

Effective Enhancement of the Electron-Phonon Coupling Driven by Nonperturbative Electronic Density Fluctuations

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We present a dynamical mean-field study of nonperturbative electronic mechanisms, which may lead to significant enhancements of the electron-phonon coupling in correlated electron systems. Analyzing the effects of electronic correlations on the lowest-order electron-phonon processes, we show that in the proximity of the Mott metal-to-insulator transition of the doped square lattice Hubbard model, where the isothermal charge response becomes particularly large at small momenta, the coupling of electrons to the lattice is strongly increased. This, in turn, induces significant corrections to both the electronic self-energy and phonon-mediated pairing interaction, indicating the possible onset of a strong interplay between lattice and electronic degrees of freedom even for small values of the bare electron-phonon coupling.

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Introduction—The scattering processes of electrons and lattice vibrations (electron-phonon coupling) represent an important factor in determining thermodynamic and spectroscopic properties of condensed matter systems [1–3]. It is also widely known that these processes play a crucial role in the electronic pairing in conventional superconductors both at ambient [1,2,4,5] and under high pressure [6,7]. In fact, an estimate of the magnitude of the electron-phonon (el-ph) coupling is often decisive [8] to classify the superconductivity shown by a given compound as “conventional” or “unconventional,” whereas the latter is typically driven by a purely electronic pairing mechanism. However, while the algorithmic progress of DFT-based methods in the last decades has allowed us to reach an unprecedented level of precision for quantitative estimates or the prediction of el-ph couplings and their effects [6,9], the corresponding treatment of this physics in strongly correlated electron systems [10–27] remains highly challenging and is still an active area of research [28,29].

In this Letter, we address this longstanding problem from a fundamental perspective (i) by performing a rigorous investigation of the renormalization of the el-ph coupling in the intermediate-to-strong coupling regime and (ii) by evaluating the associated effects on the electronic pairing

and self-energy. In doing this, we also aim at clarifying the partially contradicting interpretations and results obtained by different groups in very early studies of this problem [12–14,19], which were limited by the computational effort twenty years ago.

In order to achieve these goals in the most basic framework, we have performed dynamical mean-field theory (DMFT) calculations, on both the one- and two-particle level, for the (hole-doped) Hubbard model [30,31] on the square lattice with only nearest-neighbor (n.n.) hopping in the close proximity of its Mott metal-to-insulator transition (MIT). The choice of DMFT allows an explicit treatment of the nonperturbative effects of the electronic interaction [32–41], which, as we will demonstrate, play a pivotal role in the renormalization of the el-ph scattering. Further, the analytical insight recently gained on the momentum-dependent response function [38,42,43] of DMFT makes it possible to clarify the underlying origin of our numerical results and of the emerging physics.

Finally, we elaborate on the consequences and the limitations of our findings also in relation to their applicability to the physics of correlated oxides, Hund’s metals, and unconventional superconductors, and we outline the possible routes they might suggest for future investigations.

Momentum-dependent charge response—In our Letter, we focus on a typical realization of el-ph scattering where the lattice vibrations are directly coupled to the electronic density. For this reason, we start by considering the (momentum-dependent) charge response of the electronic system. This quantity describes, in general, the electronic density fluctuations, whereas its static limit (i.e., zero

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transfer frequency, $\omega = 0$, and transfer momentum $\mathbf{q} \rightarrow 0$), yields the (electronic) isothermal compressibility, $\kappa = (1/n^2)\partial n/\partial\mu = (1/n^2)\chi_{\mathbf{q}\rightarrow 0}(\omega = 0)$ [44–48], n being the electron density of the system and μ its chemical potential.

In this respect, we recall that the pioneering DMFT works of Refs. [49–52] demonstrated that the electronic compressibility may become significantly enhanced in the vicinity of the critical endpoint of the Mott MIT. Specifically, this happens in slightly doped as well as frustrated systems [49], where even a divergence of κ can be observed. At the same time, we should also note how the general understanding of the physical processes controlling this phenomenon has recently advanced by means of the combined analytical-numerical studies as reported in Refs. [38,42,43,53]. In particular, these studies identified the purely nonperturbative mechanisms controlling the significant enhancement of the uniform charge response in parameter regimes, where the on-site charge fluctuations get significantly suppressed by the strong electronic interaction.

Based on these considerations, here we extend the derivation of Refs. [38,43,54,55] to general transfer momenta, obtaining the following spectral representation, which yields a rather precise description of the lattice charge susceptibility of DMFT for the square lattice in the intermediate-to-strong-coupling regime (see Appendix A in the End Matter):

$$\chi_{\mathbf{q}}^c(\omega = 0) \equiv \chi_{\mathbf{q}}^c \simeq \sum_{\alpha} (\lambda_{\alpha}^{-1} + \beta T_{\mathbf{q}})^{-1} w_{\alpha}. \quad (1)$$

Here, λ_{α} denotes the eigenvalues of the generalized *on-site* static charge susceptibility of the system, $\chi_{\text{loc}}^{c,\nu\nu'}/\omega=0$, expressed as a matrix in the fermionic Matsubara frequency space $\{\nu, \nu'\}$, and the spectral weight w_{α} consists of the associated eigenvectors. The momentum dependence of Eq. (1) is enclosed entirely in the quantity $\beta T_{\mathbf{q}} \approx \beta t^2 [\cos(q_x) + \cos(q_y)]$ (see Appendix A and [56] for more details), with the n.n. hopping amplitude t and the inverse temperature $\beta = 1/T$.

While Eq. (1) will be quite useful for interpreting the numerical results presented below, as well as a starting point for additional derivations, it immediately allows us to define the condition for a strong enhancement of $\chi_{\mathbf{q}}^c$, namely, when $\lambda_{\alpha}^{-1} \rightarrow -\beta T_{\mathbf{q}}$, for $\omega_{\alpha} \neq 0$ [38]. In particular, according to Eq. (1), the divergence of the electronic compressibility would occur when the lowest eigenvalue of the on-site generalized charge susceptibility λ_l becomes negative enough to fulfill the condition $\lambda_l^{-1} \rightarrow -\beta T_{\mathbf{q}=0} = -2\beta t^2 < 0$. This is evidently possible only after a sign-flip of λ_l (which is typically positive at weak coupling) occurs, which features a *noninvertibility* of the Bethe-Salpeter equations for the on-site charge susceptibility [32,33,35–37,40,65–68] and marks a breakdown

of the corresponding self-consistent perturbation expansion [34,36,41,69,70]. As the eigenvalues λ_{α} decrease with the Hubbard interaction U , due to the freezing of on-site charge fluctuations induced by the preformation of local magnetic moments [39,41,66,71,72], Eq. (1) also directly clarifies [38] how a substantial increase in the $\mathbf{q} = 0$ charge response of the system can be driven, in the nonperturbative regime, by a suppression of local charge fluctuations.

Numerical results—We now turn to our numerical DMFT investigation of the evolution of the charge susceptibility as a function of the interaction U . For our DMFT calculations, we exploit the continuous time quantum Monte Carlo algorithm in the hybridization expansion as implemented in the *w2DYNAMICS* code package [73]. In particular, we consider here the case of the unfrustrated Hubbard model on the square lattice in energy units of its half-bandwidth, i.e., $4t = 1$. In order to lift the constraint of perfect particle-hole symmetry and allow for an enhancement of the compressibility, we specifically choose the filling of $n = 0.9966$. This sets us in close proximity to the critical endpoint of the Mott MIT for the value of $\beta = 55.75$ and the range of interactions U considered here.

In Fig. 1, we present the full momentum dependence of the charge susceptibility for different values of U . We note that, in the noninteracting $U = 0$ case (leftmost panel), the charge response is dominated by the contribution of the $\mathbf{q} = (\pi, \pi)$ sector, due to the perfect nesting properties of the square lattice [74] considered. Upon turning the interaction up to $U = 2.3$ (second panel), one observes, as generally expected on the basis of perturbation theory arguments (cf. RPA), a gradual, overall suppression of the charge susceptibility for all $\mathbf{q}$ values, while the predominance of larger transfer momenta is still retained. The situation changes drastically once the interaction value of $U = 2.4$ (corresponding to a parameter set very close to the half-filled MIT) is reached (third panel), where a strong enhancement of the isothermal susceptibility occurs. A sharp peak around $\mathbf{q} = (0, 0)$ emerges, signaling the tendency toward a phase separation instability. For larger U values (rightmost panel), further proceeding into the bad-metallic region, we continue to observe the peak at low transfer momenta, although with a smaller overall magnitude. The drastic difference in the momentum structure between the metallic ($U < 2.4$) and the bad-metallic ($U \geq 2.4$) regimes can be quantitatively understood in terms of the spectral representation of the charge response introduced in Eq. (1). Specifically, as explicitly illustrated in [56], the spectral weight w_l , associated with the lowest eigenvalue λ_l [responsible for the emergence of the $\mathbf{q} = (0, 0)$ peak [38]], is vanishingly small in the whole weak-coupling regime, and it obtains a sizable value only in the bad-metallic phase, explaining the sudden change in the momentum dependence of $\chi_{\mathbf{q}}^c$ observed at $U = 2.4$.

Effect on the electron-phonon vertex—After discussing the nonperturbative enhancement of the electronic charge

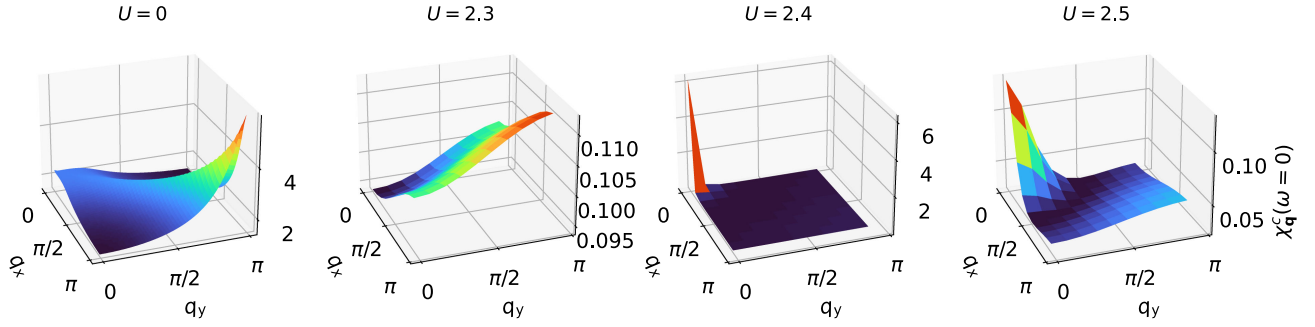


FIG. 1. Momentum dependence of the static charge susceptibility χ_q^c computed in DMFT for the 2D-Hubbard model on the square lattice for $\beta = 55.75$ and $n = 0.9966$ at the bosonic frequency $\omega = 0$ and evaluated for varying U values.

susceptibility, it is natural to pose the question of how and to what extent this phenomenon can manifest itself in the renormalization of the el-ph coupling. To this end, we consider the most simple case of optical Holstein phonons with a characteristic frequency of ω_0 and extend the Hubbard Hamiltonian by an additional interaction term with the bare, local coupling g_0 , defined as $\mathcal{H}_{\text{el-ph}} = g_0 \sum_{\mathbf{k}, \mathbf{q}} c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}} (b_{\mathbf{q}} + b_{-\mathbf{q}}^\dagger)$ where $b(b^\dagger)$ denote the bosonic annihilation (creation) operators. In the spirit of Refs. [12–14,19], we consider purely electronic corrections to the el-ph vertex linear in g_0 . In this Letter, we extend the merely electronic results of Refs. [38,43,54,55] to the renormalized el-ph coupling $\tilde{g}$ (cf. Appendix B) and derive, without additional approximations with respect to Eq. (1), an analytical expression for the dimensionless quantity $\gamma_q^\nu := \tilde{g}_q/g_0$ in terms of the on-site generalized susceptibility's eigenbasis:

$$\gamma_q^\nu \approx \sum_{\alpha} (\lambda_{\alpha}^{-1} + \beta T_{\mathbf{q}})^{-1} \tilde{w}_{\alpha}^{\nu}. \quad (2)$$

The above equation highlights the intrinsically *non-perturbative* connection between the enhancement of the $\mathbf{q} = 0$ charge response and the el-ph coupling. In fact, both quantities share the same divergence condition ($\lambda_I^{-1} \rightarrow -\beta T_{\mathbf{q}=0} = -2\beta t^2 < 0$), while only the spectral weight, $\tilde{w}_{\alpha}^{\nu}$, for the renormalized el-ph vertex gets modified with respect to that of the charge response. In fact, as explicitly shown in Appendix C, the proximity to the Mott transition, except for perfect particle-hole symmetry, will always yield a diverging compressibility *and* a strongly enhanced el-ph coupling. These arguments are based on the thermodynamic stability criteria of the Hubbard model independent of dimensionality [43,54]. Hence, they do apply but are not restricted to the DMFT data presented here.

Our DMFT results for γ_q^ν evaluated at the lowest fermionic frequency $\nu = \pi T$, obtained for the same parameter values as the charge susceptibility, are shown in Fig. 2. On the basis of Eq. (2), it is clear that the momentum differentiation between the weakly correlated metallic and

the bad metallic regimes, previously discussed for the charge susceptibility, gets also directly reflected onto the behavior of γ_q^ν . Specifically, for $U < 2.4$, an extremely reduced renormalized el-ph coupling, which is strongly suppressed $\gamma_q^{\nu=\pi T} \ll 1$ and essentially independent of the transfer momentum, is found, consistent with the conventional, gradual suppression of the charge response by increasing interactions. However, by further increasing the interaction up to $U \cong 2.4$, the renormalized el-ph vertex suddenly exhibits a huge enhancement at low transfer momenta $\mathbf{q}$. This reaches its maximum at $U = 2.4$, and then, slowly decreases with growing interaction values. Consistent with our previous discussions, we observe that this enhancement predominantly originates from the behavior of the lowest real eigenvalue λ_I of the impurity susceptibility (for details, cf. [56]), as is shown by the inset of Fig. 2, where we compare its contribution to the renormalized vertex, γ_I , with the contribution of the remaining eigenvalues, γ_R . At the same time, while the behavior of $\gamma_q^{\nu=\pi T}$ in this regime is evidently controlled by the underlying evolution of χ_q^c , we observe nonetheless a

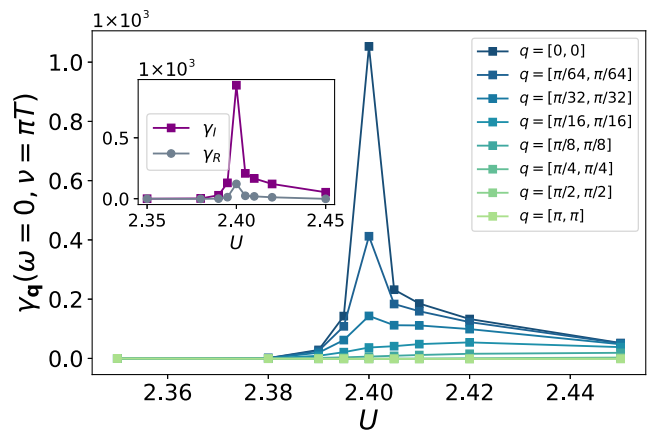


FIG. 2. Renormalized el-ph vertex $\gamma_q = \tilde{g}_q/g_0$ extracted from χ_q^c as a function of U at the lowest bosonic-fermionic frequencies at $\beta = 55.75$. Inset: Contribution of the lowest eigenvalue to γ_q (γ_I) in comparison to the contribution of the remaining eigenvalues (γ_R).

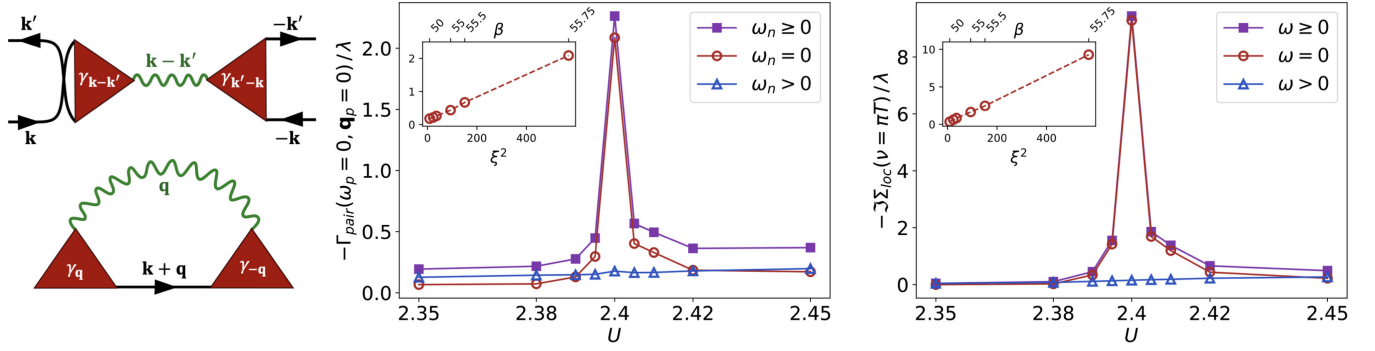


FIG. 3. Left panel: Lowest order contributions in g_0 to the phonon-mediated pairing interaction and to the electronic self-energy. Central panel: U dependence of the pairing diagram (violet) in units of λ for $\beta = 55.75$ and $\omega_0 = 0.1$, split in its contributions arising from the zero (red) and finite frequency (blue) components. Inset: Dependence of the zero-frequency contribution to the pairing diagram on the correlation length and inverse temperature. Right panel: Same plots as for the central panel, but for the self-energy corrections (see text).

relative enhancement of the renormalized el-ph coupling (with respect to the noninteracting case, where $\gamma_q^{\nu=\pi T} \equiv 1$), which is larger by 2 orders of magnitude than that for the corresponding charge response. This additional enhancement can be ascribed to the prefactor proportional to the inverse dressed DMFT bubble term $\chi_{0,q}^{\nu}$ in Eq. (B1) of Appendix B, as it gets strongly suppressed at low frequencies in the bad-metallic regime. This extra factor, required to obtain the renormalized coupling from the charge susceptibility, might have caused some contradicting interpretations in the past literature, since in the region of small but finite $\mathbf{q}$, the enhancement of $\gamma_q^{\nu=\pi T}$ can become numerically visible even *before* the corresponding increase in χ_q^c [56].

In any case, the overall similarity between γ_q^{ν} and χ_q^c in the proximity of the Mott MIT suggests that the former may display a momentum-dependence characteristic for an Ornstein-Zernike (OZ) function, which represents, in fact, a reliable parametrization for the isothermal charge compressibility computed in DMFT in the vicinity of its second-order phase transition [75]. As only $\mathcal{T}_q$ is responsible for the momentum structures of Eqs. (1) and (2), its expansion for small transfer momenta, $\mathcal{T}_q \approx t^2(2 - \frac{1}{2}\mathbf{q}^2) + \mathcal{O}(\mathbf{q}^4)$, allows us to derive an explicit expression for the correlation length of the charge response in terms of the eigenvalues of the local impurity susceptibility [56],

$$\xi^2 \simeq \frac{\sum_{\alpha} \xi_{\alpha}^2 \chi_{\alpha} w_{\alpha}}{\sum_{\alpha} \chi_{\alpha} w_{\alpha}}, \quad (3)$$

where $\chi_{\alpha} = (\lambda_{\alpha}^{-1} + \beta \mathcal{T}_{\mathbf{q}=0})^{-1}$ and $\xi_{\alpha}^2 = -(\beta t^2/2)\chi_{\alpha}$. For the renormalized el-ph vertex, we merely need to substitute $w_{\alpha} \rightarrow \tilde{w}_{\alpha}$ in Eq. (3). It is worth noting that in a first approximation close to the MIT, where the physical behaviors are dominated by the contribution of the lowest

eigenvalue λ_l , the correlation lengths of $\gamma_q^{\nu=\pi T}$ and χ_q^c become equivalent [56].

Renormalization of the electronic quantities—After addressing the effect of enhanced charge fluctuations on the el-ph coupling, we turn to analyzing the role this strong renormalization plays in the electronic system. To this end, we start by considering the effective electron-electron pairing interaction mediated by the exchange of one single phonon, taking the aforementioned vertex renormalization effects into account. The corresponding pairing diagram, depicted in the upper left panel of Fig. 3, thus can be viewed as a *perturbative* correction to the electronic scattering in the pairing up to *second order* in the bare el-ph coupling. This may provide a reasonable starting point for analyzing the regime of small, bare el-ph coupling in the presence of strong electronic correlations ($g_0 \ll U$).

For zero transfer energy and momentum in the pairing channel (i.e., $\omega_p = 0, \mathbf{q}_p = 0$), and after a change of variables in the frequency and momentum arguments, this interaction can be written as

$$\Gamma_{\text{pair}} = \frac{g_0^2}{\beta^2} \sum_{\nu\omega} \int d^2q \gamma_{-\mathbf{q}}^{-\nu,-\omega} D_0^{\omega} \gamma_{\mathbf{q}}^{\nu\omega} \quad (4)$$

$$\simeq \frac{-2g_0^2}{\omega_0\beta^2} \sum_{\nu} \int d^2q \frac{\gamma_{\mathbf{q}=0}^{\nu} \gamma_{\mathbf{q}=0}^{-\nu}}{[1 + (\xi\mathbf{q})^2]^2} + \sum_{\omega>0} \mathcal{R}(\omega), \quad (5)$$

where, in the last line, we assumed an OZ parametrization for the el-ph vertex, i.e., $\gamma_{\mathbf{q}} \propto \xi^2[1 + (\xi\mathbf{q})^2]^{-1}$ [76]. Here, $D_0^{\omega} = -2\omega_0/(\omega_n^2 + \omega_0^2)$ denotes the bare phonon propagator (with $\omega_0 = 0.1$), and $\mathcal{R}(\omega)$ is a regular function of the positive bosonic Matsubara frequencies. A quick glance at the momentum integral immediately reveals an infrared singularity for $\xi \rightarrow \infty$. This yields a divergence of Γ_{pair} that, in 2D, scales with the square of the correlation length ξ [78]. In the central panel of Fig. 3, we show our numerical

data for Γ_{pair} in units of the effective el-ph coupling strength $\lambda = (2g_0^2/\omega_0)$, evaluated using Eq. (4) as a function of U , and decompose it into the contributions arising from the static ($\omega = 0$) and dynamic ($\omega > 0$) components. We clearly observe the effect of the static contribution to the overall behavior of Γ_{pair} , namely, a prominent peak at the critical interaction value of $U = 2.4$, in contrast to a rather weak U dependence of the ($\omega > 0$) terms [79]. Moreover, we can analyze the dependence of Γ_{pair} on the correlation length by evaluating its (strongly enhanced) static contribution for different values of β (see inset of Fig. 3, central panel). As expected from the (approximated) Eq. (5), the numerical evaluation of this quantity reveals a ξ^2 dependence.

Among the several Feynman diagrams, entailing second-order corrections in g_0 to the DMFT (purely electronic) self-energy, which display the leading contribution in ξ in the proximity to the phase-separation instability [80], we focus on the one depicted in the lower left panel of Fig. 3, which was often considered in previous works [20,21,82–84] and which displays an evident diagrammatic similarity to the pairing interaction process discussed above. By following essentially the same step as for the calculations of Γ_{pair} , we get

$$\Delta\Sigma_{\mathbf{k}}^{\nu} = \frac{g_0^2}{\beta} \sum_{\omega} \int d^2q \gamma_{-\mathbf{q}}^{\nu+\omega, -\omega} G_{\mathbf{k}+\mathbf{q}}^{\nu+\omega} D_0^{\omega} \gamma_{\mathbf{q}}^{\nu\omega} \quad (6)$$

$$\cong \frac{-2g_0^2}{\omega_0\beta} \int d^2q \frac{G_{\mathbf{k}+\mathbf{q}}^{\nu} (\gamma_{\mathbf{q}=0}^{\nu})^2}{[1 + (\xi\mathbf{q})^2]^2} + \sum_{\omega>0} \mathcal{R}(\omega). \quad (7)$$

Due to the weak $\mathbf{k}$ dependence of the Green's function in the strongly correlated regime, the 2D integral will result, similarly as for Γ_{pair} , in a ξ^2 dependence. These considerations are confirmed by our numerical evaluation of Eq. (6), reported in the right panel of Fig. 3. In particular, for the sake of conciseness, we plot the local corrections to the DMFT self-energy (i.e., $\int d^2k \Delta\Sigma_{\mathbf{k}}^{\nu}$) as a function of U as well as, in the inset, its static contribution as a function of β . The former dataset indicates a huge enhancement of the el-ph corrections to the DMFT self-energy, while the latter confirms the expected ξ^2 scaling in the proximity of the nonperturbative phase-separation instability of the electronic system.

Conclusions—Our analysis, based on DMFT calculations and exact thermodynamic considerations, demonstrates that a large renormalization of an initially weak, bare el-ph coupling can be triggered by enhanced small- $\mathbf{q}$ charge fluctuations in the proximity of a Mott metal-insulator transition. This behavior contrasts the commonly expected suppression of the el-ph coupling arising from reduced charge fluctuations and the suppression of spectral weight at the Fermi surface. The intrinsically strong-coupling, nonperturbative mechanism responsible for the enhancement of the el-ph scattering identified here is

different from that active in (K-doped) BaBiO_3 , BaSbO_3 , and BaPbO_3 , where the enhancement originates instead from the long-range character of the unscreened interaction, which can be captured by *GW* and screened-hybrid-functional DFT approaches [85–87].

The enhancement of the el-ph coupling is directly reflected in a corresponding increase in the effective pairing interaction. For the single-orbital case—possibly relevant to the low-energy physics of cuprate [88–91] and nickelate superconductors [92,93]—this effect is confined to a narrow region of parameter space. The situation may, however, become substantially more favorable in multi-orbital systems [10,94–96]. In particular, we anticipate significant consequences for Hund's metals [44,97–102], where the interplay between Hund's and Hubbard interactions favors the formation of large magnetic moments in a strongly correlated yet resilient metallic phase. In this situation, DMFT-based calculations [43,103,104] show a tendency toward phase-separation instabilities in extended regions of the phase diagrams.

At the same time, the comparably large magnitude of the self-energy corrections estimated within our approach indicates that, for sufficiently large ξ , the second-order diagrammatic treatment adopted in this Letter becomes inadequate. This calls for future self-consistent investigations of the Hubbard-Holstein problem [16–18,22,28,29,105–107], for instance, based on diagrammatic extensions of DMFT [108].

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Data availability—The data that support the findings of this article are openly available [58].

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End Matter

Appendix A: Spectral representation of the generalized susceptibility in DMFT—The calculation of Bethe-Salpeter equations (BSEs) in DMFT is based on the assumption of locality of its kernel, i.e., the irreducible vertex function Γ [74,109]. For instance, in the charge sector of our interest, one can compute the corresponding static ($\omega = 0$) generalized susceptibility $\chi_{\text{loc}}^{c,\nu\nu'}$ of the self-consistently determined AIM [74] and readily extract the associated $\Gamma_c^{\nu\nu'}$ via the (inverse) BSE [108,110,111]

$$\frac{1}{\beta^2} \Gamma_c^{\nu\nu'} = [\chi_{\text{loc}}^{c,\nu\nu'}]^{-1} - [\chi_{\text{loc}}^{0,\nu\nu'}]^{-1}, \quad (\text{A1})$$

where the local bubble term is defined as $\chi_0^{\nu\nu'} = -2\beta G(\nu)G(\nu)\delta_{\nu\nu'}$, $G(\nu)$ being the local one-particle Green's function. We recall here that the physical impurity charge response can be obtained from the generalized quantity via

$$\chi_{\text{loc}}^c = \frac{1}{\beta^2} \sum_{\nu\nu'} \chi_{\text{loc}}^{c,\nu\nu'} = \sum_{\alpha} \lambda_{\alpha} w_{\alpha}, \quad (\text{A2})$$

where, in the last equality, we have decomposed the susceptibility in its spectral representation with eigenvalues λ_{α} and eigenvectors V_{α}^{ν} constituting the spectral weights $w_{\alpha} = [\sum_{\nu} V_{\alpha}^{\nu}][\sum_{\nu'} V_{\alpha}^{\nu'}]^{-1}$ [34,37].

Having determined Γ_c , the physical charge susceptibility of the lattice can be obtained from the momentum-dependent BSE,

$$\chi_{\mathbf{q}}^c = \frac{1}{\beta^2} \sum_{\nu\nu'} \left\{ [\chi_{0,\mathbf{q}}^{\nu\nu'}]^{-1} + \frac{1}{\beta^2} \Gamma_c^{\nu\nu'} \right\}^{-1}, \quad (\text{A3})$$

where the momentum-dependent bubble susceptibility is defined as $\chi_{0,\mathbf{q}}^{\nu\nu'} = -2\beta \sum_{\mathbf{k}} G_{\mathbf{k}}^{\nu} G_{\mathbf{k}+\mathbf{q}}^{\nu'} \delta_{\nu\nu'}$, with $G_{\mathbf{k}}^{\nu}$ being the

dressed DMFT Green's function. Plugging Eq. (A1) into Eq. (A3), one obtains the following expression [74]:

$$\chi_{\mathbf{q}}^c = \frac{1}{\beta^2} \sum_{\nu\nu'} \left\{ [\chi_{\text{loc}}^{c,\nu\nu'}]^{-1} + ([\chi_{0,\mathbf{q}}^{\nu\nu'}]^{-1} - [\chi_{\text{loc}}^{0,\nu\nu'}]^{-1}) \right\}^{-1}. \quad (\text{A4})$$

In the notable case of the infinite-dimensional Bethe lattice, the expression for the inverse bubble differences for the uniform and the staggered ordering vector $\mathbf{Q} = (0, 0, 0, \dots)$ and $\mathbf{Q} = (\pi, \pi, \pi, \dots)$ can be expressed analytically [38,74],

$$[\chi_{\mathbf{Q}}^{0,\nu\nu'}]^{-1} - [\chi_{\text{loc}}^{0,\nu\nu'}]^{-1} = \pm \frac{t^2}{2\beta} \delta_{\nu\nu'}, \quad (\text{A5})$$

where the plus and minus signs are associated with the uniform and staggered response functions, respectively. Since this expression is real valued and constant in the fermionic frequency space, the BSE of Eq. (A4) (for $\mathbf{q} = 0$) can be recast in the eigenbasis of the local charge susceptibility defined in Eq. (A2) [38,54,55]:

$$\chi_{\mathbf{q}=0}^c = \sum_{\alpha} \left(\lambda_{\alpha}^{-1} + \frac{\beta t^2}{2} \right)^{-1} w_{\alpha}. \quad (\text{A6})$$

Note that $\chi_{\mathbf{q}=0}^c$ can diverge if the smallest eigenvalue $\lambda_I^{-1} \rightarrow -\beta t^2/2$ unless, for symmetry reasons, w_I vanishes [e.g., for perfect particle-hole].

In the case of the 2D square lattice studied here, Eq. (A5) can be used, however, as an approximation by replacing t^2 with an effective $\mathcal{T}_{\mathbf{q}}$ term:

$$\beta^2 ([\chi_{\mathbf{q}}^{0,\nu\nu'}]^{-1} - [\chi_{\text{loc}}^{0,\nu\nu'}]^{-1}) = \beta \mathcal{T}_{\mathbf{q}}(\nu) \delta_{\nu\nu'} \approx \beta \mathcal{T}_{\mathbf{q}} \delta_{\nu\nu'}, \quad (\text{A7})$$

where now, in contrast to Refs. [38,43,54,55,112], we extend the derivation to general transfer momenta $\mathbf{q}$. Using

the above approximation in Eq. (A6), we arrive at Eq. (1) of the main text.

Importantly, the relatively large self-energy in the strong coupling limit allows a high frequency expansion of Eq. (A7) [56], resulting in the following compact expression for $\mathcal{T}_{\mathbf{q}}$:

$$\mathcal{T}_{\mathbf{q}} \approx t^2 [\cos(q_x) + \cos(q_y)]. \quad (\text{A8})$$

The above equation quantitatively captures how the sign flip of $\mathcal{T}_{\mathbf{q}}$ from $\mathbf{q} = (0, 0, \dots)$ to $\mathbf{q} = (\pi, \pi, \dots)$ occurs. Additionally, as it yields a real and frequency-independent function, it justifies employing Eq. (A7) in the strong coupling regime for the quantitative analyses of the main text.

Appendix B: Spectral representation of the renormalized electron-phonon coupling in DMFT—The renormalized electron-phonon vertex function is defined as the ratio between the renormalized and bare coupling [56]:

$$\gamma_{\mathbf{q}}^{\nu} = \tilde{g}_{\mathbf{q}}^{\nu}/g_0 = [\chi_{0,\mathbf{q}}^{\nu}]^{-1} \sum_{\nu'} \chi_{\mathbf{q}}^{c,\nu\nu'}. \quad (\text{B1})$$

We show here that, similarly to the lattice response function, the quantity of interest in our Letter, $\gamma_{\mathbf{q}}$, also can be expressed in the eigenbasis of the local susceptibility within the DMFT approach. Starting from the generalized momentum-dependent susceptibility in this eigenbasis,

$$\chi_{\mathbf{q}}^{c,\nu\nu'} \cong \beta^2 \sum_{\alpha} V_{\alpha}(\nu) (\lambda_{\alpha}^{-1} + \beta \mathcal{T}_{\mathbf{q}})^{-1} V_{\alpha}^{-1}(\nu'), \quad (\text{B2})$$

one can obtain the corresponding expression for the renormalized coupling by inserting Eq. (B2) in Eq. (B1),

$$\begin{aligned} \gamma_{\mathbf{q}}^{\nu} &\cong \beta^2 \sum_{\alpha,\nu'} (\chi_{0,\mathbf{q}}^{\nu})^{-1} V_{\alpha}(\nu) (\lambda_{\alpha}^{-1} + \beta \mathcal{T}_{\mathbf{q}})^{-1} V_{\alpha}^{-1}(\nu') \\ &= \sum_{\alpha} (\lambda_{\alpha}^{-1} + \beta \mathcal{T}_{\mathbf{q}})^{-1} \tilde{w}_{\alpha}^{\nu}, \end{aligned} \quad (\text{B3})$$

with $\tilde{w}_{\alpha}^{\nu} = \beta^2 (\chi_{0,\mathbf{q}}^{\nu})^{-1} V_{\alpha}(\nu) \sum_{\nu'} V_{\alpha}^{-1}(\nu')$ denoting the modified spectral weight.

Appendix C: Thermodynamic stability and its general consequences—The thermodynamic stability for the Hubbard model with interaction U is determined by the following conditions [43,54]:

$$\frac{\partial n}{\partial \mu} > 0, \quad -\frac{\partial n}{\partial \mu} \frac{\partial D}{\partial U} - \left[\frac{\partial n}{\partial U} \right]^2 > 0. \quad (\text{C1})$$

Here, n is the total density of the system, and $D = \langle n_{\uparrow} n_{\downarrow} \rangle$ denotes the double occupation. Of particular interest is the static ($\omega = 0$) charge response of the

system, which can be obtained from the corresponding generalized one, $\chi_{kk'\mathbf{q}}^c [k = (\nu, \mathbf{k})]$, via

$$\chi_{\mathbf{q}}^c = \frac{1}{\beta^2} \sum_{kk'} \chi_{kk'\mathbf{q}}^c = \sum_{\alpha} \lambda_{\mathbf{q}}^{\alpha} w_{\mathbf{q}}^{\alpha}, \quad (\text{C2})$$

where the last equality, differently from Appendix A, now represents the eigendecomposition of the *exact* lattice response function with (momentum-dependent) eigenvalues $\lambda_{\mathbf{q}}^{\alpha}$ and eigenvectors $V_{k\mathbf{q}}^{\alpha}$ associated with the corresponding spectral weights $w_{\mathbf{q}}^{\alpha} = [(1/\beta) \sum_k V_{k\mathbf{q}}^{\alpha}] \times [(1/\beta) \sum_{k'} V_{k'\mathbf{q}}^{\alpha-1}]$. While the isothermal compressibility is directly related to the physical charge susceptibility, $\partial n / \partial \mu = 2\chi_{\mathbf{q}}^c$, the other thermodynamic derivatives of Eq. (C1), $dn/dU := \partial n / \partial U|_{\mu}$ and $dD/dU := \partial D / \partial U|_{\mu}$, can be obtained from [43,54]

$$\frac{dn}{dU} = \frac{1}{\beta} \sum_{k\sigma} \frac{dG_{k\sigma}}{dU} \quad (\text{C3})$$

$$\frac{dD}{dU} = -\frac{D}{U} + \frac{1}{2U} \frac{1}{\beta} \sum_{k\sigma} [i\nu + \mu - \epsilon_{\mathbf{k}}] \frac{dG_{k\sigma}}{dU}, \quad (\text{C4})$$

where the derivative of the Green's function with respect to the Hubbard interaction can be directly related to the generalized charge susceptibility [43,54]:

$$\sum_{\sigma} \frac{dG_{k\sigma}}{dU} = \frac{1}{\beta} \sum_{k'} \chi_{kk'\mathbf{q}=0}^c \left(-\frac{\partial \Sigma_{k'}}{\partial U} \Big|_G \right). \quad (\text{C5})$$

The above equations precisely highlight how the Mott transition, where the double occupancy D becomes discontinuous as a function of U with a divergence of (dD/dU) at the critical endpoint of the transition, is fundamentally related to the static, uniform charge response of the system. In fact, the only singular contribution in Eqs. (C3) and (C4) originates from Eq. (C5). In turn, at finite T , such a singularity can be driven only by a divergent eigenvalue $\lambda_{\mathbf{q}=0}^{\alpha}$ of $\chi_{kk'\mathbf{q}=0}^c$, and hence, except for perfect particle-hole symmetry, by a corresponding divergence of $\chi_{\mathbf{q}=0}^c$ [cf. Eq. (C2)].

Here, we will derive the intrinsic relation linking the Mott transition and the el-ph coupling renormalization. For this, we consider a general bare coupling g_0^{kq} , for which its renormalized counterpart g^{kq} can be extracted from the generalized susceptibility of Eq. (C2),

$$\begin{aligned} g^{kq} &= (\chi_0^{kq})^{-1} \sum_{k'} \chi_{kk'\mathbf{q}}^c g_0^{k'q} \\ &= \sum_{\alpha} \lambda_{\mathbf{q}}^{\alpha} (\chi_0^{kq})^{-1} V_{k\mathbf{q}}^{\alpha} \sum_{k'} V_{k'\mathbf{q}}^{\alpha-1} g_0^{k'q} := \sum_{\alpha} g_{\alpha}^{kq}. \end{aligned} \quad (\text{C6})$$

Defining $V_{k'q}^{\alpha,-1} g_0^{k'q} := \tilde{V}_{k'q}^\alpha$, $-(\partial \Sigma_{k'}/\partial U)|_G := S_{k'}$, and by inserting $\mathbb{1} = \chi_0^{kq=0} (\chi_0^{kq=0})^{-1}$ and $\mathbb{1} = \sum_{k''} \tilde{V}_{k''q=0}^\alpha \times (\sum_{k''} \tilde{V}_{k''q=0}^\alpha)^{-1}$, we can rewrite Eq. (C5) in terms of the renormalized coupling of Eq. (C6),

$$\sum_\sigma \frac{dG_{k\sigma}}{dU} = \frac{1}{\beta} \sum_\alpha \chi_0^{kq=0} g_\alpha^{kq=0} \tilde{\sigma}_\alpha^{q=0}, \quad (C7)$$

where $\tilde{\sigma}_\alpha^{q=0} = (\sum_{k''} \tilde{V}_{k''q=0}^\alpha)^{-1} \sum_{k'} \tilde{V}_{k'q=0}^\alpha S_{k'}$. Here, we assume that particle-hole symmetry or other special symmetry constraints do not apply, such that $\sum_{k''} \tilde{V}_{k''q=0}^\alpha \neq 0$.

The extension of this important result to the more general case of a multiorbital Hubbard Hamiltonian is straightforward. To that end, we now consider a general, multiorbital electron-phonon coupling $g_{0,ab}^{kq}$, renormalized via

$$\begin{aligned} g_{ab}^{kq} &= \sum_{k',cdef} (\chi_{0,cdba}^{kq})^{-1} \chi_{cdef}^{c,kk'q} g_{0,ef}^{kq} \\ &= \sum_\alpha \lambda_q^\alpha \sum_{k',cdef} (\chi_{0,cdba}^{kq})^{-1} V_{kq,cd}^\alpha \tilde{V}_{k'q,ef}^\alpha := \sum_\alpha g_{\alpha,ab}^{kq}, \end{aligned} \quad (C8)$$

with $\tilde{V}_{k'q,ef}^\alpha = V_{k'q,ef}^{\alpha,-1} g_{0,fe}^{k'q}$. Following the same steps as for Eq. (C7), we obtain

$$\begin{aligned} \frac{dG_{k,ab}}{dU} &= \frac{1}{\beta} \sum_{k'cd} \chi_{abcd}^{c,kk'q=0} \left(\frac{-\partial \Sigma_{k',cd}}{\partial U} \Big|_G \right) \\ &= \frac{1}{\beta} \sum_{\alpha,ef} \chi_{0,abef}^{kq=0} g_{\alpha,ef}^{kq=0} \sigma_\alpha^{q=0}, \end{aligned} \quad (C9)$$

where we define $\sigma_\alpha^{q=0} := (\sum_{k'',gh} \tilde{V}_{k''q=0,gh}^\alpha)^{-1} \times \sum_{k',cd} \tilde{V}_{k'q=0,cd}^\alpha ((-\partial \Sigma_{k',cd}/\partial U)|_G)$.

With Eqs. (C7) and (C9), we derive an *exact* connection, generally valid also beyond DMFT, between the renormalized electron-phonon coupling and the thermodynamic stability criteria of the (multiorbital) Hubbard model. In particular, we show that the proximity to a Mott MIT, associated with a diverging dD/dU , will, except for peculiar high-symmetry cases, necessarily lead to a divergence of $dn/d\mu$ as well as of the renormalized electron-phonon coupling *independent* of the dimensionality of the system.