like to understand in which cases quantum effects enable, influence, or enhance the functionalities of active particles, and explore associated signatures of genuine quantum behavior. These questions naturally extend to the many-particle case of active matter, where new avenues of investigation emerge from collective quantum effects.

Very recently, a few interesting works began to address some of these questions. A description of active quantum particles in terms of a non-Hermitian quantum walk was put forward in [6], while in [7] the motion was induced by classical noise. Quantum active agents can eventually synchronize as discussed in [8]. Activity-induced collective effects were discussed in [9–12], employing both non-Hermitian [9,12] and Lindblad [10] dynamics. There are also pertinent

connections to earlier works on directed motion and motors at the nanoscale [13–20].

The purpose of this work is to find models of quantum active dynamics that are suitable for realization in synthetic systems. In particular, we introduce a class of models, which is realizable with cold atoms moving in optical lattices. The quantum particle transforms the heat exchanged in the engine into motion by coupling its internal and translational degrees of freedom, thus establishing a connection to quantum heat engines [21–24]. Quantum signatures appear in the motion of the particle and play a crucial role in the heat-to-motion conversion. Furthermore, due to the microscopic nature of the quantum heat engine, fluctuations are relevant and the stochastic nature of the heat-to-motion conversion becomes important in the self-propulsion of the active particle. In this way, we provide a natural bridge between the fields of active matter and quantum thermodynamics [25,26].

Our rather general approach applies to a large variety of specific cases. In the following, we will first discuss the general idea before providing a detailed analysis of a concrete example deep in the quantum limit: a spin-1/2 particle coupled to two heat baths. We will characterize its motion, its quantum signatures, and its stochastic nature.

The model. As sketched in Fig. 1, the active quantum particle comprises internal and translational degrees of freedom. Its internal degrees of freedom (modeled as a set of discrete levels) couple to external reservoirs, which induce transitions between the levels. The exchange of energy with the environment fuels the motion of the particle when the internal and translational degrees of freedom are coupled, e.g., by spin-orbit interactions (see Ref. [27] for a discussion of classical self-propelled particles inspired by spin-orbit coupling). Transitions between the internal levels give kicks to the particle. The rate at which the transitions take place depends on the coupling to and the state of the reservoirs, while the heat-to-motion conversion is controlled by the spin-orbit coupling. Moreover, we show that the active particle will be

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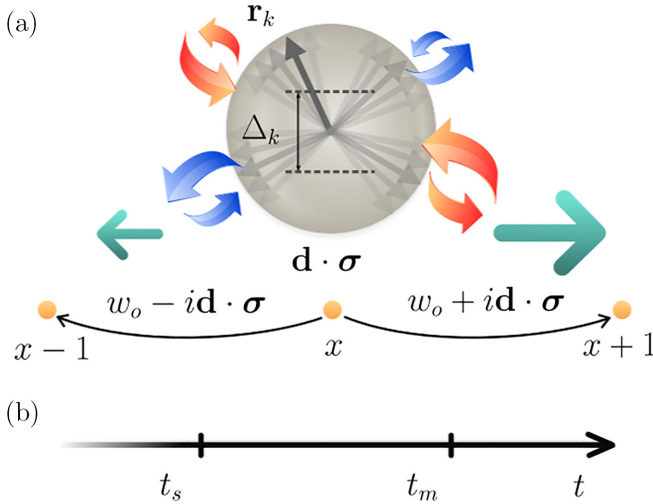


FIG. 1. Illustration of the model for an active quantum particle. (a) The particle hops with spin-dependent amplitudes (black arrows) along a chain of sites (orange dots). The particle's spin $\boldsymbol{\sigma}$ couples to its motion through the spin-orbit field $\mathbf{d}$ and is aligned by an external magnetic field, resulting in momentum-dependent spin orientation (gray arrows) and splitting Δ_k . Moreover, it interacts with hot (red) and cold (blue) reservoirs. The particle is immersed in an environment (not shown), which relaxes its momentum. (b) Hierarchy of characteristic timescales, $t_s \ll t_m$. We assume that the characteristic time t_s associated with coupling of the spin to the hot and cold reservoirs is much smaller than the momentum relaxation time t_m .

self-propelled even in a noisy environment, which accounts for damping of the translational degrees of freedom (momentum relaxation) by coupling to a phonon bath.

Directed motion of the quantum particle can be activated only under nonequilibrium conditions. We generate nonequilibrium by keeping two reservoirs at different (hot/cold) temperatures $T_{h/c} = T \pm \Delta T/2$. Thus, the internal degrees of freedom of the particle constitute the working medium of a quantum heat engine fueling the motion. As the coupling to these reservoirs is only through the internal degrees of freedom, it does not select a preferred direction of motion. Nevertheless, nonequilibrium ensures that the emission and absorption of excitations from the different baths do not balance, allowing for self-propulsion of the particle. If $T_c = T_h = T$, no directed motion takes place.

The outlined quantum particle and its coupling to the environment are modeled by the Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_p + \hat{\mathcal{H}}_B + \hat{V}_1$. The particle is described by

$$\hat{\mathcal{H}}_p = \sum_{s,s'} \varepsilon_{s,s'} |s\rangle \langle s'| - \sum_{x,s,s'} w_{s,s'} |x, s\rangle \langle x+1, s'| + \text{H.c.}, \quad (1)$$

with s labeling the set of discrete levels associated with the internal (“spin”) degrees of freedom. The constants $\varepsilon_{s,s'}$ account for the internal structure of the particle, while the $w_{s,s'}$ describe spin-dependent hopping on a lattice of sites x , thus admitting processes in which hopping is accompanied by a change in the internal state of the particle (“spin-orbit” coupling). We consider a one-dimensional lattice, but the continuum limit or the extension to higher dimensions are both straightforward. The bath Hamiltonian $\hat{\mathcal{H}}_B$ describes sets of

harmonic oscillators in thermal equilibrium at bath-dependent temperatures and $\hat{V}_1$ is the coupling to the thermal baths as specified below.

The Hamiltonian $\hat{\mathcal{H}}$ embodies the essence of the heat-to-motion conversion and the connection between active quantum particles and quantum heat engines. In the following, we capture the main features of our approach within a definite minimal model: a quantum particle with two internal states ($s = \uparrow, \downarrow$). It is subject to a Zeeman field, $\varepsilon_{s,s'} = -[\boldsymbol{\varepsilon} \cdot \hat{\boldsymbol{\sigma}}]_{s,s'}$, and hopping amplitudes $w_{s,s'} = [w_o \hat{\mathbb{1}}_s + i \mathbf{d} \cdot \hat{\boldsymbol{\sigma}}]_{s,s'}$ (with $\hat{\boldsymbol{\sigma}} = [\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z]$ the Pauli matrices and $\hat{\mathbb{1}}_s$ the identity in spin space). The (effective) spin-orbit field $\mathbf{d}$ preserves time-reversal symmetry when it is real, which we assume from now on. For the spin-1/2 particle, Eq. (1) is diagonalized in momentum space by the composition of k -dependent rotations $\hat{R}_k$. Defining the rotated spin operators $\hat{\tau}_k = \hat{R}_k^\dagger \hat{\boldsymbol{\sigma}} \hat{R}_k$, yields $\hat{\mathcal{H}}_p = \sum_k (\epsilon_k \hat{\mathbb{1}}_s + \Delta_k \hat{\tau}_{z,k}) |k\rangle \langle k|$, with $\epsilon_k = -2w_o \cos k$, $\Delta_k = |\Delta_k|$, $\Delta_k = \boldsymbol{\varepsilon} - 2\mathbf{d}_k$, and $\mathbf{d}_k = \mathbf{d} \sin k$.

We parametrize the density matrix of the k block as $\hat{\rho}_k = r_{o,k} [\hat{\mathbb{1}}_s + \mathbf{r}_k \cdot \hat{\boldsymbol{\tau}}_k]/2$, and assume that the system relaxes to thermal equilibrium at temperature $T = \beta^{-1}$ prior to applying the temperature bias. Tracing out the baths in the weak-coupling approximation leads to the Lindblad equation

$$\dot{\hat{\rho}}_k = -i[\Delta_k \hat{\tau}_{z,k}, \hat{\rho}_k] + \mathcal{D}_s[\hat{\rho}_k] + \mathcal{D}_m[\{\hat{\rho}_{k'}\}], \quad (2)$$

where the dissipator

$$\mathcal{D}_s[\hat{\rho}_k] = \sum_{\ell=\pm} \sum_{\alpha=h,c} \Gamma_{\alpha,k}^{(\ell)} \left[\hat{\tau}_{\ell,k} \hat{\rho}_k \hat{\tau}_{\ell,k}^\dagger - \frac{1}{2} \{ \hat{\tau}_{\ell,k}^\dagger \hat{\tau}_{\ell,k}, \hat{\rho}_k \} \right] \quad (3)$$

originates from the coupling

$$\hat{V}_1 = \hat{\mathcal{H}}_r + \sum_{k,n} \sum_{\alpha=h,c} |k\rangle \langle k| \otimes \hat{\tau}_{\alpha,k} \otimes (b_{\alpha,n} + b_{\alpha,n}^\dagger) \quad (4)$$

of the internal spin to the thermal baths. [$\mathcal{H}_r$ inducing momentum relaxation is defined in Eq. (7) below]. Here, $\Gamma_{\alpha,k}^{(\ell)} = \xi_{\alpha,k} [n(2\Delta_k, T_\alpha) + \delta_{\ell,-}]$ with $\delta_{\ell,\pm}$ the Kronecker symbol and $n(2\Delta_k, T_\alpha)$ the Bose function at temperature T_α . The factors $\xi_{\alpha,k} = \gamma_\alpha |\langle \uparrow | \hat{\tau}_{\alpha,k} | \downarrow \rangle|^2$ allow for couplings to the two reservoirs with different strengths and through different spin operators. We denote $\hat{\tau}_{\pm,k} = (\hat{\tau}_{x,k} \pm i\hat{\tau}_{y,k})/2$, and $\{\cdot, \cdot\}$ is the anticommutator. The dissipator $\mathcal{D}_m$ related to $\hat{\mathcal{H}}_r$ describes momentum relaxation as discussed further below. The dissipators $\mathcal{D}_s$ and $\mathcal{D}_m$ introduce two characteristic timescales—the spin and momentum relaxation times t_s and t_m , respectively. We take momentum relaxation to be the longest timescale in the problem, $t_m \gg t_s$ (see Fig. 1). Since $\mathcal{D}_s$ is diagonal in momentum, the momentum distribution $r_{o,k}$ remains constant for times short compared to t_m , even in the presence of a temperature imbalance ΔT . In contrast, the temperature bias causes nontrivial dynamics of the state of the internal degrees of freedom, as encoded in $\mathbf{r}_k(t)$. In particular, this dynamics—and hence the dynamics of the active particle—are genuinely quantum due to the k -dependent quantization axis of the spin implicit in Eq. (2).

Heat-to-motion conversion. We use Eq. (2) to analyze the dynamics of the active quantum particle. Its average velocity is defined as $\langle \hat{v}(t) \rangle = \sum_k \text{Tr}_s[\hat{\rho}_k(t) \hat{v}_k]$, where $\hat{v}_k = \partial_k \epsilon_k + (\partial_k \Delta_k) \cdot \hat{\boldsymbol{\sigma}}$ is the velocity operator. It vanishes in equilibrium, as can be verified by substituting the Boltzmann distribution.

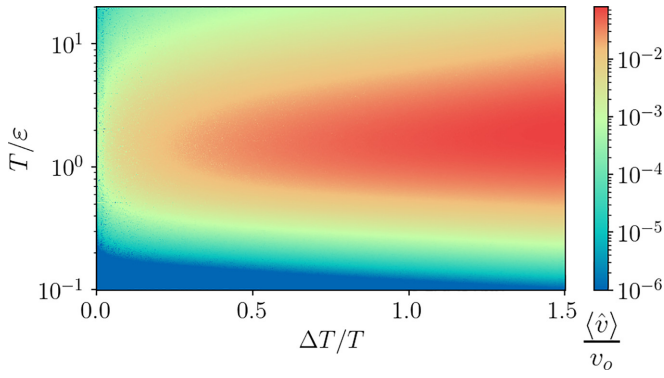


FIG. 2. Average velocity of the particle for $t_s \ll t \ll t_m$ vs equilibrium temperature and (relative) temperature bias $\Delta T/T$. Velocity scale: $v_o = \varepsilon a$. Parameters: Zeeman field $\mathbf{e} = \varepsilon(\hat{x} \cos \theta + \hat{z} \sin \theta)$, with $\theta = 3\pi/4 - \delta$ and $\delta = 0.01$, hopping energy $w_o = 2\varepsilon$, spin-orbit coupling $\mathbf{d}/\varepsilon = 0.6/\sqrt{2}(\hat{x} + \hat{z})$. The Particle couples to baths through $\hat{\tau}_{h,k} = \hat{\tau}_{x,k}$ and $\hat{\tau}_{c,k} = \hat{\tau}_{z,k}$ with $\gamma = 0.2\varepsilon$.

Under nonequilibrium conditions, the nano-engine will start to fuel the particle through heat-to-motion conversion. In linear response to a small temperature difference, and in the absence of momentum relaxation (i.e., for times $t_s \ll t \ll t_m$), we find the average steady-state velocity

$$\langle \hat{v} \rangle = \frac{\Delta T}{T^2} \sum_k r_{o,k} \frac{\xi_{h,k} - \xi_{c,k}}{\xi_{h,k} + \xi_{c,k}} \frac{\mathbf{\Delta}_k \cdot \partial_k \mathbf{d}_k}{\cosh^2(\beta \Delta_k)}. \quad (5)$$

Here, the momentum distribution $r_{o,k}$ is thermal,

$$r_{o,k}^{\text{th}} = \frac{1}{\mathcal{Z}} e^{-\beta \epsilon_k} \cosh(\beta \Delta_k), \quad (6)$$

where $\mathcal{Z} = \text{Tr} e^{-\beta \hat{H}_p}$ denotes the equilibrium partition function of the particle. In our case with only two levels, the velocity is nonzero when the particle couples to the reservoirs with different amplitudes $\xi_{h,k} \neq \xi_{c,k}$. In numerical calculations, we implement this difference by coupling to the baths through different Pauli operators, while keeping equal strengths, $\gamma_h = \gamma_c = \gamma$. Equation (5) implies that a nonzero average velocity requires that w_o , $\mathbf{e}$, and $\mathbf{d}$ are all nonvanishing (see Supplemental Material (SM) [28]).

Figure 2 shows the steady-state velocity as a function of temperature bias $\Delta T/T$ and temperature T in the absence of momentum relaxation. The steady-state velocity has an interesting T dependence, vanishing in both the high- and low-temperature limits with an intermediate optimal temperature. At low temperatures, the average velocity vanishes exponentially, $\langle \hat{v} \rangle \sim e^{-2\beta\varepsilon}$, while at high temperatures it goes to zero as $\langle \hat{v} \rangle \sim 1/T^3$. This can be understood by noting that at low temperatures, transitions are suppressed and therefore the quantum engine is unable to provide the necessary imbalance to activate the particle. With increasing temperature, the relative difference in occupations between the two reservoirs decreases and the deviations from equilibrium are less pronounced. This behavior persists beyond linear response as shown in Fig. 2. For $w_o \gg d, \varepsilon$, Eq. (5) gives an optimal temperature of 0.83ε [28].

Momentum relaxation. In general, the complex environment of the particle induces additional processes, which

randomize its momentum. This can be modeled by introducing a phonon bath at temperature T with coupling Hamiltonian

$$\mathcal{H}_r = \sum_{k,q,n} \sqrt{\frac{\lambda_q}{N}} |k\rangle \langle k+q| \otimes \hat{\mathbf{I}}_s \otimes (b_{-q,n} + b_{q,n}^\dagger). \quad (7)$$

Here, N denotes the number of sites and $b_{-q,n}$ ($b_{q,n}^\dagger$) annihilates (creates) a phonon in transverse mode n with longitudinal momentum q . Due to the k -dependent rotations R_k , momentum-relaxation processes may or may not flip the spin. We show in [28] that spin-conserving transitions dominate as long as the coupling λ_q decays rapidly with q on a scale q_0 , which is the smallest momentum scale in the problem, and the phonon density of states $\nu \sim |\omega|^p$ does not grow too rapidly with ω , namely, for $p = 1, 2, 3$. We specify to this case in the following.

Tracing out the phonon bath introduces the dissipator $\mathcal{D}_m$ into Eq. (2). We relegate explicit expressions and calculational details to [28]. We find that to lowest order in t_s/t_m , the equation for $\mathbf{r}_k$ decouples from the momentum distribution $r_{o,k}$, so that the spin distribution $\mathbf{r}_k$ is independent of the momentum distribution $r_{o,k}$. As transitions are local in momentum space, the latter obeys a drift-diffusion equation,

$$\partial_t r_{o,k} = \partial_k [v_D(k) r_{o,k} + D(k) \partial_k r_{o,k}]. \quad (8)$$

The drift velocity $v_D(k)$ and the diffusion constant $D(k)$ depend on k and on the spin distribution $\mathbf{r}_k$. The steady-state velocity in the presence of momentum relaxation is still given by Eq. (5), albeit with $r_{o,k}$ modified to be the stationary solution $r_{o,k}^\infty$ of the drift-diffusion equation. For $p = 2$, we find

$$r_{o,k}^\infty = \frac{1}{\mathcal{Z}} \exp -\frac{\beta}{2} \int_0^k dk' \text{Tr}_s (\hat{v}_k [\hat{\mathbf{I}}_s + \mathbf{r}_{k'} \cdot \boldsymbol{\sigma}]). \quad (9)$$

We give results for other values of p in Ref. [28].

We use numerical simulations to illustrate the evolution of the average velocity of the active particle across the entire range of timescales in Fig. 3, contrasting various densities of states of the phonon bath. At times short compared to t_m , the velocity is independent of the phonon bath. After an initial transient ($t_s \ll t \ll t_m$), the active particle moves at the steady-state velocity in the absence of momentum relaxation [see Eq. (5), indicated by the dashed line in the figure] by converting the heat exchanged with the baths into motion. At late times compared to the momentum relaxation time, the average velocity reaches a steady state, which is distinct from the steady-state velocity of the model without momentum relaxation. In fact, the two steady-state velocities can differ not only in magnitude, but also in sign. Remarkably, as seen in Fig. 3, momentum relaxation can induce an increase in the magnitude of the average velocity. We also observe that once phonon relaxation sets in, the average velocity depends sensitively on the phonon density of states ν . The time dependence remains qualitatively unchanged when momentum-relaxation processes with spin flips become important ($p = 4$).

Quantum effects and velocity correlations. The quantum nature of the active particle becomes apparent in the

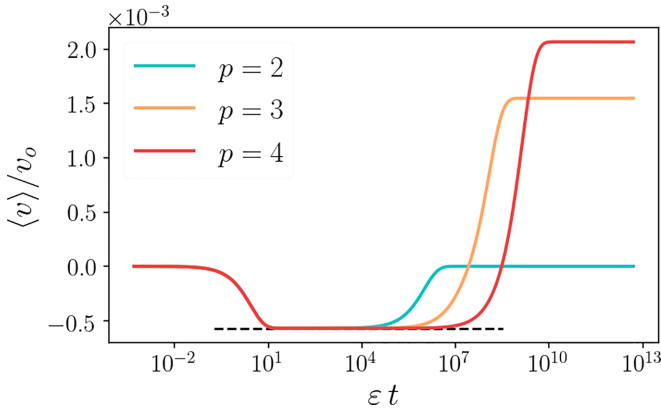


FIG. 3. Average velocity in Eq. (5) vs time, contrasting states with and without momentum relaxation. State without momentum relaxation is indicated by a black dashed line. We consider phonon baths with various densities of states $\nu \sim |\omega|^p$ (see legend). Parameters: same as in Fig. 2 with bath temperatures $T = \varepsilon$ and $\Delta T/T = 0.01$, and momentum coupling decay defined by $q_0 = 0.02\varepsilon$. Hierarchy of timescales $t_s \ll t_m$ guaranteed by $\lambda_0/N = 0.002\varepsilon \ll \gamma$.

velocity-velocity correlation function

$$g(t, \bar{t}) = \langle \delta \hat{v}(t) \delta \hat{v}(t + \bar{t}) \rangle, \quad (10)$$

where $\delta \hat{v}(t) = \hat{v}(t) - \langle \hat{v}(t) \rangle$. We compute the steady-state correlation function using the quantum regression theorem [29],

$$g(\bar{t}) = \sum_k r_{o,k} \left(e^{-\Gamma_k \bar{t}/2} \cos(2\Delta_k \bar{t}) (\hat{\Delta}_k \times \partial_k \mathbf{d}_k)^2 + 4e^{-\Gamma_k \bar{t}} \sum_{\alpha, \alpha'} \frac{\Gamma_{\alpha,k}^+ \Gamma_{\alpha',k}^-}{\Gamma_k^2} (\hat{\Delta}_k \cdot \partial_k \mathbf{d}_k)^2 \right) + g_o, \quad (11)$$

where $\Gamma_k = \sum_{\ell, \alpha} \Gamma_{\alpha,k}^{(\ell)}$ (see [28] for details) and $\bar{t} \ll t_m$. When evaluated with the appropriate momentum distribution, this expression applies to the steady states with and without momentum relaxation. The constant g_o reflects residual correlations for $t_s \ll \bar{t} \ll t_m$ due to memory of the initial momentum distribution. Momentum relaxation suppresses these correlations in the long-time limit $t, \bar{t} \gg t_m$, where $g(t, \bar{t}) \rightarrow 0$. The velocity fluctuations far exceed the average velocity, emphasizing the importance of stochasticity. Mean-square displacements can be obtained by integrating $g(\bar{t})$ (see SM [28]).

Figure 4 shows a typical time trace of the velocity correlations for $t \gg t_m$. The oscillations directly reflect the Rabi oscillations of the internal degrees of freedom in the motion of the particle. These exist in equilibrium and remain clearly visible for $\Delta T \neq 0$, when the quantum particle is active. The oscillation period and temperature scale are controlled by the Zeeman field, while the oscillations decay on the timescale t_s . These quantum features are sensitive to the relative orientation of the vectors $\mathbf{d}$ and Δ_k [see Eq. (11)]. For $\mathbf{d} \parallel \Delta_k$, energy is exchanged through incoherent transitions between the two internal states and the oscillations disappear (classical limit).

Conclusions. We set up a framework to engineer active particles in the quantum regime. Its essential ingredients are

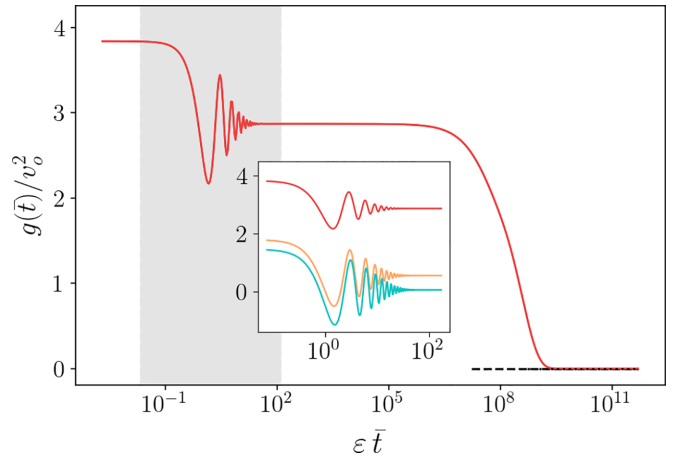


FIG. 4. Velocity correlator for $t \gg t_m$ vs relative time $\bar{t}$. Parameters: Same as Fig. 3, with $p = 3$. Inset: zoom of oscillations observed for $\bar{t} \ll t_m$ (gray background in main plot) for various equilibrium temperatures: $T = 0.02\varepsilon$ (green), $T = 0.2\varepsilon$ (orange), and $T = \varepsilon$ (red) with temperature bias $\Delta T = 0.01T$.

the presence of “spin-orbit” coupling between internal and translational degrees of freedom, breaking of time-reversal symmetry by a “magnetic” field, and an imbalance in the couplings to the energy reservoirs, which drive the system out of equilibrium. These ingredients are already available in cold-atom systems. Spin-orbit coupling in cold gases has been extensively studied both theoretically and experimentally [30–32]. The realization of the hot/cold bath can be achieved either following [33] or by putting the optical lattice in an optical cavity [34]. Selective couplings to different baths can be realized by coupling to different polarizations or cavities with multiple resonances (for multilevel systems). We hope that our work identifying the ingredients and properties of realizable, synthetic, quantum active particles stimulates the design of specific experimental setups and their detailed theoretical description.

Our work focused on the extreme quantum limit of a particle with two internal states; we explored the properties of the heat-to-motion conversion, the quantum signatures of the active motion, and the consequences of a noisy environment leading to momentum relaxation. More generally, we expect the qualitative results to extend beyond the specific model considered, making our proposed approach more amenable to experimental implementations.

So far, we focused on single-particle properties in one dimension. The model can be straightforwardly extended to include interactions between many particles as well as higher dimensional systems. These generalizations unlock a wealth of additional phenomena such as collective behavior, topological phenomena, etc. More broadly, the dynamics of these active particles bear features typical of quantum walks [35–37] and are closely related to quantum thermodynamics [25,26], which opens additional appealing bridges to other classes of phenomena.

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Data availability. The data that support the findings of this Letter are openly available [38].

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