Attractive effect of a strong electronic repulsion – the physics of vertex divergences

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While the breakdown of the perturbation expansion for the many-electron problem has several manifestations at the formal level, such as divergences of irreducible vertex functions and crossing of solutions in the Luttinger-Ward functional, here we unveil its physical effect. It corresponds to flipping the sign of the effective electronic interaction from repulsive to attractive in specific scattering channels. By decomposing the local and uniform susceptibilities of the Hubbard model in terms of their spectral representations, we prove how entering the non-perturbative regime causes an enhancement of the charge response, ultimately responsible for the phase-separation instabilities close to the Mott Hubbard MIT. Our analysis opens a new route for understanding phase-transitions in the non-perturbative regime and clarifies why attractive effects emerging from a strong repulsion can induce phase-separations, but not (s-wave) pairing or charge-density wave instabilities.

Introduction – While the many-electron problem of condensed matter and QED are similar in several respects (e.g., in their Feynman diagrammatic description), they differ in a very important point: For the former, no small expansion parameter can be identified a priori.

In fact, the possibility of applying weak-coupling approaches in condensed matter depends on how efficiently the Coulomb interaction is screened in the compounds under consideration. This variability often requires to go beyond the comfort zone of a perturbative description with important formal and algorithmic implications, as it was pointed out in the recent literature\textsuperscript{1-16}.

In this paper we demonstrate that the breakdown of perturbation theory\textsuperscript{1-3,8} should not be regarded as a mere formal issue, but that it is indeed directly linked to precise physical consequences of high importance for correlated electron systems. In particular, we will show how, and to what extent, entering the non-perturbative regime can turn a strong electrostatic repulsion into an effective attraction.

Non perturbative regime – In order to set the stage, we exploit one of the most successful many-body methods, which does not rely on perturbation theory: We will consider the dynamical mean-field theory (DMFT)\textsuperscript{17} solution of the Hubbard model. In particular, we will focus on the static charge response. Its local part is defined\textsuperscript{18,19} as

\[ \chi_{\text{loc}} = \int_0^\beta d\tau \langle \hat{n}(\tau) \hat{n}(0) \rangle - \langle \hat{n} \rangle^2, \]

which can be computed by summing the corresponding generalized two-particle susceptibility \( \chi^{\nu\nu'}(\Omega = 0) \) (at zero transfer frequency \( \Omega \)) over all the fermionic Matsubara frequencies \( \nu, \nu' \):

\[ \chi_{\text{loc}} = \frac{1}{\beta^2} \sum_{\nu, \nu'} \chi^{\nu\nu'}(\Omega = 0) = \sum_{\alpha} \lambda_{\alpha} w_{\alpha}, \]

whereas in the second line, the sum is recasted in the eigenbasis of \( \chi^{\nu\nu'}(\Omega = 0) \) (with eigenvalues \( \lambda_{\alpha} \) and spectral weight defined through the eigenvectors \( w_{\alpha} = \sum_{\nu} V_{\sigma}^{-1}(\nu) | \sum_{\nu} V_{\sigma}(\nu') \rangle \)). This spectral representation, introduced in Refs.\textsuperscript{8,16}, will be a central tool for our study.

We start from the easiest situation of a half-filled (particle-hole symmetric) model, where \( \chi^{\nu\nu'}(\Omega = 0) \) is a real, bisymmetric matrix, with real \( \lambda_{\alpha} \) and \( w_{\alpha} \geq 0 \). In this case, it was already shown that the progressive suppression of local charge fluctuations (i.e., of \( \chi_{\text{loc}} \)) by increasing \( U \) is driven by a corresponding decrease of the eigenvalues \( \lambda_{\alpha} \). In fact, while the \( \lambda_{\alpha} \) are all positive for \( U = 0 \), they start -after a certain value of \( U \)- to cross zero, becoming negative and reducing the overall value of \( \chi_{\text{loc}} \). Each sign-change of one of the \( \lambda_{\alpha} \) corresponds, per definition -to a divergence of the irreducible vertex \( \Gamma^{\nu\nu'} = [\chi^{\nu\nu'}]^{-1} - [\chi_{\text{loc}}^{\nu\nu'}]^{-1} \) or equivalently, to a non invertibility of the associated Bethe-Salpeter equation (BSE)\textsuperscript{17}.

Exactly for the same parameter sets, one also observes a crossing of solutions in the Luttinger-Ward functional\textsuperscript{3,8}. The parameters where the lowest \( \lambda_{\alpha} \) crosses zero, thus mark the end of the perturbative regime. We recall that a similar fate occurs to the local pairing fluctuations and, hence, to the BSE in the particle-particle channel.

Putting aside the important, but more technical question of how cutting-edge algorithms (especially those based on irreducible vertices\textsuperscript{20,21} or bold resummations of Feynman diagrams\textsuperscript{3,11}) get affected by this, from a physical point of view it seems natural\textsuperscript{8} to relate such non-perturbative manifestations to a suppression of the corresponding local fluctuations. However, a different viewpoint is possible\textsuperscript{22}; as the irreducible vertex \( \Gamma \) is the core of a BSE, its multiple sign-changes (driven by those of \( \lambda_{\alpha} \)) could be interpreted as a flipping of a repulsive into an attractive interaction (or vice versa). Heuristically, if we take a simple RPA-like expression \( [\Gamma^{\nu\nu'} \rightarrow \Gamma_0 > 0 \)
In the left panel of Fig. 1, shown on one side only) and embracing the critical endpoint of the MIT (blue dotted even diverges along two curves in the parameter space. κ served at finite U increasing κ while at half-filling shadow area in the n (MIT) of the Hubbard model (blue dot, topping the critical endpoint of the Mott metal-insulator transition fluctuations are strongly enhanced in the proximity of the observed major enhancement of the response in these sectors is diated by increasing U. Such a peculiar oscillatory behavior has never been reported. Instead, by looking at the DMFT results for the Hubbard model, whose phase-diagram is sketched in the left panel of Fig. 1, only one major enhancement of the response in these sectors is observed by increasing U, namely the one in the uniform charge response, the isothermal compressibility κ. A glimpse from DMFT—As known, charge fluctuations are strongly enhanced in the proximity of the critical endpoint of the Mott metal-insulator transition (MIT) of the Hubbard model (blue dot, topping the shadow area in the n = 1 plane of Fig. 1). Specifically, while at half-filling κ decreases monotonically with increasing U, a strongly enhanced compressibility is observed at finite doping on both sides of the MIT. In fact, κ even diverges along two curves in the parameter space embracing the critical endpoint of the MIT (blue dotted in the left panel of Fig. 1, shown on one side only) and marking the onset of a phase separation at lower T. As we will show, this is directly connected to the divergences of the irreducible vertex Γ found in the correlated metallic region, much before the MIT itself (sketched as red (I) and orange (II) curves, marking the location of the first two vertex singularities in the n = 1 plane). In general, the compressibility can be defined at the one particle level, as the derivative of the density w.r.t. the chemical potential (\( \frac{\partial n}{\partial \mu} \)) or at the two-particle level, as the static limit (\( q \rightarrow 0, \Omega = 0 \)) of the momentum/frequency dependent charge response function \( \chi_q(\Omega) \), obtained through the BSE:\n
\[
\chi_q(\Omega) = \frac{1}{\beta^2} \sum_{\nu \nu'} \left[ (\chi_{q}^{0}(\Omega)\delta_{\nu \nu'} + \Gamma_{\nu \nu'}^{\prime}(\Omega)) \right]^{-1},
\]

where the bubble term reads \( \chi_{q}^{0}(\Omega)\delta_{\nu \nu'} = -\beta \sum_{k} G(k, \nu) G(k + q, \nu + \Omega) \delta_{\nu \nu'} \). In DMFT, where the self-energy and the irreducible vertex Γ are both extracted from a (self-consistently determined) auxiliary impurity model, the two definitions yield per construction the same value of κ (see Ref. and). The locality of Γ in Eq. (4) makes the relation between local and collective properties particularly transparent in DMFT. In fact, by straightforwardly extending a famous result of Ref. for the charge channel, we obtain the following analytical expression:

\[
\kappa = \sum_{\alpha} \left( \frac{1}{\chi_{\alpha}^{0}} + \frac{1}{\beta^2} \right) \omega_{\alpha}^{-1},
\]

which holds exactly for the Bethe lattice case (here of halfbandwidth \( D = 2t = 1 \)), independently of its filling.
FIG. 2. Top: uniform (κ, blue empty circles from the numerical derivative of n w.r.t. μ; red squares from the BSE for χq) and local charge (χ_{loc}) susceptibility computed in DMFT for β = 53 and U = 2.4 (on a square lattice with unit D = 4t = 1). Bottom: analysis of the contributions to κ and χ_{loc} arising from the lowest two real eigenvalues (“I” in red, “II” in orange) and from all the remaining terms (“rest” in grey) for four different dopings. The light background colors are just a guide to the eye.

and, as we will discuss below, also represents a very good approximation if the DMFT is performed on other, more realistic lattices\textsuperscript{30}. A quick glance at Eq. (5) immediately shows that the only possibility for a divergence of κ is that the condition βλ = −\frac{2}{\lambda} < 0 is verified for one eigenvalue of χ^{\nu\nu}(Ω = 0). Evidently, this locates necessarily such divergences of κ on the right side of the first vertex-singularity line (red curve in Fig. 1) and poses precise constraints, calling for a quantitative analysis.

The half-filling case – We consider first the (particle-hole symmetric) half-filled Bethe-lattice case, computing the evolution of the lowest eigenvalue \lambda_I as a function of \mu for different temperatures (right panel of Fig. 1). As discussed in the literature\textsuperscript{10,16}, due to the high-symmetry of this case, \lambda_I is associated to a real, antisymmetric eigenvector (V_1(\nu) = -V_1(-\nu), hence \nu_\alpha = 0). From the data of Fig.1b, we clearly see that \lambda_I displays a minimum at intermediate \mu, in the crossover region of the Mott MIT. By reducing T the minimum gets sharper and progressively closer to the necessary condition of a divergence of κ (marked by dashed line). Remarkably, the condition gets fulfilled at the (second-order) critical end point of the MIT (at U ≃ 2.33, β ≃ 37), where the minimum of \lambda_I becomes a cusp, before one starts observing a coexistence of two solutions at lower T. We note that this behavior can alternatively be understood from the critical properties of the MIT, as independently proven by van Loon and Krien\textsuperscript{34}. At half-filling, however, the divergence of (1/\lambda_I + 1/2\beta t^2)^{-1} does not have any physical effect on κ, because the associated spectral weight \nu_I in Eq. (5) is always zero, due to the perfect antisymmetry of V_I(\nu). We note in passing that the second lowest eigenvalue (\lambda_{II}), associated with a symmetric eigenvector [V_{II}(\nu) = V_{II}(-\nu)] becomes also negative (after the orange curve in Fig. 1), but it never reaches the critical condition β\lambda_{II} = −\frac{2}{\lambda}. In fact, as its spectral weight \nu_{II} is positive, it contributes to a progressive suppression of κ.

Out of half-filling – The results above crucially depend on the high-symmetry properties\textsuperscript{16,32} of the (non-frustrated) half-filled case. As soon as those are lifted, e.g. by doping the system and/or adding a next-to-nearest hopping term (t') striking changes are observed. We consider explicitly the case of a hole doped system (\mu - \frac{U}{2} < 0, n < 1, t' = 0) on a square lattice (with half-bandwidth D = 1) rather close to the critical endpoint of the MIT (i.e., U = 2.4, β = 53, as schematically in-
that the maximum of $\kappa$ corresponds to the minimum of $\lambda_1$, where the condition $\beta \lambda_1 \simeq -\frac{U}{2}$ gets closer to be fulfilled, similarly to what happens at the critical end-point of the MIT. The difference w.r.t. the $n=1$ case is that the corresponding weight $w_1$ is now finite, and actually negative, thus contributing to an overall enhancement of the charge response. Because of the small weight $w_1$, such effect is generally mild, unless $\lambda_1$ gets negative enough to trigger a strong enhancement or even the divergence of $\kappa$. Fig. (3) also shows that the weight associated to the second lowest eigenvalue ($\lambda_{II}$) always remains positive, as at half-filling. Hence, even if both $\lambda_1$, $\lambda_{II}$ are negative, the latter is responsible for a suppression of the charge response. In fact, it is the overall sign of $\lambda_\alpha w_\alpha$ determining, in general, whether the net effect can be interpreted as repulsive or attractive in the charge sector, since the sign of $w_\alpha$ is no longer positive-definite. However, since the evolution of $w_\alpha$ is generally smooth, the sign change of $\lambda_1$, marking the first divergence\cite{1,3,8} of $\Gamma^{\nu\nu}$, flips also the net action of this contribution to the charge response from suppressing to enhancing.

We stress that having $w_1 < 0$ is crucial both for the emergence of these strong-coupling phase-instabilities and for the dichotomy between local and uniform response: The sum in Eq. (5) can be recasted as

$$\kappa = \sum_\alpha \frac{\chi_{\text{loc}}^\alpha}{1 + J_{\text{eff}}^{\alpha} \chi_{\text{loc}}^\alpha}$$

where $\chi_{\text{loc}}^\alpha = \lambda_\alpha w_\alpha$ and $J_{\text{eff}}^{\alpha} = \frac{3t^2}{4U_\alpha}$. All summands of Eqs. (2) and (6) are rather similar, except close to the phase-separation where the difference between local and uniform response is induced by the first term ($\alpha = 1$) only. In that region, as $\chi_{\text{loc}}^1 > 0$, $w_1 < 0$ implies a negative coupling\cite{38} ($J_{\text{eff}}^1 < 0$) in the charge sector.

The full momentum dependence – We now extend our analysis to the entire momentum dependence of $\chi_q$, performed at the same parameter-set where the maximal $\kappa$ is found. On the left panel of Fig. 4, where $\chi_q$ is plotted, we observe a rather sharp peak at $q = 0$. In the central

![FIG. 4. Left: Momentum-dependence of the charge susceptibility $\chi_q$ computed in DMFT on a square lattice for $U = 2.4$, $\beta = 53$ for $\mu - U/2 = -0.1$, corresponding to the maximum of the compressibility $\kappa$. Center: contribution stemming from $\lambda_1$. Right: all other contributions summed.](image-url)
and right panels, we decompose $\chi_q$ into the contributions stemming from $\lambda_I$ and from the whole rest, respectively. We immediately see that the non-perturbative enhancement of the charge response is confined to the small $q$-sector. Further we note that without the critical, effectively attractive, contribution from $\lambda_I$, the charge response would have a completely different shape, closely resembling the one at half-filling\cite{40}: a rather low $\chi_q$ with a shallow maximum at $q = (\pi, \pi)$. This selective enhancement of $\chi_q$ around $q = 0$ increases the corresponding correlation length $\xi$, which is necessary to ensure the second-order nature of the critical endpoints of the phase-separation as well as for inducing the strong dichotomy between the local and the uniform response, discussed above.

We expect the same to happen along the whole, highly non-trivial, path of the phase-separation instability computed in the DMFT phase-diagram of Ref.\cite{26}. We also want to stress, here, that the non-perturbative nature associated to the negative sign of $\lambda_I$ will prevent all approximations, where the irreducible vertices do not diverge (such as RPA, FLEX, fRG, the parquet approximations, where the irreducible vertices do not diverge) to capture this phenomenology.

**Outlook** – It is insightful to generalize our considerations by further extending Eq. (5) to the other sectors arguably reactive to attractive interactions. One can show\cite{39} that the corresponding DMFT expressions for any static particle-hole susceptibility at $q = \Pi = (\pi, \pi, \pi, \ldots)$ (e.g., the CDW in the charge sector), as well as of the pairing ($pp$) s-wave susceptibility at $q = 0$ read

$$\chi_{q=0} = \chi_{q=0}^{pp} = \sum_{\alpha} \left( \frac{1}{\chi_{\alpha} - i/2\beta t^2} \right)^{-1} w_{\alpha}. \quad (7)$$

This rules out the possibility of inducing CDW or $s$-wave pairing instabilities through a strong local repulsion: divergences of the corresponding responses can be only originated by a large and positive $\lambda_{\alpha}$, a typical hallmark\cite{16} of preformed local pairs\cite{40}, and hence, of the presence of bare attractive interaction $U < 0$. Here, we clearly see the difference between a bare (and frequency-independent) attractive interaction and an effective one, originating from non-perturbative mechanisms: the effect of the latter can be regarded as truly attractive only in specific sectors and parameter regions.

It remains to be investigated, instead, the plausible speculation that a similar, non-perturbative mechanism can be responsible for the enhanced charge fluctuations and phase-separation instabilities reported\cite{41,42} in extended parameter regions of Hund’s metal systems and, possibly, even trigger the onset of the $s_{\pm}$-pairing.

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Since $\Gamma^{\nu\nu'} \approx \lambda^\nu V^{-1}(\nu) V^\nu(\nu')$ close to a vertex divergence where $\lambda^\nu \approx 0$, a sign change of $\lambda^\nu$ also changes the sign of $\Gamma^{\nu\nu'}$.

In thermodynamics, the isothermal compressibility $\kappa$ is usually defined as $\kappa_T = -\frac{1}{V} \frac{\partial V}{\partial p} = \frac{1}{n} \frac{\partial n}{\partial \mu}$. For a more direct comparison with $\chi^{\nu\nu}(\Omega = 0)$, we define here $\kappa \equiv \frac{\partial n}{\partial \mu}$ in accordance with earlier literature. A negative $w_\alpha < 0$ can occur because $\chi^{\nu\nu}(\Omega = 0)$ is no longer hermitian (but centrohermitian) out of half-filling. For negative $w = \frac{\operatorname{Re}}{\operatorname{Re}} \left[ \sum_\nu V^{-1}_i(\nu) \right] \frac{\operatorname{Re}}{\operatorname{Re}} \left[ \sum_\nu' V^i(\nu') \right] - \frac{\operatorname{Im}}{\operatorname{Im}} \left[ \sum_\nu V^{-1}_i(\nu) \right] \frac{\operatorname{Im}}{\operatorname{Im}} \left[ \sum_\nu' V^i(\nu') \right]$ both summands yield negative contributions, whereas the latter -stemming from the imaginary part- is found to be the dominant one. Note that, due to the centrohermitian properties of $\chi^{\nu\nu}$, all $w_\alpha$ are real.

Which could be formally interpreted as a ferromagnetic coupling between the $z$-components of the pseudospin operators.

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Or local moments, if we consider the spin/magnetic sectors.

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