Stochastic dynamics of an impurity with spin-orbit coupling

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(Dated: October 6, 2022)

Brownian dynamics of a mobile impurity in a bath is affected by spin-orbit coupling (SOC). Here, we discuss a Caldeira-Leggett-type model that can be used to propose and analyze quantum simulators of this dynamics in cold Bose gases. In particular, we derive a master equation and explore it in a one-dimensional setting. To validate the standard assumptions needed for our derivation, we analyze available experimental data without SOC; as a byproduct, this analysis suggests that the quench dynamics of the impurity is beyond the Bose-polaron approach at temperatures currently accessible in a cold-atom laboratory – motion of the impurity is mainly driven by dissipation. For systems with SOC, we demonstrate that one-dimensional spin-orbit coupling can be ‘gauged out’ even in the presence of dissipation – the information about SOC is incorporated in the initial conditions. Observables sensitive to this information (such as spin densities) can be used to study formation of steady spin polarization domains during quench dynamics.

Dissipation of energy occurs naturally when a particle with finite momentum moves through a medium. This phenomenon is typically studied assuming that the momentum of the particle is decoupled from its spin degree of freedom. This is however not the case for many condensed matter systems with strong spin-orbit coupling (SOC). In particular, for externally driven setups with non-trivial topological character, such as bosonic Kitaev-Majorana chains [1, 2]. Majorana wires [3, 4], as well as systems featuring optical spin-Hall effect [5, 6], SOC is also key for explaining transport of electrons through a layer of chiral molecules [7, 8]. To understand equilibration processes in these systems and promote their use in technologies, studies of dissipative dynamics with SOC are needed. Cold-atom-based quantum simulators provide a natural testbed for such studies [9, 10] – they complement the existing research of out-of-equilibrium time evolution, see, e.g., [11–13], and SOC engineering using laser fields [14, 15].

To enjoy the potential of quantum simulators, one requires theoretical models that can be used to propose new experiments and analyze the existing data [16]. In this work, we present one such model designed to study an impurity with SOC (see also recent Ref. [17] for a discussion of a relevant Langevin-type equation). The impurity is in contact with the bath that we model as a collection of a relevant Langevin-type equation). The impurity is in contact with the bath that we model as a collection of harmonic oscillators. Using the Born and Markov approximations, we derive a master equation, which extends the result of Caldeira and Leggett [18, 19] to a spin-orbit-coupled impurity. To illustrate this equation, we focus on one-dimensional (1D) systems. First, we test it using the experimental data of Ref. [20], whose full theoretical understanding is lacking, see, e.g., Ref. [21]. We find that the Caldeira-Leggett model contains all ingredients to describe the observed breathing dynamics of the impurity assuming that the initial condition is the (only) tunable parameter. The calculations are analytical, which simplifies the analysis and allows us to gain insight into the system: relevant time scales, short- and long-time dynamics. Finally, we explore the dynamics of the system with SOC. Without magnetic fields, the 1D SOC can be gauged out so that the system can be described using the Caldeira-Leggett equation with SOC-dependent initial conditions. We present observables that are sensitive to these initial conditions and can be used to study the effect of SOC on time dynamics, for example, formation of regions with steady spin polarization. Our findings provide a convenient theoretical model that can be used to propose and benchmark quantum simulators of dissipative dynamics with SOC.

The particle-bath Hamiltonian. The Hamiltonian of the system is given by $H_{\text{tot}} = H_S + H_B + H_C$. The three terms account for, correspondingly, the (quantum) impurity, the harmonic bath and the bath-impurity coupling. We assume that $H_S$ has the form

$$H_S = \frac{p^2}{2m} + V_{SO}(\mathbf{p}, \sigma) + V_{\text{ext}}(\mathbf{q}) + \mathbf{q}^2 \sum_{j=1}^{N} \frac{c_j^2}{2m_j \omega_j^2},$$  \hspace{1cm} (1) \hspace{1cm}$$

where $m$ and $q$ are the mass and the position of the impurity, respectively. $V_{\text{ext}}$ is an external potential. $V_{SO}(\mathbf{p}, \sigma)$ is the potential that describes SOC; it depends on the Pauli vector, $\sigma$, and the momentum of the impurity, $\mathbf{p}$. A particular form of $V_{SO}$ is specified below, see also the Supplementary Material. The last term in Eq. (1) is a standard harmonic counterterm, which makes the Hamiltonian $H_{\text{tot}}$ translationally invariant if $V_{\text{ext}} = 0$ [22]. The parameters $\omega_j$ and $m_j$ are taken from the bath Hamiltonian, $H_B = \sum_j [p_j^2/(2m_j) + \frac{1}{2} m_j \omega_j^2 q_j^2]$; $c_j$ defines the strength of the bath-impurity interaction $H_C = -\mathbf{q} \cdot \sum_j c_j x_j$. For microscopic derivations that validate the form of $H_B$ and $H_C$ for weakly interacting Bose gases and Luttinger liquids, see correspondingly Refs. [23] and [24]. To summarize, we consider a single particle (impurity) linearly coupled to an environment made of non-interacting harmonic oscillators using the standard procedure [18, 25], briefly outlined below; this is a well-studied problem extended here by subjecting the impurity to SOC.

Before analyzing $H_{\text{tot}}$, we remark that there are a number of theoretical methods [26–30] that can be used for interpreting experiments with impurities in Fermi [31].
and Bose gases [20, 35, 39]. Time evolution of an impurity in a Bose gas – the focus of this work – has been studied using variational wave functions, T-matrix approximations and exact solutions in 3D at zero [40, 42] and finite temperatures [43]. Many more methods exist to address the 1D world. For example, experimentally relevant trapped systems can be studied using numerically exact approaches [44, 45], for review see Ref. [46]. In cases when those methods do not work (e.g., large energy exchange or high temperature), it has been suggested to connect a cold-atom impurity to quantum Brownian motion [23, 47, 49]. Our work provides an example when this idea leads to an accurate description of experimental data, setting the stage for testing assumptions behind theoretical models of relaxation [19, 22] in a cold-atom laboratory.

**Born-Markov master equation with SOC.** Time evolution of the impurity-bath ensemble, defined by $H_{\text{tot}}$, obeys the Von-Neumann equation: $i\hbar \dot{\rho}_{\text{tot}} = [H_{\text{tot}}, \rho_{\text{tot}}]$. To extract dynamics of the impurity from $\rho_{\text{tot}}$, we rely on the Born-Markov approximation [19, 50, 51], which leads to the equation for the (reduced) density matrix that describes the impurity, $\rho_S$:

\[
\frac{d\rho_S}{dt} = -\frac{i}{\hbar} [H_S, \rho_S] - \frac{1}{\hbar^2} \int_0^{+\infty} ds C(s) \left[ q, \{Q(-s), \rho_S\} \right] + \frac{i}{\hbar^2} \int_0^{+\infty} ds \chi(s) \left[ q, \{Q(-s), \rho_S\} \right].
\]  

We write Eq. (2) in the form standard for a Brownian particle; the contribution of SOC is conveniently hidden in $Q(t)$, which is defined as

\[
Q(t) = \frac{i}{\hbar} [H_S, q] = q - \left( \frac{p}{m} + v_{SO}(\sigma) \right) t,
\]  

where $v_{SO} = \partial_{\sigma} V_{SO}$ is the contribution to the ‘velocity’ of the particle due to SOC. Equation (2) contains the bath autocorrelation functions $C(t)$ and $\chi(t)$ in Eq. (2):

\[
C(t) = \hbar \int_0^{+\infty} dw J(\omega) \coth \left( \frac{\beta \hbar \omega}{2} \right) \cos(\omega t),
\]

\[
\chi(t) = \hbar \int_0^{+\infty} dw J(\omega) \sin(\omega t),
\]

where $\beta = 1/k_BT$ (for temperature, and $k_B$ is the Boltzmann constant). These functions assume that all recent macroscopic information is encoded in the spectral function $J(\omega)$, formally defined as $J(\omega) = \sum_j c_j^2 \delta(\omega - \omega_j) / (2m_j \omega_j)$. We choose $J(\omega) = (2m\gamma/\pi) \omega \Omega^2 / (\Omega^2 + \omega^2)$, recovering Ohmic dissipation at $\omega \to 0$; the phenomenological parameter $\Omega$ defines the high-frequency behavior. The Ohmic spectral density is a standard choice in mesoscopic [40, 42] and in cold-atom physics [24, 50, 53]. We employ it here because it leads to a local-in-time damping that agrees with the experimental data used below to validate the model (see also Refs. [24, 52] for additional details about Ohmic dissipation in 1D based upon long-wavelength approximations for superfluids). Super-Ohmic dissipation whose relevance for Bose polarons is highlighted in Refs. [23, 48] leads to strong memory effects (non-local-in-time damping), thus, we do not consider it here.

Using Eqs. (3) and (4), we derive the master equation

\[
\frac{d\rho_S}{dt} = -\frac{i}{\hbar} [H_S, \rho_S] - \frac{\gamma}{\hbar} \left[ q, \{q, \rho_S\} \right] - \frac{2m\gamma}{\beta R^2} \left[ q, \{q, \rho_S\} \right] - i m\gamma \left[ q, \{v_{SO}, \rho_S\} \right],
\]  

where $\gamma$ defines the strength of dissipation. The frequency integrals leading to Eq. (5) are discussed in the Supplementary Material. As expected, dissipative dynamics is affected by SOC (see the last term in Eq. (5)). Finally, a proper Lindblad form for Eq. (5) can be achieved by adding a minimally invasive term $-\gamma / (8m) \left[ p, \rho_S \right] / (8m)$ [19, 39]; we employ this term in our calculations.

To illustrate the master equation, we choose to consider a 1D setting parameterized by the coordinate $y$. Without loss of generality, we write the SOC term as $V_{SO} = \alpha x y$. In this case, the master equation reads as

\[
\frac{d\rho_S}{dt} = \frac{d\rho_S}{dt}\bigg|_{\alpha=0} - \alpha F[\rho],
\]

where $F[\rho] = \sigma_x \partial_{\rho} \rho + \partial_{\rho} \sigma_x \rho + \frac{i\alpha}{\hbar} (y - y') (\sigma_x \rho + \rho \sigma_x)$ with $\rho \equiv \langle y | \rho_S | y' \rangle$, and $\frac{d\rho_S}{dt}\bigg|_{\alpha=0}$ describes time evolution of the system without SOC (see the Supplementary Material). The effect of SOC is encoded in $\alpha F[\rho]$.

While the technical details leading to Eq. (5) are presented in the Supplementary Material, we recall here the standard assumptions behind the Born-Markov approximation. First, the impurity-bath density matrix is separable throughout time evolution, such that $\rho_{\text{tot}} \simeq \rho_S \otimes \rho_B$. Second, the bath is not affected by the impurity motion, namely, $\rho_B(t) \approx \rho_B^0$. This assumption is natural if the decay of bath correlations has the fastest timescale $\tau_B$; it implies that dynamical features $\sim \tau_B$ are not resolved by our approach [19, 54]. To validate these approximations, we shall demonstrate that the master equation is capable of describing experimental data of Ref. [20] that provide a benchmark point for us at $\alpha = 0$.

**Dynamics without SOC.** First, we briefly outline the main features and findings of the experiment of Ref. [20]. In that work, a potassium atom was used to model an impurity in a gas of rubidium atoms. At $t = 0$, the impurity was trapped in a tight trap created by a species-selective dipole potential (SSDP) with $\omega_{\text{SSDP}} / (2\pi) = 1$kHz. At $t > 0$, the dynamics was initiated by an abrupt removal of the SSDP; the impurity was still confined by a shallow parabolic potential, i.e., $V_{\text{ext}}(y) = \hbar^2 y^2 / 2ml^2$, where $l = \sqrt{\hbar / m \omega}$ and $\omega = (87 \times 2\pi)$Hz is the frequency of the oscillator. The experiment recorded the size of the impurity cloud $\bar{y} = \sqrt{\langle y^2 \rangle}$, and found that it can be fit using the expression

\[
\bar{y} = \bar{y}_0 + A_1 t - A_2 e^{-1\Omega t} \cos[\sqrt{1 - \Omega^2}(t - t_0)],
\]
where \(A_1, A_2, \Omega, \Gamma, \bar{y}_0, t_0\) are fitting parameters. The key experimental findings of Ref. \[20\] were: (a) \(\Omega\) (almost) does not depend on the impurity-boson interaction parametrized by \(\eta\); (b) by increasing \(\eta\) one decreases the amplitude of the first oscillation; (c) in the interacting case, besides oscillating, \(\bar{y}\) increases over time in a seemingly linear fashion; (d) at long times \(\bar{y}\) equilibrates to about the same value, which is independent of \(\eta\). Point (b) was attributed to renormalization of the mass of the impurity, i.e., to a polaron formation \[60\]. However, this posed several theoretical problems. In particular, the breathing frequency of the polaron cloud should depend on \(\eta\), which contradicts observation (a), see also discussions in Ref. \[20\]. Our results below suggest that one can understand the data of Ref. \[20\] from the perspective of dissipative dynamics.

Equation (7) leads naturally to the dynamics observed in the experiment. To show this, we assume that the initial density matrix of the impurity corresponds to a Gaussian wave packet

\[
\rho(y, y', t = 0) = e^{-\frac{y^2 + y'^2}{\pi \delta^2}} / (\sqrt{\pi l_0}),
\]

where \(l_0\) is the parameter that determines the initial distribution of the impurity momenta; Eq. (8) is standard for particles whose initial state is not precisely known.

We calculate the time dynamics for this initial condition analytically using the method of characteristics (see the Supplementary Material and Ref. \[62\]), which discovers characteristic curves where the master equation can be written as a family of ordinary differential equations \[63\]. The computed functional dependence resembles Eq. (7) with \(\Gamma \Omega = 2\gamma\) (see the Supplementary Material). Note that our calculations have only two phenomenological parameters \(\gamma\) and \(l_0\). All other parameters that appear in Eq. (7), i.e., \(A_1, A_2, \bar{y}_0, t_0\) and \(\Omega\), can be extracted from our results. For example, \(\Omega \sim 2\omega\) as in the experiment.

We present analytical results of the master equation together with the experimental data in Fig. 1. The value of \(\gamma\) is restricted to be within the errorbars of the experimentally measured value of \(\Gamma \Omega\) (so that \(\gamma \sim 40\text{Hz}\) \[64\]. The temperature is set to the value reported in the experiment, i.e., \(T = 350\text{nK}\) \[65\]. The quality of the fits in Fig. 1 is comparable to what can be obtained with Eq. (7), allowing us to conclude that the master equation provides a valuable tool for analyzing cold-atom systems.

Let us briefly discuss implications of our results for interpretation of the experiment of Ref. \[20\]. First, the weak dependence of \(\Omega\) on \(\eta\) is natural in our model: the renormalization of the frequency is given by \(\omega_{\text{eff}} \approx \omega(1 - \gamma^2/(2\omega^2))\), where \(\gamma/\omega\) is a small parameter as in the experiment. Second, the parameter \(\bar{y}\) for \(t \to \infty\) is independent of \(\gamma\) assuming that the thermal de Broglie wavelength is small. Indeed, in this case, we derive \(\bar{y} \approx \sqrt{k_BT/(\hbar \omega)}l \approx 15.42\ \mu\text{m}\) in agreement with the measurement.

The decrease of the oscillation amplitude in our analysis of the data is attributed to the initial condition, i.e., the value of \(l_0\). One can speculate that the impurity forms a polaron at \(t < 0\), and, therefore, \(l_0\) has information about renormalization of the mass of the impurity, i.e., \(m \to m_p\) at \(t = 0\) \[66\]: this might explain why theoretical calculations can produce features of the amplitude but not of the frequency \[20\]. If the impurity at \(t = 0\) has the effective mass \(m_p\), the corresponding energy scale is \(\hbar \omega_{\text{SSDP}} \sqrt{m/m_p}\). To incorporate it into Eq. (8), one should have \(l_0^2 \approx \hbar / m \omega_{\text{SSDP}} \sqrt{m/m_p}\). This expression agrees qualitatively with the outcome of our fit, see Fig. 1 (c). The obtained linear increase of \((m \omega_{\text{SSDP}} l_0^2 / \hbar)^2\) however quantitatively disagrees with calculations of the effective mass \[21\]. The agreement improves if we disregard the point with \(\eta = 30\), which (as suggested in Ref. \[20\]) is already beyond a simple one-dimensional treatment \[61\]. In any case, a further analysis of the experimental data (beyond the scope of this paper) is needed in light of our results.

Finally, we note that the inhomogeneity of the bath as well as non-Markovian physics do not appear to be important to describe dynamics discussed here. This stands in contrast to what is known about properties of the corresponding ground state \[71\] and low-energy dynamics \[57, 61, 72\], and results from a high temperature and a large energy associated with the initial impurity state.

**Dynamics with SOC.** We use the experimental protocol...
We assume that was typical in that experiment. The strength of SOC, the system from Ref. [20]. We use

\[ \gamma \]

For the sake of discussion, we take the parameters of amplitude is \( \alpha \) of position and time in the presence of SOC. The SOC amplitude is \( \alpha = 40 \text{ Hz} \cdot \mu \text{m} \). \( l_0 \) for (a,b) case corresponds to \( \omega_0/2\pi = 30 \text{ kHz} \), while \( l \) is given by \( \omega/2\pi = 87 \text{ Hz} \). All other parameters are as in Ref. [20], in particular \( T = 350 \text{nK} \).

of Ref. [20] also to study the system with SOC. The peculiarity of 1D is that the \( \alpha \)-dependent term can be gauged out from Eq. (6) via the transformation (in the position space) \( \rho = e^{-\frac{i}{\hbar} \int_0^{t} f(x) \, dx} \). The function \( f(y, t) \) then satisfies the standard Caldeira-Leggett equation and can be solved exactly as without SOC (see the Supplementary Material for details). Note that the equation for \( f \) is spin independent. Therefore, the full spin structure of the problem is contained in the initial condition \( \rho(0, \mathbf{y}) \). Spin observables depend on time, as we illustrate below for \( \sigma_y(y, t) \equiv \text{Tr}_{\text{spin}}(\sigma_y) \).

As the initial condition we take a state that is spin-polarized along the \( z \)-axis, i.e.,

\[ \rho(y', 0) = \frac{1}{2\sqrt{\pi \alpha_0} e^{-\frac{y'^2}{2\alpha_0}}} | \uparrow \rangle \langle \uparrow |. \]  

(9)

For the sake of discussion, we take the parameters of the system from Ref. [20]. We use \( \gamma = 40 \text{ Hz} \), which was typical in that experiment. The strength of SOC, \( \alpha \), can be tuned in cold-atom set-ups, see, e.g., [73–75]. We assume that \( \alpha \gamma/\omega^2 \ll 1 \) to demonstrate that even weak SOC can lead to an observable effect in dynamics.

Time evolution of \( \sigma_y(y, t) \) is shown in Fig. 2. Note that Eq. (9) is not an eigenstate of the system with SOC dynamics occurs even without a change of the trap, i.e., \( l_0 = l \) [see Figs. 2 (c) and (d)]. Without dissipation (\( \gamma = 0 \)), we observe oscillation of the spin density with \( \sigma_y > 0 \) for \( y > 0 \) and \( \sigma_y < 0 \) for \( y < 0 \) [see Figs. 2 (a) and (c)]. This effect is solely due to SOC, and can be easily calculated using a one-body Schrödinger equation. Effects of temperature and dissipation are most visible in Fig. 2 (d): the impurity is heated up by the presence of the bath, which creates regions with steady spin polarization along the \( y \) direction. Spatial extension of these regions is determined by the temperature; the time scale for their formation is given by \( 1/\gamma \) (similarly to the dynamics without SOC, see Fig. 1). To observe this effect in cold-atom systems, one will analyze the population of hyperfine states of the impurity atom.

Finally, we remark that Eq. (5) allows us to include Zeeman-type terms, which naturally appear in ultracold atoms with synthetic SOC [14, 15]. To this end, we add the term \( \mu_B \mathbf{B} \cdot \mathbf{\sigma} \) to \( H_S \). Its presence strongly modifies the spin dynamics because SOC cannot be gauged out. Theoretical analysis also becomes more involved, since we cannot solve the system analytically for all values of \( \alpha \) and \( B \). Still, we obtain closed-form expressions using tools of perturbation theory (see the Supplementary Material). The effect of the magnetic field is illustrated in Fig. 3. Initially, the dynamics with the magnetic field is similar to the dynamics presented in Fig. 2. However, at later times we observe spin precession possible only in the presence of both SOC and the magnetic field. Precession leads to change of positive and negative regions of \( \sigma_y \) with time, and can be used for engineering the spin structure.

\[ \text{Conclusion.} \]  

We analyzed Brownian-type motion of a spin-orbit coupled impurity with the goal to develop a simple theoretical tool that can be used to propose and analyze cold-atom-based quantum simulators. We introduced a master equation suitable for the problem. We tested it and illustrated its usefulness by interpreting available experimental data without SOC [20]. Our results suggested that the impurity does not experience any mass renormalization during quench dynamics at experimentally accessible temperatures. Finally, we demonstrated that systems with SOC can be studied analytically and calculated observables that measure changes in population of the hyperfine states of the impurity atom.

A comparison between results of our theoretical study and experimental data (when available) can be used to
understand the limits of applicability of a set of assumptions standard for studies of Brownian motion, such as the Markov approximation. Our findings pave the way also for studies of various condensed matter systems where SOC and dissipation play a role. For example, the chirality induced spin selectivity (CISS) effect [7, 8] is believed to require non-unitary time evolution (e.g., due to dissipation) and spin-orbit coupling, see, e.g., [76–80]. These effects are included in our model, hence, it can be developed into a testbed for studying CISS [81].

ACKNOWLEDGMENTS

We thank Rafael Barfknecht for help at the initial stages of this project; Fabian Brauneis for useful discussions; Miguel A. García-March, Georgios Koutentakis, and Simeon Mistakidis for comments on the manuscript. M.L. acknowledges support by the European Research Council (ERC) Starting Grant No. 801770 (ANGULON).

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We checked that $\gamma$ could be even fixed to the central value reported in the experiment, without affecting much the quality of the fit.

The accuracy of the fit could be slightly improved by allowing the temperature to vary within the experimental error bars. We do not do it here to avoid having an additional fitting parameter.

In this interpretation, the initial state is given by the polaron described by the Hamiltonian $-\frac{\hbar^2}{2m_p} \frac{\partial^2}{\partial y^2} + \frac{m\omega_{SSDP}^2}{2} y^2$. At $t > 0$, the polaron is destroyed, which can be due to the anomalous behavior of the residue [82] or a highly-non-equilibrium nature of the problem. To show the existence of the polaron at $t = 0$, one needs to consider ground-state properties of an impurity in a tight trap – hence with a high kinetic energy – which is beyond the scope of the present work.

Here, we calculate the expectation value of the kinetic energy for a free particle: $-\frac{\hbar^2}{2m} \langle \frac{\partial^2}{\partial y^2} \rangle$, and relate it to $\hbar \omega_{SSDP} \sqrt{m/m_p}$, which is the typical energy scale of the ‘polaron’ Hamiltonian: $-\frac{\hbar^2}{2m_p} \frac{\partial^2}{\partial y^2} + \frac{m\omega_{SSDP}^2}{2} y^2$.

One expects that large values of $\eta$ require a beyond-linear-coupling treatment of impurity-bath interactions [21, 83], which is beyond the scope of the present paper.

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