Dear SciPost Editor,

We thank you for forwarding the referee reports on our manuscript entitled "A Large-N Approach to Magnetic Impurities in Superconductors."

We are resubmitting a revised version of the manuscript with minor modifications, as suggested by the referees. We appreciate the positive feedback and constructive criticisms from both reviewers. Below we have addressed the points raised by them.

Given the ongoing effort in the Physics community to achieve a deeper understanding of the quantum phases of magnetic impurities in superconductors, we believe our paper is both timely and relevant to the field. We kindly ask that you consider it for publication in *SciPost.*

Sincerely,

Chen-How Huang, Alejandro M. Lobos, and Miguel A. Cazalilla

Reply to Report #1 by Anonymous (Referee 2)

We thank the referee for his/her time and effort in reviewing our manuscript. We also appreciate the positive feedback on our work and the suggestion to publish it in *SciPost*.

Regarding the referee's comment on the comparison between large-N and NRG calculations:

"The only point I find a bit obscure is the choice of the bandwidth for the comparison between the large-N and NRG calculations. As indicated in Eq. (25), the authors require that the density of states at the Fermi level, ρ0, should be the same in both calculations, i.e., ρ0= \frac{1}{\pi t} = \frac{1}{2D}, where t is the hopping element in the effective TB model and D is the NRG bandwidth. Thus, I would have expected that for the comparison, they choose a ratio D/t such that ρ0Δ is the same in both calculations. However, taking the values indicated in Fig. 4(a), I find ρ0/Δ=0.0005 in the NRG calculation, and ρ0/Δ=0.005/π for the large-N one. There may be some misunderstanding on my part, but in any case, it would be useful if the authors could clarify this issue in their manuscript."

We thank the referee for pointing out this apparent discrepancy. Indeed, the product of the density of states at the Fermi energy, $\rho_0 \sim 1/D$ (where D is the host bandwidth), and the superconducting gap, Δ, characterizes the superconducting host but it does not contain information about the impurity. The properties of the combined system of superconductor and impurity are scaling functions depending of the ratio of two characteristic energy scales, one being the superconducting gap of the clean superconductor Δ, and the other the Kondo temperature of the impurity in the normal state T_K. For instance, in the weak coupling limit (which is not the focus of our manuscript), the latter is well approximated by the well-known expression:

$T_K=D*\exp(-1/J*\rho_0)$

where J is the exchange coupling of the impurity with the host. In general, for $T_K \ll D$, the Kondo temperature is a function of the dimensionless product $\rho_0 * J$. Thus, in our comparison of the large-N and NRG results, the chains used for the two approaches must have the same density of states at the Fermi energy in the normal state. In the large-N method, it is more convenient to use a tight-binding model with constant hoping amplitude t resulting in a density of states given by the circle law. However, for NRG it is more convenient to use for a Wilson chain with exponentially decreasing hopping amplitude that approximates a band with constant density of states in the normal case. Assuming scaling in the parameter of Δ/T_K, we have compared the spectral properties of the impurity shown in Figs. 4a and 4b as well as Fig. 5 for the same values of the ratio Δ/T_K.

Regarding the existence of scaling, we are grateful that the referee has brought up to our attention the paper by Huang et al (Nat. Comm.), where an instance of what has been explained above is shown in their Fig. 4b. Indeed, the latter shows the scaling of the experimentally measured YSR energy with T_K/Δ. Some small deviations from the scaling are observed, which may be due to the fact that real impurities are not described by the Kondo model but by an Anderson model which is characterized by more parameters than just J or T_K. This does not apply to our calculations which have been carried out for the Kondo model for which we expect the universal scaling to be accurate. In passing, we also mention another study where some of the present authors recently found another instance where the universal scaling in terms of Δ/T_K appears when studying the YSR states induced by magnetic impurities in spin-split superconductors, see C. H. Huang et al, Phys. Rev. Res. 6, 033022 (2024).

In the revised manuscript, we have included an extended explanation of our parameter choices along the above lines together with a citation to the work of Huang et al. and to Phys. Rev. Res. 6, 033022 (2024), as examples of the universal scaling upon which were rely. See paragraph highlighted in red leading to Eq. 25, on page 5 of the revised manuscript (since it is not possible to upload the revised manuscript, we have included an snapshot of this page below).

$$\mathcal{G}_{ff}(i\nu_n) = -\int_0^\beta d\tau\, e^{i\nu_n\tau}\, \langle T_\tau f_\alpha(\tau) f_\alpha^\dagger(0)\rangle,$$
$$= \frac{1}{i\nu_n - \lambda_0 - V^2 \mathcal{G}_{cc}^{(0)}(i\nu_n)}. \quad (23)$$

Here T_τ is the imaginary-time ordering operator, and $\mathcal{G}_{cc}^{(0)}(z)$ is the Green's function of the clean insulator at site $j = 0$, whose expression for the semi-infinite one-dimensional tight-binding chain can be analytically obtained, e.g. using the recursion method [43]:

$$\mathcal{G}_{cc}^{(0)}(z) = \frac{z+\Delta}{2t^2} \pm \sqrt{\left(\frac{z+\Delta}{2t^2}\right)^2 - \frac{1}{t^2}\frac{z+\Delta}{z-\Delta}}, \quad (24)$$

where the sign must be chosen such that for $\mathrm{Im}[z] > 0$, $\mathrm{Im}\left[\mathcal{G}_{cc}^{(0)}(z)\right] < 0$. In the above expression, employing the the $\mathrm{SU}(N)$ symmetry, we have dropped the index α.

In order to compare the large-N and the NRG approaches, we assume that the properties of the impurity in the (superconducting) host are scaling functions of a single parameter, namely the ratio of gap Δ to the Kondo temperature, T_K (this scaling assumption has been verified both experimentally and theoretically, see e.g. Refs. [44, 45] and references therein). The former is an energy scale that characterizes the host in the absence of magnetic impurities, whilst the later characterizes the impurity in the normal state of the host (i.e. for $\Delta = 0$, see discussion in Sec. III A for more details about its definition). Since for $T_K \ll D$ the Kondo temperature depends on the the dimensionless coupling $\rho_0 J$, where ρ_0 is density of states of the host at the Fermi energy for $\Delta = 0$ and J the exchange coupling, we choose ρ_0 to the same in both approaches. Thus, recalling that the constant density of states used in NRG is $\rho_0 = 1/2D$ (with D the band width used in the NRG calculations), we require:

$$-\frac{1}{\pi}\mathrm{Im}\left[\mathcal{G}_{cc}^{(0)}\left(z \to \omega^+, \Delta = 0\right)\right]_{\omega=0} = \frac{1}{\pi t} = \frac{1}{2D}, \quad (25)$$

where $\omega^+ = \omega + i0^+$ (0^+ denoting a positive infinitesimal).

For illustration purposes, in Fig. 1 we show the unperturbed local density of states (LDOS) at site $j = 0$ in the chain, $\rho_c^{(0)}(\omega) = -\frac{1}{\pi}\mathrm{Im}\left[\mathcal{G}_{cc}^{(0)}(\omega^+)\right]$, both in the normal case $\Delta = 0$ (black dashed line) and superconducting case $\Delta > 0$ (continuous red line). In this latter case, we can see the presence of a gap 2Δ in the single-particle excitation spectrum. We note the asymmetry of the plot in the case $\Delta > 0$, due to the breaking of the particle-hole symmetry by the staggered potential in Eq. (11). As mentioned in the preceding section, the particle-hole symmetry of the original model can be restored undoing the transformation in Eqs. (7)-(10), and expressing the LDOS in terms of the original $d-$fermions.

Using Eq. (22), the extrema equations (18) and (19) become,

$$\frac{\partial \Delta F_{\mathrm{MF}}}{\partial V} = V\left[\frac{1}{J} + \frac{1}{\beta}\sum_{i\nu_n} \mathcal{G}_{ff}(i\nu_n)\,\mathcal{G}_{cc}^{(0)}(i\nu_n)\right] = 0, \quad (26)$$

$$\frac{\partial \Delta F_{\mathrm{MF}}}{\partial \lambda} = -q + \frac{1}{\beta}\sum_{i\nu_n} \mathcal{G}_{ff}(i\nu_n) = 0. \quad (27)$$

Note that $V = 0$ and $\lambda = 0$ always correspond to extrema, which describes a decoupled f-level from the host, or in the language of the original model, an unscreened impurity [1, 2]. At $T = 0$, the Matsubara sums above

Reply to Report #2 by Anonymous (Referee 1)

We thank the referee for her/his time and effort in reviewing our manuscript, as well as for the positive feedback and the suggestion to publish it in *SciPost*.

Regarding the main point raised by the referee, we would like to clarify that the primary goal of this work (which we hope is the first in a series) is to describe the method, benchmark its performance, and discuss its limitations, all in great detail. This alone has resulted in a manuscript of considerable length. We intentionally avoided introducing applications at this stage to maintain focus on the technical details and benchmarking of the results for the well-understood single-impurity problem. We believe that including applications would divert the attention from the core purpose as well as resulting in an extremely long manuscript.

We intend to explore applications in future works, especially for systems for which benchmarking using NRG or other numerically exact methods is not possible. Thus we believe this manuscript should serve as the main reference for the method itself.

As for the issue of the requirement of particle-hole symmetry, we acknowledge that it is a limitation of the method, as we already mentioned in the last paragraph of Sec. IV (Conclusions section, “One major limitation…”). However, we believe there is still a sufficiently broad class of models for which our method can provide useful physical insights. In this regard, it is worth comparing this limitation to the neglection of quantum fluctuations in the classical approach of Yu, Shiba, and Rusinov. Even If it is not obvious that one can neglect fluctuations, the classical approach has been widely and uncritically used to study many different models of impurities in superconductors. It took many years until the accuracy of the method was benchmarked using NRG and the conditions for its applicability were established (not only large impurity spin S, but also a large in magnitude and negative single-ion anisotropy, see R. Zitko, Physica B (2018) 536, 230-234). In our large-N approach, the benchmarking has been carried out in the present study and we hope that it can be widely applied with much more confidence despite being limited to systems with particle-hole symmetry.