Erratum: Coqblin-Schrieffer model for an ultracold gas of ytterbium atoms with metastable state [Phys. Rev. B **93**, 115143 (2016)]

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(Received 31 October 2019; revised manuscript received 25 December 2019; published 17 January 2020)

In our paper, calculation of exchange interaction is carried out for two *itinerant atoms* $^{173}\text{Yb}(^1S_0)$ and $^{173}\text{Yb}(^3P_0)$. The fact that the exchange interaction is modified when the $^{173}\text{Yb}(^3P_0)$ atom is *localized in an optical potential* was overlooked. This flaw is corrected in this Erratum, and the claim that the exchange constant is antiferromagnetic (a necessary condition for achieving the Kondo effect) is established.

DOI: [10.1103/PhysRevB.101.049906](https://doi.org/10.1103/PhysRevB.101.049906)

I. INTRODUCTION

The main conclusion of our paper is the possible realization of Coqblin-Schrieffer model in an ultracold atomic system of ^{173}Yb atoms. In this atomic gas, the atoms in the ground 1S_0 state are itinerant, whereas a few atoms in a long-lived excited 3P_0 state are localized by a specially designed optical potential and serve as a dilute concentration magnetic impurities. However, it is established that the exchange interaction between $^{173}\text{Yb}(^1S_0)$ and $^{173}\text{Yb}(^3P_0)$ atoms is proportional to the difference $a_S - a_T$ of the “singlet” (a_S) and “triplet” (a_T) scattering lengths. (The proportionality constant is negative.) The scattering lengths for free $\text{Yb}(^1S_0)$ and $\text{Yb}(^3P_0)$ atoms are [1]

$$a_S = (1878 \pm 37)a_B, \quad (1)$$

$$a_T = (219.7 \pm 2.2)a_B \quad (2)$$

[where a_B is Bohr’s radius]. Hence, the exchange interaction *between the free atoms* is ferromagnetic, and Eqs. (34)–(43) in the original paper are wrong. In order for the Kondo effect (KE) to occur, the exchange interaction should be antiferromagnetic. In the following, we show that the exchange interaction between an *itinerant* $\text{Yb}(^1S_0)$ atom and a *bound* $\text{Yb}(^3P_0)$ atom is controllable to be antiferromagnetic, and the Kondo physics is, therefore, relevant.

II. EXCHANGE INTERACTION

The strength of the exchange interaction between $\text{Yb}(^1S_0)$ and $\text{Yb}(^3P_0)$ atoms is given by

$$J = -\frac{4\pi\hbar^2(a_S - a_T)}{M}. \quad (3)$$

Thus, the exchange interaction is ferromagnetic (antiferromagnetic) when $a_S - a_T$ is positive (negative). It is crucial to note that the fact that $\text{Yb}(^3P_0)$ is trapped [whereas $\text{Yb}(^1S_0)$ is itinerant] affects the sign and value of J . The effect of trapping of $\text{Yb}(^3P_0)$ (which serves as a magnetic impurity) on the scattering lengths is analyzed in Sec. II A. It is shown there that, *for free Yb atoms*, $a_S > a_T$ and the exchange interaction is, indeed, ferromagnetic. On the other hand, if $\text{Yb}(^3P_0)$ is localized, the occurrence of confinement-induced resonances (CIRs), enables the tuning of the exchange interaction from being ferromagnetic to be antiferromagnetic and vice versa [see Fig. 1 for illustration].

A. Confinement-induced resonances

Following Ref. [2] (see also Refs. [3–5]), we obtain singlet and triplet scattering lengths for itinerant $\text{Yb}(^1S_0)$ atoms scattered on a trapped $\text{Yb}(^3P_0)$ impurity. Denoting the scattering length for two free atoms by $a_\alpha^{(0)}$, the scattering of a free atom on the localized impurity has the scattering length,

$$a_\alpha = 2a_\alpha^{(0)} \int \phi_0(r) \psi_{\text{reg}}^{(\alpha)}(r) d^3\mathbf{r}, \quad (4)$$

where $\alpha = S, T$ for the singlet and triplet two-atomic state.

Here, $\phi_0(r)$ is the wave function of the ground state of a three-dimensional (3D) harmonic-oscillator trapping potential, and $\psi_{\text{reg}}^{(\alpha)}(r)$ is defined as

$$\psi_{\text{reg}}^{(\alpha)}(r) = \lim_{\rho \rightarrow 0} \frac{\partial}{\partial \rho} \left[\rho \psi_\alpha \left(\mathbf{r} + \frac{\rho}{2}, \mathbf{r} - \frac{\rho}{2} \right) \right].$$

The itinerant and trapped atoms position vectors are $\mathbf{r}_g = \mathbf{r} + \frac{1}{2}\rho$ and $\mathbf{r}_e = \mathbf{r} - \frac{1}{2}\rho$. The two-atomic wave function $\psi_\alpha(\mathbf{r}_g, \mathbf{r}_e)$ is found from the equation,

$$\psi_\alpha(\mathbf{r}_g, \mathbf{r}_e) = \phi_0(r_B) + g_\alpha \int G_E(\mathbf{r}_g, \mathbf{r}_e; \mathbf{r}, \mathbf{r}) \psi_{\text{reg}}^{(\alpha)}(r) d^3\mathbf{r}, \quad (5)$$

where

$$g_\alpha = \frac{4\pi\hbar^2 a_\alpha^{(0)}}{M}.$$

The two-particle Green’s function is

$$G_E(\mathbf{r}_g, \mathbf{r}_e; \mathbf{r}, \mathbf{r}) = -\frac{M}{2\pi\hbar^2} \frac{1}{|\mathbf{r}_g - \mathbf{r}|} \sum_{\mathbf{n}} \phi_{\mathbf{n}}(\mathbf{r}_e) \phi_{\mathbf{n}}(\mathbf{r}) e^{-\kappa_{\mathbf{n}}|\mathbf{r}_g - \mathbf{r}|}, \quad (6)$$

where $\phi_{\mathbf{n}}(\mathbf{r})$ ’s are wave functions of the 3D harmonic oscillator in the state with harmonic numbers $\mathbf{n} = (n_x, n_y, n_z)$,

$$\kappa_{\mathbf{n}} = \sqrt{\frac{2M\Omega_e}{\hbar}} (n_x + n_y + n_z),$$

and Ω_e is the harmonic frequency of the trapped $\text{Yb}(^3P_0)$ impurity in the original paper.

Before obtaining a numerical solution of Eq. (5), we explain why the confinement can give rise to resonances. In other words, why a_α is singular. Equation (5) can be formally

FIG. 1. a_S (the blue curve) and a_T (the red curve) calculated numerically as functions of b_e . The arrows show the intervals of b_e wherein $a_T > a_S$ and the exchange interaction turns from being ferromagnetic to be antiferromagnetic.

written as

$$|\Psi_\alpha\rangle = |\Psi_0^{(\alpha)}\rangle + g_\alpha \hat{G}_\epsilon \hat{W} |\Psi_\alpha\rangle, \quad (7)$$

where the Green's function is $\hat{G}_\epsilon = (\epsilon - H_0 + i0)^{-1}$ and

$$\hat{W}\Psi\left(\mathbf{r} + \frac{\boldsymbol{\rho}}{2}, \mathbf{r} - \frac{\boldsymbol{\rho}}{2}\right) = \delta(\boldsymbol{\rho}) \frac{\partial}{\partial \boldsymbol{\rho}} \left[\rho \Psi\left(\mathbf{r} + \frac{\boldsymbol{\rho}}{2}, \mathbf{r} - \frac{\boldsymbol{\rho}}{2}\right) \right].$$

A formal solution of Eq. (7) is

$$|\Psi_\alpha\rangle = \frac{1}{1 - g_\alpha \hat{G}_\epsilon \hat{W}} |\Psi_0^{(\alpha)}\rangle. \quad (8)$$

The operator $\hat{O} = \hat{G}_\epsilon \hat{W}$ is Hermitian, having real eigenvalues λ_i ,

$$\hat{O}|e_i\rangle = \lambda_i|e_i\rangle,$$

where $|e_i\rangle$'s are eigenvectors of $\hat{O}$. Then, the scattering length (4) can be written as [2]

$$\begin{aligned} a_\alpha &= 2a_\alpha^{(0)} \langle \tilde{\psi}_0^{(\alpha)} | \frac{1}{1 - g_\alpha \hat{O}} | \tilde{\psi}_0^{(\alpha)} \rangle \\ &= \frac{M}{4\pi\hbar^2} \sum_i \frac{|\langle \tilde{\psi}_0^{(\alpha)} | e_i \rangle|^2}{g_\alpha^{-1} - \lambda_i}, \end{aligned} \quad (9)$$

where $\tilde{\psi}_0^{(\alpha)}(R) = R\Psi_0^{(\alpha)}(R, R)$. Singularity in a_α is expected when $g_\alpha^{-1} = \lambda_i$ or when

$$a_\alpha^{(0)} = \frac{M}{4\pi\hbar^2\lambda_i}.$$

Since $\lambda_i(b_e)$ is a function of b_e [the harmonic length of the trapped $\text{Yb}(^3P_0)$ atom in the original paper], the last equation allows us to expose the resonant values of b_e .

Solving Eq. (5) numerically and substituting $\psi_{\text{reg}}^{(\alpha)}(r)$ into Eq. (4), we get a_α for the singlet ($\alpha = S$) and triplet ($\alpha = T$) two-atomic states. The results of the numerical calculations are shown in Fig. 1. It is seen that for most part of the interval $100a_B < b_e < 1900a_B$, $a_S > a_T$, and the exchange interaction is ferromagnetic. However, there are two intervals, where $a_S < a_T$, and the exchange interaction is antiferromagnetic.

TABLE I. Resonant values $\Omega_n^{(S)}$ and $\Omega_n^{(T)}$ of the harmonic lengths Ω_S and Ω_T .

n	$\hbar\Omega_n^{(S)}/k_B$ (μK)	$\hbar\Omega_n^{(T)}/k_B$ (μK)
1	0.2913	21.29
2	0.1189	8.686
3	0.0747	5.456
4	0.0544	3.978

The first one is close to a resonance for the singlet state,

$$1692a_B < b_e < 1819a_B,$$

and the second one is close to a resonance for the triplet state,

$$212.8a_B < b_e < 226.7a_B.$$

The corresponding harmonic energies $\hbar\Omega_e$ are

$$0.3026 \mu\text{K} < \frac{\hbar\Omega_e}{k_B} < 0.3497 \mu\text{K}, \quad (10)$$

$$19.48 \mu\text{K} < \frac{\hbar\Omega_e}{k_B} < 22.11 \mu\text{K}. \quad (11)$$

Figure 10 in Ref. [2] [see also Table I] shows that there are additional resonances corresponding to higher values of λ_i (and shorter harmonic lengths b_e), but they are very narrow, and we do not consider them here. In the following discussion, we demonstrate the formation of CIRs for $a_\alpha^{(0)} > 0$.

B. Estimation of resonant values of Ω_e

Here, we follow Ref. [2] and calculate resonant frequencies for $a_\alpha^{(0)} \ll b_e$. In order to estimate resonant values of Ω_e , we write the two-atom Hamiltonian as

$$H = H_r + H_\rho + H_{\text{int}}, \quad (12)$$

where $\mathbf{r} = (\mathbf{r}_g + \mathbf{r}_e)/2$ is the position of the center of mass and $\boldsymbol{\rho} = \mathbf{r}_g - \mathbf{r}_e$ is the relative coordinate,

$$H_r = -\frac{\hbar^2}{4M} \frac{\partial^2}{\partial \mathbf{r}^2} + \frac{M\Omega_e^2}{2} r^2, \quad (13)$$

$$H_\rho = -\frac{\hbar^2}{M} \frac{\partial^2}{\partial \boldsymbol{\rho}^2} + g_\alpha \delta(\boldsymbol{\rho}) \frac{\partial}{\partial \rho} (\rho \cdot), \quad (14)$$

$$H_{\text{int}} = \frac{M\Omega_e^2}{8} \rho^2 - \frac{M\Omega_e^2}{2} (\mathbf{r} \cdot \boldsymbol{\rho}). \quad (15)$$

H_ρ describes the relative motion of the atoms with van der Waals potential (which is parametrized by the pointlike interaction). Consider the situation when the atoms are trapped by the van der Waals interaction and form a molecule. The energy level of the weakest-bounded s state is

$$\epsilon_r = -\frac{\hbar^2}{M(a_\alpha^{(0)})^2}.$$

H_r describes the center-of-mass motion of the molecule that is trapped by the optical lattice potential and undergoes harmonic oscillations. The corresponding harmonic frequency of the molecule is $\Omega_e/\sqrt{2}$ and the energies of the s states are

$$\epsilon_r = \frac{\hbar\Omega_e}{\sqrt{2}} \left(2n + \frac{3}{2} \right),$$

where n is a non-negative integer. Corrections to the energies from H_{int} [which are of order $\hbar\Omega_e(a_\alpha^{(0)}/b_e)^2 \ll \hbar\Omega_e$] are small and can be neglected hereafter. Within this unperturbed approximation, a_α diverges each time the energy of the oscillating molecule is equal to the ground-state energy of the pair of atoms, i.e., at the values of $\Omega_e = \Omega_n^{(\alpha)}$ that satisfy

$$\left(2n + \frac{3}{2}\right) \frac{\hbar\Omega_n^{(\alpha)}}{\sqrt{2}} - \frac{\hbar^2}{M(a_\alpha^{(0)})^2} = \frac{3}{2}\hbar\Omega_n^{(\alpha)}. \quad (16)$$

Solving Eq. (16), we find resonant harmonic frequencies,

$$\hbar\Omega_n^{(\alpha)} = \frac{\hbar^2}{M(a_\alpha^{(0)})^2} \frac{4}{[\sqrt{2}(4n+3) - 6]}. \quad (17)$$

Taking into account Eqs. (1) and (2), we get resonant frequencies for the lowest n , presented in Table I. The values for $n = 1$ are close to the values reported in Eqs. (10) and (11) calculated numerically.

III. KONDO HAMILTONIAN AND THE KONDO TEMPERATURE

Now, we consider a system composed of itinerant Yb(1S_0) atoms (a Fermi gas) and a trapped Yb(3P_0) atom (serving as a magnetic impurity). Due to the presence of a centrifugal barrier, only atoms with orbital angular momentum $L = 0$ interact with the impurity. Omitting states with $L > 0$, we write the Hamiltonian of the system as

$$H = H_0 + H_K, \quad (18)$$

where

$$H_0 = \sum_{n\mu} \varepsilon_n c_{n\mu}^\dagger c_{n\mu}, \quad (19)$$

$$H_K = J \sum_{nn'} \Psi_g^n(0) \Psi_g^{n'}(0) \sum_{\mu} Z^{\mu\mu} c_{n'\mu}^\dagger c_{n\mu} + J \sum_{nn'} \Psi_g^n(0) \Psi_g^{n'}(0) \sum_{\mu \neq \mu'} X^{\mu\mu'} c_{n'\mu'}^\dagger c_{n\mu}. \quad (20)$$

$\varepsilon_n = \hbar\Omega_g(2n+3/2)$, where Ω_g is the harmonic frequency of trapped Yb(1S_0) atoms in the original paper. Here, $c_{n\mu}$ ($c_{n\mu}^\dagger$) is the annihilation (creation) operator for an atom of the Fermi gas with harmonic quantum number n and nuclear spin quantum number $\mu = -\frac{5}{2}, -\frac{3}{2}, \dots, \frac{5}{2}$. $X^{\mu\mu'} = |\mu\rangle\langle\mu'|$'s are the Hubbard operators coupling different degenerate impurity states, and

$$Z^{\mu\mu} = X^{\mu\mu} - \frac{1}{N} \sum_{\mu'} X^{\mu'\mu'}, \quad N = 6.$$

The density of states for the Hamiltonian H_0 is as follows:

$$\varrho(\epsilon) = \sum_n |\Psi_g^n(0)|^2 \delta(\epsilon - \varepsilon_n) \approx \frac{1}{b_g^3} \frac{\sqrt{\epsilon}}{(2\hbar\Omega_g)^{3/2}} \Theta(\epsilon), \quad (21)$$

where $\Theta(\epsilon)$ is the Heaviside θ function.

Within poor man scaling formalism, the dimensionless coupling $j = J\varrho(\epsilon_F)$ satisfies the following scaling equation [6]:

$$\frac{\partial j}{\partial \ln D} = -Nj^2. \quad (22)$$

FIG. 2. Kondo temperature (27) as a function of b_e for $D_0 = T_F = T_e$ and b_e belonging to (a) the interval (24) and (b) the interval (25).

Initially, the bandwidth is $D_0 = T_e$, where

$$T_e = \frac{\hbar\Omega_e}{k_B},$$

and the reduced bandwidth D satisfies the inequalities $D_0 \geq D \gg T$. The initial value of $j(D)$, $j(D_0) \equiv j_0$ is as follows:

$$j_0 = \frac{J_0}{b_g^3} \frac{\sqrt{\epsilon_F}}{(2\hbar\Omega_g)^2} = -\frac{\pi(a_S - a_T)}{b_g} \sqrt{\frac{2\epsilon_F}{\hbar\Omega_g}}. \quad (23)$$

Equation (23) shows that the KE exists when $a_S < a_T$. Scattering lengths for the interaction of *free* Yb(1S_0) and Yb(3P_0) atoms are given by Eqs. (1) and (2) (see Ref. [1]) and yield a ferromagnetic exchange interaction. The situation is changed when the Yb(3P_0) atom is *trapped*. When the ground-state energy of the two atoms is equal to an energy of the trapped molecule, a CIR occurs [2–5]. In this case, the exchange interaction changes sign and becomes antiferromagnetic. The CIR mechanism was considered in Sec. II A where it is shown that for

$$1692a_B < b_e < 1819a_B, \quad (24)$$

$a_S < 0$, and the exchange interaction is antiferromagnetic, whereas for

$$212.8a_B < b_e < 226.7a_B, \quad (25)$$

a_T is positive and very large, and the exchange interaction is antiferromagnetic.

The scaling equation (22) has the solution,

$$j(T) = \frac{1}{N \ln(T/T_K)}, \quad (26)$$

where the Kondo temperature (the scaling invariant of the renormalization-group equation) is given by

$$T_K = D_0 \exp\left(-\frac{1}{Nj_0}\right). \quad (27)$$

The Kondo temperature (27) as a function of b_e is shown in Fig. 2 for $D_0 = T_F = T_e$. It is evident that T_K is high enough to be experimentally measured.

IV. CONCLUSIONS

In conclusion, we have shown that the exchange interaction between the itinerant Yb(1S_0) and a localized Yb(3P_0) atoms is controllable to be antiferromagnetic, and the Kondo effect can

occur. Section [III](#) in the original paper should be replaced by Secs. [II](#) and [III](#) of this Erratum. From the other side, Sec. [IV](#) in the original paper remains unchanged provided that the condition $a_S < a_T$ is obeyed and the Kondo effect occurs.

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- [1] M. Höfer, L. Riegger, F. Scazza, C. Hofrichter, D. R. Fernandes, M. M. Parish, J. Levinsen, I. Bloch, and S. Fölling, [Phys. Rev. Lett. **115**, 265302 \(2015\)](#).
 - [2] P. Massignan and Y. Castin, [Phys. Rev. A **74**, 013616 \(2006\)](#).
 - [3] T. Bergeman, M. G. Moore, and M. Olshanii, [Phys. Rev. Lett. **91**, 163201 \(2003\)](#).
 - [4] E. Haller, M. J. Mark, R. Hart, J. G. Danzl, L. Reichsöllner, V. Melezhik, P. Schmelcher, and H.-C. Nägerl, [Phys. Rev. Lett. **104**, 153203 \(2010\)](#).
 - [5] H. Moritz, T. Stöferle, K. Günter, M. Köhl, and T. Esslinger, [Phys. Rev. Lett. **94**, 210401 \(2005\)](#).
 - [6] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, UK, 1993).