On the reliability of recent Monte Carlo studies of dilute systems of localized spins interacting with itinerant carriers

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Abstract. In this paper, we discuss the magnetic properties of dilute systems of localized spins interacting with itinerant carriers. More precisely, we compare recent available Monte Carlo (MC) results with our two-step-approach (TSA) calculations. The TSA depends first on the determination of the magnetic couplings and then on a proper treatment of the resulting effective dilute Heisenberg Hamiltonian. We show an important disagreement between the MC results (in principle exact) and our TSA calculations. We analyze the origins and shed light on the reasons for those dissensions. In contrast to what one could expect, we demonstrate that the available MC calculations suffer from severe numerical shortcomings. More precisely, (i) the finite size effects appear to be huge in dilute systems, (ii) the statistical sampling (disorder configurations) was far too small and (iii) the determination of the Curie temperature was too rough. In addition, we provide new arguments to explain a recent disagreement between the MC simulations and TSA for the model study of the well-known III–V diluted magnetic semiconductor Ga\textsubscript{1−x}Mn\textsubscript{x}As. We hope that this work will motivate new systematic large-scale MC calculations.
1. Introduction

During the last decade, the study of the effects of disorder on the magnetic properties (Curie/ Néel temperatures, magnetic excitations spectrum, spin susceptibility, etc) of disordered/dilute magnetic materials became a central field of research for both theoreticians and experimentalists. It is now clear that, even for a qualitative understanding of the underlying physics, disorder, dilution and thermal fluctuations should be handled in a proper way. Among the widely studied materials one finds manganese oxides as, for example, La$_{1-x}$Sr$_x$MnO$_3$ or La$_{1-x}$Ba$_x$MnO$_3$, which exhibit the fascinating giant magneto-resistance phenomenon [1–4]. The diluted magnetic semiconductors (DMSs) as the well-known III–V compound Ga$_{1-x}$Mn$_x$As [5–8] or the II–VI compound Zn$_{1-x}$Cr$_x$Te [9] have attracted considerable attention. The interest in DMSs is partly motivated by their technological potential for spintronics. One can also mention the so-called d$^0$ materials as the wide band gap oxides HfO$_2$, ZrO$_2$, CaO, ZnO, or the irradiated graphite layers, etc [10–14]. These new materials may become an alternative for spintronic applications. The Heusler alloys, such as Ni$_{2+x}$Mn$_{1-x}$Sn [15, 16], or the double perovskites, such as Sr$_2$FeMoO$_6$ [17, 18], are also materials in which disorder clearly plays a crucial role.

Ab initio-based studies have provided the most efficient and reliable tool to allow a theoretical and quantitative investigation of the magnetic properties without adjusting parameters. As an example, it was possible to study in great detail and quantitatively the magnetic properties of the III–V DMS Ga$_{1-x}$Mn$_x$As, in both the presence and absence of additional compensating defects [19–21]. In order to test the interest in a particular material for technological applications, the $ab$ initio approach provides the most appropriate tool. However, because it is material specific and very complex, it does not allow one to draw general conclusions that could be valid for a whole family of materials. The study of a relevant minimal model is crucial and allows one to fill this gap. The model approach is essential to understand the influence of a particular physical free parameter. It can also help in the determination of potential spintronic candidates. The minimal one-band model that describes itinerant carriers (holes/electrons) interacting with localized moments reads as [39]

$$H = -\sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i p_i S_i \cdot s_i + \sum_{i\sigma} \epsilon_i c_{i\sigma}^\dagger c_{i\sigma}. \quad (1)$$

In the first term, $t_{ij} = t$ if $i$ and $j$ are nearest neighbors, otherwise it is 0. The random variable $p_i$ is one if the site is occupied by a magnetic impurity, otherwise it is 0; we denote
$x$ as the concentration of impurities. $s_i = \frac{1}{2} c_i^\dagger \hat{\sigma}_{ab} c_i^b$, where $\hat{\sigma}$ denotes the Pauli matrix vector $(\sigma_x, \sigma_y, \sigma_z)$. $S_i$ is the localized impurity spin at site $i$. For most of the materials, $S$ is large enough. We consider here the case of classical spins only. Moreover, in ferromagnets, the quantum fluctuations are not relevant. In the case of manganites, $p_i = 1$ (one Mn per site), $J_i$ is the Hund coupling ($J_{H}$) between the itinerant $e_g$ carriers and the localized $t_{2g}$ magnetic moments ($S = 3/2$). In DMSs, $J_i$ is the local p–d coupling ($J_{pd}$). The additional last term describes the effects of the disorder induced by the substitution of a cation by another one. Note that this term includes, in particular, the electrostatic contribution that originates from the difference of charge between the substituted cation and the original one.

In this paper, all the calculations are performed on a simple cubic lattice. We also neglect the last term in equation (1). The case of finite on-site potential will be discussed elsewhere [22]. We expect the more realistic case of a multi-band Hamiltonian to lead to similar conclusions to those that are presented in this paper.

2. The two-step-approach predictions

Reliable calculations require several crucial conditions to be fulfilled. In other words, one should treat (i) the local coupling in a non-perturbative way, (ii) the thermal and transverse spin fluctuations properly and (iii) the disorder and dilution effects exactly (beyond an effective medium approach). The last condition allows for the localization of the itinerant carriers. This will strongly affect both magnetic and transport properties. The full Monte Carlo (MC) method is a priori the best procedure, since localized spins degrees of freedom and itinerant carriers are treated exactly, simultaneously and on equal footings. Note that the word full is added to avoid confusion with the MC treatment of the effective Heisenberg Hamiltonian in the two-step-approach procedure presented below. An alternative approach that fulfils these requirements is the two step approach (TSA) [39]. TSA is in spirit similar to what is widely used in the ab initio-based studies. It consists of two different stages. First, for a given configuration of disorder, at $T = 0$ K, one diagonalizes the Hamiltonian given by equation (1). This provides the spin-resolved one-particle Green’s function of the itinerant carrier (GF) $G_{\sigma i j}(\omega)$ (where $\sigma = \uparrow$ or $\downarrow$). In this first step, the appropriate magnetic texture for localized spins is used. For the ferromagnetism, all localized spins are parallel. Note that the calculations are done without any approximations at $T = 0$ K; thus vertex corrections and the multiple scattering of the carriers on the magnetic impurities are included exactly. From $G_{\sigma i j}(\omega)$, one then calculates the magnetic couplings between the localized moments (integrates out the carriers degrees of freedom). We end up with the disordered/dilute Heisenberg Hamiltonian, which reads

$$H_{\text{Heis}} = -\sum_{i,j} p_i p_j J_{i j} S_i \cdot S_j,$$

where the magnetic couplings are given by the well-known expression [23, 24]

$$J_{i j} = -\frac{1}{4 \pi} \Im \left( \int_{-\infty}^{+\infty} f(\omega) \Delta_i G_{\uparrow i j}(\omega) \Delta_j G_{\downarrow i j}(\omega) d\omega \right),$$

where $f(\omega) = 1/(e^{\beta(\omega - E_F)} + 1)$ ($E_F$ is the Fermi energy). In the present case, $\Delta_i = \Delta_j = J_{pd}$ (exchange splitting). The second step of the TSA consists of diagonalizing reliably the effective disordered Heisenberg Hamiltonian (equation (2)). Note that the diagonalization can be performed either by an MC treatment (as mentioned above) or within the semi-analytical method called self-consistent local RPA (SC-LRPA) [20]. Once again, to avoid
any confusion, we underline and distinguish between the full MC study (no mapping to the Heisenberg Hamiltonian) and the MC that can be used to diagonalize Hamiltonian (2) in the TSA. It is important to recall that the TSA has already been successfully used for the study of various realistic materials. In these studies, the first step of the TSA was provided by \textit{ab initio} calculations (realistic exchange integrals). The agreement between calculated Curie temperatures and experimental data was excellent [21, 25–27]. Concerning the second step, it has also been shown that, for a given set of exchange integrals, the SC-LRPA is as accurate as MC calculations [28–30]. As will be seen in the following, one great advantage of the TSA is the very large system sizes that can be handled, but that are still inaccessible within the full MC method. Thus, in this paper the second step of the TSA is performed within SC-LRPA.

2.1. Results for non-dilute systems

Before discussing the case of dilute magnetic systems, it is important to discuss the non-dilute case, e.g. \( x = 1 \). A comparison between the full MC treatment and the TSA has been done in the limit \( JS = \infty \) (double exchange (DE) limit) [29]. In this case, the nearest-neighbor coupling between localized moments reads \( J_{ij} S^2 = t_{ij} \langle c^\dagger_i c_j \rangle \), the spin index \( \sigma \) is irrelevant in this case, and the fermion operators correspond to the majority spin. The comparison was performed in the presence of Anderson disorder; e.g. the variables \( \epsilon_i \) in equation (1) were chosen randomly in the interval \([ -V/2, V/2] \), where \( V \) denotes the strength of the disorder. Even in the presence of disorder, an excellent agreement between the full MC calculations and the TSA was achieved, and the difference in the Curie temperature was within 10\%. We now show that finite size effects are very small for the non-dilute case. This will explain the agreement found between TSA calculations performed on large systems and full MC simulations done with much smaller clusters. In figure 1, the nearest-neighbor magnetic coupling (\( J_1 \)) between impurities as a function of \( 1/N \) (\( N \) is the number of sites) is plotted. It is clearly observed that \( J_1 \) depends very

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Nearest-neighbor coupling as a function of \( 1/N \) (where \( N \) is the number of sites) for different \( \gamma \) (the hole density is \( p_h = \gamma x \)) in the case of a non-dilute (e.g. \( x = 1 \)) and non-disordered system (\( V = 0 \)), in the DE limit (\( JS = \infty \)).}
\end{figure}
weakly on system size. The finite size effects are negligible at any carrier density ($p_h = \gamma x$). In Figure 2, we have plotted Curie temperature as a function of carrier density per magnetic moment ($\gamma$). We recall that in the clean limit the local SC-RPA reduces to the standard RPA calculation. In the case of classical spins, the Curie temperature is given by $T_C = \frac{2}{3} \left( \frac{1}{N} \sum_{q \neq 0} 1/E(q) \right)^{-1}$, and the magnon excitation dispersion is $E(q) = J_S^2 \left( 1 - \frac{1}{3} (\cos(q_x a) + \cos(q_y a) + \cos(q_z a)) \right)$. We clearly observe that the finite size effects are completely negligible, even for very small systems. For the smallest system ($N = 4^3$), the Curie temperature is already accurate within less than 2%. Thus, in the case of clean systems and in the DE regime ($J_S = \infty$), the finite size effects are indeed completely negligible. Similar conclusions have been reached in the case where the on-site disorder ($V \neq 0$ in the previous Hamiltonian) is also included [22]. We have even obtained that the average over only a few configurations of disorder is enough to provide an accurate value. Thus, one can understand the success of the full MC simulations to provide accurate Curie temperatures for the study of the non-dilute DE model, even though in these studies the system sizes are typically of the order of $N \approx 5^3$ sites. The restriction to such small clusters is in fact due to the very large CPU time and memory costs of the standard full MC simulations.

However, as will be seen in the following subsection, for dilute systems, the use of too small system sizes and too weak statistical sampling affects the results in a dramatic way.

2.2. Results for dilute systems

For simplicity and to allow a direct comparison with the available full MC data, we set the impurity concentration as $x = 0.065$. We will vary both the amplitude of $J$ (its sign is irrelevant for classical spins) and the carrier density. Figure 3 shows the DOS for various couplings $J_S$. We observe that the impurity band (IB) splits from the valence band for values of $J_S \gtrsim W$. In the strong coupling regime, $J_S = 2W$, the IB is completely separated from the valence band, and the magnetic couplings are expected to be dominated by the DE mechanism. Figure 4 shows the couplings as a function of impurity distance for two different carrier concentrations.
Figure 3. Spin-resolved density of states for a fixed concentration of magnetic impurities $x = 0.065$ and different values of the local coupling $J_S$. The spin down (respectively, up) band is represented by the continuous (respectively, dotted) line. Energies are in units of the bandwidth $W = 12t$.

and different values of $J_S$. Note that the calculations were performed on a sufficiently large cluster ($N = 20^3$) to neglect the finite size effects. The discussion of the finite size effects will be done in a forthcoming paragraph. First, we observe in figure 4 that the couplings are all ferromagnetic and of relatively short range. For $x = 0.065$, the typical average distance between magnetic impurities is $\bar{d} \approx 2.4a$. It corresponds to the distance between impurities on the ordered underlying super-lattice. For the smallest values of $J_S$, the couplings are small at any distance, and this should lead to very small Curie temperatures. As $J_S$ is increased, the nearest-neighbor coupling increases strongly until it saturates, while the range of the couplings decreases (clearly seen in the insets). For very large $J_S$ ($J_S \gg W$), the couplings are essentially reduced to the nearest-neighbor coupling only, as expected in the DE limit. The limiting value is expected to be independent of carrier density and corresponds roughly to the kinetic energy of a single hole hopping between two sites. Note that there are also some additional contributions coming from one hole localized on three sites, two holes on three sites, and so on. One can already say that, in the large $J_S$ limit, the Curie temperature is expected to vanish since the average distance between impurities is larger than the range of the couplings. In other words, the system is below the percolation threshold. For $J_S \approx 2W$ (see DOS in figure 1), the couplings at distances near $\bar{d}$ are tiny; thus one expects very small Curie temperatures.

In figure 5, we have plotted the Curie temperature as a function of $J_S$. The carrier density is the same as used in figure 4. We again recall that the MC treatment of this Hamiltonian would
lead to similar results, as has already been shown in several publications [19, 28]. For both values of $\gamma$, we observe that $T_C$ increases until it reaches a maximum; it then decreases until it vanishes beyond a critical value, which depends on the magnetic impurity concentration. Note that the maximum is located at $JS \approx 0.5$ for $\gamma = 0.125$ and at $JS \approx 0.6$ for $\gamma = 0.25$. The highest $T_C$ values are, respectively, $T_C^{\text{max}}(\gamma = 0.125) \approx 3 \times 10^{-4}$ W and $T_C^{\text{max}}(\gamma = 0.25) \approx 5 \times 10^{-4}$ W. For small values of $J$ (perturbative limit), one notices that, within SC-LRPA, $T_C \propto J^2$, as expected from equation (3). In figure 6, we evaluate the role of disorder and the importance of thermal fluctuations. For that purpose, we compare $T_C$ calculated within SC-LRPA to the mean field virtual crystal approximation (MF-VCA) value. We recall that the MF-VCA value is $T_C^{\text{MF-VCA}} = \frac{2}{3}x \sum_{i \neq 0} J_{ii}$. Within this approximation, both thermal and transverse fluctuations and disorder are treated at the lowest order. In fact, the disorder (dilution) is neglected and just appears as a trivial prefactor ($x$) in the expression of $T_C$. In the limit of very small $J$ (inset of figure 6), we
Figure 5. Curie temperature within SC-LRPA (in units of the bandwidth $W = 12t$) as a function of $JS/W$. The magnetic impurity concentration is fixed at $x = 0.065$. The hole concentration per impurity is (a) $\gamma = 0.125$ and (b) $\gamma = 0.25$. The insets represent the MC calculations from [31] done for a two-band model ($N_b = 2$) in which (a) $\gamma = 0.5$ and (b) $\gamma = 0.25$.

observe a good agreement between SC-LRPA and MF-VCA. Within the perturbative limit, and for relatively weak densities of carriers only, one could indeed expect such a behavior (similar results are observed for $\gamma = 0.25$ of figure 5(a)). As we increase $JS$, we observe important quantitative and qualitative differences, as $T_C^{MF-VCA} \gg T_C^{SC-LRPA}$.

Let us now show that $T_C$ is in fact mainly controlled by the typical coupling, namely $J(\bar{d})$, where $\bar{d}$ was defined previously. For $x = 0.065$, we recall that the average distance between impurities is $d = \bar{d} \approx 2.4a$. In figure 7, we have plotted the variation of this coupling as a function of $JS/W$. We clearly see that the shape of the calculated curve is very similar to that obtained in figure 5(a). We find that the ratio $R = T_C/J(\bar{d})S^2$ is almost independent of $JS$ and $R \approx 4$. On the other hand, the non-monotonic behavior of $J(\bar{d})$ is qualitatively different from the monotonic increase in $J_1$, as seen in the inset. The limiting value of $J_1$ (for $JS \to \infty$) is
Figure 6. MF-VCA and full SC-LRPA calculations of the Curie temperature as a function of $J S$. The magnetic impurity concentration is $x = 0.065$ and the density of the hole per carrier is $\gamma = p_h/x = 0.125$.

Figure 7. $J (\bar{d}) S^2$ in units of $t$ as a function of the local coupling, $J S/W$. The density of holes is fixed and set to $p_h = 0.125x$. In the inset, we have plotted the nearest-neighbor coupling, $J_1 S^2$, as a function of $J S/W$.

expected to be close to that of the clean system as plotted in figure 1. For large $J S$, $J_1$ dominates and leads to unrealistic MF-VCA critical temperatures (see figure 6).

3. Comparison with available full MC calculations

In this section, we propose comparing our results with recent full MC simulation results available in the literature. We see that the quoted full MC results are questionable because they have severe numerical shortcomings. To our knowledge, the only available full MC study of the diluted Hamiltonian given by equation (1) was performed by Popescu et al [31]; no other group has performed similar studies in the dilute regime. In the full MC simulations,
Popescu et al also consider the particular case of two identical independent bands filled with a density of holes $p$. Hence, in this case, the relation between the couplings in two bands and the one-band model is $J_{ij}^{2\text{bands}}(p) = 2J_{ij}^{1\text{band}}(p/2)$. Then for the Curie temperatures one obtains $T_{C}^{2\text{bands}}(p) = 2T_{C}^{1\text{band}}(p/2)$. Thus both $T_{C}$ and the hole density used in their simulations are divided by two for comparison with our single-band calculations. The MC data of Popescu et al [31] are shown in the insets of both figures 5(a) and (b). The MC critical temperatures were obtained for systems with $N = 5^3$ to $6^3$ sites, and the average disorder was performed over seven configurations of disorder only. Let us note that a system of size $N = 5^3$ (respectively, $6^3$) contains only eight (respectively, 14) magnetic impurities; thus for a density of carriers per impurity $\gamma = 0.25$, such small systems respectively contain only 2 and 3 holes in the whole cluster. As seen in figure 5, several crucial differences appear immediately with respect to our results. First, we notice that for both carrier densities ($\gamma = 0.125$ and 0.25) the MC simulations predict critical $T_{C}$ much higher than those obtained within the two-step approach. Indeed, if one refers, for example, to figure 5(a), one observes that the MC values are 15–60 times larger! In particular, the highest $T_{C}$ values are typically at least 20 times larger than our results. For small values of $J S$, one notices that SC-LRPA and the MC simulations do not predict the same behavior (quadratic in $J$ in our case).

For large $J S$, while our calculated $T_{C}$ is strongly suppressed and vanishes for values of $J S \geq J_{c} S$, where $J_{c} S \approx 2 W$, the MC value decreases much more slowly and seems to saturate at large $J S$ (see figure 5(a)). For example, for $\gamma = 0.125$ and $J S = 1.2 W$ (or $p_{h} = 0.25$ for the two-band MC calculations), $T_{C}^{MC}/N_{b} = 3 \times 10^{-3} W$, while we find $T_{C}^{LRPA} = 7.5 \times 10^{-5} W$; thus the ratio $T_{C}^{MC}/T_{C}^{LRPA} = 40$, which is huge! Additionally, there is another unexpected and surprising result. The MF-VCA Curie temperature that should, in principle, be an upper bound is in fact smaller than the MC value. This is in conflict with the opposite and natural expectation. We recall that the MC method treats both disorder effects and thermal fluctuations exactly. For example, from figure 6 and for $J S = 0.4 W$, we find that $T_{C}^{MF-VCA} = 4 \times 10^{-4} W$ and $T_{C}^{MC} = 50 \times 10^{-4} W$. Additionally, it has already been shown several times in the literature, especially for the study of DMSs, that $T_{C}^{MF-VCA}$ largely overestimates the real Curie temperature, and this clearly puts a question mark on the validity of the full MC results.

On the basis of what was previously discussed, we now address the reasons that may explain the huge differences with TSA and why the MF-VCA becomes a lower bound with respect to the full MC results. To be more specific, it will be shown that the available MC results suffer from several combined effects: (i) strong finite size effects, (ii) an insufficient sampling (too few disorder configurations) and (iii) an inaccurate and approximative procedure for the determination of the Curie temperature.

4. Origins of the dissensions between TSA and MC simulations

In this section, we discuss both the importance of statistical sampling and finite size effects. In figures 8(a) and (b) ($\gamma = 0.25$ and 0.125), we have plotted the variation of $J_{ij} S^2$ as a function of the distance between impurities, for different system sizes ($N = L^3$, where $L$ varies from 4 to 16). We observe that the couplings are larger for the smallest systems and that finite size effects are especially strong at distances near the typical and relevant one, $d$. Thus, we already expect the Curie temperature to be strongly size dependent. In figure 9, the average Curie temperature as a function of $J S/W$ is shown for various sizes. The hole density (per carrier) is set to $\gamma = 0.125$. Note that each averaged $T_{C}$ is obtained using the associated
Figure 8. Magnetic couplings $J_{ij}(r)S^2$ in units of $t$ as a function of the distance between impurities $r/a$. The magnetic impurity concentration is fixed at $x = 0.065$, $JS = 5t$ and (a) $\gamma = 0.125$ and (b) $\gamma = 0.25$. The calculations are performed with clusters of size $N = L^3$, where $L = 4$, 8, 10, 12, 14 and 16.

couplings, e.g. calculated for the corresponding system. Note also that the average was properly performed, and we have used a sufficiently large number of disorder configurations (a few thousand for the smallest systems and a few hundred for the largest). We now analyze the importance of statistical sampling. For a given value of $JS$, we observe beyond $N = 14^3$ an insignificant variation in the averaged Curie temperature: beyond this size the thermodynamic limit is properly described. Because within the standard full MC method the systems are usually restricted to relatively small sizes [31–35], of the order of $N = 4^3$, let us perform the comparison between the calculations done with the smallest and largest systems. For instance, we consider $JS = 0.7$ W. We see that the Curie temperature for $L = 5$ is $T_C = 10.5 \times 10^{-4}$ W, while in the thermodynamic limit $T_C = 2.0 \times 10^{-4}$ W (500% difference!).

We now show that the sampling over disorder is also crucial and should be done properly, especially in dilute systems. Note, for instance, that Franceschetti et al [36], in their
Figure 9. Averaged Curie temperature (in units of the bandwidth $W$) as a function of the parameter $JS/W$. The magnetic impurity concentration is fixed at $x = 0.065$. The hole concentration per impurity is $\gamma = 0.125$. The calculations are carried out with clusters of size $N = L^3$, where $L = 5, 6, 12, 16$ and $20$. A systematic average over a few thousand configurations has been done for the smaller systems and a few hundred for the largest.

$ab\ initio$-based study, have shown important fluctuations in the Curie temperature from sample to sample. In figure 10, we have plotted the distribution of the Curie temperatures obtained using different system sizes. To facilitate the discussion, we have plotted in figure 11 the averaged Curie temperatures, $\overline{T_C} = \int_{-\infty}^{+\infty} T_C P_L(T_C) dT_C$, and the widths at mid height of the distributions ($\Delta T_C/W$) as a function of $1/N$. For the smallest system ($N = 4^3$), one observes a very important spreading of the critical temperatures distribution; they can vary from at least one order of magnitude! From figure 11, for this case, $\Delta T_C/W$ is rather close to the corresponding average value. For these small systems, one understands easily that 10 configurations of disorder are definitely insufficient to provide a reliable average. In other words, the calculated averaged Curie temperature over a small number of configurations (a few tens) could easily lead to critical temperatures 10–20 times larger than that calculated properly (averaged over a few thousand configurations). This implies, for example, that the Curie temperatures shown in figure 9 could easily be 50 times larger than those calculated in the thermodynamic limit if the average had been taken over only a few configurations.

As the system size increases, one gradually observes a decrease in $\Delta T_C$, which then rapidly tends to zero (thermodynamic limit), while $\overline{T_C}$ tends towards a constant value (see figure 11). One can already consider that the thermodynamic limit value of $T_C$ is reached for $L \geq 16$. In the light of the results presented in this paper, a criterion to obtain reasonable results would consist in considering system sizes where $L$ is at least five to six times larger than the typical distance between impurities. This criterion is only rough; in the case of long-range magnetic couplings, such as RKKY exchanges, the finite size effects can be even more drastic. In addition, only ten configurations of disorder for small systems are definitely insufficient to get the average value of $T_C$ in a reliable manner. It is obvious that these numerical requirements are very difficult to fulfill within standard MC calculations, but they are definitely essential.
Figure 10. Distribution of the calculated Curie temperatures (the $x$-axis is $T_C$ in units of $W$) for different system sizes $N = L^3$, where $L$ varies from 4 to 20. The parameters are $x = 0.065$, $V = 0$, $\gamma = 0.25$ and $JS = 0.5W$.

Figure 11. Width ($\Delta T_C$) and average ($\bar{T}_C$) of the Curie temperatures distribution calculated for various simple cubic lattices of size $N = L^3$ as a function of $1/N$. The parameters are the same as those of figure 10.
In addition, in the presence of inhomogeneities, temperatures are also expected to be even more sensitive to both finite size effects and statistical sampling [37]. Moreover, the way of extracting the Curie temperature is essential. Within SC-LRPA, the problem does not arise. The critical temperatures are directly given by a semi-analytical equation solved in a self-consistent way, and no extrapolation from the magnetization curve is used. Concerning the MC simulations of Popescu et al [31], the method used to extract $T_C$ from the magnetization curve is not very accurate (see figures 4(a) and (b) of [31]). Potential errors related to this method are added to the uncertainties coming from both finite size effects and the insufficiency of statistical sampling. A more accurate way of obtaining the Curie temperatures in MC simulations is based on the method of Binder cumulants [38], but this method represents an additional cost in terms of computing time since it needs a finite size effect analysis. Unfortunately, in spite of the small system sizes and the small number of configurations of disorder considered in [31], the MC simulations already need a huge resource in terms of CPU time and memory.

In a recent paper based on MC simulations, Yildirim et al studied the diluted Kondo model applied to the case of Ga$_{1-x}$Mn$_x$As by including the realistic band structure of the host material [33] (see also [40] for a comment). They calculated the Curie temperature as a function of the local coupling $J$ for systems containing $x = 8.5\%$ of magnetic impurities and $p_h = 0.75$ hole per impurity. We underline here that their numerical MC approach suffers from the same numerical shortcomings as those previously discussed. The system considered in this letter contains typically 20 localized spins only and the average is calculated using just five configurations of disorder. Additionally, the value of $J$ considered in [33] corresponds to the perturbative regime. Thus, on the basis of the present study, we argue that within this limit the couplings should exhibit RKKY oscillations, which should lead in the thermodynamic limit to small Curie temperatures or eventually to no ferromagnetic phase [41]. Unfortunately, and as previously noticed, the smallness of the cluster considered in the MC calculations hides the effects of the asymptotic RKKY tail, thus leading to finite and large Curie temperatures. We argue that by improving the statistics and increasing the size of the systems, the Curie temperature should vanish when the frustration becomes effective. Furthermore, we argue that the large MC critical temperatures found in the large $JS$ regime (see figure 1 of [33]) are in fact a numerical artifact due again to the insufficient statistical sampling and finite size effects. Indeed, in this regime the DE mechanism dominates, and thus very small or vanishing Curie temperatures are expected; see the corresponding densities of states in figure 4 of [33], where the IB is separated from the valence band.

5. Conclusion

To conclude, in this work we have shown that the study of the diluted magnetic systems requires a rigorous numerical treatment. We have shed light on the origins of the disagreements between MC and TSA for the study of diluted magnetic systems. In contrast to the non-dilute systems, the finite size effects as well as the importance of the statistical sampling appear to be crucial. We have shown that available MC simulations for the diluted model Hamiltonian (1) suffer from severe numerical insufficiencies. MC simulations are in principle exact. However, because the calculations are unfortunately restricted to relatively small systems and weak statistical sampling, the obtained Curie temperatures are often largely overestimated. In addition, limiting regimes (strong and weak couplings) are not properly described. It would be of great interest to check both the importance of statistical sampling and the finite size effects...
within new large-scale MC studies. Among MC simulations that allow one to reach relatively large system sizes, one can quote the hybrid Monte Carlo (HMC) method [42], the polynomial expansion Monte Carlo (PEMC) method [43] or its fastest counterpart, namely the truncated polynomial expansion Monte Carlo (TPEMC) method [44–46]. In particular, TPEMC handles higher systems up to $20^3$ sites within a reasonable CPU time (see table II of [45]).

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