<table>
<thead>
<tr>
<th>Title</th>
<th>Kondo effect on adiabatic spin pumping from a quantum dot driven by a rotating magnetic field</th>
</tr>
</thead>
<tbody>
<tr>
<td>Author(s)</td>
<td>Hattori, Kiminori</td>
</tr>
<tr>
<td>Citation</td>
<td>PHYSICAL REVIEW B. 2008, 78(15), p. 155321-1-155321-4</td>
</tr>
<tr>
<td>Version Type</td>
<td>VoR</td>
</tr>
<tr>
<td>URL</td>
<td><a href="https://hdl.handle.net/11094/3464">https://hdl.handle.net/11094/3464</a></td>
</tr>
<tr>
<td>Note</td>
<td></td>
</tr>
</tbody>
</table>

_Osaka University Knowledge Archive : OUKA_

https://ir.library.osaka-u.ac.jp/

Osaka University
The Kondo effect on adiabatic spin pumping from a quantum dot driven by a rotating magnetic field

Kiminori Hattori

Department of Systems Innovation, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan

(Received 12 June 2008; published 24 October 2008)

The adiabatic spin pumping from an interacting quantum dot driven by a rotating magnetic field is studied using the numerical renormalization-group method. From the spin-current continuity equation, we derive a general formalism for spin pumping, which proves that the rotating field generates a time-independent spin current. Following this formalism, the numerical calculation implemented in the adiabatic regime demonstrates that spin pumping is enhanced exponentially with Coulomb interaction. This mechanism is explained in terms of the Kondo resonance under the external field.

DOI: 10.1103/PhysRevB.78.155321 PACS number(s): 72.25.—b, 72.15.Qm, 73.23.—b, 73.63.Kv

The Kondo effect exhibited by a magnetic impurity in a metallic host constitutes a prototypical many-body correlation effect involving interactions between a localized spin and conduction electrons. This effect emerges similarly in the mesoscopic system consisting of an interacting quantum dot coupled to a free-electron reservoir, stimulating tremendous interests both theoretically and experimentally. An appealing feature behind this is an unequalled controllability of system parameters such as a single-particle level and hybridization couplings, which is hardly realized in bulk solids. The Kondo effect in quantum dots is also an intriguing subject of research in the field of spintronics, which aims to manipulate electron spin in solid-state systems, because of a peculiarity in the Kondo regime where charge excitations are fully quenched, whereas spin excitations are active. In this perspective, methodologies for generating a pure spin current without any charge current have been proposed to date, including parametric spin pumping in the Kondo regime by cyclic variations in system parameters, as well as spin pumping from an interacting dot in the presence of a rotating external magnetic field. The former exploits a fine tunability of the parameter space, while the latter could be applied to various other Kondo systems. (Apart from spin-pumping phenomena, there have been several theoretical works addressing charge pumping through interacting dots. The literature on this subject is included in the reference section for the benefit of readers.)

The Kondo effect on spin pumping from an interacting dot driven by the rotating field, however, is less accurately understood. The previous study employs the equation-of-motion method for elucidating the spin-current generation, suggesting a nontrivial enhancement for the interacting dot. This method consists of differentiating the one-particle Green’s function with respect to time, thereby generating this method, which is known to give accurate results for quantum impurity systems. We derive a general formalism for spin pumping from the spin-current continuity equation, based on which the NRG calculation is implemented in the adiabatic regime. The numerical calculation demonstrates that the pumped spin current increases exponentially with the strength of Coulomb repulsion on the dot. We explain this mechanism via a quasiparticle Green’s function that describes the Kondo resonance under the external field.

Throughout this paper, we shall work in units where ħ = keq = 1. We consider an interacting quantum dot coupled to an infinitely extended reservoir and subjected to a rotating transverse magnetic field \( B = B_0 e_z + e_y \) in addition to a static longitudinal field \( B_0 = B_0 e_z \), with \( e_x, e_y, e_z \) being the unit vectors in Cartesian coordinates. The model Hamiltonian \( H = H_d + H_r + H_{\text{hyb}} \) consists of the dot term \( H_d \), the reservoir term \( H_r \), and the hybridization term \( H_{\text{hyb}} \). These terms are expressed as

\[
H_d = \sum_{\sigma} \left( \frac{\sigma \omega_0}{2} \right) d_{\sigma}^\dagger d_{\sigma} + U \left( d_{\uparrow}^\dagger d_{\uparrow} d_{\downarrow}^\dagger d_{\downarrow} + \text{h.c.} \right) + \frac{\omega_1}{2} \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} \exp(-i\sigma \omega t),
\]

\[
H_r = \sum_{k\sigma} \left( \epsilon_k + \frac{\sigma \omega_0}{2} \right) c_{k\sigma}^\dagger c_{k\sigma},
\]

\[
H_{\text{hyb}} = V \sum_{k\sigma} (d_{\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger d_{\sigma}),
\]

respectively, where \( d_{\sigma} \) denotes the fermionic annihilation operator for an electron with spin \( \sigma \) in the dot, and similarly \( c_{k\sigma} \) stands for the annihilation operator for a reservoir electron. The single-particle energies in the absence of the external fields are represented by \( \epsilon_{d\sigma} \) in the dot and \( \epsilon_{k\sigma} \) in the reservoir. The Coulomb interaction for two electrons in the dot is given by \( U \), and both subsystems are coupled via the hybridization with strength \( V \). These expressions are similar to the single-impurity Anderson model, except for Zeeman interactions under the external fields characterized by the Larmor frequencies \( \omega_{q1} = \gamma B_{01} \), where \( \gamma \) is the gyromagnetic ratio. A uniform static field that spans the reservoir region is assumed in the present model.

The time dependence of the Hamiltonian \( H \) in the laboratory frame (in the following, denoted as L frame) is eliminated by the unitary transformation \( R = \exp(i\omega t S^z) \), where
\[ S^z = S^z_{\uparrow} + S^z_{\downarrow} \text{ is the total spin comprised of } S^z_{\uparrow} = (1/2) \sum_\sigma d^\dagger_\sigma d_\sigma \text{ and } S^z_{\downarrow} = (1/2) \sum_\sigma \sigma \epsilon \sigma_\downarrow, \text{ defining the Hamiltonian } H^R = HRR^{-1} - \omega S^z \text{ in the rotating reference frame. Subsequently, we consider the orthogonal transformation } \Theta = \exp(i\omega t), \text{ with } S^z = (1/2) \sum_\sigma d^\dagger_\sigma d_\sigma \text{ and } \tan \theta = \omega_1/(\omega_2 - \omega). \text{ This transformation introduces an auxiliary reference frame where the effective field becomes parallel to the spin-quantization axis so that the dot Hamiltonian is diagonalized. In this frame (hereafter, referred to as } \Theta \text{ frame), the total Hamiltonian } \\
\begin{align}
\tilde{H} &= \sum_{k\sigma} \epsilon_{k\sigma} v_\sigma d^\dagger_\sigma d_\sigma + U d^\dagger_\downarrow d_\downarrow d^\dagger_\uparrow d_\uparrow, \\
\tilde{H}_r &= \sum_{k\sigma} \epsilon_{k\sigma} e^{i\theta} c_{k\sigma}, \\
\tilde{H}_{hyb} &= V \sum_{k\sigma\sigma'} (d^\dagger_\sigma \Theta_\sigma \epsilon_{k\sigma'} c_{k\sigma'} + e^{i\theta} \epsilon_{k\sigma'} d^\dagger_{\sigma'} c_{k\sigma}),
\end{align}
\]

where the spin-dependent single-particle energies are defined by \( \epsilon_{k\sigma} = E_{k\sigma} + (\omega_2 - \omega) / 2 \) and \( \epsilon_{d,\sigma} = \epsilon_{d,\sigma} + \omega_1 / 2 \), with \( \Omega = (\sqrt{\omega_2 - \omega})^2 + \omega_1^2 \), and the matrix element \( \Theta_{\sigma\sigma'} \) is explicitly written as \( \Theta_{\sigma\sigma'} = \cos(\theta/2) \) and \( \Theta_{\sigma,\sigma';\sigma'} = \sin(\theta/2) \). In what follows, we analyze the spin current observed in the L frame, in combination with the nonequilibrium Green’s functions defined in the \( \Theta \) frame.

In terms of the Heisenberg equation, \( idS^z/dt = [S^z(t), H] \), the spin torque operator is formulated as \( G^z(t) = dS^z/dt = \omega_1 \text{ Im } d^\dagger_\sigma d_\sigma(t) \text{ exp}(\pm i\omega t) \) in the L frame, where \( \text{Im } A = (A - A^\dagger)/2i \). It is notable that this expression naturally constitutes the continuity equation \( dS^z/dt + F(t) = G^z(t) \) for the spin current flowing into the reservoir \( F(t) = dS^z/dt \) for convenience, we introduce the lesser Green’s function \( G^{\prec}_{\sigma\sigma'}(t, t') = i(d_\sigma(t') d_\sigma(t)) \) defined in the L frame.\(^7\) In this notation, the spin magnetization and the spin torque are expressed as \( \langle S^z(t) \rangle = (1/2) \sum_\sigma G^{\prec}_{\sigma\sigma}(t, t) \) and \( \langle G^z(t) \rangle = \omega_1 \text{ Re } G^{\perp}_{\sigma\sigma}(t, t) \text{ exp}(i\omega t) \), respectively. By definition, the double-time correlation function \( G^{\prec}_{\sigma\sigma'}(t, t') \) satisfies

\[ G^{\prec}_{\sigma\sigma'}(t, t') = \exp\left(-\frac{\sigma\omega t}{2}\right) \exp\left(-\frac{\sigma\omega t'}{2}\right) \times \sum_{\rho\rho'} \Theta_{\sigma\rho} G^{\succ}_{\rho\rho'}(t' - t') \Theta_{\sigma'\rho'}, \]

where \( G^{\prec}_{\sigma\sigma'}(t, t') \) represents the lesser Green’s function defined in the \( \Theta \) frame, and hence depends only on the time difference \( t - t' \). It is easily shown from (3) that \( d[d^\dagger_\sigma] / dt = d[G^z] / dt = 0 \), leading to the identity \( \langle F \rangle = \langle G^z \rangle \) in view of the spin-current continuity equation. Thus the spin current \( \langle F \rangle \) formed a quantum dot driven by the rotating field is essentially independent of time and can be calculated from the spin torque \( \langle G^z \rangle \) exerted on the dot. Following our mathematical derivation, it is essential for \( d[F]/dt = 0 \) that the time dependence of the total Hamiltonian \( H \) arising from the external field is completely eliminated by the unitary transformation into the rotating frame. Note that this elimination is possible particularly for the dot Hamiltonian \( H_d \) without intrinsic spin-mixing terms. In other words, spin nonconservation in the unperturbed dot, which is excluded from the present consideration, can be a source of transfer of spin current in the presence of the rotating field. From \( \langle G^z \rangle \) re-expressed as \( \tilde{G}_{\sigma\sigma'}(t) \), one obtains

\[ \langle F \rangle = \frac{\omega_1}{2\pi} \int_{-\infty}^{\infty} dt \text{ Re } \tilde{G}_{\sigma\sigma'}^\perp(e), \]

via \( \det \Theta = 1 \), where \( \tilde{G}_{\sigma\sigma'}^\perp(e) \) is the Fourier transform of \( \tilde{G}_{\sigma\sigma'}(t) \). Equation (4) is a compact and general formula deduced from Eq. (1) without any particular assumptions.

The lesser Green’s function is obtained by the Keldysh equation, expressed as \( \tilde{G}_{\sigma\sigma'}^\perp(e) = \Sigma_{\rho\rho'} \tilde{G}_{\sigma\rho}(e) \Sigma_{\rho\rho'}(e) \tilde{G}_{\rho\sigma'}^\perp(e) \), where \( \tilde{G}_{\sigma\rho}(e) = [\tilde{G}_{\sigma\rho}(e)]^* \) is the retarded Green’s function, and \( \Sigma_{\sigma\sigma'}(e) \) is the lesser self-energy. In the noninteracting case \( (U = 0) \), the retarded Green’s function obeys the equation of motion:

\[ (e - \epsilon_{\sigma\rho}) \tilde{G}_{\sigma\rho}(e) - V^2 \sum_{\rho\rho'} \Theta_{\sigma\rho} \tilde{G}_{\rho\rho'}^\perp(e) \tilde{G}_{\rho\sigma'}^\perp(e) = \delta_{\sigma\sigma'}, \]

where \( \epsilon_{\sigma\rho}(e) = (\epsilon_{\sigma\rho} + i\omega) / 2 \) is the retarded function of the reservoir, and \( \delta \) is a positive infinitesimal. The equation of motion is immediately solved in the wideband approximation. The solution is found to be \( \tilde{G}_{\sigma\rho}(e) = \delta_{\sigma\rho}(e - \epsilon_{\sigma\rho} + i\delta)^{-1} \), with \( \Gamma = \Gamma_\sigma V^2 \), where \( \rho_\sigma = \sum_\delta \delta e - \epsilon_{\sigma\rho} \) is the density of states in the reservoir. The diagonal form derived in the noninteracting limit simplifies the theoretical treatment for the finite-\( U \) Green’s function, which is written formally as

\[ \tilde{G}_{\sigma\sigma'}^\perp(e) = \left( e - \epsilon_{\sigma\rho} + i\Gamma - \Sigma_{\sigma\sigma'}(e) \right)^{-1}, \]

where the whole effect of many-body correlation is contained in the retarded self-energy \( \Sigma_{\sigma\sigma'}(e) \). On the other hand, the lesser self-energy is exactly calculated to be \( \Sigma_{\sigma\sigma'}(e) = 2i(\sum_\rho \Theta_{\sigma\rho} f_\rho(e) \Theta_{\rho\sigma'}) \) for \( U = 0 \), where \( f_\rho(e) = f(e + \omega_2 / 2) \) and \( f(e) \) is the Fermi function in the reservoir. This expression is still valid even for \( U \neq 0 \) if \( \text{Im } \Sigma_{\sigma\sigma'}(e) \equiv 0 \) around the Fermi level.\(^10\) Hence, the pumped spin current at low temperatures can be formulated as

\[ \langle F \rangle = -\frac{\omega_1}{2\pi\Omega} \int_{-\infty}^{\infty} dt [f_\rho(e) - f_e(e)] \text{Im } \tilde{G}_{\sigma\rho}(e) \tilde{G}_{\rho\sigma'}^\perp(e), \]

in terms of the retarded Green’s function \( \tilde{G}_{\sigma\rho}(e) \) defined in the \( \Theta \) frame. It is straightforward to show that in both adiabatic and nonadiabatic regimes, Eq. (6) reproduces the previous results for spin pumping from a noninteracting quantum dot in the presence of the rotating field.\(^11\)

The technique we use to calculate \( \tilde{G}_{\sigma\rho}(e) \) is Wilson’s NRG method. A prime ingredient of this method is a loga-
the calculation are indicated in the figure. The vertical bar marks the frequency corresponding to the Kondo temperature $T_K$.

Ninth, the calculation is expressed as $\tilde{H}_{bf}=\sum_{n} \delta_{n} f_{n}^{\dagger} f_{n}+\sum_{n} \delta_{n} f_{n}^{\dagger} \sigma_{n} f_{n}$ and $\tilde{H}_{f}=\sum_{n} f_{n}^{\dagger} f_{n}^{\dagger} f_{n}^{\dagger} f_{n}$. For $\omega=\omega_{0}$, where $f_{n}^{\dagger}$ (i.e., 0,1,2,...) is a fermionic operator in the linear-chain representation. The coupling constants are given by $v_{n}=\sqrt{2T D / \pi}$ and $\lambda_{n}=D[(1+\Lambda^{-1})/2] \Lambda^{-n / 2} \xi_{n}$, where $D$ is the reservoir bandwidth. $\Lambda>1$ is the discretization parameter, and $\xi_{n}$ is a constant of order 1. In the NRG calculation, the total Hamiltonian $\tilde{H}$ is diagonalized iteratively starting from the uncoupled dot $\tilde{H}_{d}$. A direct calculation of dynamical properties such as $G_{\alpha \beta}^{\dagger}(\omega)$ is allowed via the one-particle spectral function $\tilde{a}_{\alpha}(\omega)$ in the Lehmann representation and its Hilbert transformation into $\tilde{a}_{\alpha}(\omega)$). It may be appropriate here to restate that we postulate a slowly rotating field such that the interacting dot coupled to the reservoir can always adiabatically adjust to the instantaneous thermal equilibrium state. Physically, the longest time scale for equilibration is given by the inverse Kondo temperature $T_{K}^{-1}$, i.e., the Kondo time scale, which governs the buildup of the Kondo effect.

Therefore, the equilibrium Green’s function obtained from the NRG calculation reasonably applies in the adiabatic regime where $\omega \ll T_{K}$.

In the calculation, the bare level width of the dot $2\Gamma$ caused by the hybridization is taken as the energy unit. The number of states retained per NRG iteration is 1000, and the reservoir bandwidth is chosen as $D=100$. The calculation assumes zero temperature and the Fermi energy $\varepsilon_{F}=0$. The pumping field strength is normally $\omega_{0}=10^{-4}$, which is sufficiently small that the Kondo resonance persists. All the results shown below are obtained under the spin resonance condition $\omega=\omega_{0}$.

Figure 1 displays the pumped spin per pumping cycle, $P=\langle 2 \pi \omega_{0} / \omega \rangle \langle\tilde{O}\rangle$, calculated as a function of pumping frequency $\omega$ for the particle-hole symmetric case $\varepsilon_{d}=-U/2$. Each curve corresponds to a different strength of Coulomb interaction $U$. As shown in Fig. 1, the pumped spin is independent of frequency when $\omega \ll T_{K}$. This trend allows us to unambiguously quantify the pumped spin in the adiabatic regime. In this regime, the spin pumping takes place via the Kondo resonance at $\varepsilon=0$, in view of Eq. (6). An additional but interesting observation is that the pumped spin exhibits two resonances. The high-frequency peak observed around $\omega=U$ originates from a couple of atomic excitations centered at $\varepsilon=\varepsilon_{d}$ and $\varepsilon_{d}+U$. The low-frequency peak occurs around $\omega=T_{K}$, particularly for a large $U$. It is likely that this observation captures a dynamical aspect of spin generation, although its quantitative evaluation needs an extended study that covers the nonadiabatic regime exactly. The discussion that follows concentrates on the adiabatic regime.

Figure 2 illustrates how the pumped spin varies with the dot level position $\varepsilon_{d}$ (which is experimentally controlled by a gate potential) in the adiabatic regime. Important indications contained in this plot are as follows. The pumped spin is symmetric about and maximal at the particle-hole symmetric point $\varepsilon_{d}=-U/2$. At this point, more importantly, spin pumping is enhanced exponentially with $U$. In Fig. 2, the $U=0$ result is shown for comparison, from which we find that the Kondo-assisted enhancement is quite substantial for strongly interacting dots. Generally, the most fundamental quantity in Kondo physics is the Kondo temperature, which is analytically described by the formula of Haldane, \[ T_{K} = \sqrt{\frac{T U}{2}} \exp \left( \pi \varepsilon_{d} / (U_{2}) \right) / 2 U T. \] The Kondo temperature is minimal at $\varepsilon_{d}=-U/2$, and at this point decreases exponentially with $U$. This suggests that $T_{K}$ plays a crucial role in determining the magnitude of $P$. Figure 3 compares the numerical results shown in Fig. 2 to the Haldane formula, demonstrating that our observations are surprisingly well explained by the functional dependence of $T_{K}^{H}(\varepsilon_{d}, U)$. It is also confirmed in the numerical calculation that the pumped spin is quadratic in $\omega_{0}$ and tends to saturate when $\omega_{0} \geq T_{K}$ (not shown). The saturation is a direct consequence of the field-induced suppression of the Kondo resonance. The quadratic dependence is predicted from the perturbation theory applied to the spin torque, and is physically interpreted in terms of the photon absorption, which is involved in the spin-flip process that brings about a finite spin torque. The observations in the numerical results are eventually summarized into a simple empirical formula: $P \approx \omega_{0}^{2} / 3 T_{K}^{2}$ for $\omega_{0} \ll T_{K}$.

The numerical results described above are qualitatively accounted for in terms of the Kondo resonance under a per-
NRG calculation. At zero temperature, the spectral function renormalization factor, $K_{\text{MINORI}}$ in Hattori, Phys. Rev. B 78, 20849 (2008) is the quasiparticle part of the spectral function. For $\varepsilon \equiv 0$, the retarded Green’s function given by Eq. (5) takes the form $G_{\sigma \sigma}(\varepsilon) = z_\varepsilon(\varepsilon - E_p(\Delta_p)\varepsilon^{-1}$, where $z_\varepsilon = (1 - \text{Re } \sum_{\sigma} z_{\sigma \sigma}(\varepsilon))^{-1}$ is the renormalization factor, $E_p$ is the quasiparticle energy, and $\Delta_p$ is the corresponding level width. The level width remains of order $T_K$ for a weak field such that $\omega_1 < T_K$. In this case, Eq. (6) predicts the pumped spin given by $P_z \approx (\pi^2 \omega_1^2 \Gamma E_p / T_K)\hat{A}_{\sigma \sigma}(0)\hat{A}_{\sigma \sigma}(0)$ for $\omega = \omega_0 \approx T_K$, where $\hat{A}_{\sigma \sigma}(\varepsilon) = -\pi e^{-\varepsilon}$ is the spectral function. We assume the effective Zeeman splitting $\delta E = E_1 - E_2$ of order $\omega_1$, which does not contradict the Bethe-ansatz solution, as well as the NRG calculation. At zero temperature, the spectral function obeys the Friedel sum rule based on $\text{Im } \sum_{\sigma} x = 0$: $\hat{A}_{\sigma \sigma}(0) = \text{Im } (m_{\sigma \sigma}) / \pi T$, stating that the value of the spectral function at the Fermi energy is determined by the level occupation $m_{\sigma \sigma}$. In the Kondo regime, $\hat{n}_\uparrow \approx \hat{n}_\downarrow \approx 1/2$ is expected for a sufficiently weak field. From these considerations, we arrive at $P_z \approx \omega_0^2 / \Gamma T_K$. This expression agrees well with our observation, except for a trivial factor of 3. The pumped spin for a noninteracting dot is maximal at $\varepsilon_p = 0$, and then $P_z \approx \omega_0^2 / \Gamma^2$. Therefore, the enhancement factor amounts to $\Gamma / T_K$.

Before ending the discussion, it may be worthwhile to stress that the present spin-pumping scheme is implemented without specific modulation of system parameters, implying its extensive applicability to various Kondo systems. For instance, dilute Kondo alloys, for which the Kondo temperature spans a very wide range of $T_K \approx 10^{-3} - 10^3$ K while $\Gamma \approx 0.1$ eV, are interesting candidates, in addition to an interacting quantum dot with typically $T_K \approx 10^{-3} - 10^3$ K and $\Gamma \approx 0.1$ meV.

In summary, we have studied spin pumping from an interacting quantum dot driven by a rotating magnetic field, particularly in the adiabatic regime where the system is nearly in equilibrium. Starting from the single-impurity Anderson model into which Zeeman interactions are incorporated, a general formulation of spin current is derived in terms of the spin-current continuity equation at the operator level, proving that the pumped spin current in the presence of the rotating field is essentially time independent. In accordance with this formalism, the dc spin current generated in the adiabatic regime is analyzed using the NRG method. The NRG calculation discloses that in the Kondo regime, spin pumping is enhanced exponentially with Coulomb interaction. This anomalous behavior is basically explained via a quasiparticle Green’s function that describes the Kondo resonance under the external field. The spin-pumping scheme demonstrated in this study is not restricted to the interacting dot but also applicable to various other Kondo systems. We expect these findings to be useful for exploiting Kondo correlations in spintronics.

---