Erratum: Screened Coulomb interaction calculations: cRPA implementation and applications to dynamical screening and self-consistency in uranium dioxide and cerium [Phys. Rev. B 89, 125110 (2014)]

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The calculation reported in the original paper contains an error in the self-consistent calculation of effective Hund's coupling J. Let's call J_1 the value of J computed in the original paper and defined [in Eq. (9) of the original paper] as

$$J_1 = \frac{1}{4}\sum_{\sigma,\sigma'}\frac{1}{(2l+1)(2l)}\sum_{m_1=1}^{2l+1}\sum_{m_2=1(m_2\neq m_1)}^{2l+1} U^{\sigma,\sigma'}_{m_1,m_2,m_2,m_1}. \tag{1}$$

A more common definition of J can however be established using the expression of J_2 deduced from (see Ref. [1] or the Appendix of Ref. [2])

$$U - J_2 = \frac{1}{4}\sum_{\sigma,\sigma'}\frac{1}{(2l+1)(2l)}\sum_{m_1=1}^{2l+1}\sum_{m_2=1}^{2l+1}\left(U^{\sigma,\sigma'}_{m_1,m_2,m_1,m_2} - U^{\sigma,\sigma'}_{m_1,m_2,m_2,m_1}\right). \tag{2}$$

J_1 and J_2 are related by

$$J_2 = J_1 + \frac{U_{\text{diag}} - U}{2l} \quad \text{with} \quad U_{\text{diag}} = \frac{1}{4}\sum_{\sigma,\sigma'}\frac{1}{2l+1}\sum_{m} U^{\sigma,\sigma'}_{m,m,m,m}. \tag{3}$$

Even if Eq. (2) is more used, the choice between Eqs. (1) and (2) is a matter of convention. So the cRPA computed values of J given in the original paper are not erroneous for *non-self-consistent* calculations over U and J, they just use an unusual convention. However, for self-consistent calculations, there is an error, because the convention used for J in DFT + U in the `ABINIT` code [3] is the one of Eq. (2) and not the one of Eq. (1). So we have redone the self-consistent calculations for all interactions with the correct definition. For the sake of completeness, we recompute even the non-self-consistent values of

TABLE III. Bare (v), fully screened (W), and cRPA (U^{cRPA}) Coulomb interactions for UO_2. In cRPA, the screening is computed for the different models described in Table I of the original paper. All calculations are done in the nonmagnetic states for LDA, and ferromagnetic states for LDA + U. The calculation done in the antiferromagnetic configuration is indicated by †. Non-self-consistent (nsc) calculations of U use LDA + U with $U = 4.5$ eV and $J = 0.5$ eV.

	Model	U (eV)	J (eV)
v	f	16.0	0.6
v	fp or f-fp (a,b)	17.1	0.7
v	f-ext (b_a)	18.2	0.7
W	f	0.20	0.4
W	fp or f-fp (a,b)	0.21	0.4
W	f-ext (b_a)	0.23	0.5
U^{cRPA}	f	3.4	0.5
U^{cRPA}	f-fp (a)	3.6	0.6
U^{cRPA}	f-fp (b)	2.0	0.5
U^{cRPA}	f-ext (b_a)	1.0	0.6
U^{cRPA}	fp	6.2	0.6
$U^{\text{cRPA}}_{\text{nsc}}$	f-ext (b_a)	4.9	0.6
$U^{\text{cRPA}}_{\text{nsc}}$	f-ext (b_b)	5.3	0.6
$U^{\text{cRPA}}_{\text{nsc}}$	f-ext (b_c)	5.6	0.6
$U^{\text{cRPA}}_{\text{sc}}$	f-ext (b_a)	5.0	0.6
$U^{\text{cRPA}}_{\text{sc}}$	f-ext (b_b)	5.5	0.6
$U^{\text{cRPA}}_{\text{sc}}$	f-ext (b_c)	5.9	0.6
$U^{\text{cRPA}\dagger}_{\text{sc}}$	f-ext (b_a)	4.8	0.6

TABLE IV. Bare (v), fully screened (W), and cRPA (U^{cRPA}) Coulomb interactions for different models for cerium in LDA and LDA + U methods. The definition of Wannier functions and screening models are defined in Table II of the original paper. In [f-ext (b_i)] $_{i=1\ldots4}$, the same number of bands are used to build Wannier functions in α and γ cerium. In [f-ext (b'_1)], two more bands are used for the calculation of γ cerium in order that the same energy window is used in both phases. The last 12 rows of the table gives values of U obtained from a cRPA calculation starting from a band structure obtained with the LDA + U method. U_{nsc} are non-self-consistently computed values of U, starting from an LDA + U calculation with $U = 6$ eV and $J = 0$ eV. U_{sc} are values of U computed self-consistently with a given energy window to define the Wannier functions. The last four rows show values using DFT + U numbers of electrons following scheme $\mathrm{o_C}$ of Ref. [4].

	Model	Bands for Wanniers	γ		α	
			U (eV)	J (eV)	U (eV)	J (eV)
v	f-ext (b_1)	1-20	23.8	0.9	24.3	0.9
v	f-ext (b_2)	1-30	25.0	0.9		
v	f-ext (b_3)	1-40	25.3	0.9		
v	f-ext (b'_1)	1-22/20	24.2	0.9	24.3	0.9
W	f-ext (b_1)	1-20	0.4	0.6	0.6	0.7
U^{cRPA}	f-ext (b_1)	1-20	0.7	0.7	0.9	0.7
U^{cRPA}	f-W_1		0.5	0.7	0.7	0.7
U^{cRPA}	fdt_{2g}-ext	1-20	3.8	0.8	3.8	0.8
		LDA + U calculations				
$U^{\mathrm{cRPA}}_{\mathrm{nsc}}$	f-ext (b_1)	1-20	5.9	0.8	5.5	0.8
$U^{\mathrm{cRPA}}_{\mathrm{nsc}}$	f-ext (b_2)	1-30	6.6	0.8		
$U^{\mathrm{cRPA}}_{\mathrm{nsc}}$	f-ext (b_3)	1-40	6.7	0.8		
$U^{\mathrm{cRPA}}_{\mathrm{nsc}}$	f-ext (b_4)	1-50	6.7	0.8		
$U^{\mathrm{cRPA}}_{\mathrm{sc}}$	f-ext (b_1)	1-20	4.9	0.7	0.9	0.7
$U^{\mathrm{cRPA}}_{\mathrm{sc}}$	f-ext (b_2)	1-30	6.3	0.8	1.0	0.7
$U^{\mathrm{cRPA}}_{\mathrm{sc}}$	f-ext (b_3)	1-40	6.6	0.8	1.0	0.7
$U^{\mathrm{cRPA}}_{\mathrm{sc}}$	f-ext (b_4)	1-50	6.4	0.8	1.0	0.7
$U^{\mathrm{cRPA}}_{\mathrm{sc}}$ (scheme $\mathrm{o_C}$ of Ref. [4])	f-ext (b_1)	1-20	5.4	0.8	0.9	0.7
$U^{\mathrm{cRPA}}_{\mathrm{sc}}$ (scheme $\mathrm{o_C}$ of Ref. [4])	f-ext (b_2)	1-30	6.6	0.8	5.6	0.8
$U^{\mathrm{cRPA}}_{\mathrm{sc}}$ (scheme $\mathrm{o_C}$ of Ref. [4])	f-ext (b_3)	1-40	6.9	0.8	5.7	0.8
$U^{\mathrm{cRPA}}_{\mathrm{sc}}$ (scheme $\mathrm{o_C}$ of Ref. [4])	f-ext (b_4)	1-50	6.8	0.8	5.5	0.8

effective interactions, with the definition of Eq. (2). All results are given in the Tables III and IV for respectively UO_2 and cerium. For non-self consistent calculations, the values of J change with respect to the same table in the original paper because the definition has changed. For self-consistent calculations, both values of U and J change, because the use of the correct definition of J impacts the numerical value of J and hence the whole DFT + U band structure and screening properties are modified.

The main conclusion is that the values of J computed using Eq. (2) are larger by 0.2 eV than the value of J computed using Eq. (1). For self-consistent calculations, values of U are weakly impacted by the change of J for γ cerium and UO_2. In contrast, self-consistent values of U for α cerium are strongly impacted as can be seen in Table IV: In comparison to results of the original paper where (erroneous) values of U for f-ext(b_2), f-ext(b_3), and f-ext(b_4) models were about 5.5 eV, the self-consistent (correct) values of U are now very weak and around 1.0 eV.

It might be tempting to interpret this as a drastic change of electron interaction between phases of cerium. However, we can show that the difference of effective interaction between the two phases is weaker. Indeed and in order to put things into perspective, we carried out a new self-consistent calculation of U and J with a slight modification of the definition of the density matrix, discussed in Ref. [4] (see the last four rows of Table IV). Indeed, DFT + U implementations in PAW often [5,6] compute the number of electrons only inside the PAW spheres. As a consequence, the number of electrons are underestimated in the calculations using these implementations. The modification proposed in Ref. [4] intends to compute more accurately the number of electrons used in the DFT + U density matrix by renormalizing the density matrix. This correction is rather small for cerium, for which the f orbital is very localized. However, and even if it is small, and as can be seen in Table IV, this correction changes drastically the self-consistent values of U, and we recover large values of U for the most localized Wannier function [f-ext(b_2), f-ext(b_3), and f-ext(b_4)]. So we can be confident that the values of U are not too different for α and γ cerium. A more detailed discussion will be proposed in a future study [7].

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