Computer Simulation of Magnetic Exchange in Disordered Metals

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We investigate the RKKY interaction strength between local magnetic moments placed in a nonmagnetic host metal with disorder. We find that the average interaction strength will decrease to zero as disorder becomes strong. More importantly, we find that the distributions corresponding to different configurations of disorder are strongly dependant on the strength of disorder. These distributions will develop power-law tails, with a small, finite interaction strength. There seems to be universal power-law distribution that describes the interactions in the limit of strong disorder.

I. INTRODUCTION

We examine a system in which local magnetic moments are distributed throughout a nonmagnetic host metal. These moments are known to interact indirectly through the electrons of the host metal in a mechanism called the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. Since the RKKY interactions are long-ranged, they facilitate magnetic ordering, and contribute to the overall magnetic properties of the material.

These materials are commonly used in technological applications, such as diluted magnetic semiconductors. The effect of disorder in these systems is not well documented, especially in the regime of strong disorder. However, it is well known that the introduction of disorder to such a material will alter its electric and magnetic properties; for example, it in limit of strong disorder, electrons in the system will get bound to impurities. This process, known as Anderson localization, changes the properties of the metal to those of an insulator.[1] In order to prevent and overcome issues resulting from disorder in technological applications, we need theory to effectively predict its effects.

We approach this problem by analyzing the distributions of RKKY interaction strength corresponding to different configurations of disorder. In 1987, Jagannathan, Abrahams, and Stephen examined these distributions in the limit of weak disorder.[2] Their results can be obtained by simply assuming that the effect of disorder is to introduce a random phase shift in the susceptibility $\chi(R)$, where:

$$\chi_o(R) = \frac{2mk_F \cos(2k_F R)}{(2\pi)^3 R^3} \tag{1}$$

in the system without disorder. If one uses this assumption– that is, that disorder changes only the phase, and not the amplitude, of $\chi(R)$– then by averaging over all configurations of disorder, one would find that the average value of $\chi(R)$ acquires an exponential damping factor:

$$[\chi(R)]_{av} = \chi_o(R)e^{-R/l} \tag{2}$$

where l is the mean free path. The average interaction strength, therefore, will become negligibly small as disorder increases. However, if we look at the second moment,

$$[\chi^2(R)]_{av} = 3\left(\frac{mk_F}{(2\pi)^3}\right)^2 \frac{1}{R^6} \tag{3}$$

we find that it is independant of the disorder strength. This implies that the typical value of interaction strength will remain the same as disorder increases within the system. However, this is inconsistent with our current theory of metals; it seems that as disorder gets stronger, electrons should get bound to the impurities, and the typical strength of the interactions should become negligibly small. Thus, the idea that disorder introduces only random phase shifts in $\chi(R)$ must be incomplete.

In this paper we use a computer simulation to examine the effects of varying levels of disorder on the distributions of interaction strength.

II. SIMULATING THE SYSTEM

We approach the problem by simulating the clean and disordered systems with a FORTRAN program. The interaction energy between two moments is known to be proportional to their electronic susceptibility, so by calculating the electronic susceptibility as a function of the distance from each moment, we can calculate the interaction strength between the two moments.

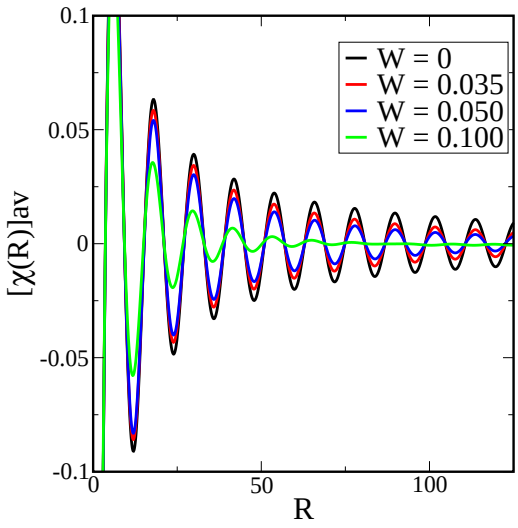

Figure 1: $[\chi(R)]_{av}$ vs R: The average interaction strength is weaker for higher disorder.

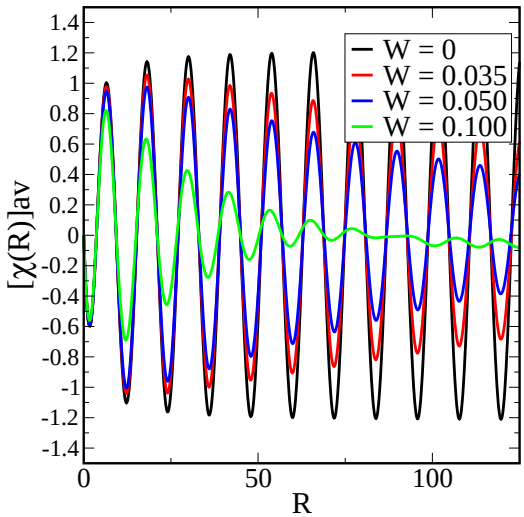

Figure 2: $[\chi(R)]_{av} \cdot R$ vs R: With the 1/R dependance gone, we can see that disorder introduces a damping factor to the average interaction strength.

To begin, we model the material as a finite one dimensional lattice. To reduce any effects that could be caused by approximating the continuous infinite system with a discrete finite system, we choose the number of lattice sites N such that N is as large as possible without being excessively computationally expensive. In our simulation, N = 500, and any possible effects of this finite size are discussed in section IV.

We construct a tight-binding Hamiltonian (TBH) of dimension NxN to represent the lattice system:

$$H = \sum_i |i > \varepsilon_i < i| + \sum_{ij} |i > V_{ij} < j| \tag{4}$$

where ε_i is the site potential at site i, and V_{ij} is the transfer matrix element between sites i and j. We take V_{ij} to be equal to V for i, j nearest neighbors and 0 otherwise. Physically, this represents a lattice system in which each electron is bound to its lattice site, but has a possibility of hopping to its neighboring sites.

We add a chemical potential μ to the diagonal elements of the Hamiltonian matrix. To introduce disorder to the system, we simply add a random value between $-W/2$ and $W/2$ to these potentials. By adjusting the parameter W, we can adjust the level of disorder in the system. The clean system, for example, corresponds to $W = 0$, and to increase the level of disorder, we increase the value of W.

Next, the simulation calculates Green's functions $G(\omega_n)$ for the system:

$$G(\omega_n) = (\omega_n - H)^{-1} \tag{5}$$

where ω_n are the Matsubara frequencies. From this result, the simulation calculates the electronic susceptibility:

$$\chi(r_1, r_2) = \frac{2}{\beta} \sum_{\omega_n} G_{w_n}(r_1, r_2) G_{w_n}(r_2, r_1) \tag{6}$$

where (r_1, r_2) correspond to the matrix elements. Finally, by defining $R = |r_1 - r_2|$, we obtain data for $\chi(R)$, where R is the distance from each moment. Running the simulation hundreds of times provides us with sufficient data to analyze the distributions of susceptibility.

III. THE RKKY INTERACTION IN A DISORDERED METAL

The simulation results for $W = 0$ agree with current theory of RKKY interactions in one-dimensional systems. That is, we find that:

$$\chi(R) \sim \frac{\cos(2k_F R)}{R} \tag{7}$$

The susceptibility in a clean system, then, is an oscillatory function that falls off with distance.

We then calculate the average susceptibility over configurations, $[\chi(R)]_{av}$, and multiply it by R to remove the $1/R$ dependence. Figures 1 and 2 show that the effect of disorder is to cause a decay in $[\chi(R)]_{av} \cdot R$. For weak disorder, we find that this relationship can be expressed as an exponential decay with R, in agreement with Eq. 2. However, since this is a known result, what we are really interested in are the distributions of $\chi(R)$ for varying levels of disorder.

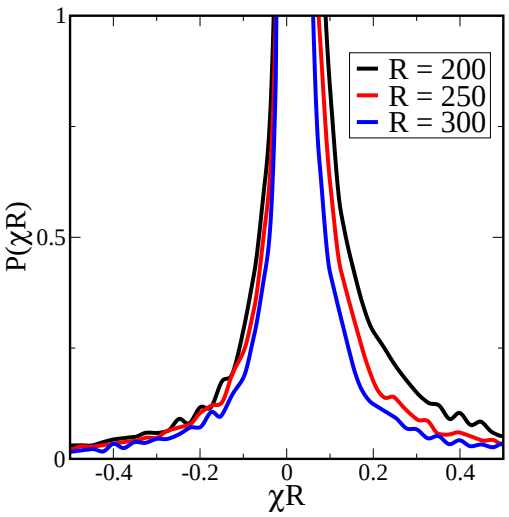

Figure 3: Unscaled $P(\chi \cdot R)$ vs $\chi \cdot R$ for W = 0.350: The width is clearly dependant on R.

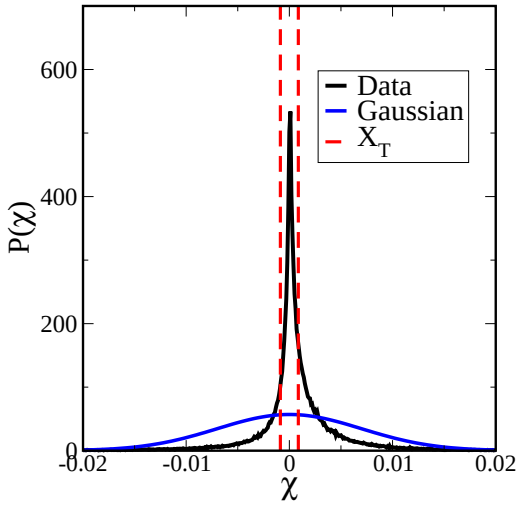

Figure 4: Distribution for $R = 100$, $W = 0.200$. X_T is a better measure of width than the Gaussian.

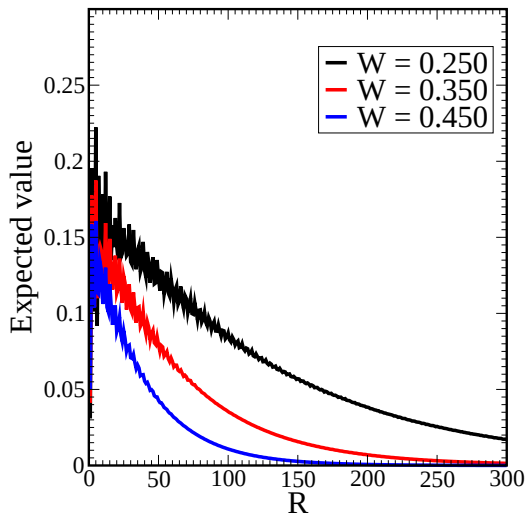

Figure 5: X_T vs R on linear axes: The width of the distributions decrease with increasing R.

Figure 3 shows that within a single level of disorder, the width of the distributions are dependant on R. Cursory examination of the data indicates that the distributions are distinctly non-Gaussian; concrete evidence of this will be provided shortly. This is important for our analysis right now, since the non-Gaussian shape of the distribution prevents us from using the standard deviation as a measure of the width of the distributions. Instead, we use X_T, the typical value of susceptibility, as a measure of the width, and we define it as:

$$X_T(R) \equiv e^{<\frac{1}{2}\ln \chi_i(R)^2>} \tag{8}$$

Here $\chi_i(R)$ refers to the value of each data point, and the notation $<>$ implies an average over all data points. Figures 4 shows a comparison of standard deviation and X_T for describing the width of the same distribution. We can see that the standard deviation is influenced by the long tails, and is far too large to be a useful description of the width. X_T, however, gives a good approximation of the width of the distribution.

Examining X_T for the distributions of $[\chi(R)]_{av} \cdot R$ for different levels of disorder (see Figures 5 and 6), we find that within each level of disorder:

$$X_T(R) \sim e^{-R/\xi} \tag{9}$$

for sufficiently large R, where ξ is the localization length. Therefore, if we define an adjusted susceptibility,

$$\chi_A(R) \equiv \chi_i(R) \cdot R \cdot e^{-R/\xi} \tag{10}$$

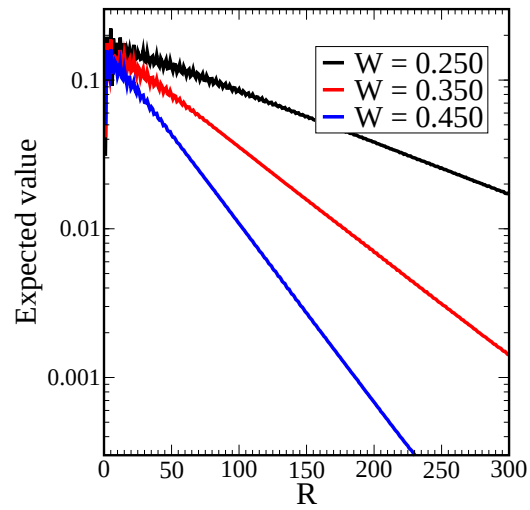

Figure 6: X_T vs R on semilogarithmic axes: Since this plot is linear, X_T must decrease exponentially with R.

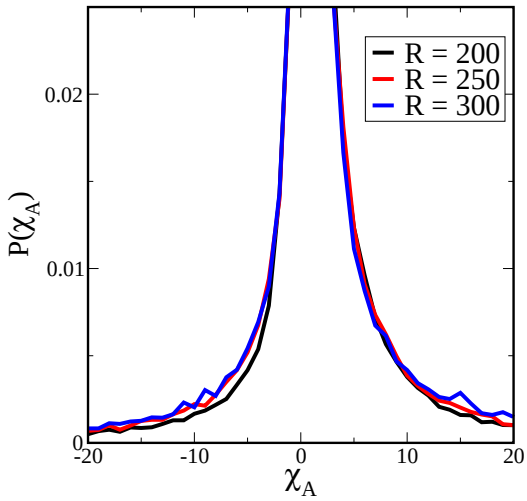

Figure 7: Scaled $P(\chi_A)$ vs χ_A for W = 0.350: After scaling, the histograms collapse.

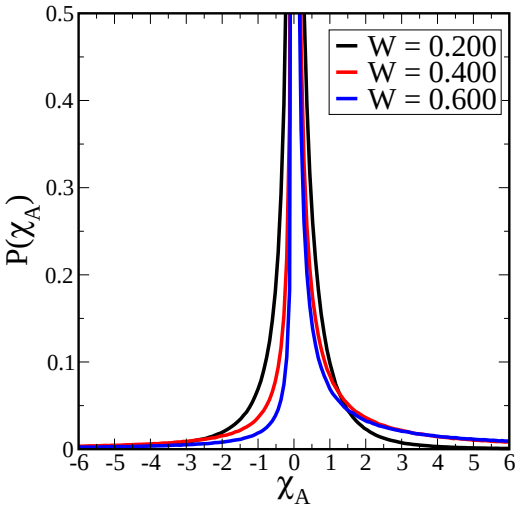

Figure 8: $P(\chi_A)$ vs χ_A for multiple values of W: The distributions are strongly peaked for higher disorder.

the distributions of $\chi_A(R)$ for large R will be entirely independent of R within each level of disorder. Figures 3 and 7 illustrate that the use of this adjusted susceptibility causes these distributions all collapse to describe a single distribution. Since each of these distributions is the same, we can combine the data from them all, and thereby obtain more robust distributions for each level of disorder.

Now each level of disorder has a single characteristic distribution formed by combining all $\chi_A(R)$. as shown in Figure 8. We then plot the tails of the distributions and find that for higher levels of disorder, these tails are linear on log-log axes, as shown in Figure 9. This shows that the tails decay as a power-law for higher disorder, and fall off more rapidly for lower disorder.

The existence of these long tails indicates that the width of the distributions for higher disorder cannot be accurately characterized by their moments. The moments of such a distribution would be extremely large, while the typical value is in fact small. Therefore, when understanding the magnetic properties of such a material, we can consider the long range part of the RKKY interactions to be irrelevant if the material is sufficiently disordered.

Using data from multiple levels of disorder, we calculate the magntiude of the slopes of these tails on the log-log axes α such that:

$$P(\chi_A) \sim \chi_A^{-\alpha} \tag{11}$$

We then plotted α versus W (see Figure 10). α seems to decay asymptotically towards some finite value, suggesting that there is a universal value that describes this distribution in the limit of very high disorder.

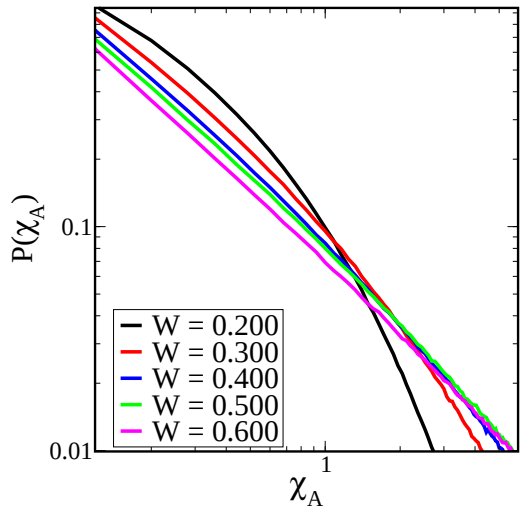

Figure 9: Tails of distributions on log-log axes: For higher disorder, the tails decrease as a power-law.

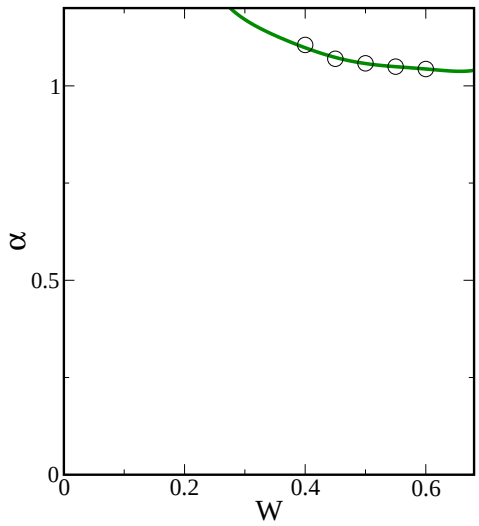

Figure 10: α vs W: α seems to approach a finite value for strong W, suggesting that there is a universal value for this slope in the limit of strong disorder.

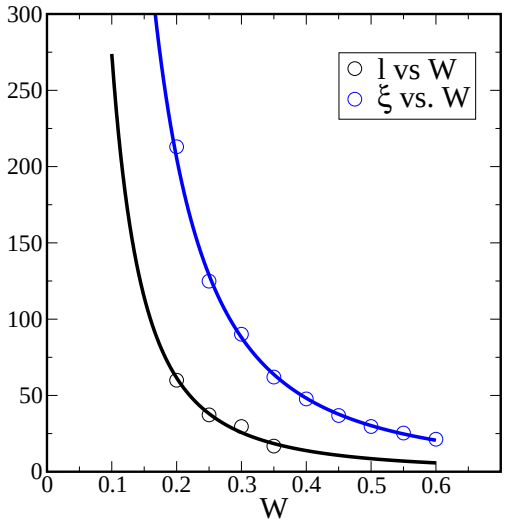

Figure 11: l vs W and ξ vs W: Both the mean free path and the localization length are proportional to W^{-2}.

We also obtained data for l from Eq. 2 and ξ from Eq. 9. Plotting l vs. W and ξ vs. W (see Figure 11), we find that l and ξ are both proportional to W^{-2}, and therefore, l and ξ must be directly proportional to each other. We find that $\xi/l \approx 3.685$, which agrees with the analytical approximation $\xi/l \approx \pi$.

IV. POSSIBLE FINITE-SIZE EFFECTS

We would like to very briefly dispel concern that our results are an artifact of using a finite-size lattice rather than an infinite lattice. If the results are, in fact, influenced by the size of the lattice, then we could simulate the system for increasingly large lattices, and then extrapolate the results for the infinite lattice. This would be extremely computationally demanding, but fortunately, we have sufficient evidence to deem this unnecessary. Performing a simulation on a system size $N = 1000$, which is one hundred perfect larger than our initial system size, we find a negligible change in our results. part of which we can attribute to statistical error. Therefore, we assert that our results are an accurate approximation of the infinite system.

V. CONCLUSION

We have determined that distributions of interaction strength are strongly dependant on the level of disorder in the system. These distributions are distinctly non-Gaussian, with long tails that decay with a power-law. We have evidence that as disorder increases, these distributions will all fall off with the same power-law, suggesting that there is a universal distribution with a small, finite typical value in the limit of strong disorder.

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