Model for overscreened Kondo effect in ultracold Fermi gas

I. Kuzmenko,¹ T. Kuzmenko,¹ Y. Avishai,¹ and K. Kikoin²

¹Department of Physics, Ben-Gurion University of the Negev, Beer-Sheva, Israel

²Raymond and Beverly Sackler Faculty of Exact Sciences, School of Physics and Astronomy, Tel Aviv University, 69978 Tel Aviv, Israel

(Received 11 March 2014; revised manuscript received 6 April 2015; published 27 April 2015)

The feasibility of realizing the overscreened Kondo effect in ultracold Fermi gas of atoms with spin $s \ge \frac{3}{2}$ in the presence of a localized magnetic impurity atom is proved realistic. Specifying (as a mere example) a system of ultracold ²²Na Fermi gas and a trapped ⁶Li impurity, the mechanism of exchange interaction between the Na and Li atoms is elucidated and the exchange constant is found to be positive (antiferromagnetic). The corresponding exchange Hamiltonian is derived, and the Kondo temperature is estimated at the order of 500 nK. Within a weak-coupling renormalization group scheme, it is shown that the coupling renormalizes to the non-Fermi-liquid fixed point. An observable displaying multichannel features even in the weak-coupling regime is the impurity magnetization that is *negative* for $T \gg T_K$ and becomes positive with decreasing temperature.

DOI: 10.1103/PhysRevB.91.165131

PACS number(s): 37.10.Jk, 31.15.vn, 33.15.Kr

I. INTRODUCTION

The experimental discovery of Bose-Einstein condensation back in 1996 opened the way to study a myriad of fundamental physical phenomena that were otherwise very difficult to realize (see Ref. [1] for a review). A few years afterward, fabrication and control of a cold gas of *fermionic atoms* has been realized [2–23]. This revelation opens the way to study the physics of a gas of fermions with (half integer) spin $s \ge \frac{3}{2}$. The main axis of the present study relates to the question whether the occurrence of this new state of matter exposes a new facet of Kondo physics.

The single-channel Kondo effect in cold atom physics has been studied in Refs. [24–28]. In Ref. [29], the possibility of observing multichannel Kondo effect has been explored for ultracold *bosonic atoms* coupled to an atomic quantum dot, as well as for a system composed of superconducting nanowires coupled to a Cooper-pair box. Recently, non-Fermiliquid behavior has been predicted for gold monatomic chains containing one carbon atom as a magnetic impurity [30].

In this work we propose a realization of the non-Fermiliquid Kondo effect in cold atom systems. The idea is to localize an atom with spin *S* in a Fermi gas of cold atoms of spin $s \ge \frac{3}{2}$ trapped in a combination of harmonic and periodic potentials. If an exchange interaction $Js \cdot S$ with J > 0 exists, the underlying Kondo physics is equivalent to the multichannel Kondo effect with large *effective number* N_s of *spin*- $\frac{1}{2}$ *channels* [31] that easily satisfies the Nozières-Blandin inequality $N_s > 2S$, leading to over-screening [32]. To be concrete, we consider the ⁶Li atom [33] (atomic spin $S = \frac{1}{2}$) as an impurity trapped in a Fermi gas of ²²Na atoms (atomic spin $s = \frac{5}{2}$). An ultracold gas of atoms of ²³Na may be achieved by first laser cooling of ²²Na atoms, followed by sympathetic cooling in a mixture with ²³Na atoms [20].

The paper is organized as follows: In Sec. II we describe the optical potential which localizes ultracold atoms. Atomic quantum states in the optical potential are described in Sec. III. Exchange interaction between atoms of Na and Li is derived in Sec. IV. In Sec. V we derive the Kondo Hamiltonian and get Kondo temperature. The impurity magnetization is estimated in Sec. VI. The results are summarized in Sec. VII. Analysis of the exchange interaction between atoms of Na and Li is relegated to the Appendix.

II. MODEL

Typically, ultracold Fermi gas is stored in optical dipole traps that rely on the interaction between an induced dipole moment in an atom and an external electric field, $\mathbf{E}(\mathbf{r},t)$. Such oscillating electric (laser) field induces an oscillating dipole moment in the atom. Usually, the trapping potential is formed by three pairs of laser beams of wavelength ~1 μ m with the use of an acousto-optic modulator, creating a time-averaged optical potential [34–39]. This technique gives an anisotropic three-dimensional (3D) trap with trapping potential

$$V_{\rm 3D}(\mathbf{R}) = \sum_{i=1,2,3} V_{\rm 1D}^i(X_i),\tag{1}$$

where $X_{1,2,3}$ are Cartesian coordinates of an atom. Each term on the right-hand side contains a high-frequency wave which forms the oscillating potential and a low-frequency wave which forms the harmonic potential [34–38] (see Fig. 1):

$$V_{1D}^{i}(X_{i}) = \alpha \lim_{T \to \infty} \frac{1}{T} \int_{0}^{T} dt |2\mathbf{E}_{f}(X_{i},t) + 2\mathbf{E}_{i}(X_{i},t)|^{2}$$

= $V_{f} \sin^{2}(k_{f}X_{i}) + V_{i}(k_{p}X_{i})^{2},$ (2)

where α is the electric polarizability of atoms, $V_f = 2\alpha |\mathbf{E}_f|^2$, and $V_i = 2\alpha |\mathbf{E}_i|^2$ are the lattice potential depths which can be controlled by varying the intensities \mathbf{E}_f or \mathbf{E}_i of the laser field or the low-frequency waves. The potential parameters are tuned such that

$$V_1 k_1^2 \lesssim V_2 k_2^2 \lesssim V_3 k_3^2 \ll V_f k_f^2. \tag{3}$$

To be concrete, we henceforth consider fermionic ²²Na atoms (spin $\frac{5}{2}$) and ⁶Li impurities (spin $S = \frac{1}{2}$). The potential well is filled with ²²Na atoms and with sparsely distributed ⁶Li atoms. We adopt that the Na and Li atoms are trapped by electromagnetic waves with different wavelengths and amplitudes. The short-wavelength well V_f^{Li} should be deep enough to trap the Li atom, whereas V_f^{Na} is so shallow that it



FIG. 1. (Color online) (a) Filling of the energy levels in the potential well $V_{1D}^i(X_i)$ (2) by fermionic atoms. The filled area denotes the occupied energy levels (blue lines), whereas the energy levels in the unfilled area are unoccupied. (b) Short-wavelength potential $V_{1D}^i(X_i)$ (purple curve) trapping the lithium atom (the red circle).

cannot trap the Na atoms. As a result, we get an atomic Fermi gas with a low concentration of localized magnetic impurities.

III. ATOMIC QUANTUM STATES IN THE POTENTIAL WELL

We consider a neutral atom (nucleus plus core) as a positively charged rigid ion (with filled shell) and one electron on the outer orbital (i.e., 3s orbital in the Na atom or 2s orbital in the Li atom). The positions of the ion and the outer electron are respectively specified by vectors **R** and **r** (Fig. 2). In the adiabatic approximation (which is natural in atomic physics), the wave function of the atom is a product of the corresponding wave functions $\Psi(\mathbf{R})$ and $\psi(\mathbf{r})$ describing the stationary states of the ion and the outer electron. In order



FIG. 2. (Color online) Two atoms. Position of electron of the lithium or sodium atom is \mathbf{r}_1 or \mathbf{r}_2 ; the radius vector between the nuclei is **R**.

to find the wave functions and energies of the ²²Na and ⁶Li ions in the anisotropic 3D potential well, we need to solve the following Schrödinger equation for $\Psi(\mathbf{R}) = \Psi^{\text{Li,Na}}(\mathbf{R})$:

$$-\frac{\hbar^2}{2M}\frac{\partial^2\Psi(\mathbf{R})}{\partial\mathbf{R}^2} + V_{3\mathrm{D}}(\mathbf{R})\Psi(\mathbf{R}) = \varepsilon\Psi(\mathbf{R}).$$
(4)

Consider first $\Psi^{\text{Li}}(\mathbf{R})$. When the corresponding energy level ε_{imp} is deep enough, the wave function of the bound state near the potential minimum at $\mathbf{R} = \mathbf{0}$ can be approximated within the harmonic potential picture as

$$\Psi^{\rm Li}(\mathbf{R}) = \frac{1}{\left(\pi a_f^2\right)^{3/2}} \exp\left(-\frac{R^2}{2a_f^2}\right),\tag{5}$$

where

$$k_f a_f = \sqrt{\frac{\hbar \omega_f}{V_f^{\text{Li}}}}, \quad \omega_f = \sqrt{\frac{2V_f^{\text{Li}}k_f^2}{M_{\text{Li}}}}, \quad \varepsilon_{\text{imp}} = \frac{3\hbar \omega_f}{2}.$$

Second, consider the wave function of the ²²Na ions, for which the shallow potential wells are not deep enough to form bound states. For studying the Kondo effect we need to focus on quantum states at energies ε within the deep well close to ϵ_F , that is, $\varepsilon \gg V_f^{\text{Na}}$. In that case we can neglect the "fast" potential relief $V_f^{\text{Na}} \sin^2(k_f x)$, and the solution of Eq. (4) becomes

$$\Psi_{\mathbf{n}}^{\text{Na}}(\mathbf{R}) = \prod_{i=1,2,3} \Phi_{n_i}^{(i)}(X_i), \quad \mathbf{n} = (n_1, n_2, n_3).$$
(6a)

Denoting $\xi_i \equiv X_i/a_i$, the wave function $\Phi_{n_i}^{(i)}(X_i)$ is

$$\Phi_{n_i}^{(i)}(X_i) = \frac{1}{\left(\pi a_i^2\right)^{1/4}} \frac{1}{\sqrt{2^{n_i} n_i!}} H_{n_i}(\xi_i) e^{-\xi_i^2/2}, \qquad (6b)$$

where $H_n(\xi)$ is the Hermite polynomial, $n_i = 0, 1, 2, ...$ is harmonic quantum number, and

$$k_i a_i = \sqrt{\frac{\hbar \omega_i}{V_i}}, \quad \omega_i = \sqrt{\frac{2V_i k_i^2}{M_{\text{Na}}}}.$$
 (6c)

The corresponding energy levels are

$$\varepsilon_{n_1 n_2 n_3} = \sum_{i=1,2,3} \hbar \omega_i \left(n_i + \frac{1}{2} \right). \tag{7}$$

When $\omega_{1,2,3}$ are incommensurate, the energy levels are not degenerate. The inequalities (3) imply $\omega_1 \leq \omega_2 \leq \omega_3 \ll \omega_f$. The Fermi energy ϵ_F is such that $\epsilon_F \geq \hbar \omega_f$, hence the Fermi gas is 3D.

The potential well is filled by ²²Na atoms (fermions) and one impurity atom ⁶Li. The latter occupies the lowest-energy level (6) of the potential well and its wave function is well concentrated around the point $\mathbf{R} = \mathbf{0}$. Hence, regarding it as a localized impurity is justified.

IV. EXCHANGE INTERACTION

When the distance between a ²²Na atom and the ⁶Li impurity is of the order of R_0 (the atomic size), there is an exchange interaction between their open electronic *s* shells [40]. It includes a direct exchange term of strength J_d (due to antisymmetrization of the electronic wave functions where

electrons do not hop between atoms), and an indirect exchange term of strength J_p (due to contribution from polar states, where electrons can hop between atoms). Unlike the case of a hydrogen molecule where the direct part dominates, here both of them should be considered since their orders of magnitude are found to be comparable. Evaluating the exchange interaction between Na and Li atoms involves four wave functions: Two of them, $\Psi^{\text{Li}}(\mathbf{R})$ [Eq. (5)] and $\Psi_{\mathbf{n}}^{\text{Na}}(\mathbf{R})$ [Eq. (6a)] pertain to the corresponding atoms as being structureless particles in the optical potential (2). The other two, $\psi_{\text{Na}}(\mathbf{r})$ and $\psi_{\text{Li}}(\mathbf{r})$, pertain to electronic wave functions of the 3s orbital in Na and the 2s orbital in Li,

$$J_{\mathbf{n},\mathbf{n}'} = -\frac{2}{(2s+1)(2S+1)} \int_{R_{12}>R_0} d^3 \mathbf{R}_1 d^3 \mathbf{R}_2 \times V(R_{12}) |\Psi^{\text{Li}}(\mathbf{R}_1)|^2 [\Psi_{\mathbf{n}}^{\text{Na}}(\mathbf{R}_2)]^* \Psi_{\mathbf{n}'}^{\text{Na}}(\mathbf{R}_2), \qquad (8)$$

where \mathbf{R}_1 or \mathbf{R}_2 is the position of the ion of Li or Na, $R_{12} = |\mathbf{R}_1 - \mathbf{R}_2|$. We assume here that $R_{12} > R_0$, since Coulomb repulsion between the electron clouds of the Na and Li atoms prevents the atoms from approaching closer than $R_0 \approx r_{\text{Na}} + r_{\text{Li}}$ (which is approximated by the sum of the corresponding atomic radii).

$$V(R) = V_{\rm d}(R) + \frac{W_{\rm p}^2(R)}{U},$$

where $V_d(R)$ is a direct exchange interaction, $W_p(R)$ is the hybridization term, and U is a Coulomb blockade. Explicitly they are (see Ref. [41] and the Appendix for details)

$$\begin{aligned} V_{\rm d}(R_{12}) &= \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 \psi_{\rm Li}(\mathbf{r}_1 - \mathbf{R}_1) \psi_{\rm Na}(\mathbf{r}_2 - \mathbf{R}_2) \\ &\times \psi_{\rm Na}(\mathbf{r}_1 - \mathbf{R}_2) \psi_{\rm Li}(\mathbf{r}_2 - \mathbf{R}_1) \\ &\times \left\{ \frac{e^2}{r_{12}} + V_{12}(R_{12}) + \sum_{i=1}^2 V_i(r_{ii}) \right\}, \end{aligned}$$
$$W_{\rm p}(R_{12}) &= \frac{1}{2} \int d^3 \mathbf{r} \sum_{i=1}^2 V_i(|\mathbf{r} - \mathbf{R}_i|) \\ &\times \psi_{\rm Li}(\mathbf{r} - \mathbf{R}_1) \psi_{\rm Na}(\mathbf{r} - \mathbf{R}_2), \\ \frac{1}{U} &= \frac{1}{U_{\rm Na} + \varepsilon_{\rm Na} - \varepsilon_{\rm Li}} + \frac{1}{U_{\rm Li} + \varepsilon_{\rm Li} - \varepsilon_{\rm Na}}. \end{aligned}$$

Here \mathbf{r}_1 or \mathbf{r}_2 is the position of the electron, $r_{ii} = |\mathbf{r}_i - \mathbf{R}_i|$ and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. $V_1(r)$ or $V_2(r)$ describes the electron-ion interaction for Li or Na, and $V_{12}(R)$ is the interaction between ions. $\varepsilon_{\text{Na}} = -5.14 \text{ eV}$ and $\varepsilon_{\text{Li}} = -5.39 \text{ eV}$ are single-electron energies of the sodium and lithium atoms; $U_{\text{Na}} = 5.69 \text{ eV}$ and $U_{\text{Li}} = 6.01 \text{ eV}$ are the Coulomb interactions preventing two-electron occupation of the outer orbitals of atoms.

The electronic wave functions decrease rapidly when the distance between the atoms exceeds the atomic radius, so that the exchange interaction may be approximated by a pointlike interaction. Moreover, the wave function $\Psi^{\text{Li}}(\mathbf{R})$, Eq. (5), has its maximum at $\mathbf{R} = \mathbf{0}$ and it vanishes for $R \gg a_f$. The wave function $\Psi_{\mathbf{n}}^{\text{Na}}(\mathbf{R})$, Eq. (6a), varies slowly on the distance scale of a_f . Then $|\Psi^{\text{Li}}(\mathbf{R})|^2$ can be approximated by the δ function. Taking into account that $\Phi_{n_i}^{(i)}(0) = 0$ for n_i odd [see Eq. (6b)], we get the following estimate of the exchange constant for

atoms near the Fermi level: $J_{\mathbf{n},\mathbf{n}'} = J$ for all n_i and n'_i even and $J_{\mathbf{n},\mathbf{n}'} = 0$ otherwise, where

$$I = \frac{2(g_{\rm d} + g_{\rm p})}{(2s+1)(2S+1)} \left(\frac{3M_{\rm Na}}{2\pi\hbar^2\epsilon_F}\right)^{3/2} \prod_{i=1,2,3} \hbar\omega_i, \quad (9)$$

where g_d and g_p are couplings of the direct and indirect exchange interactions. Expressions for g_d and g_p in terms of the potentials of the direct and indirect exchanges as well as the explicit form for the exchange potentials are standard and can be found in textbooks [see, e.g., Refs. [41–43] and Eqs. (A12) and (A13) in the Appendix]. Numerical estimations yield $g_d \approx$ 0.0301 eV nm³ and $g_p = 0.1256$ eV nm³. In Refs. [41,43] it was shown that $J_d > 0$. Since $J_p > 0$ (always), the total exchange interaction is antiferromagnetic.

V. KONDO HAMILTONIAN AND THE KONDO TEMPERATURE

Equation (9) indicates that, due to symmetry of the atomic wave function (6b), only atoms with even n_i interact with the impurity. Omitting the odd values of the quantum numbers n_i for brevity, we write the Hamiltonian of the system as $H = H_0 + H_K$, where

$$H_0 = \sum_{\mathbf{n}\mu} \varepsilon_{\mathbf{n}} c^{\dagger}_{\mathbf{n}\mu} c_{\mathbf{n}\mu}, \quad H_K = J \left(\mathbf{S} \cdot \mathbf{s} \right).$$
(10)

Here $c_{\mathbf{n}\mu}$ or $c_{\mathbf{n}\mu}^{\dagger}$ is the annihilation or creation operator of a sodium atom in the state with the harmonic quantum numbers $\mathbf{n} = (2n_1, 2n_2, 2n_3)$ (where $n_i \ge 0$ are integers), $\varepsilon_{\mathbf{n}}$ is given by Eq. (7), μ denotes atomic spin projection, **S** is the impurity spin, and

$$\mathbf{s} = \sum_{\mathbf{nn}',\mu\mu'} c^{\dagger}_{\mathbf{n}\mu} \mathbf{t}_{\mu\mu'} c_{\mathbf{n}'\mu'},$$

where $\hat{\mathbf{t}}$ is the vector of the spin-*s* matrices. The density of states for the Hamiltonian H_0 is

$$\rho(\epsilon) = \sum_{\nu=0}^{\infty} \delta(\epsilon - \varepsilon_{\mathbf{n}}) = \frac{\epsilon^2}{8} \vartheta(\epsilon) \prod_{i=1,2,3} (\hbar \omega_i)^{-1}, \quad (11)$$

where $\vartheta(\epsilon)$ is the Heaviside theta function.

Within poor man scaling formalism for multichannel Kondo effect, the dimensionless coupling $j = J\rho(\epsilon_F)$ satisfies the following scaling equation [32]:

$$\frac{\partial j(D)}{\partial \ln D} = -j^2(D) + N_s j^3(D),$$
 (12)

with $N_s = \frac{2}{3}s(s+1)(2s+1)$ being an *effective number of channels* [31]. Initially, the bandwidth is $D_0 \ge D \gg T$ and the initial value of j(D), $j(D_0) \equiv j_0$, is

$$j_0 = \frac{g_0}{(2s+1)(2S+1)} \sqrt{\frac{\epsilon_F}{2}} \left(\frac{3M_{\rm Na}}{4\pi\hbar^2}\right)^{3/2}.$$

The solution of Eq. (12) is

$$\ln\left(\frac{D_0}{D}\right) = \frac{1}{j_0} - \frac{1}{j} + N_s \ln\frac{j(1 - N_s j_0)}{j_0(1 - N_s j)}.$$
 (13)

When $D \to 0$, j(D) renormalizes to the weak-coupling fixed point $j^* = 1/N_s$. When $|j(D) - j^*| \ll j^*$, the solution for



FIG. 3. (Color online) T_K , Eq. (15), as a function of T_F for $D_0 \leq \epsilon_F$.

j(D) reduces asymptotically to

$$\frac{j^* - j(D)}{j^*} = \frac{j^* - j_0}{j_0} \left(\frac{DT^*}{D_0 T_K}\right)^{j^*}$$
(14)

(see Ref. [44]), where

$$T^* = D_0 \exp\left(-\frac{1}{j^*}\right), \quad T_K = D_0 \exp\left(-\frac{1}{j_0}\right).$$
 (15)

The scaling equation (12) accounts for the evolution of j(D) only when the atomic spin $s \ge \frac{3}{2}$. The Kondo temperature (15) as a function of $T_F = \epsilon_F/k_B$ (where k_B is the Boltzmann constant) is shown in Fig. 3 for $D_0 \le \epsilon_F$. It is seen that T_K changes from 60 to 450 nK for $T_F = 0.5-1.5 \ \mu$ K, so that the ratio $\frac{T_K}{D_0} \approx 0.1-0.3$ is really small, whereas $T \sim T_K$ may be experimentally reachable. Indeed, more than a decade ago, 40 K atoms were cooled to a temperature of 50 nK [35]; later the 133 Cs atoms were cooled to a temperature of 40 nK [36,38].

VI. IMPURITY MAGNETIZATION

Having elaborated upon the theory, we are now in a position to carry out perturbation calculations of experimental observables. It is sometimes argued that the interesting physics in the overscreened Kondo effect is exposed only in the strong-coupling regime. Here we show that peculiar behavior emerges also in the weak coupling regime. The reason is that the weak-coupling fixed point j^* is small, and in most cases, the initial value is $j(D_0) > j^*$. As the temperature T is reduced toward T_K , j(D) decreases toward j^* and as a result, some physical observables display an unusual dependence on temperature. Consider, for example, the impurity magnetization $\mathbf{M}_{imp}(T) = M_{imp}(T)\hat{\mathbf{B}}$ in response to an external magnetic field **B**. Experimentally it requires immersing a small concentration n_i of impurity atoms in the gas of fermionic atoms. Within third order perturbation theory, we have

$$M_{\rm imp} = \frac{B \chi_0 T^*}{T} \bigg\{ \frac{S}{S+1} - \frac{SN_s}{s+1} \bigg[j + j^2 (1-jN_s) \ln \bigg(\frac{D_0}{T}\bigg) \bigg] \bigg\},$$
(16)

where

$$\chi_0 = \frac{g_e^2 \mu_B^2 n_i}{12T^*},$$

 $g_e \approx 2$ is the electronic spin g factor, and μ_B is the Bohr magneton.

Due to the logarithmic terms, which, strictly speaking, are not small either, the terms proportional to j^2 and j^3 are not small as compared with *j*. Hence, expansion up to the third order in *j* is inadequate. Instead, we derive an expression for the impurity related magnetization in the leading logarithmic approximation using the renormalization group equations (12). The condition imposing invariance of the magnetization under "poorman's scaling" transformation has the form [44]

$$\frac{\partial}{\partial D} \left[j + j^2 (1 - jN_s) \ln\left(\frac{D}{T}\right) \right] = 0.$$
 (17)

Equation (17) yields the scaling equation (12). The renormalization procedure should proceed until the bandwidth D is reduced to the temperature T. The expression for the impurity related magnetization then becomes

$$M_{\rm imp} = \frac{B\chi_0 T^*}{T} X(T),$$

$$X(T) = \frac{S}{S+1} - \frac{S}{s+1} \frac{j(T)}{j^*}.$$
(18)

The function X(T) consists of two terms. The first one describes the Zeeman interaction of the impurity with the external magnetic field and results in Curie's law. The second one corresponds to the exchange interaction of the impurity with atoms (the atomic magnetization is parallel to the external magnetic field). When the exchange interaction of the impurity is stronger than the Zeeman interaction, the function X(T) is negative and the impurity magnetization is antiparallel to the external magnetic field. This occurs when j(T) exceeds some critical value j_c ,

$$j_c = j^* \frac{s+1}{S+1}.$$

Figure 4 illustrates X(T) for different values of T_F . It is seen that at high temperatures when $j(T) > j_c$, X is negative, and the impurity magnetization is antiparallel to the external magnetic field. With reducing the temperature, the effective coupling j(T) reduces as well. At temperature T_c satisfying $j(T_c) = j_c$, X(T) changes sign from negative for $T > T_c$ to positive for $T < T_c$. For the given parameter values, $T_c \ll T_K$ and, strictly speaking, cannot be estimated within the framework of the poor man's scaling technique.



FIG. 4. (Color online) The function X(T), Eq. (18), for $T_F = 0.5$, 1, and 1.5 μ K [curves (a)–(c)]. The dots correspond to $T = T_K$.

VII. CONCLUSIONS

The non-Fermi-liquid Kondo effect can be accessed within the realm of cold atom physics. Exchange Hamiltonian is derived and scaling equations are solved for an ultracold gas of ²²Na with ⁶Li impurity. The dimensionless coupling *j* is not extremely small even though the coupling *J*, Eq. (9), is small. Such over-screened Kondo effect by fermions of large spin may be exposed even in the weak-coupling regime through the temperature dependence of the impurity magnetization.

ACKNOWLEDGMENTS

We would like to thank N. Andrei, O. Parcollet, Y. Castin, C. Salomon, and R. Folman for important discussions and numerous suggestions during the early stages of this research. This work is supported by Grant No. 400/2012 of the Israel Science Foundation (ISF).

APPENDIX: EXCHANGE INTERACTION

Here we expand upon the derivation of exchange constants between ²²Na and ⁶Li that are required to arrive at the Kondo Hamiltonian (10). First we elucidate the direct exchange and then the indirect one. As it turns out, both of them are positive for realistic interatomic distance R_{12} and they are of the same order of magnitude.

1. Direct exchange contribution

Let atoms of lithium and sodium be at positions \mathbf{R}_1 and \mathbf{R}_2 , with the distance between them $R_{12} = |\mathbf{R}_1 - \mathbf{R}_2|$. Then the direct exchange interaction $V_d(R_{12})$ between the atoms is (see Ref. [29])

.

$$V_{\rm d}(R_{12}) = \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 \psi_{\rm Li}(\mathbf{r}_1 - \mathbf{R}_1) \psi_{\rm Na}(\mathbf{r}_2 - \mathbf{R}_2) \times \psi_{\rm Na}(\mathbf{r}_1 - \mathbf{R}_2) \psi_{\rm Li}(\mathbf{r}_2 - \mathbf{R}_1) \times \left\{ \frac{e^2}{r_{12}} + V_{12}(R_{12}) + V_1(r_{11}) + V_2(r_{22}) \right\}.$$
 (A1)

Here \mathbf{r}_1 or \mathbf{r}_2 is the position of the electron (see Fig. 2), $r_{ii} = |\mathbf{r}_i - \mathbf{R}_i|$ (i = 1, 2) and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. We assume here that $R_{12} > R_0$, since Coulomb repulsion between the electron clouds of the Na and Li atoms prevents the atoms from approaching closer than $R_0 \approx r_{\text{Na}} + r_{\text{Li}}$ (which is approximated by the sum of the corresponding atomic radii). In Eq. (A1), $V_1(r)$ or $V_2(r)$ describes the electron-ion interaction for Li or Na, and $V_{12}(R)$ is the interaction between ions. When the interatomic distance exceeds R_0 , we can write

$$V_1(r) \approx V_2(r) pprox - rac{e^2}{r}, \quad V_{12}(R) pprox rac{e^2}{R}.$$

The function $V_d(R)$ calculated numerically for the electronic wave functions $\psi_{Na}(\mathbf{r})$ and $\psi_{Li}(\mathbf{r})$ given by Eq. (A16) is shown in Fig. 5 (dashed green curve). It is negative for any $R > R_0$ (where $R_0 \approx 4.1$ Å for the atoms of sodium and lithium), so that the exchange interaction is antiferromagnetic.



FIG. 5. (Color online) Direct exchange interaction $V_d(R)$ [Eq. (A1), dashed green curve], indirect exchange interaction $V_p(R)$ [Eq. (A2), dashed and dotted blue curve], and the total exchange interaction V(R) [Eq. (A5), solid red curve] as functions of the distances *R* between the nuclei.

2. Indirect exchange contribution

Indirect exchange interaction between the atoms Na and Li separated by distance R_{12} is

$$V_{\rm p}(R_{12}) = -\frac{W_{\rm p}^2(R_{12})}{U},$$
 (A2)

where

$$\frac{1}{U} = \frac{1}{U_{\mathrm{Na}} + \varepsilon_{\mathrm{Na}} - \varepsilon_{\mathrm{Li}}} + \frac{1}{U_{\mathrm{Li}} + \varepsilon_{\mathrm{Li}} - \varepsilon_{\mathrm{Na}}},$$

 $\varepsilon_{\rm Na} = -5.14$ eV and $\varepsilon_{\rm Li} = -5.39$ eV are single-electron energies of the sodium and lithium atoms, and $U_{\rm Na} = 5.69$ eV and $U_{\rm Au} = 6.01$ eV are the Coulomb interactions preventing two-electron occupation of the outer orbitals of atoms.

The hybridization term $W_p(R)$ in Eq. (A2) is given explicitly as

$$W_{\rm p}(R) = \frac{1}{2} \int d^3 \mathbf{r} \Big\{ V_1(|\mathbf{r}|) + V_2(|\mathbf{r} - \mathbf{R}|) \Big\}$$
$$\times \psi_{\rm Li}(\mathbf{r}) \psi_{\rm Na}(\mathbf{r} - \mathbf{R}). \tag{A3}$$

The function $V_p(R)$ calculated numerically for the electronic wave functions $\psi_{Na}(\mathbf{r})$ and $\psi_{Li}(\mathbf{r})$ given by Eq. (A16) is shown in Fig. 5 (dashed and dotted blue curve). It is always negative, so that the indirect exchange interaction is antiferromagnetic.

3. Projecting the exchange interaction onto the states with a given total spin

The exchange interaction Hamiltonian can be written as

$$H_{\rm ex}(R_{12}) = -2V(R_{12})(\mathbf{s}_1 \cdot \mathbf{s}_2), \qquad (A4)$$

where

$$V(R) = V_{\rm d}(R) + V_{\rm p}(R). \tag{A5}$$

 s_1 or s_2 is the spin operator for the outer *s* electron of the lithium or sodium atom,

$$\mathbf{s}_{j} = \frac{1}{2} \sum_{\sigma\sigma'} d_{j\sigma}^{\dagger} \boldsymbol{\tau}_{\sigma\sigma'} d_{j\sigma'},$$

where $\hat{\boldsymbol{\tau}}$ is a vector of the Pauli matrices, and $d_{j\sigma}$ or $d_{j\sigma}^{\dagger}$ is the annihilation or creation operator of electron with spin $\sigma = \uparrow, \downarrow$.

An atom of ⁶Li has the nuclear spin $s_{Li} = 1$, so the quantum state of an atom, $|\sigma, \mu\rangle$, is described by projection of the nuclear spin μ on the axis z and electronic spin σ . Antiferromagnetic hyperfine interaction couples nuclear and electron spins in total atomic spin $S = s_{Li} - \frac{1}{2} = \frac{1}{2}$. The wave function $|S,m\rangle$ of the state with the total spin S and the projection of the spin m on the axis z is

$$|S,m\rangle = \sqrt{\frac{S+1-m}{2(S+1)}} \uparrow ,m - \frac{1}{2} \rangle$$
$$-\sqrt{\frac{S+1+m}{2(S+1)}} \downarrow ,m + \frac{1}{2} \rangle.$$
(A6)

Projecting out the electronic spin operator s_1 onto the quantum states (A6), we get

$$\mathbf{s}_{1} \rightarrow \sum_{mm'} |S,m\rangle \langle S,m|\mathbf{s}_{1}|S,m'\rangle \langle S,m'| = \frac{\mathbf{S}}{2S+1},$$

$$\mathbf{S} = \sum_{mm'} \mathbf{T}_{mm'} X_{\mathrm{Li}}^{mm'},$$

(A7)

where $\hat{\mathbf{T}}$ is a vector of the spin-*S* matrices,

$$X_{\text{Li}}^{mm'} = |S,m\rangle \langle S,m'|.$$

Similarly, the nuclear spin of ²²Na is $s_{Na} = 3$, and the total atomic spin is $s = 3 - \frac{1}{2} = \frac{5}{2}$. The wave function $|s,m\rangle$ of the quantum state with the total spin *s* and projection *m* of the spin on the *z* axis is given by Eq. (A6) with $S \rightarrow s$. Then projecting out the electronic spin operator s_2 onto the quantum states (A6), we get

$$\mathbf{s}_{2} \rightarrow \sum_{mm'} |s,m\rangle \langle s,m|\mathbf{s}_{1}|s,m'\rangle \langle s,m'| = \frac{\mathbf{s}}{2s+1},$$

$$\mathbf{s} = \sum_{mm'} \mathbf{t}_{mm'} X_{\mathrm{Na}}^{mm'},$$
 (A8)

where $\hat{\mathbf{t}}$ is a vector of the spin-s matrices,

$$X_{\mathrm{Na}}^{mm'} = |s,m\rangle \langle s,m'|.$$

Finally, the exchange Hamiltonian (A4) takes the form

$$H_{\rm ex}(R_{12}) = -\frac{2V(R_{12})}{(2s+1)(2S+1)} (\mathbf{s} \cdot \mathbf{S}).$$
(A9)

4. Derivation of the coupling *J*

Atoms of sodium and lithium are placed in the external potential given by Eq. (1). The wave function $\Psi^{\text{Li}}(\mathbf{R})$ of the atom of lithium is given by Eq. (5), whereas the wave functions $\Psi^{\text{Na}}_{\nu m 0}(\mathbf{R})$ of the atoms of sodium are given by Eq. (6a). Then the coupling is

$$J_{\mathbf{n},\mathbf{n}'} = -\frac{2}{(2s+1)(2S+1)} \int_{R_{12} \ge R_0} d^3 \mathbf{R}_1 d^3 \mathbf{R}_2 V(R_{12})$$
$$\times |\Psi^{\text{Li}}(\mathbf{R}_1)|^2 [\Psi_{\mathbf{n}}^{\text{Na}}(\mathbf{R}_2)]^* \Psi_{\mathbf{n}'}^{\text{Na}}(\mathbf{R}_2), \qquad (A10)$$

where V(R) is given by Eq. (A5). The sign of $J_{n,n'}$ is chosen in such a way that positive coupling strength corresponds to antiferromagnetic interaction. The integration on the righthand side of Eq. (A10) is restricted by the condition $R_{12} > R_0$, since Coulomb repulsion between the electron clouds of the Na and Li atoms prevents the atoms from approaching closer than R_0 .

The function V(R) is negative for any $R > R_0$, so that the exchange interaction is antiferromagnetic. |V(R)| has its maximum at some value $R \sim R_0$ and vanishes when $R \gg R_0$. The atomic wave functions $\Psi^{\text{Li}}(\mathbf{R})$ and $\Psi_{\mathbf{n}}^{\text{Na}}(\mathbf{R})$ change slowly at a range of R_0 . Therefore, the following approximations are justified: (1) changing the limits of integration on the righthand side of Eq. (A10) from $R_0 \leq R_{12} < \infty$ to $0 \leq R_{12} < \infty$ and (2) approximating V(R) by a δ function,

$$V(R_{12}) \approx -g_0 \delta(\mathbf{R}_{12}),$$

$$g_0 = -4\pi \int_{R_0}^{\infty} V(R) R^2 dR = g_d + g_p,$$
(A11)

where g_d and g_p are couplings for the direct and indirect exchange interactions,

$$g_{\rm d} = -4\pi \int_{R_0}^{\infty} V_{\rm d}(R) R^2 dR,$$
 (A12)

$$g_{\rm p} = -4\pi \int_{R_0}^{\infty} V_{\rm p}(R) R^2 dR.$$
 (A13)

Numerical estimates with electronic wave functions $\psi_{\text{Na}}(\mathbf{r})$ and $\psi_{\text{Li}}(\mathbf{r})$ of the form of Eq (A16), $V_1(r) \approx V_2(r) \approx -\frac{e^2}{r}$ and $V_{12}(R) \approx \frac{e^2}{R}$, yields $g_d \approx 0.0301 \text{ eV} \text{ nm}^3$ and $g_p = 0.1257 \text{ eV} \text{ nm}^3$.

The Li wave function $\Psi^{\text{Li}}(\mathbf{R})$ [Eq. (5)] has its maximum at $\mathbf{R} = \mathbf{0}$ and it vanishes for $R \gg a_f$. The wave function $\Psi_{\mathbf{n}}^{\text{Na}}(\mathbf{R})$ [Eq. (6a)] changes slowly on the distance scale of a_f . Then the function $|\Psi^{\text{Li}}(\mathbf{R})|^2$ in Eq. (A10) can be approximated by the δ function,

$$|\Psi^{\text{Li}}(\mathbf{R})|^2 \approx \delta(\mathbf{R}). \tag{A14}$$

Substituting Eqs. (A11) and (A14) into Eq. (A10), we get the following estimate of the exchange constant:

$$J_{\mathbf{n},\mathbf{n}'} = \frac{2(g_{\rm d} + g_{\rm p})}{(2s+1)(2S+1)} \Psi_{\mathbf{n}}^{\rm Na}(0) \Psi_{\mathbf{n}'}^{\rm Na}(0).$$

For the energy levels close to the Fermi level ϵ_F , $\Psi_{\mathbf{n}}^{\text{Na}}(0)\Psi_{\mathbf{n}'}^{\text{Na}}(0)$ can be approximated as

$$\Psi_{\mathbf{n}}^{\mathrm{Na}}(0)\Psi_{\mathbf{n}'}^{\mathrm{Na}}(0) \approx \left(\frac{3M_{\mathrm{Na}}}{2\pi\hbar^2\epsilon_F}\right)^{3/2} \prod_{i=1,2,3}\hbar\omega_i$$

Then we can write

$$J_{\mathbf{n},\mathbf{n}'}\approx J_{\mathbf{n}}$$

where J is given by Eq. (9).

5. Electronic wave functions $\psi_{\text{Na}}(r)$ and $\psi_{\text{Li}}(r)$

The wave function of the outer electron in the atom of Na or Li satisfies the Schrödinger equation,

$$-\frac{\hbar^2}{2m_e}\Delta\psi_i(r) + V_i(r)\psi_i(r) = -\varepsilon_i\psi_i(r), \quad (A15)$$

where i = 1, 2 (i = 1 corresponds to the atom of lithium and i = 2 denotes the atom of sodium), $|\varepsilon_i|$ is the ionization energy ($\varepsilon_1 = 5.1391$ eV and $\varepsilon_2 = 5.3917$ eV), m_e is the mass of electron, and $V_i(r)$ is the effective potentials of interaction between the electron and the atomic core.

When the distance *r* from the nucleus exceeds the radius of the inner orbitals (which is smaller than the atomic radius), $V_i(r)$ is of the Coulomb type,

$$V_i(r) \approx -\frac{e^2}{r}.$$

The asymptotic behavior of $\psi_i(r)$ is

$$\psi_i(r) \sim (\kappa_i r)^{(1/\alpha_i)-1} e^{-\kappa_i r},$$

where

$$\kappa_i = \frac{\sqrt{2m_e\varepsilon_i}}{\hbar}, \quad \alpha_i = \kappa_i r_B, \quad r_B = \frac{\hbar^2}{m_e e^2}$$

 $\kappa_1 = 1.1602 \text{ Å}^{-1}, \alpha_1 = 0.61440, \kappa_2 = 1.1884 \text{ Å}^{-1}, \text{ and } \alpha_2 = 0.62932.$

The electronic cloud of the outer orbital is located mainly out of the electronic cloud of the inner orbitals (which is about 1 Å for Li and Na). Therefore we will assume the following expression for the wave functions:

$$\psi_i(r) = \mathcal{N}_i(2\kappa_i r)^{(1/\alpha_i)-1} e^{-\kappa_i r}, \qquad (A16)$$

where the normalization factor is

$$\mathcal{N}_i = \sqrt{\frac{2\kappa_i^3}{\pi\,\Gamma\left(\frac{2+\alpha_i}{\alpha_i}\right)}}$$

- I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
- [2] T. Bourdel, J. Cubizolles, L. Khaykovich, K. M. F. Magalhães, S. J. J. M. F. Kokkelmans, G. V. Shlyapnikov, and C. Salomon, Phys. Rev. Lett. **91**, 020402 (2003).
- [3] S. J. J. M. F. Kokkelmans, G. V. Shlyapnikov, and C. Salomon, Phys. Rev. A 69, 031602 (2004).
- [4] C. A. Regal and D. S. Jin, Adv. At., Mol., Opt. Phys. 54, 1 (2006).
- [5] Q. J. Chen, C. A. Regal, M. Greiner, D. S. Jin, and K. Levin, Phys. Rev. A 73, 041601 (2006).
- [6] Wenhui Li, G. B. Partridge, Y. A. Liao, and R. G. Hulet, Nucl. Phys. A 790, 88c (2007).
- [7] J. T. Stewart, J. P. Gaebler, and D. S. Jin, Nature (London) 454, 744 (2008).
- [8] W. Li, G. B. Partridge, Y. A. Liao, and R. G. Hulet, Int. J. Mod. Phys. B 23, 3195 (2009).
- [9] S. Nascimbne, N. Navon, K. J. Jiang, F. Chevy, and C. Salomon, Nature (London) 463, 1057 (2010).
- [10] R. Jördens, N. Strohmaier, K. Günter, H. Moritz, and T. Esslinger, Nature (London) 455, 204 (2008).
- [11] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, C. Chin, J. H. Denschlag, and R. Grimm, Phys. Rev. Lett. 91, 240402 (2003).
- [12] Z. Idziaszek, L. Santos, M. Baranov, and M. Lewenstein, Phys. Rev. A 67, 041403(R) (2003).
- [13] A. G. Truscott, K. E. Strecker, W. I. McAlexander, G. B. Partridge, and R. G. Hulet, Science 291, 2570 (2001).
- [14] M. W. Zwierlein, A. Schirotzek, C. H. Schunck, and W. Ketterle, Science 311, 492 (2006).
- [15] F. Schreck, G. Ferrari, K. L. Corwin, J. Cubizolles, L. Khaykovich, M.-O. Mewes, and C. Salomon, Phys. Rev. A 64, 011402(R) (2001).
- [16] Z. Hadzibabic, S. Gupta, C. A. Stan, C. H. Schunck, M. W. Zwierlein, K. Dieckmann, and W. Ketterle, Phys. Rev. Lett. 91, 160401 (2003).
- [17] S. Gupta, Z. Hadzibabic, M. W. Zwierlein, C. A. Stan, K. Dieckmann, C. H. Schunck, E. G. M. van Kempen, B. J. Verhaar, and W. Ketterle, Science 300, 1723 (2003).

- [18] J. K. Chin, D. E. Miller, Y. Liu, C. Stan, W. Setiawan, C. Sanner, K. Xu, and W. Ketterle, Nature (London) 443, 961 (2006).
- [19] J. F. Bertelsen, Ph.D. thesis, Danish National Research Foundation Center for Quantum Optics (QUANTOP) and University of Aarhus, 2007.
- [20] Z. Hadzibabic, C. A. Stan, K. Dieckmann, S. Gupta, M. W. Zwierlein, A. Görlitz, and W. Ketterle, Phys. Rev. Lett. 88, 160401 (2002).
- [21] W. Ketterle, Rev. Mod. Phys. 74, 1131 (2002).
- [22] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 80, 1215 (2008).
- [23] N. Navon, S. Nascimbne, F. Chevy, and C. Salomon, Science 328, 729 (2010)
- [24] A. Recati, P. O. Fedichev, W. Zwerger, J. von Delft, and P. Zoller, arXiv:cond-mat/0212413.
- [25] A. J. Heinrich, J. A. Gupta, C. P. Lutz, and D. M. Eigler, Science 306, 466 (2004).
- [26] Yao-Hua Chen, Wei Wu, Hong-Shuai Tao, and Wu-Ming Liu, Phys. Rev. A 82, 043625 (2010).
- [27] Y. Nishida, Phys. Rev. Lett. 111, 135301 (2013).
- [28] Johannes Bauer, Christophe Salomon, and Eugene Demler, Phys. Rev. Lett. 111, 215304 (2013).
- [29] S. Lal, S. Gopalakrishnan, and P. M. Goldbart, Phys. Rev. B 81, 245314 (2010).
- [30] S. Di Napoli, A. Weichselbaum, P. Roura-Bas, A. A. Aligia, Y. Mokrousov, and S. Blügel, Phys. Rev. Lett. 110, 196402 (2013).
- [31] A. M. Sengupta and Y. B. Kim, Phys. Rev. B **54**, 14918 (1996).
- [32] P. Nozières and A. Blandin, J. Phys. (Paris) 41, 193 (1980).
- [33] C. Silber, S. Gunther, C. Marzok, B. Deh, P. W. Courteille, and C. Zimmermann, Phys. Rev. Lett. 95, 170408 (2005).
- [34] D. C. McKay and B. DeMarco, Rep. Prog. Phys. 74, 054401 (2011).
- [35] C. A. Regal, C. Ticknor, J. L. Bohn, and D. S. Jin, Nature (London) 424, 47 (2003).
- [36] F. Ferlaino, S. Knoop, M. Berninger, M. Mark, H.-C. Naegerl, and R. Grimm, arXiv:0904.0935.

- [37] G. Barontini, C. Weber, F. Rabatti, J. Catani, G. Thalhammer, M. Inguscio, and F. Minardi, Phys. Rev. Lett. 103, 043201 (2009).
- [38] S. Knoop, F. Ferlaino, M. Mark, M. Berninger, H. Schoebel, H.-C. Naegerl, and R. Grimm, Nat. Phys. 5, 227 (2009).
- [39] M. Greiner, Ph.D. thesis, Ludwig Maximilian University of Munich, 2003.
- [40] E. A. Andreev, Theor. Chim. Acta 30, 191 (1973).

- [41] A. S. Davydov, *Quantum Mechanics* (Pergamon, New York, 1965).
- [42] A. G. Sitenko, *Scattering Theory* (Springer-Verlag, Berlin, 1991).
- [43] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, A Course of Theoretical Physics Vol. 3 (Pergamon, New York, 1965).
- [44] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, UK, 1993).