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Disorder effect on the spin susceptibility of the two-dimensional one-valley electron gas

S De Palo[1,2], **S Moroni**[1,3] **and G Senatore**[1,2]

[1] INFM DEMOCRITOS National Simulation Center, Trieste, Italy
[2] Dipartimento di Fisica Teorica, Università di Trieste, Strada Costiera 11, 34014 Trieste, Italy
[3] SISSA, International School for Advanced Studies, via Beirut 2-4, 34014 Trieste, Italy

E-mail: depalo@democritos.sissa.it

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Abstract
Starting from the quantum Monte Carlo (QMC) prediction for the ground-state energy of a clean two-dimensional one-valley (2D1V) electron gas, we estimate the energy correction due to scattering sources present in actual devices such as AlAs quantum wells and GaAs heterostructures. We find that the effect of uncorrelated disorder, in the lowest (second) order in perturbation theory, is to enhance the spin susceptibility leading to its eventual divergence. In the density region where the Born approximation is able to reproduce the experimental mobility, the prediction for the spin susceptibility yielded by perturbation theory is in very good agreement with the available experimental evidence.

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1. Introduction

The two-dimensional electron gas that can be realized in quantum wells or at the interface of semiconducting heterostructures has attracted a lot of interest over the years [1, 2]. Such interest has recently been renewed by the discovery of an apparent metallic phase which is at variance with the predictions of the scaling theory of localization for non-interacting 2D systems at zero magnetic field [3]. The strictly two-dimensional electron gas (2DEG) embedded in a uniform neutralizing background has often been used to describe the physics of these devices [1, 2]. However it has recently been found that the 2DEG model is too simple to provide quantitative account of experiments, which can only be achieved through the inclusion in the model of essential device details, such as the finite transverse thickness [4], the in-plane anisotropic mass [5], the valley degeneracy present for instance in Si-based devices [6], the scattering sources (disorder) which determine the mobility [4, 6].

Here, we discuss the effect of disorder on the ground-state energy and the spin susceptibility of narrow AlAs quantum wells (QW) [7] and a GaAs HIGFET [8], analyzing as well the role of different scattering sources. We stress that an accurate treatment of electron correlation is crucial in the present approach, which is based on the properties of the ideally clean interacting electron gas; in particular on its ground-state energy and static response functions, the latter being a key ingredient in the evaluation of the ground-state energy shift due to disorder. Moreover, some of the parameters modeling the disorder are not known from experiments and we choose to fix them by fitting the experimental mobility within the Born approximation. The set of parameters determined in such a way is then used to estimate the effect of disorder on the ground-state energy, within second-order perturbation theory.

In the first section, we introduce the model and give some details on our estimate of the (wavevector and spin-polarization dependent) density–density response function. We then present our results for the mobility, obtained by using the Born approximation, in the second section. Finally, we discuss the effect of disorder on the spin susceptibility enhancement and the ground-state energy in the third section and offer some conclusions.

2. Model and theory

Our starting point is the strictly 2D1V electron gas (2D1VEG), whose state at zero temperature and magnetic field can be fixed by just two dimensionless parameters: the coupling $r_s = 1/\sqrt{\pi n} a_B$ and the spin polarization $\zeta = (n_\uparrow - n_\downarrow)/n$. Above, $n_\uparrow$ and $n_\downarrow$ denote the spin-up and spin-down areal densities, $n = n_\uparrow + n_\downarrow$, and specific parameters of the solid state device appear only in the effective Bohr radius $a_B = \hbar^2\epsilon/m_b e^2$, via the dielectric constant ϵ and the band mass m_b.

In this work, we assume that the ground state of the 2D1VEG in the presence of disorder provides a first reasonable approximation to the observed metallic phase; we assume as well that, with respect to the ideally clean system, the ground state is not strongly altered by a weak disorder—at least far from the metal–insulator transition—and therefore the effect of scattering sources can be accounted for by perturbation theory. We note in passing that a realistic description of these systems must necessarily take into account disorder, in order to predict a finite (or vanishing) mobility.

The energy per particle of the 2D1VEG in the presence of a weak uncorrelated disorder reads, at the lowest (second) order in perturbation theory,

$$\begin{aligned} E(r_s,\zeta) &= E_{2D}^{QMC}(r_s,\zeta) + \frac{1}{2n}\sum_q \chi_{nn}(q,\zeta)\langle|U_{imp}(q)|^2\rangle_{dis} \\ &\equiv E_{2D}^{QMC}(r_s,\zeta) + \Delta(r_s,\zeta), \end{aligned} \tag{1}$$

where $U_{imp}(q)$ is the Fourier transform (FT) of the random scattering potential and $\langle\ldots\rangle_{dis}$ denotes the average on the disorder configuration distribution. Above, $E_{2D}^{QMC}(r_s,\zeta)$ and $\chi_{nn}(q,\zeta)$ are respectively the energy and the density–density linear response of the ideally clean system. $E_{2D}^{QMC}(r_s,\zeta)$ can readily be calculated from the analytical parametrization of quantum Monte Carlo energies given in [9]. We describe how to construct $\chi_{nn}(q,\zeta)$, which is accurately known only at $\zeta = 0, 1$ [15], in subsection 2.1.

For the extremely clean HIGFET the random scattering comes from the unintentional doping of the GaAs channel by charged impurities with density N_d and/or from the charged scatterers in the $Al_{0.32}Ga_{0.68}As$ barrier. The U_{imp} for these scatterers are taken from [11]. The unknown densities of charged scatterers (N_d and N_{AlGaAs}) are obtained from a fitting of the mobility as described in section 2. Here, we just mention that the depletion density N_d is

expected to be negligible in these systems and indeed our best mobility fit is compatible with $N_d = 0$.

Many scattering sources contribute to the finite mobility of the QW [10]: remote impurities due to the intentional *delta* doping, the three-dimensional homogeneous background doping with density N_b in the AlGaAs, possible unintentional doping in the AlAs channel with density N_c and above all fluctuations of the quantum well width, which is usually modeled with a contribution to $\langle|U_{\rm imp}(q)|^2\rangle_{\rm dis} \propto \Delta^2\Lambda^2 {\rm e}^{-q^2\Delta^2/4}$ [12]. The first source can be modeled as the scattering coming from a sheet of randomly distributed charged impurities of areal density n_i, separated from the side of the QW by an AlGaAs spacer of width d (in this case $n_i = 5 \times 10^{12}$ cm^{-2} and $d = 756A$ [7, 10]). The unknown parameters Δ, Λ, N_b and N_c are fixed through the mobility fit. For completeness, we need to add that here we considered the background doping only in the spacer between the QW and the delta doping sheet.

2.1. Density–density response function

The density–density linear response function for a partially spin polarized system can be written in terms of local-field factors (LFF) depending on the wavevector q, as well as on charge and magnetization densities, respectively n and m [2]:

$$\chi_{nn}(q,\zeta) = \frac{\chi_0^{\uparrow} + \chi_0^{\downarrow} + 4\chi_0^{\uparrow}\chi_0^{\downarrow}G_{mm}(q)v_{2d}(q)}{D}, \tag{2}$$

$$D = 1 + v_{2d}(q)\big[(-1 + G_{mm} - 2G_{nm} + G_{nn})\chi_0^{\downarrow} + (-1 + G_{mm} + 2G_{nm} + G_{nn})\chi_0^{\uparrow} + 4\big(-G_{mm} - G_{nm}^2 + G_{mm}G_{nn}\big)\chi_0^{\downarrow}\chi_0^{\uparrow}v_{2d}(q)\big], \tag{3}$$

where $\chi_0^{\sigma}(q,\zeta)$ ($\sigma = \uparrow, \downarrow$) is the spin resolved density–density response function for the non-interacting system [2, 13], $v_{2d}(q)$ is the Fourier transform of the Coulomb interaction and $G_{\alpha,\beta}(q,\zeta)$ are the LFF.

A complete description of the response functions relies on the knowledge of the LFF in the whole momentum region. We note here that the exact low-momentum behavior ($q \to 0$) of the LFF is known in terms of the exchange-correlation energy $\epsilon_{\rm xc}$ [2]:

$$G_{nn}(q) = -\frac{1}{v_{2d}(q)}\left(2\frac{\partial\epsilon_{\rm xc}}{\partial n} + n\frac{\partial^2 n\epsilon_{\rm xc}}{\partial n^2}\right), \tag{4}$$

$$G_{nm}(q) = -\frac{1}{v_{2d}(q)}\left(\frac{\partial\epsilon_{\rm xc}}{\partial m} + n\frac{\partial^2\epsilon_{\rm xc}}{\partial n\partial m}\right), \tag{5}$$

$$G_{mm}(q) = -\frac{1}{v_{2d}(q)}\left(n\frac{\partial^2\epsilon_{\rm xc}}{\partial m^2}\right), \tag{6}$$

with $m = n_{\uparrow} - n_{\downarrow} = n\zeta$. The simplest approximation would be to extend the low-momenta linear behavior $\left(v_{2d}^{-1} \propto q\right)$ of the LFF to all momenta. We have tested the effect on the response of the linear approximation (LA) for G_{nn} and G_{mm}, at zero polarization, with available QMC data [15]. Deviations from the LA become more evident as the system becomes more strongly interacting. We report in figure 1 results for χ_{nn} and χ_{mm} at $r_s = 10$ and $\zeta = 0$ where the deviation of the LA from the QMC data is more evident. Note that for $\zeta = 0$, χ_{nn} (χ_{mm}) only involves G_{nn} (G_{mm}). For the charge case (the left panel in figure 1) the LA for G_{nn} works quite well at least up to $2k_F$. For the spin case (the right panel in figure 1) the χ_{mm} obtained from the LA for G_{mm} shows important deviations from the QMC results over the whole range $0 \leqslant q \leqslant 2q_F$, while a much better and in fact satisfactory agreement is obtained with the exponential approximation, whereby $G_{mm}^{\rm EA}(q,\zeta) = G_{mm}^{\rm LA}(q,\zeta) \times \exp[-\alpha(q/q_F)]$

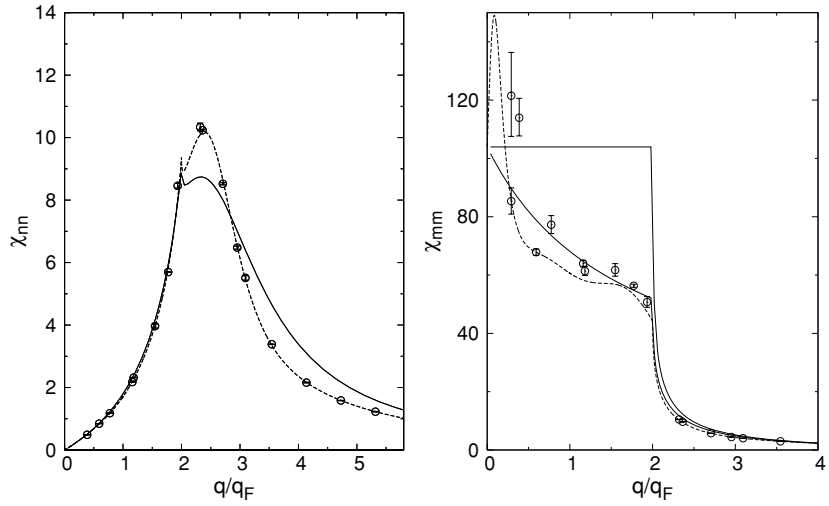

Figure 1. Linear response of the 2DEG in Ry^{-1}/n. Open dots are charge (χ_{nn}) and spin (χ_{mm}) response functions from QMC simulations [15], the dashed lines are response functions using analytical parametrizations from [14] the solid lines are the results of the LA. For the spin case (right panel) the EA is also shown (thick solid line). For the definition of the LA and EA see the text.

and $\alpha = 0.1$. An analytical parametrization of the LFF [14] embodying the exact known behavior at small and large momenta is available for $\zeta = 0$ and $0 \leqslant r_s \leqslant 10$. However, while it could be used for the calculation of mobility (see below) it is of no use for the calculation of the spin susceptibility, which requires the ζ-dependence of the LFF.

In computing the ζ-dependent correction to the ground-state energy, we have used the LA for G_{nn} and G_{nm} and the EA for G_{mm}. We do not discuss in detail here the behavior of G_{nm}, which appears to be one order of magnitude smaller than the other two LFFs and therefore should not affect the results in an appreciable manner.

3. The mobility

Quite generally, not all parameters entering the modeling of the scattering sources are known from experiments and we take the customary approach in which the unknown ones are fixed through a global fit of the experimental mobility. The relaxation time τ at the lowest order in the scattering potential is given by the Born approximation [16]:

$$\frac{1}{\tau} = \frac{\hbar^{-1}}{2\pi\epsilon_F}\int_0^{2k_F} \mathrm{d}q\, \frac{q^2}{\left(4k_F^2 - q^2\right)^{1/2}} \frac{\langle |U_{\mathrm{imp}}(q)|^2\rangle_{\mathrm{dis}}}{\epsilon_P(q)^2}, \tag{7}$$

where $\epsilon_P(q) = 1 - v_c(q)(1 - G_{nn}(q))\chi_0(q) = \epsilon_P^{\mathrm{RPA}}(q) + v_c(q)G_{nn}(q)\chi_0(q)$. The integrand in equation (7) is peaked around $2k_F$ because of the combined effect of the factors $\left(4k_F^2 - q^2\right)^{-1/2}$ and $\epsilon_P(q)^{-2}$, the latter being strongly enhanced by $G_{nn}(q)$ with respect to its RPA expression. An accurate estimate of $G_{nn}(q)$ in this region of momenta is therefore crucial: the disorder parameters can increase by almost an order of magnitude if one replaces $\epsilon_P(q)$ with $\epsilon_P^{\mathrm{RPA}}(q)$ in the mobility fit.

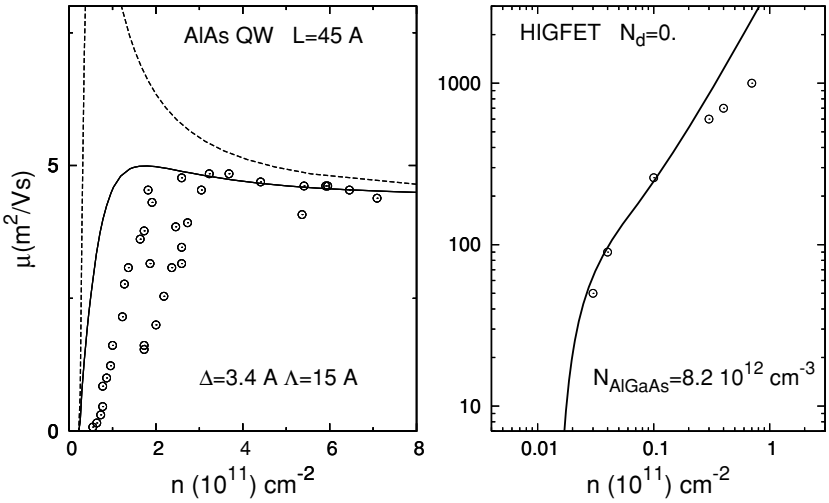

Figure 2. 2DEG mobility in actual devices. Open dots are experimental data for the AlAs QWs of [7] (left panel) and for the HIGFET heterostructure [8] (right panel). Solid lines are the fitted mobility using equation (7). For the QWs the mobility obtained including only roughness scattering is also shown (dashed line).

Here, we use G_{nn} for a strictly two-dimensional system and accordingly we set $v_c(q) = v_{c,}(q) = 2\pi e^2/\epsilon q$. This may look at first a very crude assumption for the HIGFET [8], which is characterized by a sizeable thickness. However we have checked, within RPA, that while the fitted disorder parameters change appreciably in going from the $v_{c,2D}(q)$ to $v_{c,\text{thick}}(q)$, the energy shift due to disorder does not change sensibly provided the same consistent combination of $v_c(q)$ and the disorder parameters used for the mobility is also used for the energy shift calculation. The same applies to the ensuing spin susceptibility.

Mobility results for the two devices considered are shown in figure 2. In the QW the surface roughness plays a major role in determing the mobility at high densities ($\Delta = 3.4A$, $\Lambda = 15A$) in agreement with the existing literature [12] (see the left panel of figure 2). At low density, however, roughly below $n \simeq 2.5 \times 10^{11}$ cm^{-2}, the Born approximation is no longer able to reproduce the experimental data. This is a density region where the charged impurities ($N_b = N_c = 2 \times 10^{14}$ cm^{-3}) become effective. In the right panel of figure 2 we display results for the HIGHFET with $N_d = 0$ and $N_{\text{AlGaAS}} = 8.2 \times 10^{12}$ cm^{-3}. The discrepancy of these disorder parameters with those in [4] is due to the replacement, with respect to the previous calculation, of $v_{c,\text{thick}}$ with $v_{c,2D}$. The effect of such a change on the spin susceptibility is however barely visible, as it can be checked by comparing the results in figure 3 with those in [4]. We should mention that both in the present calculations and those of [4] we have chosen the form of U_{imp} appropriate to a thick electron gas.

4. The spin susceptibility

The spin susceptibility enhancement of the systems under investigation is [4]

$$\frac{\chi_s}{\chi_0} = \left[\frac{\partial^2 E_0(r_s,\zeta)}{\partial\zeta^2}\right]_{\zeta=0}\left[\frac{\partial^2 E^{\text{QMC}}(r_s,\zeta)}{\partial\zeta^2} + \frac{\partial^2 \Delta E(r_s,\zeta)}{\partial\zeta^2}\right]^{-1}_{\zeta=0}, \tag{8}$$

where $E_0(r_s,\zeta)$ is the energy of the non-interacting system, $\Delta E(r_s,\zeta)$ is the energy shift due to disorder defined in equation (1) and $E^{\text{QMC}}(r_s,\zeta)$ is the energy of the clean system, which

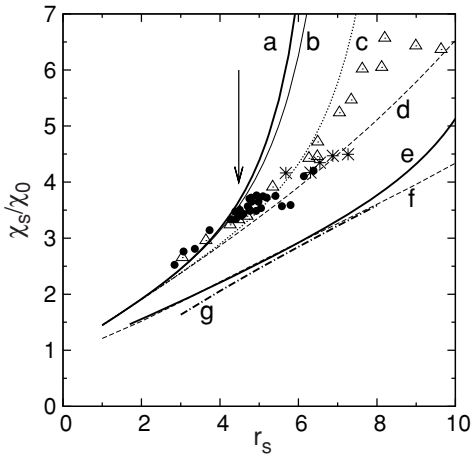

Figure 3. Spin susceptibility enhancement of the 2DEG in actual devices. Experimental results for the thin QW of [7] and for the HIGHFET of [8] are respectively represented by points (different symbols correspond to different samples [7]) and by the line labeled **g**. Line **d** reports the QMC prediction for the clean 2DEG [9], while lines **f** and **e** give the QMC-based predictions for the *clean* and *dirty* quasi-2DEG in the HIGHFET [4], respectively. The arrow indicates the density at which the Born approximation for the QW mobility fails. Line **a** is our prediction for χ_s/χ_0 in the QW including both surface roughness and charged impurities scattering; the predictions obtained including only surface roughness or only charged impurities are given by lines **b** and **c**, respectively.

may include, if necessary, the effect of thickness. As mentioned above, the results of this calculation strongly depend on the LFF in the region around $2q_F$, the region where $\chi_{nn}(q,\zeta)$ has a sizeable change when varying ζ around zero. We stress that the parameters describing the disorder are fixed by a fit of the experimental mobility and depend on G_{nn} at zero polarization; while $\Delta E(r_s,\zeta)$ requires the knowledge of all LFFs and their ζ-dependence.

Before examining in detail our results for the spin susceptibility, summarized in figure 3, we make some general comments on the effect of disorder. Apart from the surface roughness at a very high density ($r_s \leqslant 1$), where it induces a negligible reduction of spin susceptibility, the effect of all scattering sources is to enhance χ_s/χ_0, once the electron correlation is included in the response function, even at the RPA level. A calculation employing the response function $\chi_0(q,\zeta)$ of non-interacting electrons and including only the roughness scattering, for example, predicts a suppression of the spin susceptibility at all densities. On lowering the electron density the relative contribution of disorder to the second derivative of the energy, with respect to ζ, increases in size and being negative leads to the eventual divergence of the spin susceptibility. We note that quite generally the transverse thickness reduces the spin susceptibility of 2D electron systems, while disorder generally enhances it [4].

As is clearly seen in figure 3, in the extremely clean case of the HIGHFET, the inclusion of disorder does not alter the agreement between the theoretical prediction (obtained including thickness) and measurements, throughout the whole experimental density range[4]. If one neglects thickness and uses the disorder parameters fitted to the experimental mobility of the

[4] The apparent discrepancy between theory as end experiment at high density (one would expect χ_s/χ_0 to go to 1 as $r_s \to 0$, while the expression fitted to experiments in [8] tends to 0 in this limit) is eliminated once band structure effects, modifying the band mass and g-factor, are duly taken into account [17]. We do not report here the data of [17] for χ_s/χ_0, which are obtained from a different sample for which we do not know all relevant physical parameters.

HIGHFET, as specified above, the energy shift due to the disorder makes the ferromagnetic state of the strictly 2DEG energetically favorable with respect to the normal state at $r_s \simeq 12.5$.

In contrast, the same procedure using the disorder parameters appropriate to the thin electron gas realized in AlAs QWs [7] predicts a transition toward a partially polarized state at $r_s \simeq 7$, namely a second-order phase transition. We should stress, however, that for this system the fitting of the experimental mobility in the Born approximation breaks down at low densities (corresponding to $r_s \gtrsim 4$), as clearly shown in figure 2. Yet, up to $r_s \lesssim 4$, our prediction for the spin susceptibility is only moderately affected by the disorder (thick solid line (a) in figure 3), with an enhancement with respect to the clean system of at most 20%, which results in a very good agreement with experiments. By looking at the theoretical prediction for the spin susceptibility enhancement obtained by including only the scattering by charged impurities (dotted line (c)) or only that by roughness (thin solid line (b)), it is evident that the major role is played by roughness at all densities, as well as the negligible effect of charged scatterers at high density (due to screening). At low densities, though being quite smaller than that of roughness, the effect of charged impurities on χ_s becomes however sizeable. Within second-order perturbation theory, lowering the density, disorder becomes more and more effective enhancing the spin susceptibility and finally driving it to diverge. A strong enhancement is found also in the experiments, however we cannot push our quantitative comparison between the experiments and our predictions in density regions where the level of disorder cannot be reliably related to the experimental mobility using the Born approximation.

We stress that the accuracy of the prediction of the spin susceptibility of the clean 2D1V electron gas is crucial in the present approach, as suggested by the comparison between theory and experiment for the thin electron gas realized in narrow AlAs QWs [7], for which the effect of thickness is negligible [4]. In this respect, we recall that RPA predicts for the 2D1V electron gas a first-order ferromagnetic transition already at $r_s \simeq 5.5$ and a χ_s/χ_0 divergence in the paramagnetic phase at $r_s \simeq 7.3$ [18]. Evidently the inclusion of disorder in RPA would push the Bloch and Stoner transitions [18] to a higher density, well inside the experimental range.

5. Conclusions

We have studied the effect of disorder on the spin susceptibility of 2D electron systems realized in semiconductor heterostructures, considering narrow AlAs-based QWs and a GaAs-based HIGHFET, systems which have an in-plane isotropic mass and no valley degeneracy. We take as reference, in assessing the effect of disorder, the ideally clean 2D1V electron gas, whose spin susceptibility is known with great accuracy, thanks to QMC simulations [9]. We found that the effect of a weak uncorrelated disorder is to enhance the spin susceptibility, at the lowest order in perturbation theory, with correlation seemingly playing a crucial role. The disorder parameters which were not known from experiments were determined through a fit of the experimental mobility over the whole experimental density range, in the Born approximation, and then used without any change in the spin susceptibility calculation. We discovered that at densities where the Born approximation is capable of fitting the experimental mobility, our prediction of the spin susceptibility in the *dirty* system turns out to be very accurate; while it appreciably deviates from the experiment at densities where the Born approximation breaks down, or more precisely, is unable to fit the experimental mobility.

Thus, the really weak disorder present in the GaAs HIGFET of [8] has a small effect on the spin susceptibility and does not change qualitatively the phase diagram of the 2D1V electron gas. Evidently, the disorder in the AlAs QWs of [7] is much stronger and it can be possibly treated in perturbation theory only at densities not too low. It is anyhow reassuring that when the perturbative approach is capable of quantitatively fitting the experimental mobility,

the resulting prediction of the spin susceptibility enhancement is in good agreement with experiments.

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