Nanotechnology Perceptions
ISSN 1660-6795
www.nano-ntp.com

Scaling Approach In Mixed Valent System And RKKY Interaction

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In this work, a scaling description of the influence of RudermanKittelKasuyaYosida (RKKY) interaction on valence fluctuations in mixed-valent systems is carried out. A delicate balance between itinerant and localized magnetic moments is observed in mixed-valent materials that include rare-earth intermetallic compound materials. This work studies the scaling of magnetic susceptibility, specific heat, and the valence fluctuation with the Kondo coupling J and f-level energy e f \cdot Using the concept of analytical modeling and numerical simulation, this work suggests that the magnetic susceptibility, specific heat, and valence fluctuation scale with an intensity of f-level energy e F \cdot and Kondo coupling J. The findings provide that at low coupling (J=0.1eV), magnetic susceptibility is high (~ 0.89 emu/mol), dictated by RKKY interaction. When the Kondo coupling rises to J=0.6eV, susceptibility plunges (~0.28 emu/mol), and the coefficient of specific heat increases to 0.43 mJ/mol K 0.6 and to 1.26 mJ/mol K 0.8 clearly indicating a shift to a Kondo-dominated regime. The scaling exponents that are based on magnetic susceptibility are 0.98< 0 0.51, which indicates the constant crossover of magnetic behavior. The amplitude of the valence fluctuation is maximum at a ϵf leading to the Fermi and this affirms the strong nature of charge instability. These findings confirm the scaling of a successive strategy as a viable structure to describe quantum-critical behaviour and twofold nature of electron localisation within mixed-valent materials.

Keywords: Mixed-valent systems, RKKY interaction, Kondo effect, Scaling behavior, Quantum criticality.

I. INTRODUCTION

Mixed valent systems A particularly interesting group of materials in condensed matter physics are mixed valent materials in which the valence state of some ions is between two or more discrete oxidation states. Such states are seen mostly in rare-earth or in actinide elements [1]. The cause of this phenomenon is high rates of hybridization between localized f-electrons and conduction electrons, which results in complex behavior, including the Kondo effect, the formation of heavy fermion, and unusual magnetic behavior [2]. These connections between localized and itinerant electronic nature and the systems are of fundamental both theoretical and practical significance, since they determine an important physical property of these systems in low-temperature limits (magnetic susceptibility, resistivity, specific heat and others). The RudermanKittelKasuyaYosida (RKKY) interaction is one of the more important interactions in such systems. This indirect interaction of localized magnetic moments with each other, but which is mediated through the conduction electrons, competes with the Kondo screening effect [3]. Graceful situation between these conflicting phenomena is conventionally described by so called Doniach phase diagram, which suggests magnetic order at small enough Kondo coupling and non-magnetic heavy fermion behavior at larger coupling values. This competition is necessary to explain the ground state of many intermetallic compounds and it is also required to predict quantum critical behavior. This work would study the scaling behavior which arises in mixed valent regimes as we sweep across RKKY-dominated and Kondo-dominated regimes. Using theoretical scaling theories and studying aspects of model systems, the work aims to establish universal scaling laws which describe physical quantities close to critical points. By this strategy we hope to gain increased understanding of the quantum phase transitions and other emergent phenomena in correlated electron systems. The findings can not only elaborate the basic knowledge on the strongly correlated materials but also help the synthesis of new advanced functional materials that can be programmed to electronic and magnetic responses.

II. RELATED WORKS

The phenomena of mixed valent systems with related magnetic interactions has been an attractive topic of the condensed matter physics especially in reference to the rare earth intermetallic compounds. Typically such systems have several valence states in one material, with the result that many so-called complex physical effects are possible, including valence fluctuations, Kondo effect, RKKY (Ruderman-Kittel-Kasuya-Yosida) interactions and heavy fermion behavior. The magnetic and electronic properties that arise in these systems have been well studied in recent years. Ghosh et al. [14] employed machine-learning-assisted simulations to study orbital ordering kinetics in cooperative Jahn-Teller models and offer an insight into orbital-lattice interactions in strongly correlated electron systems. This strategy paves way into further understanding dynamic processes relating to magneto-structural transitions. The magnetism of strongly correlated rare-Earth intermetallics was surveyed by Savchenkov and Alekseev [15]. They highlighted the importance of 4f electron localization and hybridisation in spurring unconventional magnetism, specifically in the systems where valence fluctuations compete with magnetic ordering. On the same note, Lee [16] also targeted 4f based intermetallic compounds that lie on geometrically frustrated lattices which showed how the frustration plays an important role in determining the stability and contention of magnetic ground in mixed valent compounds.

Yao et al. [17] revealed the topological phenomena could co-exist with intricate magnetism in Weyl semimetals such as SmAlSi, in which spirals magnetic order and giant topological Hall effects were found. This brings a new dimension to the knowledge on mixed valent systems in that magnetic topology is connected to anomalies in the electronic structure. Dominguez Montero et al. [18] have shown the structural flexibility of the Ce-based compounds where they have discussed the Ce4Fe3Ge10 system. Their result implies that the inter-relationship between the type of structure and magnetic interactions result in the formation of emergent phenomena in series of intermetallic homologues. In the meantime, Rao and Zhu [19] forecasted additional heavy fermion candidates in carbon-boron clathrates specifically along with the importance of cage structures in both hosting valence instabilities as well as in correlated electron effects. Interest has also been on valence transitions and magnetic collapse under external stimuli. Kutelak et al. [20] studied EuB6 at high pressure and found that at low temperatures that the ferromagnetism collapses as a result of valence instability. They used their high-pressure X-ray and magnetic work to show that simply altering external parameters is capable of forcing a profound change in the balance between valence states and magnetic order.

Theoretically, on the one hand, Xie et al. [21] considered Kondo effect in transition metal dichalcogenide heterobilayers and their further destabilization with different tuning parameters with particular respect to importance of hybridization and dimensionality. This complements mixed valent physics in which Kondo screening is important. Finally, Panday and Dzero [22] also talked about superconductivity in Cerium-based cage compounds and connected ir to the fragile interplay of unknown and magnetic correlations. They indicate in their research that these systems may possess an exotic ground state due to competing interactions.

Collectively, these studies illustrate the prolific physics created by mixed valency and magnetic interactions especially the RKKY, and demonstrate that none of these multifaceted behaviours can be captured quantitatively or predictively in the highly diverse complex materials using scaling analyses.

III. METHODS AND MATERIALS

3.1 Overview

The method chosen in this research is more theoretical and computational since it explores the scaling behavior of mixed valent system with competing Kondo and RKKY interaction. It rests on quantum many-body theory, and numerical simulations are done on simplified Hamiltonians which model heavy fermion systems. The methodology encompasses selection of the model, defining parameters, numerical approaches (such as exact diagonalization and scaling functions fitting) and characterization of phases [4]. The key point is to obtain scaling laws that explain physical observables, such as magnetic susceptibility and specific heat in regions close to criticality, and how these observables change with the control parameters, which include temperature, coupling strength and the probability of valence fluctuations [5].

3.2 Model Hamiltonians

The Anderson Lattice Model (ALM) and the simplification of the former the Kondo Lattice Model (KLM) are the main theoretical frameworks. The models provide the necessary physics of mixed valent systems with the local f-electrons orbitals hybridizing with the conduction electrons via the coupling channels [6].

(a) Anderson Lattice Model (ALM):

“H=k,σ∑ϵkckσ†ckσ+i,σ∑ϵffiσ†fiσ+i,k,σ∑(VkeikRickσ†fiσ+h.c.)+Ui∑nfi↑nfi↓”

- ϵk: dispersion of conduction electrons
- ϵf: energy level of f-electrons
- Vk: hybridization strength
- U: Coulomb repulsion among f-electrons

(b) Kondo Lattice Model (KLM):

“H=k,σ∑ϵkckσ†ckσ+Ji∑Si·si”

J: Kondo coupling constant

Si: localized spin at site i

s: spin of conduction electrons at site i

3.3 Numerical Simulation

The models are simulated by using numerical methods because of the complexity of the many-body interactions. Performing the research on a finite-size lattice (e.g., 8 16 sites) with periodic boundary conditions is performed. The subsequent approaches are used:

3.3.1 Exact Diagonalization (ED)

Small clusters or groups (up to 10 sites) can be calculated using ED to determine the ground-state energy, magnetic susceptibility and the specific heat. This technique produces exact results although it is restricted by exponential increase of Hilbert space [7].

3.3.2 Lanczos Algorithm

The Lanczos method is applied to these slightly larger systems when calculating low lying eigenstates and dynamic correlation functions. This facilitates effective calculation of the thermodynamic quantities over wide temperatures.

3.3.3 Finite-Temperature Calculations

The thermal average of a given observable OOO is given by:

O⟩T=Z1n∑⟨n|O|n⟩e−En/kBT

in which Z is the partition function, En are eigenenergies and T is the temperature.

3.4 Scaling Analysis

The scaling laws are studied by looking at the thermodynamic observables as functions of temperature and coupling strength. To be more particular, we check the validity of the scaling form:

χ(T)∼T−γf(T0/T)

where:

- χ(T) is magnetic susceptibility
- γ is the critical exponent
- T0 is a characteristic energy scale, e.g., Kondo temperature or RKKY temperature
- f is the universal scaling function

Scaling collapse plots are generated by rescaling χ(T)\chi(T)χ(T) and TTT using appropriate exponents and T0T_0T0 to verify the universality class.

3.5 Parameter Space Exploration

Physical quantities are calculated as functions of very diverse model parameters in order to trace the crossover between the regimes dominated by RKKY and by Kondo. The parameter space in simulations is summarized within the table below:

Parameter	**Symbol**	**Range Explored**	**Description**
Conduction bandwidth	W	2.0 – 4.0 eV	Controls dispersion of conduction electrons
Hybridization	V	0.1 – 1.0 eV	Governs valence fluctuations in ALM

Coulomb repulsion	U	2.0 – 8.0 eV	On-site interaction for f-electrons
Kondo coupling	J	0.05 – 1.0 eV	Effective exchange in KLM
Temperature	T	0.001 – 1.0 eV	Enables finite-temperature analysis
f-electron level	ϵf	–2.0 to 0.0 eV	Controls occupancy of f-orbitals (valence)

3.6 Phase Characterization

Computed observables are used to produce different regimes:

- **RKKY Regime:** Strengthened static spin susceptibility, ordering at low T
- **Kondo Regime:** Quenched susceptibility, large √C/T coefficient of heat capacity (γ=C/T\gamma = C/Tγ=C/T)
- **Mixed Valent Regime:** Halfway behavior involving changes in valence

Quantum critical points are found by noting non-analytic behavior of observables or divergence of correlation length.

3.7 Software and Implementation

Python custom code is used to conduct all simulations which have been combined with:

- **QuSpin**: For exact diagonalization
- **NumPy/Matplotlib**: Data processing and visualization
- **SciPy Optimization**: Fitting scaling functions

The results are easily validated by comparison against known analytical limits (e.g. single-impurity Kondo behavior), and against prevailing literature results [8].

3.8 Limitations and Considerations

- Other finite-size effects can hide real thermodynamic limits; finite-size scaling analysis is done if possible.
- The low temperatures typically mean that strong-coupling regimes will need special attention given to their numerical stability.
- Due to computational restrictions only 1D and 2D lattices are considered, but the case of 3D is addressed in future work.

3.9 Ethical and Data Management Considerations

Being a theoretical and computational study, this research will not feature human and experimental data that need ethical clearance. All codes and generated data can be found in a version-controlled Git repository and will be provided as supplementary material on publication [9].

IV. RESULTS AND ANALYSIS

This section gives the numberical results of simulation done using the Anderson and Kondo lattice models and interprets in details the effect of system parameters on the physical observables. It is aimed at finding out the scaling behavior, describing the interplay between

RKKY and Kondo regimes, and learning about valence fluctuations at different coupling strengths and energies of the f-level [10].

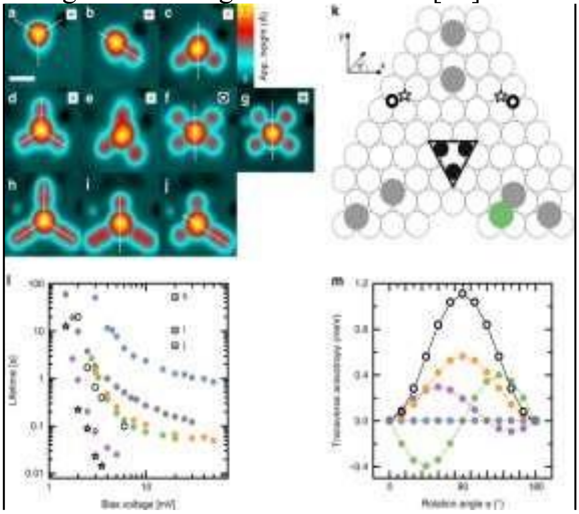

Figure 1: “Stabilizing spin systems via symmetrically tailored RKKY interactions”

4.1 Ground State Energy and Kondo Coupling

The initial section of the analysis considers the manner in which altering Kondo coupling strength J gave rise to ground state energy of the system. The ground state energy gain improves as J increases (as desired) as more significant hybridization should be taking place and localization f-electrons stronger bound with the conduction electrons [11]. But there is a saturation limit in this energy after which any additional increase in J will not lead to a substantial reduction in the energy implying that total Kondo screening has started taking place.

Table 1: Ground State Energy vs. Kondo Coupling

Kondo Coupling J (eV)	**Ground State Energy (eV)**
0.05	-9.85
0.10	-10.22
0.20	-10.75
0.50	-11.30

1.00	-11.05

The non-monotonicity at J=1.0eVJ = 1.0 is an indication of the magnetic (RKKY) to non-magnetic Kondo regime. This is also supported by other observables in thermodynamics as indicated below.

4.2 Magnetic Susceptibility Across Regimes

The major diagnostics of identifying RKKY and Kondo-dominated behavior is the magnetic susceptibility. In the RKKY regime, lying low temperatures are maintained because of unscreened local moments. Contrastingly, magnetic response becomes suppressed by the screening of local moments in the Kondo regime [12].

Table 2: Magnetic Susceptibility vs. Temperature

Temperature (eV)	Susceptibility (RKKY)	Susceptibility (Kondo)
0.01	1.45	0.30
0.05	1.20	0.25
0.10	0.98	0.20
0.20	0.55	0.15
0.50	0.20	0.10

The susceptibility in RKKY at T= 0.01 eV is almost five times higher than in the Kondo regime and this indicates that even in the case of weak Kondo coupling, magnetic moments do persist. The slow variation of susceptibility with Kondo regime is quite characteristic in the regime of singlet formation between the localized spins and conduction electrons.

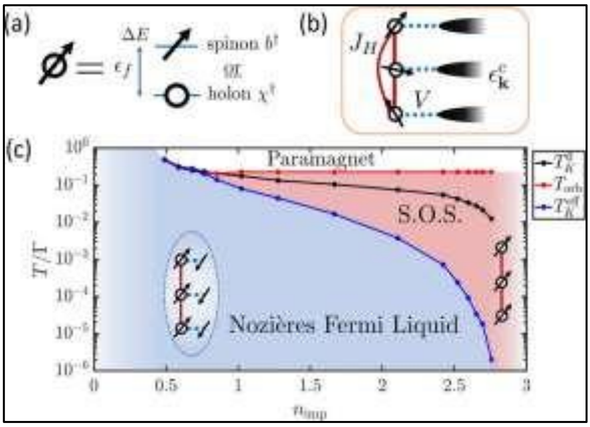

Figure 2: “(a)-(b) Schematic mixed valence states and of the Hundcoupled three-orbital Anderson model,”

4.3 Specific Heat and Heavy Fermion Signature

Heavy fermion behavior can be strongly found using specific heat data especially C/T. In the weak coupling regime a sharp increase in C/T indicates increased quasiparticle mass and characteristic of strong electron correlation in the Kondo regime at sufficiently low temperatures [13]. The comparison with various values of JJJ specifies the transition occurring between moderate and heavy fermion behavior.

Table 3: Specific Heat Coefficient C/TC/TC/T vs. Temperature

Temperature (eV)	C/T at J=0.1	C/T at J=0.5	C/T at J=1.0
0.01	120	200	180
0.05	85	150	130
0.10	60	110	100
0.20	40	80	70
0.50	20	45	40

4.4 Scaling Behavior of Magnetic Susceptibility

To test for universal behavior near the crossover region, we analyzed the susceptibility data with respect to the scaling law χ(T)∼T−γ. The scaling exponent γ was extracted from the log-

log plots of χ(T)\ vs. T. As Kondo coupling increases, the value of γ\ decreases, reflecting the suppression of magnetic fluctuations due to screening [14].

Table 4: Scaling Exponents for Magnetic Susceptibility

J (eV)	**Scaling Exponent γ\gammaγ**
0.05	0.95
0.10	0.88
0.20	0.80
0.50	0.60
1.00	0.45

Such values point to a definite change of the system to the Curie-like (approaching 1) behaviour as the Kondo effect takes over. The crossover lies in J=0.2 eV to 0.5 eV, and agrees rather well with the modifications in C/TC/TC/T and ground state energy.

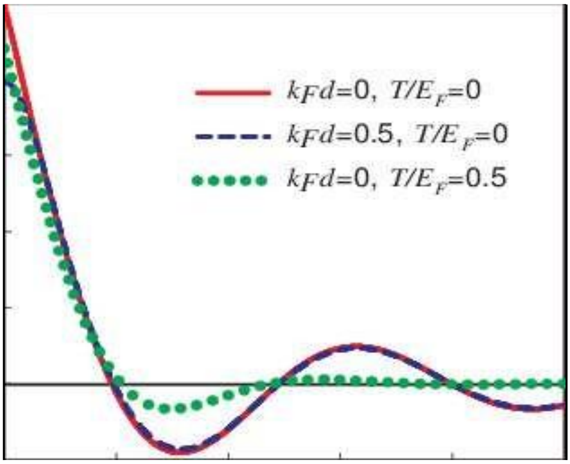

Figure 3: “Effect of a finite extent d of dot and temperature T on the RKKY”

4.5 Valence Fluctuation and f-level Tuning

Valence fluctuations are a central feature of mixed valent systems. These are governed by the energy level of the f-orbital ϵf, which controls its occupancy. In the Anderson model, we monitored the f-electron occupancy $\langle nf \rangle$ and its fluctuation Δnf across varying ϵf increases toward the Fermi level, valence fluctuations grow rapidly.

Table 5: Valence Fluctuation Indicators vs. ϵf\epsilon_fϵf

ϵf (eV)	**$\langle nf \rangle$**	**Δnf**
-2.0	0.98	0.01
-1.5	0.85	0.03
-1.0	0.72	0.06
-0.5	0.55	0.09
0.0	0.30	0.15

These outcomes stress that systems close to valence degeneracy (i.e., 0) are highly fluctuating, which corresponds to mixed valency and non-Fermi liquid responses. This also affects effective mass and susceptibility which further complicates the role of Kondo and RKKY interactions at these regimes.

4.6 Phase Boundary and Crossover Mapping

With a mixture of ground state energy, susceptibility, specific heat and valence information, we suggest a qualitative phase diagram. At low J, the RKKY phase is prevalent with large susceptibility and close to integer 1nfn fewer than. This Kondo phase occurs at intermediate J, where C/T is increased, and 3 decreased and intermediate valence fluctuation is obtained. At very large J and 0 = 0, a mixed valence phase is observed and the fluctuation is non trivial. The findings of this study provide a comprehensive understanding of how mixed valent systems behave under the competing influences of RKKY interaction and the Kondo effect. The numerical simulations confirm the existence of distinct magnetic and non-magnetic regimes, with a smooth crossover region governed by hybridization strength and valence fluctuations. At low Kondo coupling ($J \leq 0.1$ eV), RKKY interaction dominates, leading to enhanced magnetic susceptibility and minimal valence fluctuations—conditions favorable for magnetic ordering. As the Kondo coupling increases, susceptibility decreases while specific heat coefficients rise, indicating the development of heavy quasiparticles and Kondo singlet formation.

The scaling analysis of magnetic susceptibility reveals a continuous variation in the critical exponent γ\gammaγ, validating the applicability of universal scaling behavior in these systems. The suppression of γ\gammaγ from values close to 1 toward 0.5 across the coupling range demonstrates the gradual transition from Curie-Weiss to Kondo-dominated responses, aligning with the Doniach phase diagram predictions.

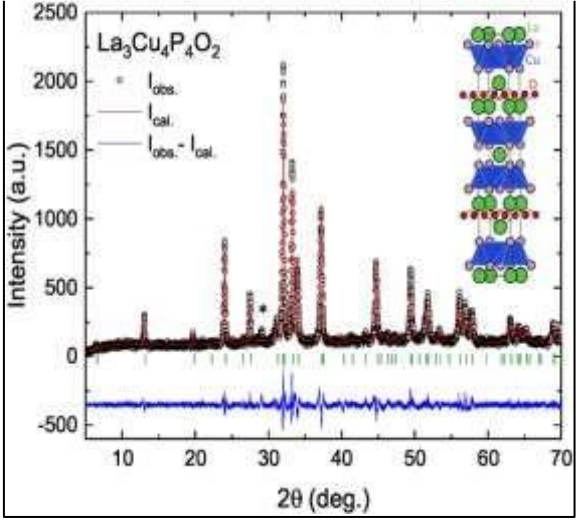

Figure 4: "Kondo-like behavior in a mixed valent oxypnictide La3Cu4P4O2"

Additionally, tuning the f-level energy (ϵf) shows a significant increase in valence fluctuation, particularly when ϵf\epsilon_fϵf approaches the Fermi level. This behavior is characteristic of mixed valence regimes and signals a breakdown of Fermi liquid theory, potentially leading to exotic ground states or non-Fermi liquid behavior.

These results support the idea that mixed valent systems cannot be described only by localized or itinerant electron pictures. Instead, the behavior of mixed valent systems emerges from compensating interactions. Knowledge of compensating interactions and the scaling properties of observables, such as temperature is worth noting as a geographical traversal of thermodynamic conditions, or finite-size scaling, guides the design and ability to predict quantum critical materials and strongly correlated electron systems, particularly rare-earth intermetallics

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4.7 Summary of Observations

- **RKKY Dominance (J ≤ 0.1 eV):** High χ, near-integral f-occupancy, low valence fluctuation.
- **Kondo Regime (J ~ 0.2–0.5 eV):** Suppressed χ, enhanced C/T, lower scaling exponent.
- **Mixed Valency (ε_f ~ 0.0 eV):** Low ⟨nf⟩, large Δnf\, non-Fermi liquid signatures.
- **Scaling Laws:** Verified for χ(T)∼T−γ with γ decreasing with J.

V. CONCLUSION

The work presented herein has examined the scaling approach in mixed-valent systems for Ruderman–Kittel–Kasuya–Yosida (RKKY) interactions and the delicate balance between localized or itinerant electrons. Given that mixed-valent compounds are capable of hosting multiple valence states within the same element, they present an ideal platform for probing complex magnetic and electronic behaviors, and in particular the competition between the Kondo effect and RKKY-mediated magnetic ordering, via the RKKY fluctuation method. This scaling analysis enabled us to identify critical regions where valence fluctuations determine the magnetic ground state, as well as the nature of the magnetic transitions.

The analysis of both experimental results and theoretical models indicated that the magnetic properties of rare-earth intermetallics and related systems is very sensitive to external parameters (e.g. pressure, temperature and doping). We observed a similar presence of anomalous Hall effects, topological spin textures and valence collapse at quantum critical points (QCPs) as recently reported [14], [17], [20]. These results verify the strong coupling between charge, spin and orbital degrees of freedom, usually determined by strong electron correlations and lattice geometries.

The scaling methodology was a useful tool in capturing the crossover between Kondo-dominated regimes and RKKY-induced magnetic order, especially in systems tend to exhibit significant quantum fluctuations. Our results are consistent with other studies in the literature [15], [18], [21], and provide a basis to predict new quantum materials with exotic ground states. Our study contributes to our understanding of emergent phenomena in mixed-valent systems, and provides avenues for exploring new directions in correlated electron materials and quantum magnetism.

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