

Analytical expression for π -ton vertex contributions to the optical conductivity

Juraj Kršnik,^{1,2*} Anna Kauch,¹ and Karsten Held¹

¹ Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

² Department for Research of Materials under Extreme Conditions, Institute of Physics, HR-10000 Zagreb, Croatia

* juraj.kršnik@tuwien.ac.at

Abstract

Vertex corrections from the transversal particle-hole channel, so-called π -tons, are generic in models for strongly correlated electron systems and can lead to a displaced Drude peak (DDP). Here, we derive the analytical expression for these π -tons, and how they affect the optical conductivity as a function of correlation length ξ , fermion lifetime τ , temperature T , and coupling strength to spin or charge fluctuations g . In particular, for $T \rightarrow T_c$, the critical temperature for antiferromagnetic or charge ordering, the dc vertex correction is algebraic $\sigma_{VERT}^{dc} \propto \xi \sim (T - T_c)^{-\nu}$ in one dimension and logarithmic $\sigma_{VERT}^{dc} \propto \ln \xi \sim \nu \ln(T - T_c)$ in two dimensions. Here, ν is the critical exponent for the correlation length. If we have the exponential scaling $\xi \sim e^{1/T}$ of an ideal two-dimensional system, the DDP becomes more pronounced with increasing T but fades away at low temperatures where only a broadening of the Drude peak remains, as it is observed experimentally. Further, we find the maximum of the DPP to be given by the inverse lifetime: $\omega_{DDP} \sim 1/\tau$. These characteristic dependencies can guide experiments to evidence π -tons in actual materials.

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23 1 Introduction

24 The phenomenon of a displaced Drude peak (DDP) in metallic systems, characterized by a
 25 maximum in the optical absorption at a finite frequency (unlike in normal metals where the
 26 maximum occurs at zero frequency), has been observed over the past few decades across a
 27 diverse range of compounds including cuprates, transition metal oxides, organic conductors,
 28 and Kagome metals [1–23]. Despite the variety of these materials, a universal experimental
 29 feature is that the DDP frequency is an increasing function of temperature, $\omega_{DDP} \sim T^\alpha$, with
 30 the coefficient α in the range $0 < \alpha < 3/2$ [24]. This striking universal temperature depen-
 31 dence immediately raises an important question: Is there a microscopic mechanism common
 32 to all these materials that gives rise to a displaced Drude peak? In addressing this question,
 33 it is important to note the key similarities that these materials share: they are predominantly
 34 strongly correlated electron systems, many showing effectively two-dimensional (2D) physics
 35 and hosting strong spin and/or charge fluctuations.

36 Although several theories have been proposed in the past decade to explain the mecha-
 37 nism behind the Drude peak displacement on a broader level [24–27], our understanding of
 38 the phenomenon remains relatively limited. For example, Ref. [25] explains it in terms of the
 39 hydrodynamics of short-range quantum critical fluctuations of incommensurate density wave
 40 order. Another established scenario involves the transient localization mechanism [27], which
 41 originates from quantum localization corrections due to slow phononic fluctuations [24] or
 42 charge fluctuations mediated by long-range Coulomb interaction coexisting with lattice frus-
 43 tration [26] in low-dimensional systems. More recently, however, a novel mechanism involving
 44 π -ton vertex contributions [28–31] has been identified as another potential cause of the Drude
 45 peak displacement [32].

46 The significance of π -ton vertex contributions in shaping the optical spectrum of 2D cor-
 47 related electron systems was first emphasized in Refs. [28–30] for a variety of different mod-
 48 els of strongly correlated electron systems. These works provide a comprehensive analysis
 49 of different vertex contributions in correlated electron systems based on the two-particle re-
 50 ducibility, which was possible due to recent methodological advances in using the parquet
 51 equations [33–35] within the dynamical vertex approximation (D Γ A) [36–38] and the parquet
 52 approximation [33]. In particular, it was observed that the dominant vertex contributions in
 53 prototypical models of strongly correlated electrons originate from the transversal particle-hole
 54 ($p\bar{h}$) channel. Despite the negligibly small transfer momentum of the photon, these vertex con-
 55 tributions can pick up bosonic fluctuations at an arbitrary wave vector, and in particular strong

antiferromagnetic (AFM) or charge density wave fluctuations at $\mathbf{k} - \mathbf{k}' \approx (\pi, \pi, \dots)$ associated with correlated systems, thus the name π -tons [29]. The aforementioned vertex contributions from quantum localization, in contrast, emerge from the particle-particle (pp) channel.

Shortly after the numerical papers [28–30], π -tons were investigated in the simplified random phase approximation (RPA) [31, 32, 39, 40]. These studies sought to better understand the behavior of π -ton vertex contributions in the weakly correlated regime of the Hubbard model across a broader temperature range, particularly near the paramagnetic-to-antiferromagnetic transition boundary. While it was first reported in Ref. [31] that the RPA π -ton vertex contributions are small compared to the bubble contribution in the 2D case, in Refs. [39, 40] their nonnegligible contributions were recognized in one-dimensional (1D) systems until finally it was realized in Ref. [32] that they may lead to the DDP. Specifically, it was shown that, in the 1D case close to the paramagnetic-to-antiferromagnetic transition, the coupling of strong AFM fluctuations via the RPA π -ton vertex contributions to low-energy quasiparticle excitations shifts the Drude peak to a finite frequency [32]. Similar qualitative features were observed in the 2D case, but the magnitude of the π -ton vertex contributions was orders of magnitude smaller than in 1D, resulting in only a broadening of the Drude peak. It is important to note, however, that the study in Ref. [32] was purely numerical, and achieving convergence of the π -ton vertex contributions in the 2D case near the transition boundary proved to be a formidable task.

Building on these findings, in this paper, we further investigate the impact of π -tons in 2D systems with strong AFM fluctuations by conducting an analytical evaluation of the π -ton vertex contributions and by leveraging the cuba package [41] for adaptive integration. The analytical approach allows us to examine π -ton vertex contributions arbitrarily close to the transition boundary, while the improved adaptive integration (compared to Ref. [32]) enables us to benchmark our analytical results over a broader temperature range. To accomplish this, we are taking only the basic ingredients required to obtain the DDP via π -tons as noted in Ref. [32]: (i) low-energy fermionic quasiparticle excitations described by Green's function [42]

$$G(\mathbf{k}, i\nu_m) = \frac{1}{i\nu_m - \varepsilon_{\mathbf{k}} + \frac{i}{2\tau} \text{sgn } \nu_m}, \quad (1)$$

and (ii) AFM fluctuations resembling the Ornstein-Zernike form [43–45]

$$\chi_{\text{OZ}}(\mathbf{q}, i\omega_m) \sim \frac{A}{\xi^{-2} + (\mathbf{q} - \mathbf{Q})^2 + \lambda |\omega_m|}, \quad (2)$$

with $\mathbf{Q} = (\pi, \pi, \dots)$. In the following, we adopt the notation $G^{e/h}(\mathbf{k}, i\nu_m) \equiv \frac{1}{i\nu_m - \varepsilon_{\mathbf{k}} \pm \frac{i}{2\tau}}$, associated with the propagation of an electron and a hole with $\nu_n > 0$ and $\nu_n < 0$, respectively. Furthermore, we assume a D -dimensional half-filled hypercubic lattice with N sites and only the nearest-neighbor hoppings t , for which the electron dispersion equals $\varepsilon_{\mathbf{k}} = -2t \sum_{i=1}^D \cos(k_i)$. We set $t \equiv 1$ as the unit of energy, as well as $\hbar \equiv 1$, $k_B \equiv 1$, electric charge $e \equiv 1$, and lattice constant $a \equiv 1$. For the fermion lifetime τ , we assume the quadratic-in-temperature Fermi liquid form [42] $\tau^{-1} \sim a + bT^2$, where the constant term may originate from impurity or some other source of scattering.

With $G(\mathbf{k}, i\nu_m)$ fully specified, we can further evaluate the Lindhard function and with it the RPA π -ton vertex function, assuming a Hubbard repulsion $U \leq 2$ between fermions [31]. We then seek the paramagnetic-to-antiferromagnetic transition temperature T_c by identifying the temperature at which the vertex function (proportional to magnetic susceptibility) diverges. Finally, for temperatures $T > T_c$, we can fit the vertex function calculated in RPA to the Ornstein-Zernike form for obtaining the temperature dependence of the parameters ξ , A , and λ , giving us all the necessary quantities to evaluate π -ton vertex contributions to the optical conductivity. This whole procedure for $U = 2$ in the 1D case and for $U = 1.9$ in the

100 2D case with $\tau^{-1} = 0.1547 + 1.637 T^2$ has been already carried out in Refs. [32] and [31],
 101 respectively. Here, we instead use these fitted temperature dependencies and substitute them
 102 in the analytical expression for π -tons to (i) perform benchmark calculations against numeri-
 103 cal results, and (ii) investigate scenarios with the Drude peak displacement in 2D. Please note
 104 that while our present consideration specifically considers AFM fluctuations in the π -ton ver-
 105 tex contributions, these fluctuations can actually be of any origin, e.g., also stem from charge
 106 fluctuations, provided they are well described by the Ornstein-Zernike form in Eq. (2).

107 The paper is structured as follows: In Sec. 2.1, we recall the evaluation of the Drude optical
 108 conductivity from the bubble contribution, prior to the evaluation of the π -ton vertex contri-
 109 butions in Sec. 2.2. In Sec. 3, we first discuss general qualitative features of the analytically
 110 obtained π -ton vertex contributions, after which in Sec. 3.1 we benchmark our analytical re-
 111 sults with the results of the adaptive integration in 1D and 2D. We present our key findings on
 112 the potential pathways to the DDP in the presence of π -tons in 2D systems in Sec. 3.2. Lastly,
 113 we compare the π -ton vertex contributions to the (quantum) localization vertex contributions
 114 in Sec. 3.3, before concluding our findings in Sec. 4.

115 2 Analytical evaluation of the optical conductivity

116 2.1 Bubble contribution

117 Since similar concepts will be applied in calculating the π -ton vertex contributions, we first
 118 recall the textbook derivation [42] of the Drude optical conductivity [46, 47] from the bubble
 119 (BUB) contribution to the current-current correlation function. In terms of the fermion Green's
 120 functions $G(\mathbf{k}, i\nu_m)$, fermion velocity $v_{\mathbf{k}} = \frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}}$ [48], and temperature $T(\beta^{-1})$, the latter can
 121 be expressed in the long-wavelength limit $\mathbf{q} \rightarrow 0$ as [31]

$$\chi_{BUB}(i\omega_n) = -\frac{2}{\beta N} \sum_{i\nu_m} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 G(\mathbf{k}, i\nu_m) G(\mathbf{k}, i\nu_m + i\omega_n). \quad (3)$$

122 where we consider $\omega_n \geq 0$. This implies $\omega_n > -\nu_m > 0$, since otherwise two electrons or two
 123 holes would be created by an incident photon. In particular, $G(\mathbf{k}, i\nu_m) \equiv G^h(\mathbf{k}, i\nu_m)$ describes
 124 the propagation of a hole, while $G(\mathbf{k}, i\nu_m + i\omega_n) \equiv G^e(\mathbf{k}, i\nu_m + i\omega_n)$ the propagation of an
 125 electron, see the left-hand side of Fig. 1.

126 Fermions in the vicinity of the Fermi surface (FS) contribute the most to the current fluctu-
 127 ations. For that reason, we replace the momentum summation in Eq. (3) by an energy integral
 128 in which the fermion density of states g is approximated by a constant, i.e., the value at the
 129 Fermi level $g(\varepsilon_F)$ [42]

$$\frac{1}{N} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 u_{\mathbf{k}} = \int_{-\infty}^{+\infty} v^2(\varepsilon) g(\varepsilon) u(\varepsilon) d\varepsilon \approx g(\varepsilon_F) \langle v^2 \rangle_{FS} \int_{-\infty}^{+\infty} u(\varepsilon) d\varepsilon, \quad (4)$$

130 with $\langle v^2 \rangle_{FS}$ being the fermion velocity averaged over the Fermi surface, holding for an arbitrary
 131 function $u_{\mathbf{k}}$. This further gives, see Appendix A for details on the integral evaluation:

$$\begin{aligned}
\chi_{BUB}(i\omega_n) &= -\frac{2}{\beta} g(\varepsilon_F) \langle v^2 \rangle_{FS} \sum_{\omega_n > -\nu_m > 0} \int_{-\infty}^{+\infty} d\varepsilon \left[\frac{1}{i\omega_n + i\nu_m - \varepsilon + \frac{i}{2\tau}} \right] \left[\frac{1}{i\nu_m - \varepsilon - \frac{i}{2\tau}} \right] \\
&= -\frac{2}{\beta} g(\varepsilon_F) \langle v^2 \rangle_{FS} \frac{2\pi i}{i\omega_n + \frac{i}{\tau}} \sum_{\omega_n > -\nu_m > 0} 1 = -2g(\varepsilon_F) \langle v^2 \rangle_{FS} \frac{1}{i\omega_n + \frac{i}{\tau}} i \frac{2\pi n}{\beta} \\
&= -2g(\varepsilon_F) \langle v^2 \rangle_{FS} \frac{i\omega_n}{i\omega_n + \frac{i}{\tau}},
\end{aligned} \tag{5}$$

132 where we note that the sum over ν_m in the second row gave the index n of the Matsubara
133 frequency ω_n . Analytic continuation, $i\omega_n \rightarrow \omega + i0^+$, now readily yields

$$\chi_{BUB}(\omega) = -2g(\varepsilon_F) \langle v^2 \rangle_{FS} \frac{\omega}{\omega + \frac{i}{\tau}}, \quad \text{and} \quad \text{Im}\chi_{BUB}(\omega) = 2g(\varepsilon_F) \langle v^2 \rangle_{FS} \tau \frac{\omega}{1 + \omega^2 \tau^2}. \tag{6}$$

134 Since the optical conductivity is given in terms of the current-current correlation function on
135 the real frequency axis as $\sigma(\omega) = \frac{\text{Im}\chi(\omega)}{\omega}$ [31], we recover the Drude result

$$\sigma_{BUB}(\omega) = \frac{\sigma_{BUB}^{dc}}{1 + \omega^2 \tau^2}, \tag{7}$$

136 where we have identified $\sigma_{BUB}^{dc} \equiv 2g(\varepsilon_F) \langle v^2 \rangle_{FS} \tau$. For the practical purposes of this paper,
137 we obtain σ_{BUB}^{dc} by performing adaptive integration of the bubble contribution on the real
138 frequency axis, as outlined in Ref. [31].

139 2.2 π -ton vertex contributions

140 The total vertex (VERT) contribution to the current-current correlation function reads

$$\begin{aligned}
\chi_{VERT}(\mathbf{q}, i\omega_n) &= -\frac{2}{(\beta N)^2} \sum_{i\nu_m, i\nu_{m'}} \sum_{\mathbf{k}, \mathbf{k}'} v_{\mathbf{k}, \mathbf{q}} v_{\mathbf{k}', -\mathbf{q}} G(\mathbf{k}, i\nu_m) G(\mathbf{k} + \mathbf{q}, i\nu_m + i\omega_n) \\
&\quad \times G(\mathbf{k}', i\nu_{m'}) G(\mathbf{k}' + \mathbf{q}, i\nu_{m'} + i\omega_n) F_d(\mathbf{k}, \mathbf{k}', \mathbf{q}, i\nu_m, i\nu_{m'}, i\omega_n),
\end{aligned} \tag{8}$$

141 whose evaluation requires knowledge of the full density component of the two-particle vertex
142 $F_d(\mathbf{k}, \mathbf{k}', \mathbf{q}, i\nu_m, i\nu_{m'}, i\omega_n)$ [35, 49]. Assuming the predominance of the π -ton vertex contribu-
143 tions, it is, however, reasonable to approximate the entire density component using only the
144 $p\hbar$ contribution $F_d(\mathbf{k}, \mathbf{k}', \mathbf{q}, i\nu_m, i\nu_{m'}, i\omega_n) \approx F_{d, p\hbar}(\mathbf{k}, \mathbf{k}', \mathbf{q}, i\nu_m, i\nu_{m'}, i\omega_n)$.

145 Within the RPA framework, the vertex function $F_{d, p\hbar}(\mathbf{k}, \mathbf{k}', \mathbf{q}, i\nu_m, i\nu_{m'}, i\omega_n)$ can be fur-
146 ther simplified, as the RPA π -ton vertex function depends only on a single transfer momen-
147 tum/energy, $F_{d, p\hbar}(\mathbf{k}, \mathbf{k}', \mathbf{q}, i\nu_m, i\nu_{m'}, i\omega_n) \equiv F_{p\hbar}(\mathbf{k}' - \mathbf{k}, i\nu_{m'} - \nu_m)$ [31, 32, 39, 40]. Further, close
148 to the paramagnetic-to-antiferromagnetic phase transition, the π -ton vertex function can be
149 well approximated with the Ornstein-Zernike form [31, 32]

$$F_{p\hbar}(\mathbf{k}' - \mathbf{k}, i\nu_{m'} - i\nu_m) \approx F_{OZ}(\mathbf{k}' - \mathbf{k}, i\nu_{m'} - i\nu_m) = \frac{A}{\xi^{-2} + (\mathbf{k}' - \mathbf{k} - \mathbf{Q})^2 + \lambda |\nu_{m'} - \nu_m|}, \tag{9}$$

150 with $\mathbf{Q} = (\pi, \pi, \dots)$ corresponding to the strong AFM fluctuations. Here, ξ is the AFM correla-
151 tion length, λ represents the damping of AFM fluctuations, while $A \sim g^2$ contains the coupling
152 strength g of fermions to AFM fluctuations. Considering the momentum and frequency charac-
153 teristics of F_{OZ} , it is evident that the π -ton contributions are most significant when the energy

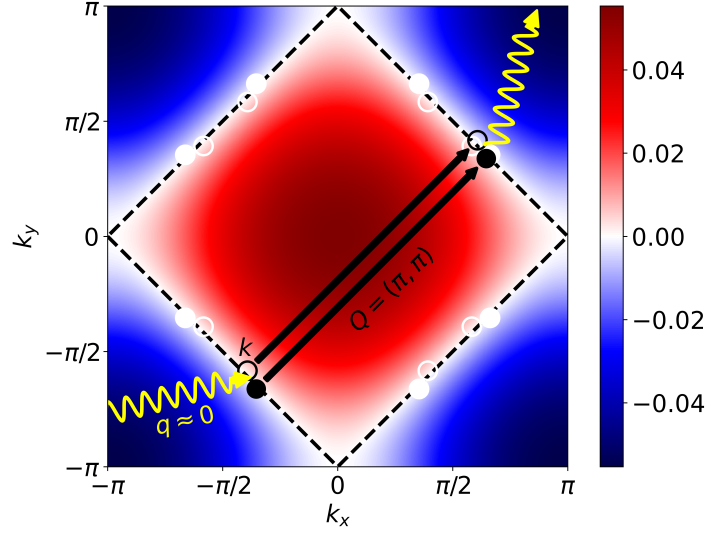


Fig. 1: Sketch of the dominant π -ton process for the case with weakly interacting fermions on a half-filled square lattice. The yellow wiggled line denotes the incoming (and outgoing) photon with the transfer momentum $\mathbf{q} \approx 0$, which excites an electron-hole pair represented by the full and empty black circles, respectively. The excited hole (electron) with wave vector \mathbf{k} ($\mathbf{k} + \mathbf{q}$) is scattered via antiferromagnetic fluctuations with wave vector $\mathbf{Q} = (\pi, \pi)$ (black arrows) across the Fermi surface (black dashed line) forming a second electron-hole pair that eventually recombines to emit the outgoing photon. The full (empty) white circles show the equivalent eightfold symmetric electron-like (hole-like) states. The red (blue) color region denotes hole-like (electron-like) states.

154 transfer is approximately zero, i.e., $\nu_{m'} - \nu_m \approx 0$, and the momentum transfer is close to \mathbf{Q} , i.e.,
 155 $\mathbf{k}' - \mathbf{k} \approx \mathbf{Q}$. Thus, it is convenient to rewrite Eq. (8) with a change of variables $\mathbf{k}' = \mathbf{k} + \mathbf{Q} + \tilde{\mathbf{q}}$,
 156 yielding

$$\chi_{VERT}(i\omega_n) = -\frac{2}{(\beta N)^2} \sum_{i\nu_m, i\nu_{m'}} \sum_{\mathbf{k}, \tilde{\mathbf{q}}} \nu_{\mathbf{k}} \nu_{\mathbf{k} + \mathbf{Q} + \tilde{\mathbf{q}}} G(\mathbf{k}, i\nu_m) G(\mathbf{k}, i\nu_m + i\omega_n) \quad (10)$$

$$\times G(\mathbf{k} + \mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'}) G(\mathbf{k} + \mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'} + i\omega_n) F_{OZ}(\mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'} - i\nu_m),$$

157 where we again focus only on the long-wavelength limit $\mathbf{q} \rightarrow 0$.

158 Analogously as for the bubble contribution, we evaluate in the following $\chi_{VERT}(i\omega_n)$ only
 159 for non-negative Matsubara frequencies $\omega_n \geq 0$. This implies again $\omega_n > -\nu_m > 0$, as
 160 well as $G(\mathbf{k}, i\nu_m) \equiv G^h(\mathbf{k}, i\nu_m)$, and $G(\mathbf{k}, i\nu_m + i\omega_n) \equiv G^e(\mathbf{k}, i\nu_m + i\omega_n)$. To determine the
 161 causality properties of the remaining two Green's functions in Eq. (10), we utilize the particle
 162 conservation law. With the initial assumption of $\omega_n \geq 0$, the only way to comply with the
 163 particle conservation law is to restrict $\nu_{m'}$ to $\omega_n > -\nu_{m'} > 0$, which automatically imposes
 164 $G(\mathbf{k} + \mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'}) \equiv G^h(\mathbf{k} + \mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'})$, $G(\mathbf{k} + \mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'} + i\omega_n) \equiv G^e(\mathbf{k} + \mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'} + i\omega_n)$.
 165 Following the visual representation of a dominant π -ton process depicted in Fig. 1, we note
 166 that these latter constraints on the Green's functions are feasible due to the finite scattering
 167 rate τ^{-1} which smears the fermion states around the Fermi surface. This ensures that the
 168 scattered hole (electron) is within reach of the hole-like (electron-like) states. Otherwise, the
 169 entire contribution would vanish at finite frequencies, similar to how the Drude contribution
 170 collapses to a delta function at zero frequency when there are no momentum relaxation pro-
 171 cesses.

172 In order to proceed, we note that the $\tilde{\mathbf{q}}$ dependence in Green's functions is weak in compar-
 173 ison with the $\tilde{\mathbf{q}}$ dependence of the vertex function in Eq. (9), so we keep it only in the vertex
 174 function peaked at $|\tilde{\mathbf{q}}| \approx 0$, decoupling thus the two momentum summations. Furthermore,
 175 for analogous reasons, we set $\nu_{m'} = \nu_m$ in Green's functions while retaining for now the full
 176 dependence on ν_m and $\nu_{m'}$ in the vertex function. For the π -ton vertex contributions to the
 177 current-current correlation function, we thus have for $\xi \gg 1$

$$\begin{aligned} \chi_{VERT}(i\omega_n) = & -\frac{2}{\beta^2} \sum_{\omega_n > -\nu_m, -\nu_{m'} > 0} \frac{1}{N} \sum_{\mathbf{k}} v_{\mathbf{k}} v_{\mathbf{k}+\mathbf{Q}} G^h(\mathbf{k}, i\nu_m) G^e(\mathbf{k}, i\nu_m + i\omega_n) \\ & \times G^h(\mathbf{k} + \mathbf{Q}, i\nu_m) G^e(\mathbf{k} + \mathbf{Q}, i\nu_m + i\omega_n) \frac{1}{N} \sum_{\tilde{\mathbf{q}}} F_{OZ}(\mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'} - i\nu_m). \end{aligned} \quad (11)$$

178 Lastly, we use the eightfold symmetry depicted in Fig. 1 to set $G^h(\mathbf{k} + \mathbf{Q}, i\nu_m) \rightarrow G^h(\mathbf{k}, i\nu_m)$,
 179 $G^e(\mathbf{k} + \mathbf{Q}, i\nu_m + i\omega_n) \rightarrow G^e(\mathbf{k}, i\nu_m + i\omega_n)$, and importantly $v_{\mathbf{k}+\mathbf{Q}} \rightarrow -v_{\mathbf{k}}$ in Eq. (11), leading
 180 finally to

$$\begin{aligned} \chi_{VERT}(i\omega_n) = & \frac{2}{\beta^2} \sum_{\omega_n > -\nu_m > 0} \frac{1}{N} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 [G^h(\mathbf{k}, i\nu_m)]^2 [G^e(\mathbf{k}, i\nu_m + i\omega_n)]^2 \\ & \times \sum_{\omega_n > -\nu_{m'} > 0} \frac{1}{N} \sum_{\tilde{\mathbf{q}}} F_{OZ}(\mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'} - i\nu_m). \end{aligned} \quad (12)$$

181 Just as with the bubble contribution, we use the fact that the dominant contributions to
 182 the current fluctuations come from the states at the Fermi level, allowing us to again replace
 183 the summation over \mathbf{k} with an energy integral. Using further the assumed form of the Green's
 184 function in Eq. (1), this yields

$$\begin{aligned} & \frac{1}{N} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 [G^h(\mathbf{k}, i\nu_m)]^2 [G^e(\mathbf{k}, i\nu_m + i\omega_n)]^2 \\ & \approx g(\varepsilon_F) \langle v^2 \rangle_{FS} \int_{-\infty}^{+\infty} d\varepsilon \left[\frac{1}{i\nu_m - \varepsilon - \frac{i}{2\tau}} \right]^2 \left[\frac{1}{i\nu_m + i\omega_n - \varepsilon + \frac{i}{2\tau}} \right]^2. \end{aligned} \quad (13)$$

185 This integral over ε can be readily evaluated in the complex plane, as outlined in Appendix A,
 186 resulting in

$$\int_{-\infty}^{+\infty} d\varepsilon \left[\frac{1}{i\nu_m - \varepsilon - \frac{i}{2\tau}} \right]^2 \left[\frac{1}{i\nu_m + i\omega_n - \varepsilon + \frac{i}{2\tau}} \right]^2 = -4\pi i \frac{1}{(i\omega_n + \frac{i}{\tau})^3}, \quad (14)$$

187 which indicates that the ν_m dependence in the Green's functions has again been lost, appearing
 188 only in the vertex function, giving

$$\chi_{VERT}(i\omega_n) = -\frac{8\pi i}{\beta^2} g(\varepsilon_F) \langle v^2 \rangle_{FS} \frac{1}{(i\omega_n + \frac{i}{\tau})^3} \sum_{\omega_n > -\nu_m, -\nu_{m'} > 0} \frac{1}{N} \sum_{\tilde{\mathbf{q}}} F_{OZ}(\mathbf{Q} + \tilde{\mathbf{q}}, i\nu_{m'} - i\nu_m). \quad (15)$$

189 What remains is to evaluate the summations over the Ornstein-Zernike vertex function

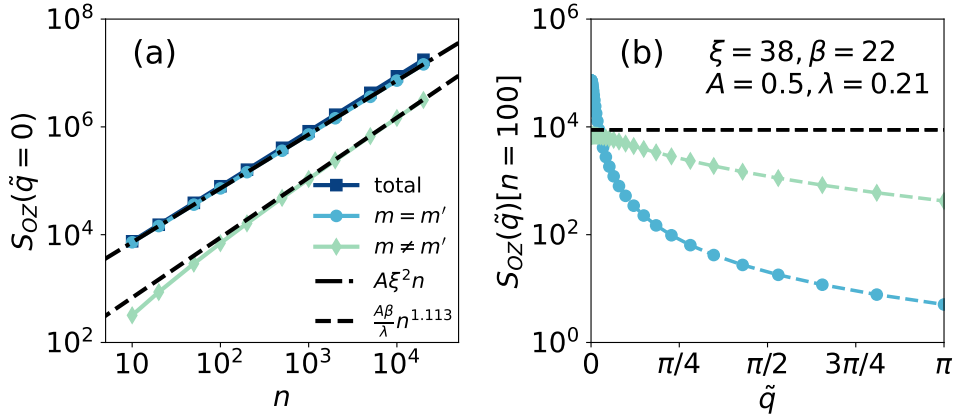


Fig. 2: (a) Total (dark blue line), diagonal $m = m'$ (light blue line), and non-diagonal $m \neq m'$ (light green line) Matsubara frequency summation contributions over the Ornstein-Zernike vertex function, Eq. (16), at $\tilde{q} = 0$ for different numbers of the largest negative Matsubara frequencies ν_m and ν'_m taken in the sums. The black dashed-dotted line represents the diagonal contribution equal to $nA\xi^2$, while the black dashed line represents the upper bound on the non-diagonal contribution of $n^c \frac{A\beta}{\lambda}$ with $c \approx 1.113$ for considered n values. (b) Momentum dependence of the diagonal, $m = m'$ (light blue), and non-diagonal, $m \neq m'$ (light green), Matsubara frequency summation contributions over the Ornstein-Zernike vertex function, summed over $n = 100$ largest negative Matsubara frequencies ν_m and ν'_m . The inverse temperature is $\beta = 22$, while the Ornstein-Zernike parameters read $\xi = 38$, $A = 0.5$, and $\lambda = 0.21$ [32].

$$\begin{aligned}
 S_{OZ} &= \frac{1}{N} \sum_{\tilde{\mathbf{q}}} \sum_{\omega_n > -\nu_m, -\nu'_m > 0} F_{OZ}(\mathbf{Q} + \tilde{\mathbf{q}}, i\nu'_m - i\nu_m) \\
 &= \frac{1}{N} \sum_{\tilde{\mathbf{q}}} \sum_{\omega_n > -\nu_m, -\nu'_m > 0} \frac{A}{\xi^{-2} + \tilde{q}^2 + \lambda |\nu'_m - \nu_m|}.
 \end{aligned} \tag{16}$$

190 We begin by addressing the Matsubara frequency sums. For this purpose, we separate the
 191 diagonal, $m = m'$, and the non-diagonal, $m \neq m'$, contributions, where for the diagonal con-
 192 tribution $S_{OZ}^{m=m'} = \frac{1}{N} \sum_{\tilde{\mathbf{q}}} \frac{A}{\xi^{-2} + \tilde{q}^2}$ trivially follows. Here, n is the number of negative Matsubara
 193 frequencies ν_m included in the sum where $|\nu_m| < \omega_n$.

194 To tackle the non-diagonal contribution, in Fig. 2(a) we plot the Ornstein-Zernike ver-
 195 tex function summed over the Matsubara frequencies ν_m and ν'_m for different numbers n of
 196 the largest negative Matsubara frequencies included in the sums for $\tilde{q} = 0$. Specifically, we
 197 present the total contribution (dark blue line), the diagonal $m = m'$ (light blue line), and the
 198 non-diagonal $m \neq m'$ contribution (light green line) for the inverse temperature $\beta = 22$ and
 199 Ornstein-Zernike parameters $\xi = 38$, $A = 0.5$, and $\lambda = 0.21$ [32]. For this set of parameters
 200 and the considered values of n , we observe that the total sum is predominantly determined by
 201 the diagonal contribution. Interestingly, however, we empirically find that in the case $\xi \gg 1$
 202 the non-diagonal contribution is bounded by $n^c \frac{A\beta}{\lambda}$ with $c \approx 1.113$, see Fig. 2(b), for the con-
 203 sidered n values. This bound is approached for $\tilde{q} = 0$ already when $n \sim 10^3$ as indicated
 204 in Fig. 2(a). The latter observation suggests that as $n \rightarrow \infty$, the non-diagonal contribution
 205 may eventually surpass the diagonal term. Nevertheless, it is important to recall that the Mat-
 206 subara frequency sums are limited by $\omega_n > -\nu_m, -\nu'_m > 0$, which restricts n to finite values.
 207 Considering the condition $\xi \gg 1$, which holds close to the paramagnetic-to-antiferromagnetic

208 transition boundary, we can then roughly estimate the relative importance of the diagonal and
 209 non-diagonal contributions by comparing $S_{OZ}^{m=m'}/n = A\xi^2$ and $S_{OZ}^{m\neq m'}/n^a \approx A\beta/\lambda$. In particu-
 210 lar, providing that $\xi \gg \sqrt{\frac{\beta}{\lambda}}$ roughly holds, we can approximate the total Matsubara frequency
 211 sums by considering only the diagonal contribution. Assuming the weak temperature depen-
 212 dence of λ [31, 32], this translates to the correlation length growing faster than $\beta^{\frac{1}{2}} = T^{-\frac{1}{2}}$.
 213 In all the subsequent cases this condition will indeed be met, so we keep only the diagonal
 214 contribution in Eq. (16), i.e., $S_{OZ} \approx S_{OZ}^{m=m'}$.

215 Let us finish the discussion about the Matsubara frequency sums by recalling again that
 216 they are restricted by $\omega_n > -\nu_m, -\nu'_m > 0$. This implies that in the evaluation of $\chi_{VERT}(i\omega_n)$
 217 for a given ω_n , n in $S_{OZ}^{m=m'}$ is the index of the corresponding bosonic Matsubara frequency,
 218 $i\omega_n = i\frac{2\pi n}{\beta}$, analogously as was the case for the bubble contribution. Taking that into account,
 219 we then have

$$\chi_{VERT}(i\omega_n) \approx -\frac{4g(\varepsilon_F)\langle v^2 \rangle_{FS}}{\beta} \frac{i\frac{2\pi n}{\beta}}{(i\omega_n + \frac{i}{\tau})^3} \frac{S_{OZ}^{m=m'}}{n} = -\frac{4g(\varepsilon_F)\langle v^2 \rangle_{FS}}{\beta} \frac{i\omega_n}{(i\omega_n + \frac{i}{\tau})^3} s_{OZ}^{m=m'}, \quad (17)$$

220 where we have introduced $s_{OZ}^{m=m'} \equiv \frac{S_{OZ}^{m=m'}}{n} = \frac{1}{N} \sum_{\tilde{\mathbf{q}}} \frac{A}{\xi^{-2} + \tilde{q}^2}$. Analytic continuation, $i\omega_n \rightarrow \omega + i\eta$,
 221 now gives

$$\chi_{VERT}(\omega) = -\frac{4g(\varepsilon_F)\langle v^2 \rangle_{FS}}{\beta} \frac{\omega}{(\omega + \frac{i}{\tau})^3} s_{OZ}^{m=m'}, \quad (18)$$

222 and correspondingly

$$\text{Im}\chi_{VERT}(\omega) = 2\frac{2g(\varepsilon_F)\langle v^2 \rangle_{FS}}{\beta} \tau^2 \frac{(3\omega^2\tau^2 - 1)\omega}{(1 + \omega^2\tau^2)^3} s_{OZ}^{m=m'}, \quad (19)$$

223 so we get for the optical conductivity $\sigma(\omega) = \frac{\text{Im}\chi(\omega)}{\omega}$

$$\sigma_{VERT}(\omega) = -2\frac{\sigma_{BUB}^{dc}}{\beta} \tau^2 \frac{1 - 3\omega^2\tau^2}{(1 + \omega^2\tau^2)^3} s_{OZ}^{m=m'}. \quad (20)$$

224 In Appendix B, we evaluate the summation over the momentum $\tilde{\mathbf{q}}$ in $s_{OZ}^{m=m'}$ for the 1D and 2D
 225 cases. This yields the π -ton vertex contributions to the optical conductivity

$$\sigma_{VERT}(\omega) = -A T \tau^2 \sigma_{BUB}^{dc} \frac{1 - 3\omega^2\tau^2}{(1 + \omega^2\tau^2)^3} \begin{cases} \xi/\pi & \text{in 1D,} \\ \ln(\pi\xi)/\pi^3 & \text{in 2D,} \end{cases} \quad (21)$$

226 which is the main result of our paper.

227 3 Discussion

228 To help us keep track of upcoming discussions, it is convenient to introduce

$$\sigma_{VERT}^{dc} \equiv -A T \tau^2 \sigma_{BUB}^{dc} \begin{cases} \xi/\pi, & \text{in 1D} \\ \ln(\pi\xi)/\pi^3, & \text{in 2D} \end{cases} < 0, \quad (22)$$

229 keeping in mind that $\xi \gg 1$. This σ_{VERT}^{dc} gives the dc value of the π -ton vertex contribu-
 230 tions, which is negative and thus suppresses the Drude conductivity at small frequencies. For
 231 large frequencies, on the other hand, $3\omega^2\tau^2$ in the numerator of Eq. (21) becomes large, and
 232 correspondingly $\sigma_{VERT}(\omega)$ is positive and asymptotically decays to zero as

$$\lim_{\omega \rightarrow \infty} \sigma_{VERT}(\omega) = \frac{3}{\omega^4 \tau^4} |\sigma_{VERT}^{dc}|. \quad (23)$$

233 This further implies that the sign of the π -ton vertex contributions changes at the zero of
 234 Eq. (21), $\sigma_{VERT}(\omega_0) = 0$, which is given solely by the fermion lifetime, $\omega_0 = \frac{1}{\sqrt{3}}\tau^{-1}$. Addi-
 235 tionally, the maximum of $\sigma_{VERT}(\omega)$ is at the frequency $\omega_{MAX} = \tau^{-1}$, with the value of the
 236 maximum $\sigma_{VERT}(\omega_{MAX}) = \frac{1}{4} |\sigma_{VERT}^{dc}|$ independent of dimension.

237 Such shape of the π -ton vertex contributions together with the Drude contribution may
 238 result in the DDP in the total optical conductivity, $\sigma_{TOT}(\omega) = \sigma_{BUB}(\omega) + \sigma_{VERT}(\omega)$. Given
 239 that we have closed-form analytical expressions for both contributions, we can determine the
 240 criterion for the DDP appearance, as well as the DDP frequency and height. The details of these
 241 calculations can be found in Appendix C, while here we just highlight the final expression for
 242 the DDP frequency

$$\omega_{DDP} = \frac{1}{\tau} \sqrt{\sqrt{3 \frac{|\sigma_{VERT}^{dc}|}{\sigma_{BUB}^{dc}} \left(3 \frac{|\sigma_{VERT}^{dc}|}{\sigma_{BUB}^{dc}} + 4 \right) - \left(1 + 3 \frac{|\sigma_{VERT}^{dc}|}{\sigma_{BUB}^{dc}} \right)}}. \quad (24)$$

243 The Drude peak will be displaced to the finite frequency ω_{DDP} when there exists a real solution
 244 of Eq. (24), which is given by the criterion $6 |\sigma_{VERT}^{dc}| > \sigma_{BUB}^{dc}$. In the case when the π -ton
 245 contributions become particularly strong, $6 |\sigma_{VERT}^{dc}| \gg \sigma_{BUB}^{dc}$, Eq. (24) indicates that the DDP
 246 frequency would be determined solely by the fermion lifetime $\omega_{DDP} \approx \tau^{-1}$, giving for the DDP
 247 height $\sigma_{TOT}(\omega_{DDP}) = \sigma_{BUB}^{dc} - \frac{1}{4} |\sigma_{VERT}^{dc}|$. Note, however, that $|\sigma_{VERT}^{dc}| > \sigma_{BUB}^{dc}$ can give an
 248 unphysical negative dc conductivity, so the criterion for the applicability of our results and the
 249 appearance of the DDP can be put into the inequality $\sigma_{BUB}^{dc}/6 < |\sigma_{VERT}^{dc}| < \sigma_{BUB}^{dc}$.

250 Finally, we would especially like to emphasize that the π -ton vertex contributions in Eq. (21)
 251 comply with the optical sum rule following from the Ward identities [50,51]. Namely, with the
 252 Green's function given in Eq. (1), the full optical spectral weight is entirely given by the bubble
 253 contribution. By integrating the π -ton vertex contributions in Eq. (21) over frequencies it read-
 254 ily follows that the corresponding optical spectral weight vanishes, i.e., $\int_0^\infty d\omega \sigma_{VERT}(\omega) = 0$.
 255 Thus, such contributions may only shift, but not add any additional optical spectral weight.

256 3.1 Comparison of analytical and adaptive integration results

257 Before going into the consideration of DDP caused by π -tons in the 2D case, we first bench-
 258 mark our analytical results against those obtained from the adaptive integration of the π -ton
 259 vertex contributions formulated¹ on the real frequency axis in Refs. [31,32]. In particular,
 260 the Ornstein-Zernike form of the vertex function is assumed, whose parameters are obtained
 261 within the RPA. We compare separately the dc values, σ_{VERT}^{dc} , as well as the full frequency
 262 dependence of the π -ton vertex contributions. The two quantities are shown in Figs. 3(a,b)
 263 and (c,d) for the 1D case and the 2D case, respectively.

¹See Appendix A of Ref. [32] for the expressions for the π -ton vertex contributions to the current-current correlation function on the real frequency axis.

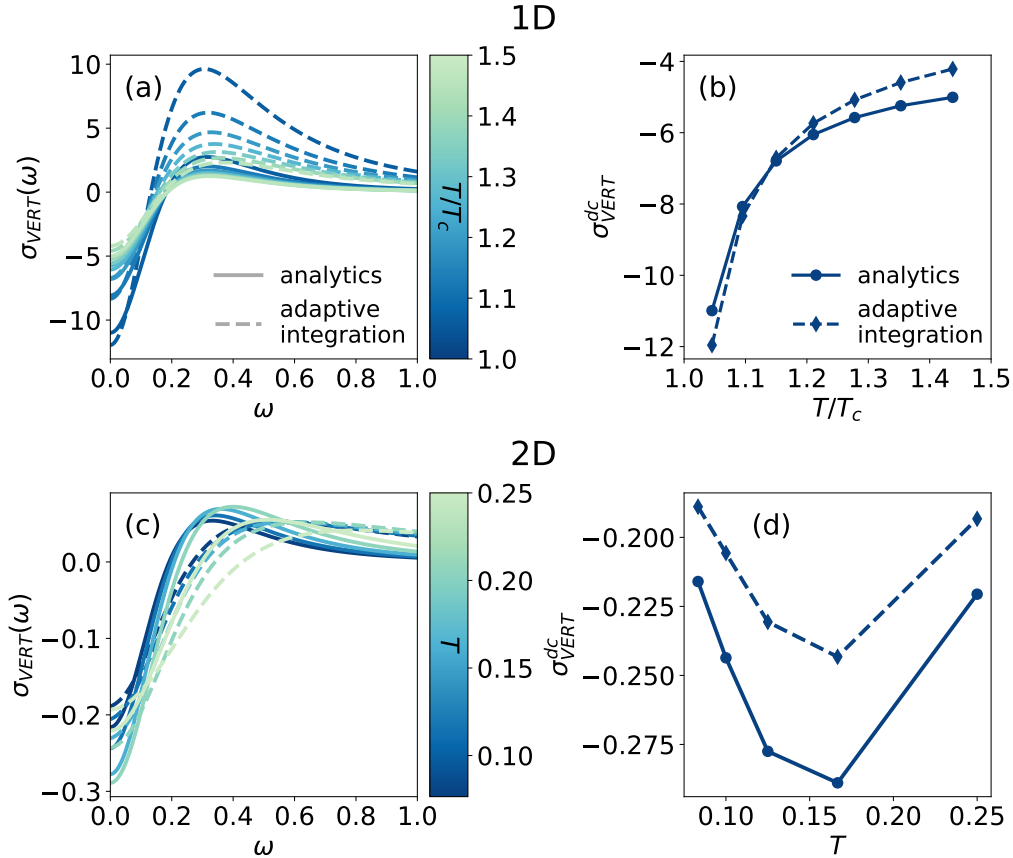


Fig. 3: (a,c) Analytical results [solid lines, Eq. (21)] vs adaptive integration [dashed lines] for the vertex correction to the optical conductivity. Several temperatures are discriminated by color. (b,d) dc value of the vertex correction as a function of temperature [Eq. (22)]. Here, the temperature dependencies of the fermion lifetimes and Ornstein-Zernike parameters have been taken from Ref. [32] in the 1D case (a,b) and from Ref. [31] in the 2D case (c,d).

264 3.1.1 1D case

265 For the 1D case, the parameterization of the Ornstein-Zernike vertex function within the RPA
 266 with the Hubbard interaction $U = 2$ and $\tau^{-1} = 0.1547 + 1.637 T^2$ as well as the adaptive
 267 integration of the corresponding π -ton vertex contributions has been already carried out in
 268 Ref. [32]. In such an approximation, the correlation length increases algebraically with T
 269 approaching T_c : $\xi \sim (T - T_c)^{-\nu}$, where $T_c \approx 1/23$ for these specific parameters. Please note
 270 that we assume finite τ at T_c throughout the paper. These numerical results for the frequency
 271 dependence of the π -ton vertex contributions and their dc values are shown as dashed lines
 272 for temperatures approaching the transition temperature T_c in Figs. 3(a) and (b), respectively.
 273 For the same set of parameters, the analytical results in Eqs. (21) and (22) are shown for
 274 comparison as solid lines in Fig. 3(a) and in Fig. 3(b), respectively.

275 By focusing first on the dc values in Fig. 3(b), we note that our analytical results show
 276 excellent qualitative and quantitative agreement with the numerical results obtained by adap-
 277 tive integration. The two lie almost on top of each other near the transition temperature. As
 278 the frequency increases, both results predict a sign change of π -ton vertex contributions and
 279 a broad maximum at some finite frequency, see Fig. 3(a). However, both the position and
 280 height of the maximum differ between the two calculations, where the analytical calculations

281 show the maximum at a lower frequency with a significantly smaller value. Such discrepan-
 282 cies at larger frequencies are not so surprising since in the analytical evaluation we considered
 283 only small energy transfer processes, giving a better description of π -ton vertex contributions
 284 around the dc values. Overall, taking into account the number of approximations and sim-
 285 plifications imposed in evaluating the analytical results, the qualitative frequency behavior of
 286 the π -ton vertex contributions and their dc values match astonishingly well with the adaptive
 287 integration results in the 1D case.

288 3.1.2 2D case

289 Next, we compare analytical and adaptive integration results for the 2D case. As in the 1D
 290 case, we take for the fermion lifetime $\tau^{-1} = 0.1547 + 1.637 T^2$. At this point, we should note
 291 that this temperature dependence of τ stems from the fitting of the quasiparticle peak to the
 292 parquet DGA results [29, 31]. For this specific temperature dependence of τ , the 2D Ornstein-
 293 Zernike parameters within the RPA and for $U = 1.9$ have been fitted as thoroughly discussed
 294 in Ref. [31]. Here, we only briefly outline the end result (see also Appendix D)

$$\xi = \frac{0.30}{T} + 10^{-3} \exp^{\frac{0.51}{T}}, \quad A = 0.41 + 13T^{1.03}, \quad \text{and} \quad \lambda = 0.38 + 10.6T^{1.29}. \quad (25)$$

295 It should be noted that the correlation length ξ in Eq. (25), although derived using the RPA with
 296 nominally algebraic temperature dependence of the correlation length, was fitted in Ref. [31]
 297 with an exponential function. This fitting resembles the ideal 2D zero temperature phase
 298 transition behavior according to the Mermin-Wagner theorem [52], with the exponential di-
 299 vergence of the correlation length as zero temperature is approached. The scenario of a finite
 300 T_c with the algebraic temperature dependence of the correlation length, as is the case in our
 301 1D modeling, is for 2D also discussed in Sec. 3.2.2.

302 Integrating the π -ton vertex contributions over four momenta and two frequencies in the
 303 real frequency formulation [31, 32] poses significant challenges in ensuring proper conver-
 304 gence in the 2D case, even when using adaptive integration methods. Here, we overcome
 305 these challenges using the vegas method from the cuba package [41]. The results of this
 306 adaptive integration for the frequency dependence of the π -ton vertex contributions for sev-
 307 eral temperatures are shown in Fig. 3(c) with dashed lines, while their dc values with the blue
 308 line in Fig. 3(d). For the same 2D parameter set (τ , ξ , A , and λ), the corresponding analytical
 309 results are shown as full lines in Fig. 3(c) and as solid green lines Fig. 3(d).

310 For the dc values, there is again an excellent qualitative agreement between the analyt-
 311 ical and adaptive integration results regarding the temperature dependence. Quantitatively,
 312 though, the analytical values are slightly larger. One possible explanation for this lies in the
 313 velocity factor, see Appendix B, which favors momenta in the nodal region of the Fermi sur-
 314 face, while the analytical evaluation assumed a constant value across the whole Fermi surface
 315 equal to the average fermion velocity. Similarly like in the 1D case, the discrepancies are also
 316 present in the high-frequency regions, where now analytical results predict slightly larger val-
 317 ues of the π -ton vertex contributions maxima. It is essential to highlight, however, that the
 318 overall magnitude of the π -ton vertex contributions agree well in both analytical and adaptive
 319 integration calculations. This agreement is particularly important when comparing the 1D and
 320 2D cases, where the analytical calculations corroborate the orders of magnitude differences in
 321 π -ton contributions between the two cases, as previously reported numerically in Ref. [32].
 322 This then carries important implications for the potential formation of the DDP in the 2D case,
 323 as discussed further in Sec. 3.2 below.

3.2 2D π -ton vertex contributions

Because the 2D π -ton vertex contributions shown in Fig. 3(c) are of relatively small magnitude, their inclusion to the Drude optical conductivity results only in a broadening of the Drude peak. This is depicted in Figs. 4(a)-(c), showing the Drude contribution of the bubble term, the π -ton vertex contributions, and their sum for several temperatures, respectively. Unlike the 1D case, where the π -ton contributions continuously increase in magnitude as the temperature decreases [32], the 2D π -ton vertex contributions in Figs. 4(b) initially increase in magnitude with decreasing temperature, though not enough to produce the DDP, but eventually, these contributions begin to get weaker and finally saturate as zero temperature is approached. This is due to the distinctive characteristics of the 2D case, where the π -ton contributions depend logarithmically on the correlation length [$\ln(\pi\xi)$ in Eq. (21)]. The correlation length ξ in turn exponentially diverges as the temperature approaches zero, $\xi \sim \exp(1/T)$ [Eq. (25)]. Combining both gives a factor β , which however cancels out the factor β in the denominator of Eq. (21) coming from the Matsubara sums. At the same time, Eq. (25) suggests that A and λ go to constant as $T \rightarrow 0$, leaving the 2D π -ton vertex contributions temperature independent at low temperatures, thus explaining the saturation of the π -ton contributions.

The 2D (temperature behaviors of) Ornstein-Zernike parameters in Eq. (25) apparently proved not to yield large enough π -ton contributions to result in the DDP. However, since we have a closed analytical expression for π -tons, we can tweak the Ornstein-Zernike parameters in such a way as to give larger π -ton contributions and explore possible routes for the appearance of the DDP in the 2D case. Thus, we can identify scenarios where π -tons are present in 2D systems.

3.2.1 Scenario I: Enhanced coupling strength to antiferromagnetic fluctuations

Since the magnitude of the π -ton contributions is directly proportional to the Ornstein-Zernike parameter A , the most straightforward way to increase it is by increasing the parameter A . Physically, this corresponds to enhancing the coupling strength g between fermions and AFM fluctuations. In particular, we consider the scenario where the coupling g is uniformly increased by a factor of $\sqrt{2}$ across all temperatures. This results in A being enhanced by a factor of 2, which doubles the magnitude of the π -ton vertex contributions while maintaining their qualitative temperature behavior as described in Sec. 3.2.

Such enhanced π -ton vertex contributions are shown in Fig. 4(d) and the resulting total optical conductivity in Fig. 4(e). The Drude peaks in the total optical conductivity are now shifted to finite frequencies, with the DDP frequency being an increasing function of temperature, $\omega_{DDP} \propto T^\alpha$, where $0 < \alpha < 1$, as can be seen in Fig. 4(f). Interestingly, as the temperature decreases, the height of the DDP increases, but the overall shape of the DDP becomes less distinct. This behavior is reminiscent of the experimental observations reported in Refs. [1–23], and contrasts with the DDP features associated with π -tons in the 1D case [32]. In the latter case, as the transition temperature T_c is approached, the displacement of the Drude peak becomes increasingly pronounced. As explained in Sec. 3.2, these discrepancies arise due to the peculiar temperature behavior of π -tons in the 2D case: At low temperatures, the π -ton contributions reach a saturation point, while the Drude peak of the bubble contribution sharpens, indicating a crossover from the displaced to the broadened Drude peak behavior in the optical conductivity as the temperature decreases in the enhanced coupling strength scenario.

3.2.2 Scenario II: Finite temperature phase transition

In Ref. [32], it was reported that the magnitude of the 2D π -ton vertex contributions increases monotonically and logarithmically as the transition temperature is approached, which is in

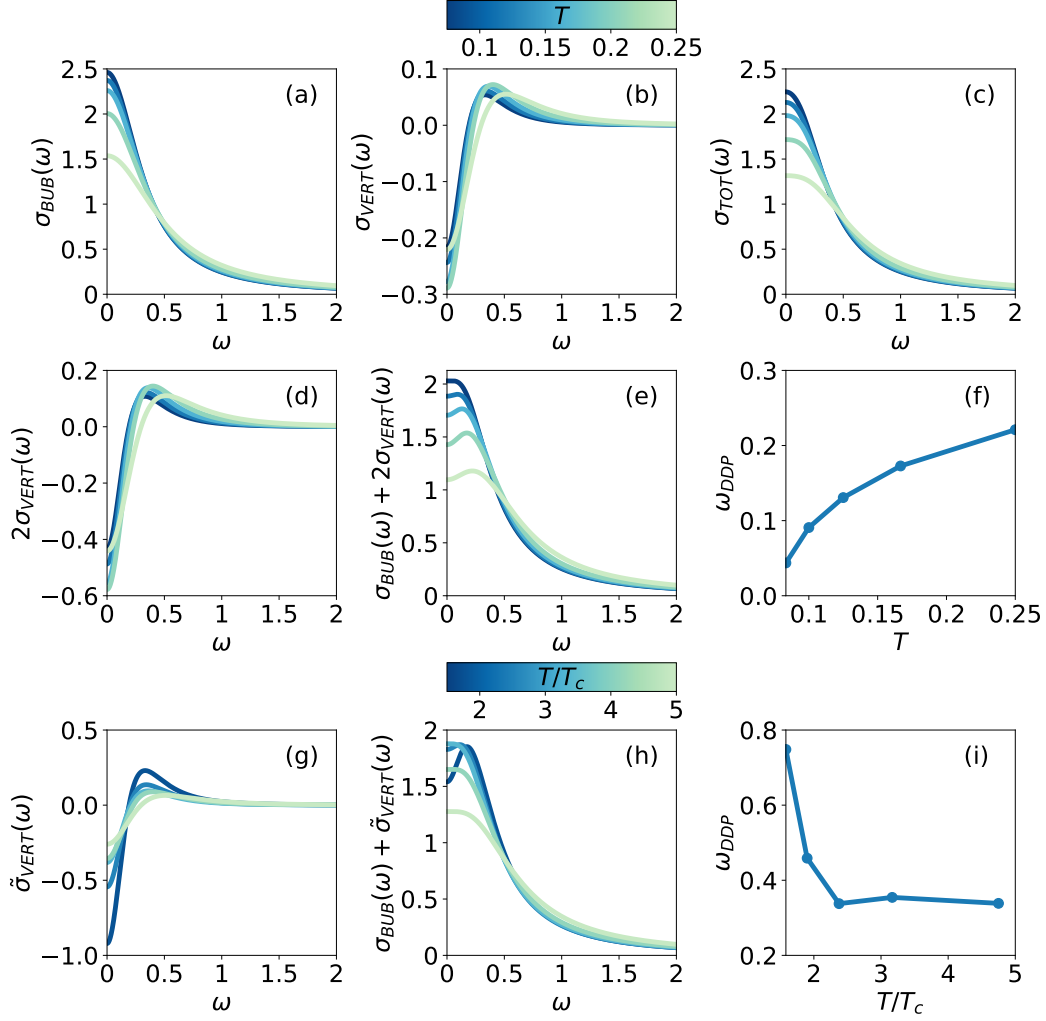


Fig. 4: (a) Bubble, (b) π -ton vertex, and (c) total contribution to the optical conductivity for several temperatures T for the 2D case with the fermion lifetime $\tau^{-1} = 0.1547 + 1.637 T^2$ and the Ornstein-Zernike parameters in Eq. (25). (d, e) π -ton contribution and total optical conductivity for Scenario I: twice the magnitude A of the π -ton vertex contributions. (g, h) π -ton contribution and total optical conductivity for Scenario II: a finite temperature phase transition at $T_c \approx 1/19$ and a power-law divergence of the correlation length, $\xi \sim (T - T_c)^{-1}$. (f, i) Temperature dependence of the displaced Drude peak frequency for the latter two cases.

371 sharp contrast to the behavior of the 2D π -ton contributions discussed so far in Secs. 3.2
 372 and 3.2.1. To this end, we note, however, that in Ref. [32], (1) the phase transition appeared
 373 at the finite temperature $T_c \approx 1/19$, and (2) the correlation length diverged with a power-law
 374 dependence on temperature rather than exponentially as in Eq. (25). To mimic such a scenario,
 375 in the following, we modify the temperature behavior of the correlation length in Eq. (25) to
 376 $\xi = \frac{0.30}{T-T_c} + 10^{-3} \exp^{\frac{0.51}{T}}$ [we turn back to the original coupling strength with the Ornstein-
 377 Zernike parameter A given in Eq. (25)]. Now the power-law term in the correlation length
 378 outweighs the exponential term in the vicinity of T_c , causing the π -ton vertex contributions
 379 to diverge logarithmically with temperature according to Eq. (21) as $\sigma_{VERT} \propto \ln(T - T_c)$.
 380 Analogously then, as in Ref. [32], the magnitude of π -ton vertex contributions monotonically
 381 increases all the way down to the transition boundary as shown in Fig. 4(g).

382 Similar to the enhanced coupling strength scenario, the corresponding total optical conduc-
 383 tivity in Fig. 4(h) also features the DDP, but with a qualitatively different temperature behavior
 384 compared to that in Fig. 4(e) and discussed in Sec. 3.2.1. Specifically, at high temperatures,
 385 the π -ton vertex contributions are small, leading only to the broadening of the Drude peak.
 386 As the temperature decreases, the π -ton contributions eventually become strong enough to
 387 displace the Drude peak, which becomes more pronounced as the temperature approaches T_c .
 388 Notably, Fig. 4(i) illustrates that in this scenario, starting from low temperatures, the DDP fre-
 389 quency initially decreases as the temperature increases, then increases within an intermediate
 390 temperature range, before decreasing again at higher temperatures.

391 Finally, we want to emphasize that while the overall qualitative frequency behavior of the
 392 π -ton vertex contributions does not depend on the peculiarities of the Ornstein-Zernike pa-
 393 rameters, their qualitative and quantitative temperature dependence does. These temperature
 394 dependencies are primarily governed by the correlation length, which allows for various sce-
 395 narios for the appearance of the DDP due to the π -ton contributions in the 2D case. Here we
 396 consider just two of them. Scenario I with a relatively strong coupling of fermions to AFM
 397 fluctuations and an exponential divergence of the correlation length at zero temperature. In
 398 this scenario, the displacement of the Drude peak appears at high temperatures and gradu-
 399 ally transitions to a simple broadening of the Drude peak at low temperatures with the DDP
 400 frequency increasing with temperature as in some experiments [1–23]. In Scenario II, with
 401 a finite temperature phase transition and a power-law divergence of the correlation length at
 402 a finite T_c , the magnitude of the π -ton vertex contributions continuously increases as T_c is
 403 approached. A DDP is observed in such a case, however, only close to T_c .

404 3.3 π -ton vs localization vertex contributions

405 Besides the displacement of the Drude peak through π -ton vertex contributions, it is well
 406 known that the DDP can also arise from the localization vertex corrections [24, 26, 27, 42, 53,
 407 54]. It is therefore fitting to wrap up with a brief discussion of the distinctions between these
 408 two types of vertex contributions.

409 The first key difference arises from the underlying microscopic source giving rise to the ver-
 410 tex corrections. Specifically, the π -ton vertex contributions stem from interactions of fermions
 411 with a soft critical boson (cf. below), whereas the core source of localization vertex correc-
 412 tions is static disorder. It should be, however, emphasized that in the recent studies on tran-
 413 sient localization [24, 26, 55], the initial model Hamiltonian did not include disorder from the
 414 outset; instead, an effectively disordered environment was generated through fermion-boson
 415 interactions. The latter involves the destructive interference of the electron wave function,
 416 which, when classified according to the two-particle reducibility, falls into the category of
 417 particle-particle reducible vertex contributions. In contrast, the π -ton vertex contributions are
 418 reducible in the transversal particle-hole channel.

419 This brings us to the second important difference: the topologies of the Feynman diagrams

420 associated with these two types of vertex corrections are distinct. This distinction further
 421 affects how momentum and frequency summations couple the fermion Green's functions and
 422 the vertex function in the current-current correlation function. In particular, for the π -ton
 423 vertex contributions, the frequency behavior is determined primarily by the fermion Green's
 424 functions, as follows from Eqs. (12) and (14), whereas in the case of localization, the vertex
 425 function governs the frequency behavior of the optical conductivity [42, 53].

426 Regarding the vertex function, the third important point is that in both cases, the vertex
 427 function resembles the form of an overdamped boson mode. In the context of localization
 428 physics, this boson is the diffuson with the form of the vertex function $F(\mathbf{q}, i\omega_m) \sim \frac{1}{D|\mathbf{q}|^2 + |\omega_m|}$
 429 [56], whereas, in the present consideration of π -ton effects, the boson represents AFM fluc-
 430 tuations with $F(\mathbf{q}, i\omega_m) \sim \frac{1}{\xi^{-2+|\mathbf{q}-\mathbf{Q}|^2 + \lambda|\omega_m|}}$. The crucial difference between these two vertex
 431 functions is that the π -ton vertex function possesses a mass term determined by the correlation
 432 length, which is absent in the case of the diffuson. Because of that mass term, the strength
 433 of the π -ton vertex contributions scales with the correlation length of the critical fluctuations,
 434 with the specific scaling behavior depending on the system dimension. In the 1D case, the
 435 strength of the π -ton vertex contributions scales linearly, while in the 2D case, it scales loga-
 436 rithmically with the correlation length. This correlation length scaling, along with the relation
 437 between Drude peak displacement and proximity to the phase transition, may be used in ex-
 438 periments to discriminate π -tons from other mechanisms, particularly localization corrections,
 439 leading to the DDP.

440 4 Conclusion

441 A displaced Drude peak originating from π -tons was recently found numerically in the weakly
 442 correlated metallic regime in one-dimension near the paramagnetic-to-antiferromagnetic tran-
 443 sition boundary [32]. Although qualitatively similar π -ton contributions have been observed
 444 in two dimensions, their logarithmic temperature scaling prevented unambiguous numerical
 445 statements.

446 Here, we derive the analytical expression Eq. (21) for π -ton vertex contributions and
 447 Eq. (24) for the peak position of the DDP, and validate these against an improved, adaptive
 448 numerical integration. Our assumptions to arrive at these analytical expressions are that: we
 449 are at small frequencies, the correlation length is large, and—in 2D—the optical conductiv-
 450 ity mainly stems from nodal momenta where the velocity is largest. We find that a displaced
 451 Drude peak due to the π -tons may appear in 2D systems with a relatively strong coupling of
 452 the electrons to antiferromagnetic spin fluctuations or for a finite temperature phase transi-
 453 tion. In the former case, the displaced Drude peak gradually diminishes as the temperature
 454 decreases, while in the second scenario, the effect will be the opposite.

455 With the identified characteristic dependencies of the π -ton vertex contributions in 1D
 456 and 2D [see Eq. (21), Eq. (24), and the Abstract], we have laid the foundations for observ-
 457 ing π -tons also in experiments. We find, as in some experiments, an enhancement of the
 458 DDP with increasing temperature if we have the ideal 2D case with an exponential scaling of
 459 the correlation length with $1/T$ and strong coupling to spin or charge fluctuations. An even
 460 more clear-cut proof would be to study the DDP upon approaching a finite temperature phase
 461 transition at T_c . In such scenarios, we predict an algebraic, $\sigma_{VERT}^{dc} \propto \xi \sim (T - T_c)^{-\nu}$, and
 462 logarithmic, $\sigma_{VERT}^{dc} \propto \ln \xi \sim \nu \ln(T - T_c)$, enhancement of π -tons in 1D and 2D, respectively,
 463 which should be contrasted with $\ln T$ dependence of localization corrections in 2D.

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468 A Contour integrations

469 We solve the integral

$$\mathcal{I}_1 = \int_{-\infty}^{+\infty} d\varepsilon \left[\frac{1}{i\omega_n + i\nu_m - \varepsilon + \frac{i}{2\tau}} \right] \left[\frac{1}{i\nu_m - \varepsilon - \frac{i}{2\tau}} \right] = \int_{-\infty}^{+\infty} d\varepsilon u_1(\varepsilon), \quad (\text{A.1})$$

470 appearing in the bubble contribution to the current-current correlation function, Eq. (5), by
471 performing the contour integration in the complex plane. In particular, we choose the contour
472 \mathcal{C} running from $+\infty$ to $-\infty$ on the real axis enclosed by the arc Γ of infinite radius in the
473 lower half of the complex plane, so that we can write

$$\oint_{\mathcal{C}} dz u_1(z) = -\mathcal{I}_1 + \int_{\Gamma} dz u_1(z) = 2\pi i \operatorname{Res} \left(u_1, i\nu_m - \frac{i}{2\tau} \right). \quad (\text{A.2})$$

474 Note that $z = i\nu_m - \frac{i}{2\tau}$ is the only pole (of order one) in the lower half of the complex plane due
475 to the constraint $\omega_n > -\nu_m > 0$. The arc that closes the contour does not give a contribution
476 because the integrand is decaying faster than $1/|z|$, while the corresponding residue reads

$$\begin{aligned} \operatorname{Res} \left(u_1, i\nu_m - \frac{i}{2\tau} \right) &= \lim_{z \rightarrow i\nu_m - \frac{i}{2\tau}} \left[z - \left(i\nu_m - \frac{i}{2\tau} \right) \right] \left[\frac{1}{i\omega_n + i\nu_m - z + \frac{i}{2\tau}} \right] \left[\frac{1}{i\nu_m - z - \frac{i}{2\tau}} \right] \\ &= -\frac{1}{i\omega_n + \frac{i}{\tau}}. \end{aligned} \quad (\text{A.3})$$

477 This yields the required integral

$$\mathcal{I}_1 = \frac{2\pi i}{i\omega_n + \frac{i}{\tau}}. \quad (\text{A.4})$$

478 For the evaluation of the π -ton vertex contributions, we additionally need to compute

$$\mathcal{I}_2 = \int_{-\infty}^{+\infty} d\varepsilon \left[\frac{1}{i\nu_m + i\omega_n - \varepsilon + \frac{i}{2\tau}} \right]^2 \left[\frac{1}{i\nu_m - \varepsilon - \frac{i}{2\tau}} \right]^2 = \int_{-\infty}^{+\infty} d\varepsilon u_2(\varepsilon). \quad (\text{A.5})$$

479 The only difference between \mathcal{I}_1 and \mathcal{I}_2 is that in the latter the pole $z = i\nu_m - \frac{i}{2\tau}$ is of order
480 two, so the corresponding residue reads

$$\begin{aligned}
& \text{Res}\left(u_2, i\nu_m - \frac{i}{2\tau}\right) \\
&= \lim_{z \rightarrow i\nu_m - \frac{i}{2\tau}} \frac{d}{dz} \left\{ \left[z - \left(i\nu_m - \frac{i}{2\tau} \right) \right]^2 \left[\frac{1}{i\omega_n + i\nu_m - z + \frac{i}{2\tau}} \right]^2 \left[\frac{1}{i\nu_m - z - \frac{i}{2\tau}} \right]^2 \right\} \quad (\text{A.6}) \\
&= \lim_{z \rightarrow i\nu_m - \frac{i}{2\tau}} (-2) \left[\frac{1}{i\omega_n + i\nu_m - z + \frac{i}{2\tau}} \right]^3 (-1) = 2 \left[\frac{1}{i\omega_n + \frac{i}{\tau}} \right]^3.
\end{aligned}$$

481 This gives for the integral \mathcal{I}_2

$$\mathcal{I}_2 = -4\pi i \frac{1}{\left(i\omega_n + \frac{i}{\tau}\right)^3}. \quad (\text{A.7})$$

482 B Momentum summation over the Ornstein-Zernike vertex function

483

484 We are interested in evaluating the sum

$$s_{OZ}^{m=m'} = \frac{1}{N} \sum_{\tilde{\mathbf{q}}} \frac{A}{\xi^{-2} + \tilde{q}^2}, \quad (\text{B.1})$$

485 for the 1D and the 2D case. In the 1D case, we simply have, keeping in mind $\xi \gg 1$

$$s_{OZ}^{m=m',1D} = \frac{1}{2\pi} \int_{-\pi}^{+\pi} d\tilde{q}_x \frac{A}{\xi^{-2} + \tilde{q}_x^2} \xrightarrow{\xi \rightarrow \infty} \frac{1}{2\pi} 2A\xi \frac{\pi}{2} = \frac{A\xi}{2}. \quad (\text{B.2})$$

486 Furthermore, by following Fig. 1 and the accompanying discussion, we note that in principle
487 only $\tilde{\mathbf{q}}$ which retains the scattered electron-hole pair close to the Fermi surface (accounting for
488 the smearing) should contribute to the sum. In the simplest approximation, this introduces a
489 correction factor given by the relative size of the Fermi surface to the whole Brillouin zone.
490 In the 1D case, there are only two momenta contributing to the Fermi surface in the whole
491 Brillouin zone of length 2π . Thus introducing a factor of $2/2\pi$ gives the final result

$$s_{OZ}^{m=m',1D} = \frac{A\xi}{2\pi}. \quad (\text{B.3})$$

492 In the 2D case, the integrals are a little bit more involved

$$s_{OZ}^{m=m',2D} = \frac{1}{(2\pi)^2} \int_{-\pi}^{+\pi} d\tilde{q}_x \int_{-\pi}^{+\pi} d\tilde{q}_y \frac{A}{\xi^{-2} + \tilde{q}_x^2 + \tilde{q}_y^2}. \quad (\text{B.4})$$

493 However, for $\xi \gg 1$ we can approximate the integral over the Brillouin zone with the integral
494 over the circle of radius π , which, importantly, contains the whole Fermi surface in the half-
495 filled case. In that case, we simply have

$$s_{OZ}^{m=m',2D} \approx \frac{1}{(2\pi)^2} \int_0^{2\pi} d\phi \int_0^\pi d\tilde{q} \tilde{q} \frac{A}{\xi^{-2} + \tilde{q}^2} \xrightarrow{\xi \rightarrow \infty} \frac{A}{2\pi} \ln(\pi\xi). \quad (\text{B.5})$$

496 Similar to the 1D case, we should correct this result with the ratio of the length of the Fermi
 497 surface to the area of the entire Brillouin zone. In the 2D case, the situation is a little bit more
 498 involved due to the velocity contribution $v_{\mathbf{k}}^2 \sim \sin^2 k_x$, which favors momenta around $k_x \sim \pm \frac{\pi}{2}$.
 499 In the simplest approximation, we can assume that four momentum points, $(\pm \frac{\pi}{2}, \pm \frac{\pi}{2})$, on the
 500 Fermi surface give the largest contributions, introducing a correction factor of $4/(2\pi)^2$. This
 501 is a possible source of the difference between analytical and numerical results in Fig. 3(c,d).
 502 We then have in 2D

$$s_{OZ}^{m=m', 2D} \approx \frac{A \ln(\pi \xi)}{2\pi^3}. \quad (\text{B.6})$$

503 To summarize, we obtained

$$s_{OZ}^{m=m'} \approx \frac{A}{2} \begin{cases} \xi/\pi, & \text{in 1D,} \\ \ln(\pi \xi)/\pi^3, & \text{in 2D.} \end{cases} \quad (\text{B.7})$$

504 C Displaced Drude peak frequency and height

505 In order to determine the displaced Drude peak frequency, we take derivatives of Eqs. (7)
 506 and (21) with respect to frequency. For the bubble contribution, we have

$$\frac{d\sigma_{BUB}(\omega)}{d\omega} = -\frac{2\omega\tau^2\sigma_{BUB}^{dc}}{(1+\omega^2\tau^2)^2}, \quad (\text{C.1})$$

507 while for the π -ton vertex contributions we get

$$\begin{aligned} \frac{d\sigma_{VERT}(\omega)}{d\omega} &= |\sigma_{VERT}^{dc}| \frac{6\omega\tau^2(1+\omega^2\tau^2)^3 - (3\omega^2\tau^2 - 1)6\omega\tau^2(1+\omega^2\tau^2)^2}{(1+\omega^2\tau^2)^6} \\ &= |\sigma_{VERT}^{dc}| 12\omega\tau^2(1+\omega^2\tau^2)^2 \frac{1-\omega^2\tau^2}{(1+\omega^2\tau^2)^6}. \end{aligned} \quad (\text{C.2})$$

508 By adding up the two contributions, $\sigma_{TOT}(\omega) = \sigma_{BUB}(\omega) + \sigma_{VERT}(\omega)$, we obtain

$$\frac{d\sigma_{TOT}(\omega)}{d\omega} = \frac{|\sigma_{VERT}^{dc}| 12\omega\tau^2(1+\omega^2\tau^2)^2(1-\omega^2\tau^2) - 2\omega\tau^2\sigma_{BUB}^{dc}(1+\omega^2\tau^2)^4}{(1+\omega^2\tau^2)^6}. \quad (\text{C.3})$$

509 The maximum is at $\frac{d\sigma_{TOT}(\omega)}{d\omega} = 0$ and given by the equation

$$6|\sigma_{VERT}^{dc}|(1-\omega^2\tau^2) - \sigma_{BUB}^{dc}(1+\omega^2\tau^2)^2 = 0. \quad (\text{C.4})$$

510 We do not consider a trivial solution $\omega = 0$. By introducing $a = 6|\sigma_{VERT}^{dc}|/\sigma_{BUB}^{dc} > 1$ and
 511 $x = \omega^2\tau^2$, we may write

$$x^2 + (2+a)x + (1-a) = 0, \quad (\text{C.5})$$

512 whose solutions are

$$x_{1,2} = \frac{-(2+a) \pm \sqrt{a(a+8)}}{2}. \quad (\text{C.6})$$

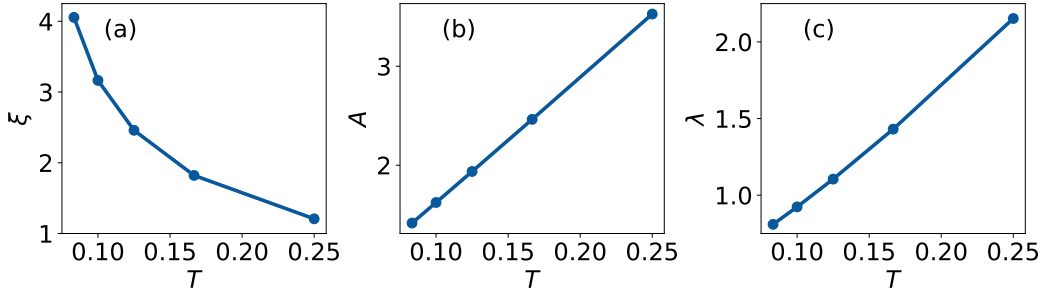


Fig. 5: Temperature dependence of the 2D Ornstein-Zernike parameters ξ , A , and λ from Ref. [31], extracted by fitting the Ornstein-Zernike form in Eq. (9) to the RPA π -ton vertex function.

513 We are interested only in positive x , so we can immediately discard the solution with the minus
 514 sign. For the solution with the plus sign to be positive, $a > 1$ needs to hold, so the criterion for
 515 the appearance of the displaced Drude peak reads $6 \left| \sigma_{VERT}^{dc} \right| > \sigma_{BUB}^{dc}$. The frequency associated
 516 with the displaced Drude peak is then equal to

$$\omega_{DDP} = \frac{1}{\tau} \sqrt{\sqrt{3 \frac{\left| \sigma_{VERT}^{dc} \right|}{\sigma_{BUB}^{dc}} \left(3 \frac{\left| \sigma_{VERT}^{dc} \right|}{\sigma_{BUB}^{dc}} + 4 \right)} - \left(1 + 3 \frac{\left| \sigma_{VERT}^{dc} \right|}{\sigma_{BUB}^{dc}} \right)}, \quad (C.7)$$

517 which in the limit $6 \left| \sigma_{VERT}^{dc} \right| \gg \sigma_{BUB}^{dc}$ reduces to $\omega_{DDP} = \tau^{-1}$. In the latter case, the height of
 518 the displaced Drude peak equals

$$\sigma_{TOT}(\omega_{DDP}) = \sigma_{BUB}^{dc} - \frac{1}{4} \left| \sigma_{VERT}^{dc} \right|. \quad (C.8)$$

519 D Temperature dependence of the Ornstein-Zernike parameters

520 In Fig. 5, we show the temperature dependence of the Ornstein-Zernike parameters ξ , A , and
 521 λ extracted in Ref. [31] by fitting the Ornstein-Zernike vertex form to the RPA π -ton vertex
 522 function for the case with the fermion lifetime $\tau^{-1} = 0.1547 + 1.637 T^2$ in the 2D case. The
 523 corresponding temperature dependencies respectively read

$$\xi = \frac{0.30}{T} + 10^{-3} \exp \frac{0.51}{T}, \quad A = 0.41 + 13T^{1.03}, \quad \text{and} \quad \lambda = 0.38 + 10.6T^{1.29}. \quad (D.1)$$

524 Note that although the correlation length is extracted from the RPA π -ton vertex function
 525 showing a finite transition temperature at $T_c \approx 1/19$, it is fitted with an exponential function,
 526 resembling the true 2D exponential divergence of the correlation length as zero temperature
 527 is approached.

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