Influence of Rashba spin-orbit coupling on the Kondo effect

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An Anderson model for a magnetic impurity in a two-dimensional electron gas with bulk Rashba spin-orbit interaction is solved using the numerical renormalization group under two different experimental scenarios. For a fixed Fermi energy, the Kondo temperature $T_K$ varies weakly with Rashba coupling $\alpha$, as reported previously. If instead the band filling is low and held constant, increasing $\alpha$ can drive the system into a helical regime with exponential enhancement of $T_K$. Under either scenario, thermodynamic properties at low temperatures $T$ exhibit the same dependences on $T/T_K$ as are found for $\alpha = 0$. Unlike the conventional Kondo effect, however, the impurity exhibits static spin correlations with conduction electrons of nonzero orbital angular momentum about the impurity site. We also consider a magnetic field that Zeeman splits the conduction band but not the impurity level, an effective picture that arises under a proposed route to access the helical regime in a driven system. The impurity contribution to the system’s ground-state angular momentum is found to be a universal function of the ratio of the Zeeman energy to a temperature scale that is not $T_K$ (as would be the case in a magnetic field that couples directly to the impurity spin), but rather is proportional to $T_K$ divided by the impurity hybridization width. This universal scaling is explained via a perturbative treatment of field-induced changes in the electronic density of states.

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I. INTRODUCTION

The field of spintronics has primarily been driven by the idea of manipulating spin states to create new, spin-based electronic devices.1,2 Rashba spin-orbit (SO) coupling3 has been proposed as a mechanism for spin-control, not only because of the possibility of its external manipulation, but also because it is the physical origin of spin-dependent phenomena such anisotropic magnetoresistance4 and the spin-Hall effect.5 Interest in SO interactions has also been motivated by the recent discovery of large Rashba spin-splittings in Bi2Se3 topological insulators6,7, where the Rashba parameter can be an order of magnitude higher than in standard III-V semiconductors.

The study of Kondo correlations in the presence of SO interactions can be traced back more than 40 years to experiments that seemed to demonstrate suppression of the Kondo effect by Pt impurities.8 However, early theoretical studies of Anderson and Kondo models including SO scattering from heavy nonmagnetic impurities reached opposing conclusions as to whether SO interactions cut off the Kondo $\ln(T/T_K)$ term in the resistivity.8,10,11 Subsequent magnetoresistance measurements were interpreted as providing evidence for coexistence of SO scattering and the Kondo effect.11 A similar conclusion was reached on the basis of time-reversal symmetry12, although this assertion has recently been challenged.13

In recent years, several theoretical works have investigated the effect of SO interaction of the Rashba type on the Kondo temperature $T_K$. An analysis of the Kondo model for a magnetic impurity in an otherwise clean two-dimensional electron gas (2DEG) concluded that $T_K$ remains essentially unchanged by Rashba coupling.14 A numerical renormalization-group (NRG) study of an Anderson model describing the same physical situation similarly predicted weak enhancement or depression of $T_K$, depending on the energy of the impurity level relative to the Fermi energy.15 A variational treatment of the Kondo problem for arbitrary band dispersion and a general SO coupling also found no significant change of $T_K$, although it was claimed that the impurity is only partially screened.16 By contrast, a mapping via a generalized Schrieffer-Wolff transformation17 of an Anderson impurity in a two-dimensional host to an effective Kondo model led to the prediction18 of an exponential enhancement of $T_K$. In the specific context of adatoms on graphene, it was shown19 that Kondo physics survives the presence of bulk Rashba coupling, with a Kondo temperature that can change faster or slower with tuning of the chemical potential than would be the case in the absence of SO interaction (where the low-energy excitations are massless Dirac fermions).

This paper revisits the Kondo problem in the presence of Rashba SO interaction from a different perspective. We focus on two different scenarios under which the Rashba coupling in a 2DEG might be externally tuned: (1) an open electron system with a Fermi level pinned to that of external reservoirs, and (2) an isolated system with a constant band filling and a Fermi energy that varies with the Rashba coupling. The ap-
proper model for a magnetic impurity in a Rashba-coupled host is mapped exactly to effective two-channel and one-channel Anderson models without SO interaction but with conduction-band densities of states that are modified to account for the Rashba coupling. For the specific case of quadratic band dispersion (in the absence of SO interaction) and local impurity-band hybridization, we use the NRG technique to solve the effective one-channel model to calculate thermodynamic properties, from which we extract the Kondo temperature. For fixed Fermi energy, the case considered in previous work, we reproduce the conclusions of Ref. [13] that many-body screening of the impurity is complete, thermodynamic properties have conventional Kondo temperature dependencies, and varying the Rashba coupling produces only modest changes in the many-body scale $T_K$. In the helical regime, thermodynamics retain their conventional nature, but with a characteristic scale $T_K$ that is exponentially enhanced.

We also solve numerically the effective two-channel Anderson model, which retains angular-momentum information that is discarded in the one-channel model. Calculations of static angular-momentum correlations provide explicit confirmation of the expectation from previous works [14, 16, 18, 19] that the SO interaction induces an indirect coupling between the impurity and electrons of nonzero orbital angular momentum.

Entry to the helical regime requires very strong Rashba couplings and/or low carrier densities [22]. There has been considerable recent progress in fabrication of very low-density and clean two-dimensional hole gases [23], but here Coulomb interactions will likely replace disorder as a barrier to reaching the helical regime. However, it has been suggested that this regime may be accessed in a driven system by using circularly polarized light to create an effective Zeeman field that opens a gap between the two Rashba bands [21]. (Similar ideas have been proposed for engineering topological states in insulators [22, 23].) Although the breaking of time-reversal symmetry is inimical to the Kondo effect, this proposed experiment offers an opportunity to study Kondo physics in the presence of an effective magnetic field that couples directly only to the bulk electrons.

A real magnetic field would couple both to the spin of the bulk electrons and to the impurity spin, with respective $g$ factors $g_b$ and $g_i$ that need not be equal. There have been numerous studies of Anderson and Kondo models in fields that couple equally to the bulk and impurity spins ($g_b = g_i$) or only to the impurity ($g_b = 0$). Moreover, it has been shown [24] how to map between Kondo models having different pairs ($g_b$, $g_i$) and ($g_b'$, $g_i'$) so long as $g_i \neq 0$ and $g_i' \neq 0$. It is well understood [25] that in such cases, Kondo correlations are destroyed once the conduction-band Zeeman splitting $2\epsilon_Z$ becomes comparable $2\Gamma$ to $T_K$. By contrast, the proposal of Ref. [21] corresponds to a case $g_i = 0$ that has received little attention until now. Under these circumstances, we find (through NRG solution of an effective one-channel Anderson model) that the impurity contribution to the total angular momentum of the system’s ground state is a universal function, not of $\epsilon_Z/T_K$, but rather of $\int \Gamma \epsilon_Z / T_K D$, where $\Gamma$ is the hybridization width of the impurity level, $D$ is a measure of the conduction-band width, and the dimensionless quantity $f$ depends on other model parameters: the impurity level energy and on-site Coulomb repulsion, as well as (in this particular realization) the Rashba coupling. A perturbative treatment of field-induced changes in the effective densities of states for electrons with different components of the total angular momentum allows the scaling to be interpreted in terms of an effective spin-splitting of the impurity level by an energy proportional to $\Gamma \epsilon_Z / D$. A similar picture should hold for any realization of the Anderson impurity model with $g_i = 0$, as seems likely to be achievable in lateral quantum dots [23].

The remainder of the paper is organized as follows. Section II describes the Anderson model for a magnetic impurity in a two-dimensional host with bulk Rashba SO interaction, and outlines the mapping of the problem to a one-channel Anderson model with a hybridization function that depends on energy and, in the presence of a bulk Zeeman splitting as proposed in Ref. [21] also on the component of the electron’s total angular momentum parallel to the Zeeman field. Explicit expressions for the hybridization function are provided for cases where the band dispersion in the absence of Rashba coupling is purely quadratic. Section III presents numerical results for such cases, focusing on the effect of the Rashba coupling on the Kondo temperature $T_K$ and on static angular-momentum correlations, as well as the variation of the impurity polarization with bulk Zeeman field. We summarize our results in Sec. IV. Appendix A describes a perturbative method used to analyze the effects of Rashba coupling (in Sec. IIIA) and of a bulk Zeeman splitting (in Sec. IIIB). Details of the calculation of angular-momentum correlations appear in Appendix B.

II. MODEL AND PRELIMINARY ANALYSIS

A. Anderson model with Rashba coupling

We consider an Anderson impurity in a two-dimensional electron gas in the presence of Rashba SO coupling, modeled by the Hamiltonian [13, 18]

$$ H = H_{\text{bulk}} + H_{\text{imp}} + H_{\text{hyb}}, $$

Here, $H_{\text{bulk}} = H_0 + H_{\text{Rashba}}$, where

$$ H_0 = \sum_{k, \sigma} \epsilon(k) c_{k, \sigma}^\dagger c_{k, \sigma} $$

describes the conduction band in the absence of SO interaction, with operator $c_{k, \sigma}$ destroying a band electron
of two-dimensional wave vector $k = k_x \hat{x} + k_y \hat{y}$, spin $z$ component $\sigma = \pm 1/2$ (or $\uparrow$, $\downarrow$), and energy $\epsilon(k)$. The second term in $H_{\text{bulk}}$ represents the effect of the Rashba SO interaction $\lambda_R \vec{z} \cdot \vec{\sigma} \times \vec{k}$, where $\vec{\sigma}/2$ is the electron spin operator:

$$H_{\text{Rashba}} = i\lambda_R \sum_k k e^{-i\phi_k} c_{k,\uparrow}^\dagger c_{k,\downarrow} + \text{H.c.}, \quad (3)$$

where $k = |\vec{k}|$, $\phi_k = \text{atan}(k_y/k_x)$ are the polar components of $\vec{k}$, and $\lambda_R$ is the SO coupling (assumed in our analysis to be non-negative).

In isolation, the nondegenerate impurity level is described by

$$H_{\text{imp}} = (\epsilon_d + \mu)(d_{\uparrow}^\dagger d_{\uparrow} + d_{\downarrow}^\dagger d_{\downarrow}) + U d_{\uparrow}^\dagger d_{\uparrow} d_{\downarrow}^\dagger d_{\downarrow}, \quad (4)$$

where $d_{\sigma}$ destroys an electron with spin $z$ component $\sigma$ and energy $\epsilon_d$ relative to the chemical potential $\mu$, and $U$ is the on-site Coulomb repulsion. The impurity state is assumed to exhibit axial symmetry about $\vec{z}$.

The last term in Eq. (1), representing tunneling of electrons between the impurity and the bulk, is

$$H_{\text{hyb}} = \frac{1}{\sqrt{N_c}} \sum_{k,\sigma} V(k)(c_{k,\sigma}^\dagger d_{\sigma} + \text{H.c.}), \quad (5)$$

where $N_c$ is the number of unit cells in the host (and hence the number of distinct $k$ values in the first Brillouin zone) and the hybridization matrix element $V(k)$ can be taken to be real and non-negative. We note that although the orbital motion of the conduction electrons is constrained to two dimensions, all spin vectors are fully three-dimensional.

For simplicity, we consider a jellium host such that the band dispersion and the hybridization matrix element are isotropic in $k$ space, i.e., $\epsilon(k) = \epsilon(k)$ and $V(k) = V(k)$.

B. Mapping to a two-channel Anderson model

This section lays out an exact transformation of the Hamiltonian (1) into the form of an effective two-channel Anderson model for a magnetic impurity hybridizing with two bands in which the SO interaction has been subsumed into a modification of the density of states. The mapping generalizes the one presented in Ref. 15 to allow for arbitrary forms of $\epsilon(k)$ and $V(k)$.

We take the thermodynamic limit in the standard manner by letting the unit-cell number $N_c \to \infty$ and the system area $A \to \infty$ in such a way that $A/N_c \to A_c$, a finite unit-cell area. Each summation $\sum_k f(k)$ over a discrete wave vector $k$ can be replaced by an integral $(A_c/4\pi^2) \int d^2k f(k)$.

In the absence of SO coupling, it is natural to adopt a basis of states having a definite $z$ component of the orbital angular momentum about the impurity site. The transformation

$$c_{k,\sigma} \to \sum_{m=-\infty}^{\infty} \sqrt{\frac{2\pi}{A_c}} \epsilon^{i(m\phi_k - \pi/2)} c_{k,m,\sigma}, \quad (6)$$

where $\{c_{k,m,\sigma}, c_{k',m',\sigma'}^\dagger\} = \delta(k-k') \delta_{m,m'} \delta_{\sigma,\sigma'}$, allows one to rewrite Eq. (2) in the diagonal form

$$H_0 = \sum_{m,\sigma} \int dk \epsilon(k) c_{k,m,\sigma}^\dagger c_{k,m,\sigma} + \text{H.c.}, \quad (7)$$

while the hybridization term becomes

$$H_{\text{hyb}} = \frac{\sqrt{A_c}}{2\pi} \int dk \sqrt{k} V(k) (c_{k,0,\sigma}^\dagger d_{\sigma} + \text{H.c.}), \quad (8)$$

in which the impurity couples only to the $m = 0$ mode.

The Rashba Hamiltonian term, which becomes

$$H_{\text{Rashba}} = \lambda_R \int dk \sum_m c_{k,m,\uparrow}^\dagger c_{k,m+1,\downarrow} + \text{H.c.}, \quad (9)$$

is not diagonal in the ($k, m, \sigma$) basis because Rashba SO interaction couples spin and orbital degrees of freedom. However, since $H_{\text{Rashba}}$ mixes only pairs of states ($k, m, \uparrow$) and ($k, m + 1, \downarrow$), $H_{\text{bulk}}$ conserves $\tau = m + \sigma$, the $z$ component of total (orbital plus spin) angular momentum. The bulk Hamiltonian also commutes with the helicity operator

$$\hat{h} = \vec{z} \cdot \vec{\sigma} \times \vec{k} = \int dk \sum_m c_{k,m,\uparrow}^\dagger c_{k,m+1,\downarrow} + \text{H.c.}. \quad (10)$$

It is therefore convenient to perform a canonical transformation to a new complete basis of fermionic operators

$$\tilde{c}_{k,h,\tau} = \frac{1}{\sqrt{2}} \left(h^{\tau-1/2} c_{k,\tau-1/2,\uparrow} + h^{\tau+1/2} c_{k,\tau+1/2,\downarrow} \right), \quad (11)$$

each of which annihilates an electron in a state of well-defined $\tau = \pm 1/2, \pm 3/2, \ldots$ and definite helicity $h = \pm 1$ (abbreviated $h = \pm$ at certain points below).

This transformation diagonalizes the bulk Hamiltonian, yielding

$$H_{\text{bulk}} = \sum_{h,\tau} \int dk \epsilon_h(k) \tilde{c}_{k,h,\tau}^\dagger \tilde{c}_{k,h,\tau} \quad (12)$$

with a helicity-dependent (but total-angular-momentum-independent) dispersion

$$\epsilon_h(k) = \epsilon(k) + h\lambda_R k. \quad (13)$$

The two operators $c_{k,h\tau}$ to which the impurity couples in Eq. (8) can be represented in terms of four operators $\tilde{c}_{k,h,\tau}$, namely those with $h = \pm$ and $\tau = \pm 1/2$. Since these four operators also involve $c_{k,-1,\uparrow}$ and $c_{k,1,\downarrow}$, one sees that the Rashba SO interaction creates an indirect coupling of the impurity to conduction electrons with nonzero orbital angular momentum [14][18].

One can drop the uninteresting contribution to $H_{\text{bulk}}$ from electrons having total angular momentum $z$ component $|\tau| > 1/2$, thereby reducing Eq. (1) to a two-channel Anderson Hamiltonian with the helicity $h$ acting.
as a channel index:

\[
H = \sum_{k, \tau} \int dk \, \epsilon_k (k) \, \tilde{c}_{k, h, \tau} \tilde{c}_{k, h, \tau}^\dagger + H_{\text{imp}}
\]

\[
+ \frac{A_c}{4\pi} \sum_{k, \tau} \int dk \, \sqrt{k} \, V(k) (\tilde{c}_{k, h, \tau} \tilde{c}_{k, h, \tau}^\dagger + H.c.).
\]

Due to the difference \(\epsilon_+ (k) - \epsilon_- (k) = 2\lambda_R k\), the two helicities enter Eq. (17) in an inequivalent manner; in particular, they have different Fermi wave vectors. It is also important to bear in mind that the index \(\tau = \pm 1/2\) (or \(\uparrow, \downarrow\)) labels the \(z\) component of the total angular momentum, although this reduces to \(z\) component of spin for the impurity operators \(d_r\).

Equation (14) can be transformed to an energy representation by defining

\[
\tilde{c}_{\epsilon, h, j, \tau, \tau'} = |\epsilon'_j (k_j)|^{-1/2} \ \tilde{c}_{k_j, h, \tau},
\]

where \(\epsilon'_j = d\epsilon_h / dk\) and \(k_j (\epsilon, h), j = 1, \ldots, n_h (\epsilon)\) are the numerically distinct roots of the equation \(\epsilon_h (k_j) = \epsilon\). If \(\epsilon_h (k)\) is a monotonically increasing function of \(k\), as would be the case for free fermions in the absence of SO interaction, then \(n_h (\epsilon) = 0\) for \(\epsilon < \epsilon_h (0)\) and \(n_h (\epsilon) = 1\) for \(\epsilon \geq \epsilon_h (0)\). However, as discussed in greater detail in Sec. III B the presence of Rashba SO interaction creates an energy range within which \(n_{-} (\epsilon) = 2\).

The operators defined in Eq. (15) obey the canonical anticommutation relations

\[
\{ \tilde{c}_{\epsilon, h, j, \tau, \tau'}, \tilde{c}_{\epsilon', h', j', \tau', \tau'}^\dagger \} = \delta (\epsilon - \epsilon') \ \delta_{h, h'} \ \delta_{j, j'} \ \delta_{\tau, \tau'}
\]

and allow Eq. (15) to be rewritten

\[
H = \sum_{h, \tau} \int d\epsilon \ n_h (\epsilon) \ \tilde{c}_{\epsilon, h, \tau} \tilde{c}_{\epsilon, h, \tau}^\dagger + H_{\text{imp}}
\]

\[
+ \sum_{h, \tau} \int d\epsilon \ n_h (\epsilon) \ \sqrt{\Gamma_{h, j} (\epsilon)} / \pi \ (\tilde{c}_{\epsilon, h, \tau} \tilde{c}_{\epsilon, h, \tau}^\dagger \ d_r + H.c.),
\]

where

\[
\Gamma_{h, j} (\epsilon) = \frac{A_c k_j}{4 |\epsilon'_j (k_j)|} V(k_j)^2
\]

is the contribution to the helicity-\(h\) hybridization function at energy \(\epsilon\) that arises from wave vector \(k = k_j (\epsilon, h)\).

Equation (17) is an exact restatement of Eq. (14), and allows full recovery of dependences on the radial coordinate measured from the impurity site, as obtained via Fourier transformation with respect to \(k\). Further transformations of the Hamiltonian described in Sec. III C below serve to simplify the calculation of certain thermodynamic properties, but necessarily entail loss of information about radial or angular momentum degrees of freedom that could be inferred from a complete solution of Eq. (17).

### C. Further reduction of the model

One simplification of Eq. (17) arises from noting that for energies \(\epsilon\) where \(n_{-} (\epsilon) > 1\), the impurity couples to a single linear combination of the operators \(\tilde{c}_{\epsilon, h, \tau}, j = 1, 2, \ldots, n_h (\epsilon)\). Defining

\[
\sqrt{\Gamma_{h} (\epsilon)} \ \tilde{c}_{\epsilon, h, \tau} = \sum_{j=1}^{n_h (\epsilon)} \sqrt{\Gamma_{h, j} (\epsilon)} \ \tilde{c}_{\epsilon, h, \tau}
\]

with a helicity-\(h\) hybridization function

\[
\Gamma_{h} (\epsilon) = \sum_{j=1}^{n_h (\epsilon)} \Gamma_{h, j} (\epsilon)
\]

allows one to write

\[
H = \sum_{h, \tau} \int d\epsilon \ \epsilon \ \tilde{c}_{\epsilon, h, \tau} \tilde{c}_{\epsilon, h, \tau}^\dagger + H_{\text{imp}}
\]

\[
+ \sum_{h, \tau} \int d\epsilon \ \sqrt{\Gamma_{h} (\epsilon)} / \pi \ (\tilde{c}_{\epsilon, h, \tau} \ d_r + H.c.),
\]

from which have been dropped diagonal terms involving \(n_{-} (\epsilon) - 1\) linear combinations of the operators \(\tilde{c}_{\epsilon, h, \tau}\) that are orthogonal to \(\tilde{c}_{\epsilon, h, \tau}\). The mapping from \(n_{-} (\epsilon) > 1\) operators \(\tilde{c}_{\epsilon, h, \tau}\) to a single \(\tilde{c}_{\epsilon, h, \tau}\) involves loss of radial information since the latter operator cannot be associated with any single wave vector \(k\).

Another simplification can be made by combining the \(h = +\) and \(h = -\) states of the same energy that couple to the impurity. Defining

\[
\sqrt{\Gamma_{+} (\epsilon)} \ \tilde{c}_{\epsilon, \tau} = \sqrt{\Gamma_{+} (\epsilon)} \ \tilde{c}_{\epsilon, +, \tau} + \sqrt{\Gamma_{-} (\epsilon)} \ \tilde{c}_{\epsilon, -, \tau}
\]

with a total hybridization function

\[
\Gamma (\epsilon) = \Gamma_{+} (\epsilon) + \Gamma_{-} (\epsilon),
\]

one can again discard decoupled degrees of freedom [here, associated with \(\sqrt{\Gamma_{-} (\epsilon)} \ \tilde{c}_{\epsilon, +, \tau} - \sqrt{\Gamma_{+} (\epsilon)} \ \tilde{c}_{\epsilon, -, \tau}\)] to arrive at an effective one-impurity Anderson model

\[
H = \sum_{\tau} \int d\epsilon \ \epsilon \ \tilde{c}_{\epsilon, \tau} \tilde{c}_{\epsilon, \tau}^\dagger + H_{\text{imp}}
\]

\[
+ \sum_{\tau} \int d\epsilon \ \sqrt{\Gamma (\epsilon)} / \pi \ (\tilde{c}_{\epsilon, \tau} \ d_r + H.c.).
\]

That the original model in Eq. (11) can be reduced to a one-channel Anderson impurity model was shown previously in Ref. 13 for the specific case of a quadratic \(c (k)\) and a local (\(k\)-independent) \(V (k)\). However, the derivation above makes clear that the price paid for going from Eq. (21) to Eq. (24) is the loss of the ability to distinguish between the spin and orbital angular momenta within a bulk state of given \(z\) component of the total angular momentum. For this reason, Sec. III D presents not only...
impurity properties calculated from Eq. [24], but also impurity-bulk angular-momentum correlations obtained via numerical solution of Eq. [21].

In the absence of the impurity, the bands entering Eqs. [21] and [24] would be filled at temperature $T = 0$ up to a chemical potential $\mu = \epsilon_F$. (As will be emphasized in Secs. [11E] and [11I] the Fermi energy $\epsilon_F$ may or may not take the same value as for $\alpha = 0$, depending on the experimental setup being described.) In cases where $\Gamma(-\epsilon_d) \ll -\epsilon_d$ and $\Gamma(U + \epsilon_d) \ll U + \epsilon_d$, it is appropriate to apply a generalized Schrieffer-Wolff transformation [17] to map the two- and one-channel Anderson models to two- and one-channel Kondo models, respectively. In general, the resulting Kondo models [18] will not be the same as those obtained by starting with a Kondo Hamiltonian for a magnetic impurity in a 2DEG and then incorporating a bulk Rashba SO interaction.

D. Model with bulk Zeeman field

In a recent paper, Ojans and Kitagawa [21] proposed to realize a helical system through irradiation of a two-dimensional electron gas containing Rashba SO interaction by light in the THz frequency range. After time-averaging over a period of the electromagnetic radiation, the bulk electrons experience an effective Zeeman coupling of tunable strength $\epsilon_Z = (\lambda_{\text{eff}} E_0)^2/\Omega^2$, where $E_0$ and $\Omega/2\pi$ are the magnitude and frequency of the applied electric field. Provided that the characteristic rate $k_B T_K/2\pi$ [24] of spin flips involved in Kondo screening is much slower than $\Omega/2\pi$, the impurity will effectively interact with the time-averaged band structure. This regime spans $T_K \ll 50K$ for $\Omega/2\pi = 1$ THz and $T_K \ll 500K$ for $\Omega/2\pi = 10$ THz, conditions that will be readily satisfied in most experiments. We also note that for the values of $E_0$ envisioned in Ref. [21], the magnetic component of the circularly polarized light is so small as to have negligible effect.

With this motivation, we consider the Hamiltonian [11] augmented by a term

$$H_{\text{Zeeman}} = 2\epsilon_Z \sum_{k,\sigma} \sigma c_{k,\sigma}^\dagger c_{k,\sigma},$$

where $\sigma = \pm 1/2$ or $\uparrow$, $\downarrow$, depending on the context, and we assume below that $\epsilon_Z \geq 0$. The model can again be mapped to effective two-channel and one-channel Anderson models via a sequence of steps along the lines laid out in Secs. [11B] and [11C].

In order to diagonalize $H_{\text{bulk}} = H_0 + H_{\text{Rashba}} + H_{\text{Zeeman}}$, the operator transformation in Eq. [11] must be generalized to

$$\tilde{c}_{k,h,\tau} = \frac{1}{\sqrt{2}} \left[ \begin{array}{c} h^{\tau-1/2} \beta_+ h(k) c_{k,\tau-1/2,\tau} \\ h^{\tau+1/2} \beta_- h(k) c_{k,\tau+1/2,\tau} \end{array} \right],$$

where

$$\beta_{\pm 1}(k) = \sqrt{1 \pm \frac{\epsilon_Z}{(\lambda_{\text{eff}}^2 k^2 + \epsilon_Z^2)^{1/2}}}.$$

This yields Eq. [12] with a helicity-dependent dispersion

$$\epsilon_h(k) = \epsilon(k) + h \sqrt{\lambda_{\text{eff}}^2 k^2 + \epsilon_Z^2}$$

that features a gap $2\epsilon_Z$ at $k = 0$, while the impurity-bulk hybridization becomes

$$H_{\text{hyb}} = \sqrt{\frac{A}{4\pi}} \sum_{h,\tau} \int dk \sqrt{k} V(k) \beta_{2\tau} h(k) (\tilde{c}_{k,h,\tau}^\dagger d_{\tau} + \text{H.c.}),$$

where the value of the product $2\tau h = \pm 1$ selects between the two functions $\beta_{\pm 1}(k)$ defined in Eq. [21]. After further transformation to an energy representation, the problem maps to a generalized two-channel Anderson model

$$H = \sum_{h,\tau} \int d\epsilon \epsilon \tilde{c}_{\epsilon,h,\tau}^\dagger \tilde{c}_{\epsilon,h,\tau} + H_{\text{imp}}$$

$$+ \sum_{h,\tau} \int d\epsilon \sqrt{\Gamma_{h,\tau}(\epsilon)/\pi} \left( \tilde{c}_{\epsilon,h,\tau}^\dagger d_{\tau} + \text{H.c.} \right),$$

containing a helicity- and angular-momentum-dependent hybridization function

$$\Gamma_{h,\tau}(\epsilon) = \sum_{j=1}^{n_{\text{h}}(\epsilon)} \frac{A_k k_j}{4|\epsilon_h(k_j)|} [\beta_{2\tau} h(k_j) V(k_j)]^2.$$
where it is convenient to define a Rashba wave vector \( k_R = \frac{m^* \lambda_R}{2} \), and a Rashba energy \( \epsilon_R = k_R^2/2m^* = m^* \lambda_R^2/2 \), such that \( \epsilon_0 = \epsilon_0 - \epsilon_R \) is the energy at a parabolic minimum in \( \epsilon_- (k) \) located at \( k = k_R \).

These dispersions, plotted schematically in Fig. 1(a), yield helicity-resolved densities of states (per unit cell, per total angular momentum \( z \) component)

\[
\rho_h(\epsilon) = \begin{cases} 
0 & \text{for } \epsilon_0 < \epsilon < \epsilon_0, \\
\frac{\epsilon_R}{\sqrt{\epsilon_R (\epsilon - \epsilon_0)}} & \text{for } \epsilon_0 < \epsilon < D_h, \\
\frac{\epsilon_0}{2} \left[ 1 - \frac{\epsilon_R}{\sqrt{\epsilon_R (\epsilon - \epsilon_0)}} \right] & \text{for } \epsilon_0 < \epsilon < D_-, \\
0 & \text{otherwise.}
\end{cases}
\]

The upper cutoff of the helicity-\( h \) band has shifted from \( D \) to \( D_h = \epsilon_h (k_{\max}) = D + 2h \sqrt{\epsilon_R (D - \epsilon_0)} \) such that \( \int_{-\infty}^{\infty} \rho_h(\epsilon) \, d\epsilon = \frac{1}{h} \). The densities of states \( \rho_h(\epsilon) \) are plotted schematically in Fig. 1(b). When compared with \( \frac{1}{2} \rho_0(\epsilon) \) [to which \( \rho_+ (\epsilon) \) and \( \rho_- (\epsilon) \) reduce for \( \epsilon_R = 0 \)], the most striking features are (i) the shift of \( h = + \) states to higher energies \( D < \epsilon < D_+ \), resulting in a monotonic depression of \( \rho_+ (\epsilon) \) to zero as \( \epsilon \to 0^+ \), and (ii) the shift of \( h = - \) states from \( D_- < \epsilon < D \) to lower energies, and particularly the \( 1/\sqrt{\epsilon - \epsilon_0} \) variation of \( \rho_- (\epsilon) \) over the range \( \epsilon_0 < \epsilon < 0 \). The van Hove singularity in \( \rho_- (\epsilon) \) at \( \epsilon = \epsilon_0 \) arises from the parabolic minimum in \( \epsilon_- (k) \) at \( k = k_R \).

Figure 1(b) also shows (dashed line) the density of states \( \rho(\epsilon) = \rho_+ (\epsilon) + \rho_- (\epsilon) \) for the effective one-channel Anderson problem defined in Eq. (24). This function is identical to its counterpart in the absence of Rashba interaction over a wide energy window \( 0 \leq \epsilon < D_- \), with \( \rho(\epsilon) \) differing from \( \rho_0 \) only in the redistribution of weight around the upper band edge \( \epsilon > D_- \), with part of that weight being transferred into the low-energy upturn spanning \( \epsilon_0 < \epsilon < 0 \).

In Sec. II, we examine the effect of increasing the Rashba energy \( \epsilon_R \), as might be achieved experimentally by increasing the strength of an electric field applied perpendicularly to the two-dimensional electron gas. We consider two scenarios:

1. The Fermi energy is fixed at \( \epsilon_F = 0 \), as would be the
In addition, below these densities of states coincide with the Rashba energy range in such a way that the overall filling fraction increases linearly with $\epsilon_R$:

$$\eta = \frac{1}{2}(\eta_+ + \eta_-) = \frac{2\epsilon_R - \epsilon_0}{D - \epsilon_0}. \quad (39)$$

The overall band filling is held constant, as would occur if the system were isolated from any external source of electrons. In this case, as illustrated in Fig. 2(b), varying the Rashba coupling still leads to changes in $\eta_+$ and $\eta_-$, but it does not alter their mean $\eta = -\epsilon_0/(D - \epsilon_0)$. This comes about because with increasing $\epsilon_R$, the Fermi energy decreases according to

$$\epsilon_F(\epsilon_R) = \begin{cases} -2\epsilon_R & \epsilon_R < \frac{\epsilon_0}{2}, \\ \epsilon_0 - \epsilon_R + \frac{\epsilon_0^2}{4\epsilon_R} & \epsilon_R \geq \frac{\epsilon_0}{2}. \end{cases} \quad (40)$$

For $\epsilon_R > \frac{\epsilon_0}{2}$, the Fermi energy lies below $\epsilon_0$, with two important consequences. First, the occupied bulk states all have $h = -$, resulting in the formation of an unconventional, helical metal. Second, the total density of states at the Fermi level is $\rho(\epsilon_F) = 2\rho_0|\epsilon_0|/\epsilon_0|$, which is enhanced over its value $\rho_0$ for $\epsilon_R = 0$. This situation is unlikely to be realized in standard III-V semiconductor heterostructures \cite{3}, since it would require very high Rashba couplings or very low carrier densities that will be affected by disorder or Coulomb interactions. However, driven systems may allow investigation of this interesting regime provided that one takes into account the effective Zeeman splitting of the helicity-resolved bands \cite{21}.

In the presence of a bulk Zeeman field as well as Rashba interaction, the helicity-$h$ dispersion in Eq. (25) can be expressed as

$$\epsilon_h(k) = \epsilon_0 + \frac{(\sqrt{k^2 + k_Z^2} + \hbar k_R)^2}{2m^*}, \quad (41)$$

where $k_Z = \epsilon_Z/\lambda_R$ and we have redefined

$$\epsilon_0 = \epsilon_0 - \epsilon_R - \frac{\epsilon_0^2}{4\epsilon_R} = \epsilon_0 - \epsilon_Z - \frac{(2\epsilon_R - \epsilon_Z)^2}{4\epsilon_R}. \quad (42)$$

Equation (41) implies that $\epsilon_+(k)$ rises monotonically with increasing $k$ from $\epsilon_+(0) = \epsilon_0 + \epsilon_Z$. If $k_F < k_R$, which is equivalent to the condition $\epsilon_Z < 2\epsilon_R$, the $h = -$ dispersion has a parabolic minimum at a nonzero wave vector $k = \sqrt{k_Z^2 - k_R^2}$, as shown schematically in Fig. 4(a); otherwise, $\epsilon_-(k)$ rises monotonically from $\epsilon_-(0) = \epsilon_0 - \epsilon_Z$, with a small-$k$ behavior that is quartic in $k$ for $\epsilon_Z = 2\epsilon_R$ but quadratic for any $\epsilon_Z > 2\epsilon_R$ [see Fig. 3(b)].

The helicity- and angular-momentum-resolved densities of states entering Eq. (35) become

$$\rho_{h,\tau}(\epsilon) = \begin{cases} \frac{\epsilon_0}{\sqrt{\epsilon_R(\epsilon - \epsilon_0)}} \Theta(2\epsilon_R - \epsilon_Z) \delta_{h,-} & \text{for } \epsilon_0 < \epsilon < \epsilon_0 - \epsilon_Z, \\ \frac{\epsilon_0}{2} \left[1 - \frac{\epsilon_0 - \epsilon_R - \epsilon_Z}{\sqrt{\epsilon_R(\epsilon - \epsilon_0)}}\right] & \text{for } \epsilon_0 + \hbar \epsilon_Z < \epsilon < D_h, \\ 0, & \text{otherwise}, \end{cases} \quad (43)$$

where $D_h = D + 2\hbar \sqrt{\epsilon_R (D - \epsilon_R - \epsilon_0)}$. For weak Zeeman splittings $\epsilon_Z \leq 2\epsilon_R$, $\rho_{-\tau}(\epsilon)$ features a van Hove singularity at $\epsilon = \epsilon_0$, associated with the minimum in $\epsilon_+(k)$. By contrast, for strong Zeeman splittings $\epsilon_Z > 2\epsilon_R$, there is no divergence of any $\rho_{h,\tau}(\epsilon)$.

Figures 3 also shows schematic plots of the angular-momentum-resolved densities of states $\rho_\tau(\epsilon) = \sum_h \rho_{h,\tau}(\epsilon)$, which determine $\Gamma_+(\epsilon)$ entering Eq. (34). These densities of states coincide with $\rho_0(\epsilon)$ over the energy range $\epsilon_0 + \epsilon_Z < \epsilon < D_0$. For $\epsilon_Z \leq 2\epsilon_R$, each density of states, plotted schematically in Fig. 3(c), inherits a van Hove singularity at $\epsilon = \epsilon_0$ from the divergence of $\rho_{-\tau}(\epsilon)$. In addition, $\rho_{-1/2}(\epsilon)$ exhibits a jump as the energy drops below $\epsilon = \epsilon_0 - \epsilon_Z$ due to the onset of contributions from $h = -$ states close to $k = 0$. [There is no corresponding jump in $\rho_{1/2}(\epsilon)$ because $\beta_{-1}(k)$ vanishes at $k = 0$.] For $\epsilon_Z > 2\epsilon_R$, by contrast, $\rho_{1/2}(\epsilon)$ approaches zero and $\rho_{-1/2}(\epsilon)$ rises smoothly to a constant limiting value as $\epsilon$ approaches $\epsilon_0 - \epsilon_Z$ from above, and both densities of states vanish for $\epsilon < \epsilon_0 - \epsilon_Z$, as sketched in Fig. 3(d).

III. NUMERICAL RESULTS

In order to study Hamiltonians \cite{24}, \cite{25}, and \cite{63} with the densities of states defined in Eqs. (35) and (43), we have applied the numerical renormalization-group (NRG) method for the solution of the Anderson model \cite{29}, as adapted to treat arbitrary densities of states \cite{30,31}. We set the Wilson discretization parameter to $\Lambda = 2.5$, retaining at least 2000 many-body states after each iteration. Results are shown for $\epsilon_0 = -0.08D$ and various combinations of $U$, $\epsilon_d$, and the hybridization width $\Gamma \equiv \pi\rho_0 V^2$. Any value of $\Gamma$ employed in
an NRG calculation should be equivalent in the continuum limit to a hybridization width $\Gamma_{\text{eff}} = \Gamma/A_\Lambda$, where $A_\Lambda = \frac{1}{\ln \Lambda} (\Lambda + 1)/(\Lambda - 1) \approx 1.069$ accounts for a reduction in the density of states that arises from the NRG discretization [29].

The results shown in Sec. III A 3 were obtained by solving the two-channel Anderson model [Eq. (21)]. All other data presented in this section come from calculations performed on a one-channel model [either Eq. (24) or Eq. (34)].

A. Results without a Zeeman field

1. Thermodynamic properties

We begin by showing the temperature variation of the impurity contribution to two thermodynamic quantities calculated using the effective one-channel Anderson model [Eq. (21)]: the magnetic susceptibility $\chi_{\text{imp}}$ (calculated for equal impurity and band $g$ factors, $g_i = g_b$) and the entropy $S_{\text{imp}}$. To reduce NRG discretization errors, we employed interleaved averaging over three different band discretizations.

In order to investigate the universality of the low-temperature physics, Fig. 4 shows $T_{\chi_{\text{imp}}}$ and $S_{\text{imp}}$ for a symmetric impurity ($U = -2e_d = 0.1D$, $\Gamma = 0.005D$) as functions of $T/T_K$. Note that we have defined $\chi_{\text{imp}}$ to be the impurity contribution to the static part of the correlation function for the $z$ component of the total angular momentum, which reduces to the customary static spin susceptibility in the case $\epsilon_R = 0$. The Kondo temperature $T_K$ was determined via the conventional criterion $\lim_{T \to 0} T_{\chi_{\text{imp}}} = 0$, or equivalently, via the condition $S_{\text{imp}}(T_K) = 0.383$. The fact that for $T \lesssim T_K$ the curves for $\epsilon_R/D = 0.04$ and $0.08$, calculated both for fixed Fermi energy (dotted lines) and for constant band-filling (dashed lines), lie on top of the curve for $\epsilon_R = 0$ (solid line) provides evidence that the low-temperature thermodynamic properties are those of a conventional Kondo effect, with $\lim_{T \to 0} T_{\chi_{\text{imp}}} = 0$ and $\lim_{T \to 0} S_{\text{imp}} = 0$ indicating complete ground-state screening of the impurity degree of freedom.

Even well above the Kondo temperature, four of the five curves in each panel of Fig. 4 are virtually indistinguishable, exhibiting both a high-temperature free-impurity regime (in which $T_{\chi_{\text{imp}}} \approx 1/8$, $S_{\text{imp}} \approx \ln 4$) and an intermediate-temperature local-moment regime (where $T_{\chi_{\text{imp}}} \approx 1/4$, $S_{\text{imp}} \approx \ln 2$). The only exception is the curve for $\epsilon_R = 0.08D$ at constant band filling. Here, the Fermi energy is pushed down into the van Hove singularity in the effective one-channel density of states. The enhanced hybridization width drives the system from its local-moment regime into mixed valence, where $T_{\chi_{\text{imp}}}$ never rises close to $1/4$ and with decreasing temperature $S_{\text{imp}}$ drops from $\ln 4$ to $0$ with at most a weak shoulder around $\ln 2$.

2. Kondo temperature

Given that the low-temperature physics is characterized by a single scale $T_K$, we now examine more closely the effect of Rashba coupling on the Kondo temperature. Figures 4(a) and 4(a) plot the ratio of the Kondo tem-
FIG. 5. (Color online) (a) Scaled Kondo temperature $T_K/T_K^0$ vs Rashba energy $\epsilon_R$ for fixed Fermi energy $\epsilon_F = 0$ and for different values of $\epsilon_d$ expressed in the legend in units of $D$. Symbols represent NRG data and lines are the result of the perturbative treatment described in the text. (b) Perturbative shifts $\tilde{\epsilon}_d - \epsilon_d$ and $\tilde{U} - U$ in the effective impurity parameters vs $\epsilon_R$ for the same cases shown in (a). Data are for $\epsilon_0 = -0.08D$, $U = 0.1D$, and $\Gamma = 0.005D$.

Temperature $T_K$ at Rashba energy $\epsilon_R$ to its value $T_K^0$ in the absence of SO interaction.

Figure 5 treats the scenario of fixed Fermi energy $\epsilon_F = 0$ for $\epsilon_0 = -0.08D$, $U = 0.1D$, and $\Gamma = 0.005D$. The Kondo temperature in the absence of SO interaction varies with $\epsilon_d$, taking its smallest value around $\epsilon_d = -U/2 = -0.05D$, for which case $T_K^0 \simeq 1.7 \times 10^{-6}D$. This is very close to the value $1.4 \times 10^{-6}D$ given by substituting $\Gamma(\epsilon_F) = \Gamma_{\text{eff}}$ into Haldane’s estimate $\rho(\epsilon_F)$ vs $\epsilon_F$.

$T_K \simeq 0.29\sqrt{U \Gamma(\epsilon_F)} \exp\left[\frac{\pi \epsilon_d (U + \epsilon_d)}{2U \Gamma(\epsilon_F)}\right]$. (45)

for the Kondo temperature of an Anderson impurity in the limit that $0 < \Gamma(\epsilon_F) \ll U + \epsilon_d$, $-\epsilon_d \ll D$.

The data symbols in Fig. 5(a) show $T_K$ to be only weakly affected by Rashba coupling, just as was found in Ref. 15. The Kondo scale displays a quasi-linear $\epsilon_R$ dependence $\epsilon_d$ with a slope that is positive for $\epsilon_d < -U/2$, negative for $\epsilon_d > -U/2$, and essentially vanishing for $\epsilon_d = -U/2$ (also in agreement with Ref. 15). Since the effective density of states $\rho(\epsilon)$ is independent of $\epsilon_R$ in a window of energies around $\epsilon_F$, any modification of $T_K$ must arise from changes in the total density of states near the band edges.

One can attempt to analyze the effect of density of states changes via a perturbative treatment along the lines of Haldane’s derivation of poor-man’s scaling equations for the Anderson impurity model $25$. This treatment, described further in Appendix A can be used to map the Anderson impurity model with density of states $\rho(\epsilon)$ onto another Anderson impurity model with the Rashba density of states $\rho_R(\epsilon)$, but with the impurity parameters $\epsilon_d$ and $U$ replaced by modified values $\tilde{\epsilon}_d$ and $\tilde{U}$ chosen so as to preserve (approximately) the same low-energy impurity properties as the original model. As explained in Appendix A, the hybridization matrix element $V$ remains unchanged under this approach.

For purely quadratic band dispersion in the absence of Rashba SO interaction, expressions for the renormalized parameter $\tilde{\epsilon}_d$ and $\tilde{U}$ can be obtained in closed form, but they are too cumbersome to reproduce here. Instead, Fig. 5(b) shows the evolution with $\epsilon_R$ of the shifts $\tilde{\epsilon}_d - \epsilon_d$ and $\tilde{U} - U$ for each of the three $\epsilon_d$ values illustrated in Fig. 5(a). An upward shift in the level energy and a downward shift in the on-site interaction both grow with $\epsilon_R$ and with $-\epsilon_d$, becoming 10% corrections in the most extreme case shown. Upon substitution into the Haldane formula $| \epsilon_F(\epsilon_R) |$, these shifts in $\tilde{\epsilon}_d$ and $\tilde{U}$ have opposite effects on $T_K$, so any overall change in $T_K$ is the result of a subtle balance. The predicted curves for $T_K/T_K^0$ vs $\epsilon_R$ [solid lines in Fig. 5(a)] display the correct trends with growing $-\epsilon_d$, but the fact that NRG and perturbative curves for the same value of $\epsilon_d$ are not in close correspondence is an indication of the delicacy of the interplay between the parameter renormalizations.

Figure 5(a) shows very different behavior in cases where the band filling is fixed. For weak SO interaction, the total density of states $\rho(\epsilon)$ near the Fermi energy remains independent of $\epsilon_R$, and $T_K$ has a quasi-linear behavior similar to that found for fixed $\epsilon_F$. However, once $\epsilon_R > | \epsilon_0 | / 2$, the system enters the helical metal regime and both $\rho(\epsilon_F)$ and $\Gamma(\epsilon_F)$ rise rapidly. This rise is magnified in the Kondo temperature due to the exponential dependence of $T_K$ on $\Gamma(\epsilon_F)$ shown in Eq. (45). Figure 6(b) confirms such a dependence of the numerically determined value of $T_K$. The five lower curves exemplify the Kondo regime, where the weak deviations from linearity in this plot of $-1/\ln(T_K/D)$ vs $\rho(\epsilon_F)$ can be attributed primarily to the $\sqrt{\rho(\epsilon_F)}$ prefactor in Eq. (45). The remaining two cases ($U = 0.1D$, $\epsilon_d = 0$ and $\epsilon_d = -0.1D$) correspond to mixed valence, where the low-temperature scale is no longer expected to depend exponentially on $\Gamma(\epsilon_F)$.

3. Static angular-momentum correlations

Further insight can be gained into the nature of Kondo physics in presence of Rashba SO interaction by studying...
FIG. 7. (Color online) Static correlations between the impurity spin and the total angular momentum in different conduction-band channels, calculated for (a,c) fixed Fermi energy \( \epsilon_f = 0 \), or (b,d) constant band filling \( \eta \approx 0.074 \). The upper panels show \( \langle S_d \cdot J_h \rangle \) for helicity \( \hbar = \pm \), while the lower panels plot the correlation of \( S_d \) with \( J^{m=0} \) (the total angular momentum of all electrons with orbital angular momentum \( m = 0 \)) and with \( J^{m \neq 0} \) defined in Eq. (15). Data are for \( \epsilon_0 = -0.08D \), \( U = -2\epsilon_d = 0.1D \), and \( \Gamma = 0.005D \).

the correlations between the impurity spin

\[
S_d = \frac{1}{2} \sum_{\tau, \tau'} d^\dagger_\tau \sigma_{\tau, \tau'} d_{\tau'}^\dagger
\]

and the total angular momentum

\[
J_h = \frac{1}{2} \sum_{\tau, \tau'} \int dk \tilde{c}_{k,h,\tau} \sigma_{\tau, \tau'} \tilde{c}_{k,h',\tau'}
\]

of all conduction-band electrons that have helicity \( \hbar \) and angular momentum \( z \) component \( \pm \frac{1}{2} \). The appendix provides details of how such correlations can be obtained within the NRG treatment of the two-channel Anderson Hamiltonian [Eq. (21)]. The results presented below are static values calculated in the limit of absolute temperatures \( T \to 0 \).

Figure (a) plots \( \langle S_d \cdot J_h \rangle \) vs \( \epsilon_R \) under the scenario where the Fermi energy is fixed at \( \epsilon_f = 0 \). At zero Rashba energy, \( \langle S_d \cdot J_h \rangle \) is the same for helicities \( \hbar = \pm \). As \( \epsilon_R \) increases, the impurity spin becomes more strongly correlated with the \( \hbar = + \) channel and less strongly with the \( \hbar = - \) electrons. This can be understood as a density of states effect because the dimensionless ratio

\[
r_h = \frac{\langle S_d \cdot J_h \rangle}{\langle Dp_{h}(\epsilon_f) \rangle}
\]

(not plotted) turns out to be almost independent of \( \epsilon_R \) and \( h \). Since the combined Fermi-level density of states \( \rho(\epsilon_f) = \rho_+(\epsilon_f) + \rho_-(\epsilon_f) \) remains constant, it is therefore unsurprising that \( \langle S_d \cdot (J_+ + J_-) \rangle \) barely changes with \( \epsilon_R \).

In cases where the band filling is constant [e.g., Fig. (b)], the behavior found for Rashba energies \( \epsilon_R < -\epsilon_0/2 \) is qualitatively the same as for fixed \( \epsilon_f \). However, once the helical regime is reached \( \epsilon_R > -\epsilon_0/2 \), \( \rho_+(\epsilon_f) = 0 \) and \( \langle S_d \cdot J_+ \rangle \) almost vanishes; the impurity spin is almost exclusively correlated with the \( \hbar = - \) channel. In this parameter range, the growth of \( \rho_-(\epsilon_f) \) inside the helical regime increases the occupancy of the empty and doubly occupied impurity states and decreases the local-moment character, leading to a gradual decline in the magnitude of \( \langle S_d \cdot (J_+ + J_-) \rangle \) with increasing \( \epsilon_R \). The contrast with the fixed-\( \epsilon_f \) scenario is highlighted by the facts that \( r_+ \to \infty \) due to the numerator on the right-hand side of Eq. (15) being small but nonzero due to correlation of \( S_d \) with high-energy electrons, while \( r_- \) rapidly approaches zero with increasing \( \epsilon_R \) due to \( \langle S_d \cdot J_- \rangle \) being nearly saturated but \( \rho_-(\epsilon_f) \) still rising.

Figures (c) and (d) separate (for the fixed-\( \epsilon_f \) and constant-\( \eta \) scenarios, respectively) two contributions to the overall impurity-band angular momentum correlation \( \langle S_d \cdot (J_+ + J_-) \rangle \): (i) \( \langle S_d \cdot J^{m=0} \rangle \), where \( J^{m=0} \) is the total angular momentum of all electrons with orbital angular momentum \( m = 0 \), and (ii) \( \langle S_d \cdot J^{m \neq 0} \rangle \), where

\[
J^{m \neq 0} = J_+ + J_- - J^{m=0}.
\]

In both panels, the most striking result is the appearance of a nonzero correlation \( \langle S_d \cdot J^{m \neq 0} \rangle \) that arises, not through direct interaction with the impurity (which is confined to \( m = 0 \)), but rather indirectly through Rashba mixing of \( m = 0 \) states with \( m = \pm 1 \) states.

The results of Figs. (c) and (d) can be understood in terms of the helicity-resolved densities of states. Equation (15) shows that the operators \( \tilde{c}_{k,h,\tau} \) entering Eq. (14) contain \( m = 0 \) and \( m = \pm 1 \) components of equal magnitude with a relative phase that is opposite for \( h = + \) and \( h = - \). For \( \epsilon_R = 0 \), the two helicity channels participate equally in Kondo screening in a manner that produces complete destructive interference of correlations contributing to \( \langle S_d \cdot J^{m \neq 0} \rangle \). With increasing \( \epsilon_R \), there is a growing difference \( \rho_-\epsilon \) - \( \rho_+\epsilon \) for energies \( \epsilon \) near \( \epsilon_f \), leading to imperfect cancellation of correlations between the impurity and \( m = \pm 1 \) electrons and a gradual convergence of \( \langle S_d \cdot J^{m=0} \rangle \) and \( \langle S_d \cdot J^{m \neq 0} \rangle \). Once the system enters the helical regime \( \epsilon_R > -\epsilon_0/2 = 0.04D \) in Fig. (d), \( \rho_+\epsilon = 0 \), and the two correlation measures differ only due to contributions from electrons far from the Fermi energy.

B. Results with a Zeeman field

In order to study the combined effect of Rashba and Zeeman couplings on Kondo correlations, we have calculated the zero-temperature impurity polarization \( M_{\text{imp}} = \langle J_z \rangle - \langle J_z \rangle_0 \), where \( J_z \) is the \( z \) component of the total system angular momentum, and \( \langle \ldots \rangle \) and \( \langle \ldots \rangle_0 \) denote,
respectively, expectation values in the presence and absence of the impurity. $M_{\text{imp}}$ is the natural extension of the usual impurity spin magnetization $\langle S_z \rangle = \langle S_z \rangle_0$, to which it reduces in the absence of Rashba coupling (i.e., for $\epsilon_R = 0$).

Initially, we focus on the scenario of fixed Fermi energy $\epsilon_F = 0$. Figure 8(a) shows the zero-temperature impurity polarization $M_{\text{imp}}$ as a function of $\epsilon_Z$ for $U = -2\epsilon_d = 0.15D$, for $\epsilon_R/D = 0$ and 0.1, and for $\Gamma/D = 0.003$ and 0.005. The impurity parameters are such that for $\epsilon_R = 0$, the Kondo temperatures $T_K^0(\Gamma = 0.003 D) \approx 4.4 \times 10^{-12}D$ and $T_K^0(\Gamma = 0.005 D) \approx 2.6 \times 10^{-9}D$ differ by four orders of magnitude. As expected, $M_{\text{imp}}$ is in all cases an increasing function of $\epsilon_Z$. For a given value of $\epsilon_Z > 0$, $M_{\text{imp}}$ is a decreasing function of $\epsilon_R$. This can be understood by noting that the Zeeman field enters $\Gamma$ by four orders of magnitude. As expected, $M_{\text{imp}}$ is in all cases an increasing function of $\epsilon_Z$. For a given value of $\epsilon_Z > 0$, $M_{\text{imp}}$ is a decreasing function of $\epsilon_R$. This can be understood by noting that the Zeeman field enters $\Gamma$ by four orders of magnitude. As expected, $M_{\text{imp}}$ is in all cases an increasing function of $\epsilon_Z$. For a given value of $\epsilon_Z > 0$, $M_{\text{imp}}$ is a decreasing function of $\epsilon_R$. This can be understood by noting that the Zeeman field enters $\Gamma$ by four orders of magnitude. As expected, $M_{\text{imp}}$ is in all cases an increasing function of $\epsilon_Z$.

Figure 8(b) demonstrates a very good collapse of the polarization data in Fig. 8(a) when plotted as a function of $2\Gamma\epsilon_Z/T_K D$, where $T_K$ is the Kondo temperature for $\epsilon_Z = 0$ and $f$ is a dimensionless fitting parameter that depends on $\epsilon_R$. It is particularly notable that for given $\epsilon_R$ (including the case of no Rashba coupling), the Zeeman field is scaled by $T_K/\Gamma$ rather than by the Kondo temperature itself, as would be the case for a nonzero impurity $g$ factor. Small deviations from the scaling collapse occur only in the parameter range $\epsilon_Z \gtrsim \Gamma$.

The scaling shown in Fig. 8(b) can be understood via a second application of the perturbative treatment outlined in Appendix A. One can regard the Zeeman field as introducing a spin-dependent change $\Delta\rho_\tau = \rho_\tau(\epsilon) - \rho(\epsilon)$ in the density of states of electrons with angular momentum $z$ component $\tau$, where $\rho(\epsilon) = \rho_+(\epsilon) + \rho_-(\epsilon)$ is derived from Eq. (21). The perturbative method maps the problem to a one-channel Hamiltonian of the form of Eq. (24) in which both spin species share the same density of states $\rho(\epsilon)$ and to lowest order in $\epsilon_Z$ and $\Gamma$.

FIG. 9. (Color online). Quantity $f$ entering the scaling collapse of the impurity polarization for a system with fixed Fermi energy $\epsilon_F = 0$: (a) $f$ vs $\epsilon_R$ for different values of $U$ and $\epsilon_d$ expressed in the legend in units of $D$. Each symbol was obtained via an NRG calculation of the compensating local field for $\Gamma\epsilon_Z/T_K D = 0.1$, while the lines represent algebraic results based on Eq. (50). (b) NRG values of $f$ vs $\Gamma\epsilon_Z/T_K D$ for $U = 0.15 D$ and different values of $\epsilon_R$ and $\epsilon_d$ expressed in the legend in units of $D$. Lines are guides to the eye showing that $f$ is independent of $\epsilon_Z$ for $\Gamma\epsilon_Z/T_K D \lesssim 10$. Data in both panels are for $\epsilon_0 = -0.08 D$ and $\Gamma = 0.005 D$.

In other words, the Zeeman coupling effectively spin-splits the impurity level by an amount proportional to $\Gamma\epsilon_Z$. Just as would be the case if this splitting were caused by a magnetic field that coupled directly to the impurity spin, the Kondo correlations are destroyed when the splitting becomes comparable to $T_K$. In the present context, the result is a scaling dependence on the dimensionless quantity $\Gamma\epsilon_Z/D\Gamma K$ rather than the conventional (i.e., $g_i \neq 0$) combination $\epsilon_Z/T_K$. This conclusion is not restricted to situations involving Rashba SO interaction, and holds quite generally for realizations of the Anderson impurity model with $g_i = 0$.

Equation (A5) yields an algebraic expression for $f$ to lowest order in $\epsilon_Z/\epsilon_R$ that is rather cumbersome and will not be reproduced here. More generally, one can consider a combination of a bulk Zeeman splitting and a local field $B_{\text{loc}}$ that couples only to the impurity. After integrating out the Zeeman field, one arrives at a renormalized impurity energy $\tilde{\epsilon}_{d,\tau} = \epsilon_d - 2\Gamma f(\epsilon_R, U, \epsilon_d) \Gamma\epsilon_Z/D + \tau\Gamma_{B_{\text{loc}}}$, which allows the numerical determination of $f$ as $f = g_i B_{\text{comp}}/(2\Gamma\epsilon_Z)$, where $B_{\text{comp}}$ is the compensation value of the local field such that $\tilde{\epsilon}_{d,\tau} = \epsilon_d$ and hence $M_{\text{imp}} = 0$.

Figure 9(a) illustrates the behavior of $f$ vs $\epsilon_R$ for different combinations of $U$ and $\epsilon_d$. All cases show a monotonic decrease of $f$ with increasing $\epsilon_R$. There is also an interplay between $U$ and $\epsilon_d$, such that the $f$ value for $(U/D, \epsilon_d/D) = (0.2, -0.1)$ and $(0.15, -0.045)$ lie almost on top of each other. In all the cases shown, there is good quantitative agreement between the numerical and
algebraic values plotted using symbols and lines, respectively.

Figure 10(b) shows $f$ as a function of $\Gamma \varepsilon_Z / T_K D$ for $U = 0.15 D$ and a few selected values of $\epsilon_R$ and $\epsilon_d$. The most salient feature is that $f$ remains constant as $\Gamma \varepsilon_Z / T_K D$ is varied over four orders of magnitude, indicating the lack of dependence on $\Gamma$ and/or $\varepsilon_Z$. Deviations from universality are again seen only in the regime of very large Zeeman fields where the impurity polarization approaches saturation at $M_{\text{imp}} = 0.5$.

Finally, we consider the effect of Zeeman splitting under the scenario of constant band filling. Figure 10(a) shows $M_{\text{imp}}$ vs $\varepsilon_Z$ for $U = -2 \epsilon_d = 0.15 D$, for $\epsilon_R / D = 0.06$ and 0.08, and for $\Gamma / D = 0.003$ and 0.005. Since Rashba SO interaction changes the Fermi-energy density of states, the Zeeman energy needed to destroy Kondo correlations is exponentially sensitive to both $\epsilon_R$ and $\Gamma$. As under the fixed-$\varepsilon_Z$ scenario, all the polarization curves share a similar shape (except for $\varepsilon_Z \gtrsim \Gamma$) and a universal scaling dependence on $2\Gamma\varepsilon_Z / T_K D$ is confirmed in Fig. 10(b). In this case, however, the parameter $f$ depends not just on $\epsilon_R$, $U$, and $\epsilon_d$, but also decreases with $\Gamma$. Under the constant-filling scenario, the Fermi level lies in an energy range where the density of states is spin-split, so a perturbative approach to first order in $\Gamma$ is likely insufficient to reproduce the parameter dependences of $f$. For this reason, we focus on the numerical estimation of $f$ via the compensation field. Figure 11 plots the results for the same parameters as were used in Fig. 9. Note that $f$ exhibits a nonmonotonic dependence on $\epsilon_R$, with a maximum at $\epsilon_R = -\epsilon_0/2 = 0.04 D$. For $\epsilon_R \leq -\epsilon_0/2$, the value of $f$ under the constant-filling scenario is generally greater than for fixed Fermi energy. For $\epsilon_R > -\epsilon_0/2$, the range where the system is in its helical regime for $\varepsilon_Z = 0$, $f$ decreases rapidly with increasing Rashba coupling and may even become negative.

IV. SUMMARY

We have studied the effect of bulk Rashba SO interaction on Kondo correlations between a magnetic impurity and a two-dimensional electron gas. The low-temperature thermodynamic properties exhibit the conventional Kondo form with scaling in terms of $T / T_K$, providing evidence for complete quenching of the impurity degree of freedom as $T \to 0$. In most situations, the Kondo temperature $T_K$ is little affected by the Rashba coupling, as has been pointed out previously. However, within a helical regime that can in principle be accessed for high Rashba couplings and/or low electron densities, the Kondo temperature exhibits an exponential enhancement compared to the situation without Rashba interaction.

Our analysis of static angular-momentum correlations demonstrates and quantifies an indirect, Rashba-induced coupling of the impurity spin with conduction channels of nonzero orbital angular momentum about the impurity site. This coupling can be regarded as a manifestation of a Dzyaloshinskii-Moriya term found previously by mapping the Anderson impurity model with bulk Rashba SO interaction to an effective Kondo model. A perturbative renormalization-group analysis of this Kondo model showed an exponential enhancement of $T_K$. We should note, however, that the RG equations were solved neglecting the helicity dependence of the Fermi wave vector. A complete analysis of the effective Kondo model will be presented elsewhere.

Optical irradiation experiments seem to be good candidates to explore the helical regime of a Rashba-coupled 2DEG. Motivated by the proposal of Ref. 21, we have also investigated Kondo physics in the presence of both...
Rashba SO interaction and Zeeman splitting of the bulk electrons (but not of the impurity). The characteristic Zeeman energy scale for the destruction of the Kondo effect is not \( T_K \), as would be expected in the case of a true magnetic field that couples directly to the impurity spin, but rather \( T_K/T \) where \( T \) is the impurity hybridization width. The behavior can be accounted for to reasonable quantitative accuracy by a perturbative treatment of the Zeeman splitting of the host density of states.

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**Appendix A: Perturbative Analysis**

This appendix considers an Anderson impurity model

\[
H = \sum_{\sigma} \int d\epsilon \ (c_{\epsilon,\sigma}^\dagger c_{\epsilon,\sigma} + \sum_{\epsilon} \rho_{\sigma}(\epsilon) (c_{\epsilon,\sigma}^\dagger d_{\sigma} + H.c.)) + \sum_{\sigma} V_{\sigma} \int d\epsilon \rho_{\sigma}(\epsilon) (c_{\epsilon,\sigma}^\dagger d_{\sigma} + H.c.),
\]

(A1)

where the conduction-band density of states \( \rho_{\sigma}(\epsilon) \), the impurity level energy \( \epsilon_{d,\sigma} \), and the hybridization matrix element \( V_{\sigma} \) are all allowed to depend on \( \sigma = \uparrow, \downarrow \). The goal is to construct an approximate mapping of Eq. (A1) to a similar Hamiltonian having a different conduction-band density of states \( \tilde{\rho}_{\sigma}(\epsilon) \), and with the impurity parameters \( \tilde{\epsilon}_{d,\sigma}, \tilde{U} \), and \( \tilde{V}_{\sigma} \) chosen to ensure that the two models share the low-energy physics (at least as it pertains to the impurity properties).

Haldane, in his derivation of poor-man’s scaling equations for the Anderson model [35], used perturbation theory in the hybridization matrix element to take into account the effect of all conduction-band states in a narrow window of energies near each band edge. Here, we perform a similar calculation in order to find energy shifts arising from the density-of-states difference \( \Delta \rho_{\sigma}(\epsilon) = \rho_{\sigma}(\epsilon) - \tilde{\rho}_{\sigma}(\epsilon) \) at all energies \( \epsilon \). Like Haldane, our focus is on four many-body states \( |0\rangle, |\sigma\rangle = |d_{\sigma}\rangle |0\rangle \), and \( |2\rangle = |d_{\uparrow}\rangle |d_{\downarrow}\rangle \), formed by combining the conduction-band ground state [having \( N \) electrons of energy \( \epsilon(K) < \epsilon_F \) with one of the possible configurations of the Anderson impurity level. These many-body states have energies \( E_0, E_\sigma = E_0 + \epsilon_d \), and \( E_2 = E_\uparrow + E_\downarrow - E_0 + U \), respectively.

The state \( |0\rangle \) can decrease its energy through virtual tunneling of an electron of spin \( \sigma \) from a band state below the Fermi level to the impurity and then back to the original band state. Integrating the contribution to such processes arising just from the density of states difference \( \Delta \rho_{\sigma}(\epsilon) \), then summing over \( \sigma \), transforms the state \( |0\rangle \) to one \( |\tilde{0}\rangle \) having an energy \( \tilde{E}_0 \) that, to second order in \( V \), is

\[
\tilde{E}_0 = E_0 - \sum_{\sigma} V_{\sigma}^2 \int_{-\infty}^{\epsilon_F} \frac{\Delta \rho_{\sigma}(\epsilon)}{\epsilon - \epsilon + \epsilon_{d,\sigma}} d\epsilon. \tag{A2}
\]

Similarly, the state \( |2\rangle \) can decrease its energy through virtual tunneling of a spin-\( \sigma \) electron from the impurity to a band state above the Fermi level and then back to the impurity. The contribution to such processes arising from \( \Delta \rho_{\sigma}(\epsilon) \), when summed over \( \sigma \), transforms \( |2\rangle \) to \( |\tilde{2}\rangle \) with energy

\[
\tilde{E}_2 = E_2 - \sum_{\sigma} V_{\sigma}^2 \int_{-\infty}^{\epsilon_F} \frac{\Delta \rho_{\sigma}(\epsilon)}{\epsilon - \epsilon - U - \epsilon_{d,\sigma}} d\epsilon. \tag{A3}
\]

Lastly, the state \( |\sigma\rangle \) can lower its energy through (i) tunneling of an electron with spin \( \sigma \) from the impurity to a band state above the Fermi level and then back to the impurity, and (ii) tunneling of an electron with spin \( -\sigma \) from a band state below the Fermi energy to the impurity and then back to the original band state. The contribution to such processes arising from \( \Delta \rho_{\sigma}(\epsilon) \) transforms \( |\sigma\rangle \) to \( |\tilde{\sigma}\rangle \) with energy

\[
\tilde{E}_{\sigma} = E_{\sigma} - V_{\sigma}^2 \int_{-\infty}^{\epsilon_F} \frac{\Delta \rho_{\sigma}(\epsilon)}{\epsilon} - V_{\sigma}^2 \int_{-\infty}^{\epsilon_F} \frac{\Delta \rho_{-\sigma}(\epsilon)}{\epsilon} d\epsilon. \tag{A4}
\]

Equations (A2)–(A4) can be used to define shifted impurity parameters

\[
\tilde{\epsilon}_{d,\sigma} = \tilde{E}_{\sigma} - \tilde{E}_0 \tag{A5}
\]

and

\[
\tilde{U} = \tilde{E}_2 + \tilde{E}_0 - \tilde{E}_\uparrow - \tilde{E}_\downarrow. \tag{A6}
\]

Corrections to the hybridization matrix elements (arising as a consequence of wave-function renormalization) are found to be of order \( V^3 \), so at the level of our approximation,

\[
\tilde{V}_{\sigma} = V_{\sigma}. \tag{A7}
\]

Since \( \Delta \rho_{\sigma}(\epsilon) \) everywhere enters the above equations multiplied by \( V_{\sigma}^2 \), the analysis can be recast as the derivation of shifts in the impurity parameters \( \epsilon_d \) and \( U \) to account for a change \( \Delta \Gamma_{\sigma}(\epsilon) = \pi \Delta \rho_{\sigma}(\epsilon) V_{\sigma}^2 \) in the spin-dependent hybridization function.

We note that an equation equivalent to Eq. (A1) appears in Refs. [37] and [38] which examine the spin splitting of the impurity level arising from entirely integrating out the conduction band. In our language, this case corresponds to \( \tilde{\rho}_{d}(\epsilon) = 0 \) and \( \Delta \rho_{\sigma}(\epsilon) = \rho_{\sigma}(\epsilon) \). These earlier works did not take into account changes in the energies of the empty and doubly occupied states that can lead to a shift in the on-site interaction \( U \).
Appendix B: Computation of Angular-Momentum Correlations

This appendix describes the calculation of static correlations between the impurity spin $S_d$ defined in Eq. (12) and one of $J_h$, $J_m^\lambda=0$, and $J_m^\lambda\neq0$ representing the total angular momentum operators of helicity-$h$ electrons, of electrons having orbital angular momentum $m=0$, and of electrons with angular momentum $m \neq 0$.

Within the numerical renormalization-group treatment of the effective two-channel Anderson model described by Eq. (21), an appropriate representation of the Wilson chain $S_d \cdot J_h$ in terms of annihilation operators $f_n,m,\tau$ for orbital angular momentum eigenstates, in direct analogy with Eq. (47), is more complicated since orbital angular momentum is not a good quantum number of the bulk states. Since the NRG Lanczos procedure preserves spin and orbital angular momenta, one can write

$$ f_{n,m,\tau} = \frac{1}{\sqrt{2}} (f_{n,\tau-1/2,\uparrow} + f_{n,\tau+1/2,\downarrow}) \quad (B3) $$

in terms of annihilation operators $f_{n,m,\tau}$ for orbital angular momentum eigenstates, in direct analogy with Eq. (11). Substitution of Eq. (B3) into Eq. (12) allows one to write

$$ J_{m=0}^n + J_{m\neq0}^n, \quad (B4) $$

where

$$ J_{m=0}^n = \frac{1}{2} \sum_{\tau,\tau'} f_{n,0,\tau}^\dagger \sigma_{\tau,\tau'} f_{n,0,\tau'}, \quad (B5) $$

$$ J_{m\neq0}^n = \frac{1}{2} \sum_{\tau,\tau'} f_{n,2\tau,-\tau}^\dagger \sigma_{\tau,\tau'} f_{n,2\tau',-\tau'}, \quad (B6) $$

Equation (B6) makes clear that $J_{m\neq0}^n$ includes terms that are off-diagonal in the orbital angular momentum index.

Equation (B3) can be inverted to yield, for $m=0$, $\tau = \pm \frac{1}{2}$ and for $m=\pm1$, $\tau = \mp \frac{1}{2}$,

$$ f_{n,m,\tau} = \frac{1}{\sqrt{2}} [\tilde{f}_{n,+,\tau} + \tilde{f}_{n,-,\tau}]. \quad (B8) $$

Substitution of Eq. (B8) into Eqs. (B5) and (B6) yields

$$ J_{m=0}^n = \frac{1}{2} \sum_{n=0}^N (J_{n,+} + J_{n,-} + \tilde{J}_n) \quad (B9) $$

$$ J_{m\neq0}^n = \frac{1}{2} \sum_{n=0}^N (J_{n,+} + J_{n,-} - \tilde{J}_n), \quad (B10) $$

where

$$ \tilde{J}_n = \frac{1}{2} \sum_{h,\tau,\tau'} \tilde{f}_{n,h,\tau}^\dagger \sigma_{\tau,\tau'} \tilde{f}_{n,-h,\tau'} \quad (B11) $$

is off-diagonal in the helicity index.

Equations (B1), (B2), and (B9)–(B11) contain the prescription for constructing the total angular momentum operators in our NRG calculations. In order to obtain ground-state correlations, we took the thermal averages of $S_d$ with $J_h$, $J_{m=0}^n$, and $J_{m\neq0}^n$ in the limit of large iteration numbers corresponding to temperature scales far below $T_K$.

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