

Band-Edge Quasiparticles from Electron-Phonon Coupling and Resistivity Saturation

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We address the problem of resistivity saturation observed in materials such as the *A-15* compounds. To do so, we calculate the resistivity for the Hubbard-Holstein model in infinite spatial dimensions to second order in on-site repulsion $U \leq D$ and to first order in (dimensionless) electron-phonon coupling strength $\lambda \leq 0.5$, where D is the half bandwidth. We identify a unique mechanism to obtain two parallel quantum conducting channels: low-energy and band-edge high-energy quasi-particles. We identify the source of the hitherto unremarked high-energy quasiparticles as a positive slope in the frequency dependence of the real part of the electron self-energy. In the presence of phonons, the self-energy grows linearly with the temperature at high T , causing the resistivity to saturate. As U is increased, the saturation temperature is pushed to higher values, offering a mechanism by which electron correlations destroy saturation.

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Introduction.—Resistivity has been observed to saturate at high temperatures in certain materials, such as the *A-15* compounds, while growing without bound in others, such as the cuprates [1–8]. Resistivity saturation has been seen as a signature of electron-phonon interactions [9] and weak electron-electron interactions. Many theoretical mechanisms have been proposed to address the problem of resistivity saturation [1,10–17]. In this Letter, we offer a unique mechanism: the presence of two parallel quantum conducting channels consisting of the usual low-energy and the less obvious high-energy quasiparticles. These emergent objects derive from electron-phonon interactions. This is the main idea of our work, namely, the role of the hitherto unnoticed high-energy (i.e., band edge) quasiparticles, residing at or beyond the edge of the bare band. The demonstration of this idea requires only low order perturbation theory.

In particular, we evaluate the bare diagrams to leading order in the electron-phonon coupling. It would also have been possible to resum an infinite subset of diagrams by doing a self-consistent version of the same approximation. Moreover, for low energies, these are the only diagrams which contribute (Migdal’s theorem) [18]. However, in our work, it is in fact the high-energy quasiparticles that play a key role, and therefore the use of Migdal’s theorem is no longer justified. Therefore, all higher order diagrams enter into the series on equal footing. In the case of weak electron-phonon coupling, the approximation used here is rigorously justified, while for the case of intermediate or strong coupling, we consider it to be the most unbiased. It has also been shown in recent work that self-consistent diagrammatic approximations can lead to wrong results in certain cases [19]. Because of the nature of our approximation, we restrict $\lambda \leq 0.5$.

In the presence of phonons, the high-energy quasiparticles lead to resistivity saturation. The mechanism we propose has

a unique signature in the local density of states (LDOS), which acquires peaks at or beyond the edge of the bare band. Therefore, it can be identified experimentally using Angle resolved photoemission spectroscopy (ARPES)/Scanning Tunneling microscopy (STM) measurements. It also has a distinct signature in the optical conductivity (see the Supplemental Material, Fig. (5) [20]), and can therefore be identified using the latter as well.

We study the Hubbard-Holstein model on the Bethe lattice in the limit of infinite spatial dimensions. The electrons interact through on-site repulsion U , and couple to an Einstein phonon mode with dimensionless electron-phonon coupling strength λ . We perform perturbation theory to second order in U and to first order in λ . We compute the dc resistivity over a large range of temperature. We find that it displays resistivity saturation. In Fig. 1, we plot the resistivity ρ measured in units of $\mu\Omega$ cm, as a function of the temperature T for $T \leq 1000$ K. We computed this resistivity for three sets of parameters: $[(U/D) = 0.5; \lambda = 0.25]$, $[(U/D) = 0.5; \lambda = 0.5]$, and $[(U/D) = 1; \lambda = 0.5]$ where D is the half bandwidth.

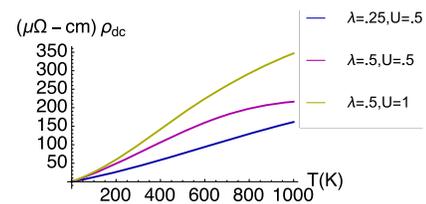


FIG. 1. The dc resistivity vs temperature for the Hubbard-Holstein model for three sets of parameters: $[(U/D) = 0.5; \lambda = 0.25]$, $[(U/D) = 0.5; \lambda = 0.5]$, and $[(U/D) = 1; \lambda = 0.5]$, with D estimated as 2000 K. The prolonged region of negative curvature found in the middle set is observed in the *A-15* compounds Nb_3Sn and Nb_3Sb [2].

These values seem compatible with the perturbative scheme employed. For the middle set of parameters, the calculated resistivity happens to be in good quantitative agreement with the resistivity observed in the *A*-15 compounds Nb₃Sn and Nb₃Sb [2]. In particular, note the negative curvature of the resistivity vs temperature curve for $T \gtrsim 500$ K. For either weaker electron-phonon coupling or stronger electron-electron interactions, the saturation temperature increases beyond the scale that is probed in experiments.

While previous studies of transport have focused on the conduction of low-energy quasiparticles, we identify a parallel quantum conduction channel, consisting of high-energy quasiparticles defined by peaks in the spectral function, at, or beyond, the edge of the bare band that are sharp enough to be identifiable under certain conditions. In contrast to the low-energy quasiparticles, which are scattered more strongly at higher temperatures, the high-energy quasiparticles are pushed to higher energies with increasing temperature, and are therefore scattered more weakly. Denoting the resistivity of the low- and high-energy quasiparticles by ρ_{ideal} and ρ_{sat} , respectively, the overall resistivity is given by the parallel resistor formula

$$\frac{1}{\rho} = \frac{1}{\rho_{\text{ideal}}} + \frac{1}{\rho_{\text{sat}}}, \quad (1)$$

where ρ_{ideal} (ρ_{sat}) is defined at all temperatures as the low (high)-frequency contribution to the integral in Eq. (5) [detailed in the Supplemental Material Eqs. (SM-1), (SM-2) [20]].

As the temperature increases, the high-energy channel short circuits the low-energy channel, and the resistivity saturates. The high-energy quasiparticles are visible in the local density of states (LDOS), which develops peaks at high energies as the temperature is increased, while the central peak, associated with the low-energy quasiparticles, simultaneously shrinks. This is a prediction of our theory which can be tested using scanning tunneling microscopy (STM). In Fig. 2, we plot the LDOS $A(\omega)$ at $T = 1000$ K for the same parameters as used in Fig. 1. The high-energy peaks are diminished by either decreasing λ or by increasing U .

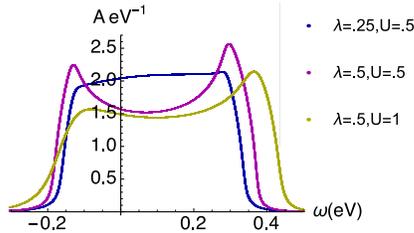


FIG. 2. The LDOS at $T = 1000$ K for the same sets of parameters as in Fig. 1. The peaks located beyond the edges of the bare band are signatures of the high-energy quasiparticles, and are a prediction of our theory which can be tested using STM. Figures 4, 8 display the T variation of A .

The model and calculation.—The Hamiltonian for our model containing disorder, interactions, and a local Einstein mode phonon [21] is the following:

$$H = \sum_k (\varepsilon_k - \mu) a_k^\dagger a_k + \omega_0 \sum_q b_q^\dagger b_q + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{g}{\sqrt{N_s}} \sum_{k,q} a_{k+q}^\dagger a_k (b_q + b_{-q}^\dagger) + \sum_j \varepsilon_j n_{j\sigma}, \quad (2)$$

where a_k is the electron destruction operator in momentum state k , ε_k is the dispersion of the lattice, b_q is the phonon destruction operator in momentum state q , ω_0 is the energy of all phonon modes, U is the on-site Hubbard repulsion, N_s is the number of sites in the lattice, and g is the electron-phonon coupling energy. The ε_j are quenched random site energies, which are treated within the Born approximation [22], whereby the impurity averaged noninteracting electron Greens function is broadened $G_0^{-1} \rightarrow G_0^{-1} + i\eta$ and $\eta = n_i \pi \mathcal{D}(\varepsilon_F) \langle \varepsilon_j^2 \rangle$.

The electrons hop on the infinite-dimensional Bethe lattice, which has the density of states for energy $\varepsilon \in [-D, D]$,

$$\mathcal{D}(\varepsilon) = \frac{2}{\pi D} \left[1 - \left(\frac{\varepsilon}{D} \right)^2 \right]^{1/2}, \quad (3)$$

where D is the half bandwidth. For the remainder of the Letter, all energies will be measured in units of $D \sim 2000$ K [23].

Following Ref. [21] (see Supplemental Material [20] for details), for $T \gtrsim \omega_0$, the electron-phonon self-energy, computed to $O(g^2)$, is expressed as

$$\rho_{\Sigma_{\text{el,ph}}}(\omega - \mu_{\text{el}}) = \frac{\pi \lambda A_{\text{el}}(\omega - \mu_{\text{el}})}{2} \times T, \quad (4)$$

where λ , defined by $g^2 \equiv [(\pi D \lambda \omega_0)/4]$, is a dimensionless measure of the electron-phonon coupling strength. For any dynamical object $Q(\omega)$, $\rho_Q(\omega) \equiv -(1/\pi) \Im m[Q(\omega)]$, and the subscript “el” refers to quantities computed in the absence of phonons ($g = 0$), using second order perturbation theory in the Hubbard U . Finally, $A(\omega)$ is the LDOS, obtained by integrating $\rho_G(\varepsilon, \omega)$ over ε , the latter obtained from $\Sigma(\omega)$ using Dyson’s equation.

The dc conductivity can be expressed in terms of the spectral function via the formula [24]

$$\sigma = \frac{2}{\pi T} \sigma_{\text{IRM}} \int d\omega f(\omega - \mu_{\text{el}}) \bar{f}(\omega - \mu_{\text{el}}) I(\omega - \mu_{\text{el}}), \quad (5)$$

where $f(\omega) \equiv [1/(e^{\beta\omega} + 1)]$, $\bar{f}(\omega) \equiv 1 - f(\omega)$, and $\beta \equiv (1/T)$. The spectral intensity $I(\omega)$ is defined as

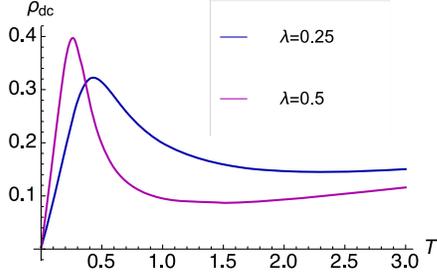


FIG. 3. ρ_{dc} vs T for $\lambda = 0.25, 0.5$, and $U = 0$. As λ increases, T_{\max} decreases, while the height of the peak increases. In the $T \rightarrow \infty$ limit, the resistivity curves collapse onto a straight line.

$$I(\omega - \mu_{el}) = \pi^2 \int d\epsilon \phi(\epsilon) \rho_G^2(\epsilon, \omega - \mu_{el}), \quad (6)$$

where $\sigma_{IRM} \equiv (1/\rho_{IRM})$, ρ_{IRM} is the Ioffe-Regel-Mott limit of the resistivity, and the transport function is given explicitly as $\phi(\epsilon) = \Theta(1 - \epsilon^2) \times (1 - \epsilon^2)^{(3/2)}$. We will measure the resistivity in units of $\rho_{IRM} \approx 258 \mu\Omega \text{ cm}$ [25]. In the limit that $\rho_{\Sigma}(\omega - \mu_{el}) \ll D$ [24,25],

$$I(\omega - \mu_{el}) \approx \frac{1}{2} \frac{\phi[R(\omega - \mu_{el})]}{\rho_{\Sigma}(\omega - \mu_{el})}, \quad (7)$$

where $\Sigma(\omega) = \Sigma_{el}(\omega) + \Sigma_{el,ph}(\omega)$, $R(\omega - \mu_{el}) \equiv \omega + \Delta\mu - \Re e \Sigma(\omega - \mu_{el})$, and $\Delta\mu \equiv \mu - \mu_{el}$ tends to 0 as $T \rightarrow \infty$. Both μ and μ_{el} are determined through the particle sum rule for the Green's function. The approximation Eq. (7) is excellent for the dominant frequency range at all temperatures.

In our treatment of Eq. (5), we eschew the popular Sommerfeld approximation [26,27] $f(\nu)\bar{f}(\nu) \rightarrow T\delta(\nu)$, since it misleadingly throws out the contribution from the high-energy peaks in $I(\nu)$. In Eq. (7), we note that the spectral intensity I can be large at any frequency where the imaginary self-energy is small, and the real part of the inverse Green's function is also small.

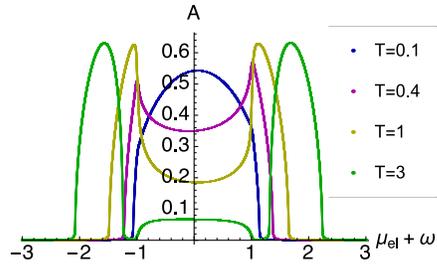


FIG. 4. The LDOS for $\lambda = 0.5$ and $U = 0$ at $T = 0.1, 0.4, 1, 3$. For $T \lesssim T_{\max}$, the central peak is a signature of the low-energy quasiparticles, while for $T \gtrsim T_{\max}$, the two high-energy peaks are signatures of the high-energy quasiparticles. The high-energy peaks get pushed to higher energies with increasing temperature. As the scattering rate of the high-energy quasiparticles decreases, so does the resistivity (Fig. 3).

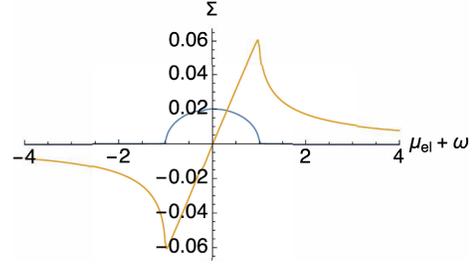


FIG. 5. ρ_{Σ} and $\Re e \Sigma$ for $\lambda = 0.5$ and $U = 0$ at $T = 0.04$. This relatively low temperature is already in the semiclassical regime ($T \gtrsim \omega_0$), where Eqs. (8) and (9) are excellent approximations. The positive slope of $\Re e \Sigma$ is responsible for the high-energy quasiparticles (Fig. 4).

Results.—We choose the parameters as follows. We set the density to $n = 0.7$. Since our calculation does not incorporate any Mott physics, the exact value of the density does not change the qualitative features of the results. We choose the phonon energy $\omega_0 = 0.015$. Since the temperature regime of interest is in the semiclassical regime ($T \gg \omega_0$), the value of ω_0 has very little bearing on the results [see Eq. (4)]. We choose the impurity scattering $\eta = 0.0012$. η is chosen to be small but finite to ensure that the resistivity does not abruptly drop to zero above a certain temperature. Once again, in the range of experimentally relevant temperatures, η has little bearing on the results. Finally, we restrict $\lambda \leq 0.5$ and $U \leq D$, so that low-order perturbation theory can be expected to give reliable results.

$U = 0$.—In the case of $U = 0$, the free electrons are scattered by phonons and impurities. In Fig. 3, we plot the resistivity for $\lambda = 0.25$ and $\lambda = 0.5$. In both cases, the resistivity displays a maximum at $T \equiv T_{\max}$, before finally increasing again at high temperatures. As λ increases, T_{\max} decreases, while the height of the peak increases. In the $T \rightarrow \infty$ limit, the resistivity curves collapse onto a straight line, whose slope is fixed by the impurity scattering of the electrons. This picture differs from the textbook discussions [28] of a monotonically increasing phononic resistivity. In the latter, the electrons are modeled as an electron gas with an infinite bandwidth, while here the narrow electronic band is a key component, leading to high-energy

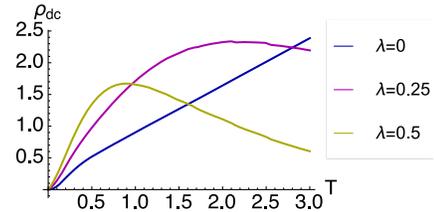


FIG. 6. The resistivity vs temperature curve for $\lambda = 0, 0.25, 0.5$, and $U = 1$. For $\lambda \neq 0$, the peak shifts to the left and becomes sharper with increasing λ . Note that when T is restricted to experimentally relevant values, i.e., $T \lesssim 0.5D$, only the left half of the peak appears, mimicking saturation (see Fig. 1).

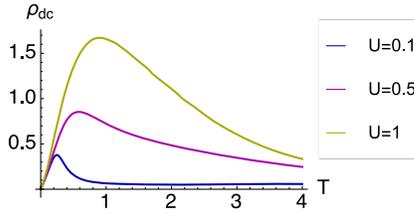


FIG. 7. The resistivity vs temperature curve for $\lambda = 0.5$ and $U = 0.1, 0.5, 1.0$. T_{\max} increases with increasing U .

quasiparticles at or beyond the edge of the bare band. The presence of the high-energy parallel conducting channel causes a rollover and hence a maximum in the curve. In fact, resistivity curves similar to those in Fig. 3 have also been found in theoretical studies of the periodic Anderson model and the Kondo lattice model [29–35], as well as the half-filled Hubbard model close to the Mott transition [36–39]. In these works, the resistivity is due entirely to electron-electron correlations, while in the present work, electron-phonon interactions are the driving force behind the maximum in the resistivity vs temperature curve.

In Fig. 4, we plot the LDOS for $\lambda = 0.5$ at $T = 0.1, 0.4, 1, 3$. For $T \lesssim T_{\max}$, the LDOS consists of a single central peak, and hence the conductivity is dominated by the low-energy channel ($\rho \approx \rho_{\text{ideal}}$). For $T \gtrsim T_{\max}$, the LDOS consists of two high-energy peaks, and hence the conductivity is dominated by the high-energy channel ($\rho \approx \rho_{\text{sat}}$). As the temperature increases past T_{\max} , the high-energy quasiparticles are pushed to increasingly higher energies and have correspondingly smaller scattering rates, causing the resistivity to decrease.

The existence of high-energy quasiparticles requires $R(\omega - \mu_{\text{el}})$ to vanish at large values of the frequency. This in turn requires that $\Re e \Sigma(\omega - \mu_{\text{el}})$ have positive slope of order unity. In Fig. 5, we plot ρ_{Σ} and $\Re e \Sigma$ at $T = 0.04$. Using Eq. (4) (for small η),

$$\rho_{\Sigma}(\omega - \mu_{\text{el}}) = \frac{\pi \lambda D(\omega)}{2} \times T, \quad (8)$$

$$\Re e \Sigma(\omega - \mu_{\text{el}}) = \pi \lambda \times T \times \omega \left(1 - \Theta(\omega^2 - 1) \sqrt{1 - \frac{1}{\omega^2}} \right). \quad (9)$$

The slope of $\Re e \Sigma(\omega - \mu_{\text{el}})$ increases linearly with T , pushing the high-energy quasiparticles to higher energies, causing their scattering rate to decrease. Meanwhile, the scattering rate of the low-energy quasiparticles grows linearly with T .

Finite- U .—In Fig. (6), we plot the resistivity vs temperature curve for $\lambda = 0, 0.25, 0.5$, and $U = 1$. For $\lambda = 0$, i.e., the Hubbard model, the resistivity is monotonic, but has a kink at $T_{\text{kink}} \approx 0.4$. For $T_{\text{FL}} < T < T_{\text{kink}}$, the resistivity is quasilinear with negative intercept, while $T > T_{\text{kink}}$, it is

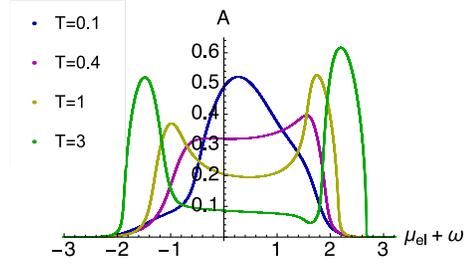


FIG. 8. The LDOS for $\lambda = 0.5$ and $U = 1$ at $T = 0.1, 0.4, 1, 3$. For $T \lesssim T_{\max}$, the central peak is a signature of the low-energy quasiparticles, while for $T \gtrsim T_{\max}$, the high-energy peaks are a signature of the high-energy quasiparticles.

quasilinear with positive intercept. Here, T_{FL} is the Fermi-liquid scale, below which the resistivity is quadratic with temperature. These features are also observed in dynamical mean-field theory studies of the Hubbard model in both the cases of small and large U [24,40–42]. For finite λ , the resistivity once again displays a maximum at T_{\max} . T_{\max} decreases and the peak becomes sharper with increasing λ . In Fig. 7, we plot the resistivity vs temperature curve for $\lambda = 0.5$ and $U = 0.1, 0.5, 1.0$. T_{\max} increases with increasing U .

In Fig. 8, we plot the LDOS for $\lambda = 0.5$ and $U = 1$ at $T = 0.1, 0.4, 1, 3$. For $T \lesssim T_{\max}$, the central peak is a signature of the low-energy quasiparticles, while for $T \gtrsim T_{\max}$, the high-energy peaks are a signature of the high-energy quasiparticles. Comparing with Fig. 4, the high-energy peak values are smaller. This is a consequence of the broadening of the imaginary part of the self-energy beyond the edges of the bare band (see Fig. 5 and Supplemental Material, Fig. 1 [20]) as U is increased. Consequently, the conductivity in the high-energy channel decreases, and T_{\max} shifts to the right with increasing U (see Fig. 7).

Conclusion.—We have computed the resistivity vs temperature curve in the Hubbard-Holstein model on the infinite dimensional Bethe lattice, with weak to intermediate electronic repulsion $U \leq D$, and electron-phonon coupling strength $\lambda \leq 0.5$. For $\lambda > 0$, it has a broad maximum, consistent with materials that display resistivity saturation. For $\lambda = 0$, it has a kink rather than a maximum.

We have identified two parallel quantum conducting channels, consisting of low- and high-energy quasiparticles. The former dominates at low temperatures, causing the resistivity to increase, while the latter dominates at high temperatures, causing the resistivity to saturate. The temperature scale of the saturation increases with both increasing U and decreasing λ .

Therefore, our theory predicts resistivity saturation in systems with narrow conducting bands, strong electron-phonon coupling, and weak to moderate electron-electron interactions.

It is possible that resistivity saturation can be achieved by more than one mechanism. The mechanism which we propose (i.e., high-energy quasiparticles) has a distinct signature in the LDOS [see Fig. (5)], which can be observed using ARPES/STM, as well as in the optical conductivity (see Fig. (5) of the Supplemental Material [20]).

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- [1] O. Gunnarsson, M. Calandra, and J. E. Han, *Rev. Mod. Phys.* **75**, 1085 (2003).
- [2] Z. Fisk and G. W. Webb, *Phys. Rev. Lett.* **36**, 1084 (1976).
- [3] J. H. Mooij, *Phys. Status Solidi A* **17**, 521 (1973).
- [4] T. Kakeshita, T. Fukuda, H. Tetsukawa, T. Saburi, K. Kindo, T. Takeuchi, M. Honda, S. Endo, T. Taniguchi, and Y. Miyako, *Jpn. J. Appl. Phys.* **37**, 2535 (1998).
- [5] Y. Ando, S. Komiya, K. Segawa, S. Ono, and Y. Kurita, *Phys. Rev. Lett.* **93**, 267001 (2004).
- [6] S. Martin, M. Gurvitch, C. E. Rice, A. F. Hebard, P. L. Gammel, R. M. Fleming, and A. T. Fiory, *Phys. Rev. B* **39**, 9611 (1989).
- [7] H. Takagi, B. Batlogg, H. L. Kao, J. Kwo, R. J. Cava, J. J. Krajewski, and W. F. Peck, *Phys. Rev. Lett.* **69**, 2975 (1992).
- [8] A. F. Hebard, T. T. M. Palstra, R. C. Haddon, and R. M. Fleming, *Phys. Rev. B* **48**, 9945 (1993).
- [9] M. Gurvitch and A. T. Fiory, *Phys. Rev. Lett.* **59**, 1337 (1987).
- [10] C. C. Yu and P. W. Anderson, *Phys. Rev. B* **29**, 6165 (1984).
- [11] M. Gurvitch, *Phys. Rev. B* **24**, 7404 (1981).
- [12] Y. Werman, S. A. Kivelson, and E. Berg, *npj Quantum Mater.* **2**, 7 (2017).
- [13] A. J. Millis, J. Hu, and S. Das Sarma, *Phys. Rev. Lett.* **82**, 2354 (1999).
- [14] W. Pickett, *J. Supercond.* **4**, 397 (1991).
- [15] H. Wiesmann, M. Gurvitch, H. Lutz, A. Ghosh, B. Schwarz, M. Strongin, P. B. Allen, and J. W. Halley, *Phys. Rev. Lett.* **38**, 782 (1977).
- [16] P. B. Allen, in *Superconductivity in D- and F-Band Metals*, edited by H. Suhl and M. B. Maple (Academic Press, New York, 1980), pp. 291–304.
- [17] R. B. Laughlin, *Phys. Rev. B* **26**, 3479 (1982).
- [18] A. B. Migdal, *Zh. Eksp. Teor. Fiz.* **34**, 1438 (1958).
- [19] E. Kozik, M. Ferrero, and A. Georges, *Phys. Rev. Lett.* **114**, 156402 (2015).
- [20] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevLett.122.026602> for details on plots of the real and imaginary parts of the self-energy, the optical conductivity, the dc conductivity vs. temperature in both the low- and high-energy channels, and the dependence of the saturation temperature on U and λ . They also contain further details of the perturbative calculation.
- [21] S. M. Girvin and M. Jonson, *Phys. Rev. B* **22**, 3583 (1980).
- [22] A. A. Abrikosov and L. P. Gor'kov, *Zh. Eksp. Teor. Fiz.* **35**, 1090 (1959).
- [23] L. F. Mattheiss and W. Weber, *Phys. Rev. B* **25**, 2248 (1982).
- [24] X. Deng, J. Mravlje, R. Žitko, M. Ferrero, G. Kotliar, and A. Georges, *Phys. Rev. Lett.* **110**, 086401 (2013).
- [25] B. S. Shastry and E. Perepelitsky, *Phys. Rev. B* **94**, 045138 (2016).
- [26] F. Bloch, *Z. Phys.* **59**, 208 (1930).
- [27] E. Grüneisen, *Ann. Phys. (Berlin)* **408**, 530 (1933).
- [28] J. M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, 1960), pp. 357–370.
- [29] H. Schweitzer and G. Czycholl, *Phys. Rev. Lett.* **67**, 3724 (1991).
- [30] S. Burdin, A. Georges, and D. R. Grempel, *Phys. Rev. Lett.* **85**, 1048 (2000).
- [31] T. Pruschke, R. Bulla, and M. Jarrell, *Phys. Rev. B* **61**, 12799 (2000).
- [32] S. Burdin and V. Zlatić, *Phys. Rev. B* **79**, 115139 (2009).
- [33] C. Grenzbach, F. B. Anders, G. Czycholl, and T. Pruschke, *Phys. Rev. B* **74**, 195119 (2006).
- [34] A. N. Tahvildar-Zadeh, M. Jarrell, and J. K. Freericks, *Phys. Rev. B* **55**, R3332 (1997).
- [35] N. S. Vidhyadhiraja, V. E. Smith, D. E. Logan, and H. R. Krishnamurthy, *J. Phys. Condens. Matter* **15**, 4045 (2003).
- [36] T. Pruschke, D. L. Cox, and M. Jarrell, *Phys. Rev. B* **47**, 3553 (1993).
- [37] N. Pakhira and R. H. McKenzie, *Phys. Rev. B* **91**, 075124 (2015).
- [38] P. Limelette, P. Wzietek, S. Florens, A. Georges, T. A. Costi, C. Pasquier, D. Jérôme, C. Mézière, and P. Batail, *Phys. Rev. Lett.* **91**, 016401 (2003).
- [39] Y. Kurosaki, Y. Shimizu, K. Miyagawa, K. Kanoda, and G. Saito, *Phys. Rev. Lett.* **95**, 177001 (2005).
- [40] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, *Rev. Mod. Phys.* **68**, 13 (1996).
- [41] W. Ding, R. Žitko, P. Mai, E. Perepelitsky, and B. S. Shastry, *Phys. Rev. B* **96**, 054114 (2017).
- [42] E. Perepelitsky, A. Galatas, J. Mravlje, R. Žitko, E. Khatami, B. S. Shastry, and A. Georges, *Phys. Rev. B* **94**, 235115 (2016).

Supplementary Material:

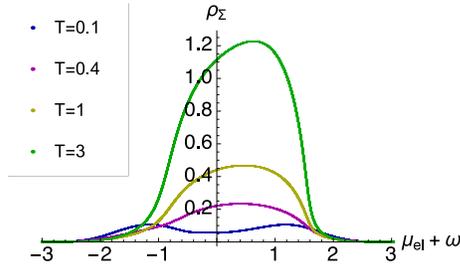
Band-edge quasiparticles from electron phonon coupling and resistivity saturation.

Edward Perepelitsky¹ and B. Sriram Shastry¹

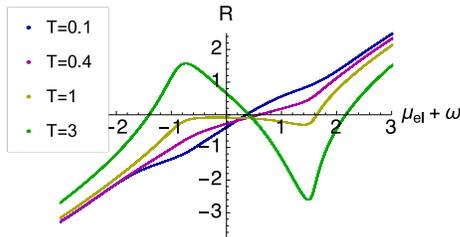
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SM-I. SELF-ENERGY IN FINITE- U CASE.

We consider once again $U = 1$. In SM-Fig. (1), we plot $\rho_\Sigma(\omega - \mu_{el})$ for $\lambda = .5$ at $T = 0.1, 0.4, 1, 3$. Just as in the case of $U = 0$, it consists of a peak centered near the origin, whose height grows in magnitude linearly with T (see Fig.(5) of the main paper). However, in the finite- U case, the tails spill over beyond the edges of the bare band, causing the resistivity to increase in the high-energy channel, and T_{max} to increase with increasing U . The corresponding $R(\omega - \mu_{el})$ is plotted in SM-Fig. (2). The maximum in $\rho_\Sigma(\omega - \mu_{el})$ causes $\Re \Sigma(\omega - \mu_{el})$ to have a broad region of positive slope. The resulting $R(\omega - \mu_{el})$ bends towards the frequency-axis at high-energies, leading to the high-energy quasiparticles.



SM-Fig 1: ρ_Σ for $U = 1$ and $\lambda = 0.5$ at $T = 0.1, 0.4, 1, 3$. Compared with the $U = 0$ case (see Fig.(5) of the main paper), the tails spill over beyond the edges of the bare band.



SM-Fig 2: R for $U = 1$ and $\lambda = 0.5$ at $T = 0.1, 0.4, 1, 3$. As the temperature is raised, $R(\omega - \mu_{el})$ bends towards the frequency axis at high-energies, leading to the high-energy quasiparticles.

SM-II. CONDUCTIVITY IN THE LOW AND HIGH FREQUENCY CHANNELS.

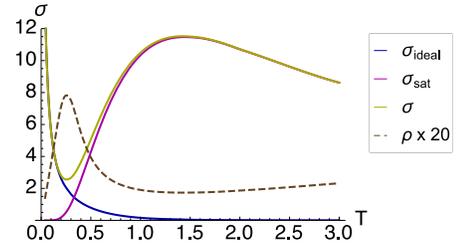
Rewriting Eq.(1) in terms of conductivities, we have

$$\sigma = \sigma_{ideal} + \sigma_{sat}, \quad (\text{SM-1})$$

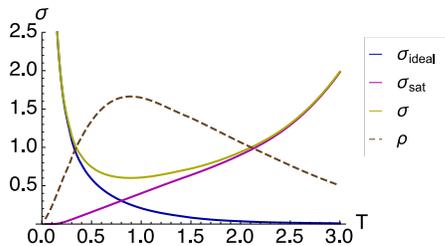
where σ_{ideal} is the conductivity of the low-energy quasiparticles and σ_{sat} is the conductivity of the high-energy quasiparticles. We can formally define each one as the low- and high- frequency contributions to the integral in Eq.(5):

$$\begin{aligned} \frac{\sigma_{ideal}}{\sigma_{IRM}} &= \frac{2}{\pi T} \int_{|\omega| < \omega_c} d\omega f(\omega - \mu_{el}) \bar{f}(\omega - \mu_{el}) I(\omega - \mu_{el}), \\ \frac{\sigma_{sat}}{\sigma_{IRM}} &= \frac{2}{\pi T} \int_{|\omega| > \omega_c} d\omega f(\omega - \mu_{el}) \bar{f}(\omega - \mu_{el}) I(\omega - \mu_{el}). \end{aligned} \quad (\text{SM-2})$$

We choose $\omega_c = 0.95$ to be slightly smaller than the edge of the bare band to capture the entire high-energy quasiparticle in σ_{sat} . In Figs. (3) and (4), we plot σ_{ideal} , σ_{sat} , and σ as a function of T for the cases of $U = 0$; $\lambda = 0.55$, and $U = 1$; $\lambda = 0.5$, respectively. At low temperatures, σ is dominated by the low-energy quasiparticles, while at high temperatures, it is dominated by the high energy quasiparticles. In both cases, the resulting resistivity vs. temperature curve has a maximum at approximately the crossover temperature.



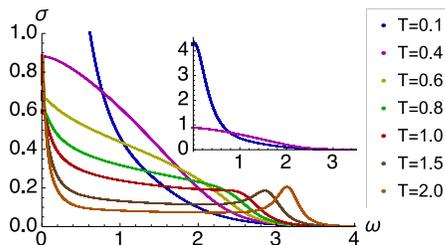
SM-Fig 3: σ_{ideal} , σ_{sat} , and σ as a function of T for the case of $U = 0$, $\lambda = 0.5$. At low temperatures, σ is dominated by σ_{ideal} , while at high temperatures, it is dominated by σ_{sat} . The crossover occurs at $T \approx T_{max}$, the location of the maximum in the resulting resistivity vs. temperature curve (plotted as the dashed brown curve (scaled by a factor of 20)).



SM-Fig 4: σ_{ideal} , σ_{sat} , and σ as a function of T for the case of $U = 1$, $\lambda = 0.5$. At low temperatures, σ is dominated by σ_{ideal} , while at high temperatures, it is dominated by σ_{sat} . The crossover occurs at $T \approx T_{max}$, the location of the maximum in the resulting resistivity vs. temperature curve (plotted as the dashed brown curve).

SM-III. OPTICAL CONDUCTIVITY

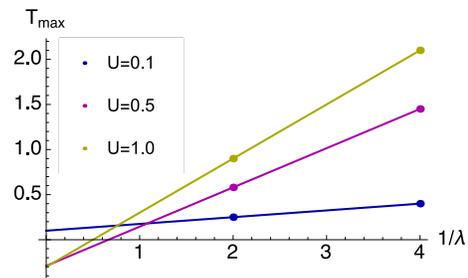
The high-energy quasi-particles have a distinct signature in the temperature-dependence of the optical conductivity (Eq. (SM-14)). In SM-Fig. (5), we plot the optical conductivity for $\lambda = 0.5$ and $U = 1$, at $T = 0.1, 0.4, 0.6, 0.8, 1.0, 1.5, 2.0$. The Drude peak, which is present at all temperatures, corresponds to zero-energy optical transitions between the central peak (in the spectral function) and itself at low temperatures, and the high-energy peaks and themselves at high-temperatures (see Fig.8 of MS). For $T \gtrsim T_{max}$ (see Fig.6 of MS), the optical conductivity develops a feature at high-frequencies, which both grows and moves to the right with increasing temperature. This corresponds to optical transitions between the high-energy peaks, which are growing and moving further apart with increasing temperature (see Fig.8 of MS).



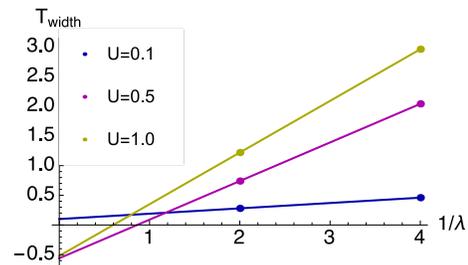
SM-Fig 5: The optical conductivity for $\lambda = 0.5$ and $U = 1$, at $T = 0.1, 0.4, 0.6, 0.8, 1.0, 1.5, 2.0$. For $T \gtrsim T_{max}$, it develops a high-frequency feature, which both grows and moves to the right with increasing temperature. This feature corresponds to optical transitions between the high-energy quasiparticle peaks in the spectral function. Therefore, the high-energy quasiparticles have a distinct and observable signature in the optical conductivity.

SM-IV. DEPENDENCE OF T_{max} ON λ AND U .

In this section, we explore the dependence of T_{max} on λ and U . Note that in the equation for the self-energy (Eq.(4) of the main paper), λ and T appear together. In addition, the Fermi functions in the definition of the conductivity (Eq.(5) of the main paper) have explicit temperature dependence (the pre-factor of $\frac{1}{T}$ does not affect the value of T_{max}). Therefore in the $T_{max} \rightarrow \infty$ ($\lambda \rightarrow 0$) limit, we expect $T_{max} \propto \frac{1}{\lambda}$. In SM-Fig. (6), plotting T_{max} vs. $\frac{1}{\lambda}$ for $U = 0.1, 0.5, 1.0$ reveals that $T_{max} = \frac{T_{width,s}}{\lambda} + T_{max,0}$, where $T_{max,0}$ and $T_{max,s}$ are undetermined fit parameters. In the $\lambda \rightarrow 0$ limit, this reproduces the expected result. Additionally, in SM-Fig. (7), we plot T_{width} vs. $\frac{1}{\lambda}$ for $U = 0.1, 0.5, 1.0$, where T_{width} is the width at half-maximum of the peak in the resistivity vs. temperature curve. Once again, we find that $T_{width} = \frac{T_{width,s}}{\lambda} + T_{width,0}$, where $T_{width,0}$ and $T_{width,s}$ are undetermined fit parameters. We summarize the values of the fit parameters for various values of U in Table I.



SM-Fig 6: T_{max} vs. $\frac{1}{\lambda}$ for $U = 0.1, 0.5, 1.0$, where T_{max} is the peak location in the resistivity vs. temperature curve. It has the form $T_{max} = \frac{T_{max,s}}{\lambda} + T_{max,0}$, where $T_{max,0}$ and $T_{max,s}$ are undetermined fit parameters.



SM-Fig 7: T_{width} vs. $\frac{1}{\lambda}$ for $U = 0.1, 0.5, 1.0$, where T_{width} is the peak width at half-maximum in the resistivity vs. temperature curve. It has the form $T_{width} = \frac{T_{width,s}}{\lambda} + T_{width,0}$, where $T_{width,0}$ and $T_{width,s}$ are undetermined fit parameters.

TABLE I: Fit Parameters

U	$T_{max,0}$	$T_{max,s}$	$T_{width,0}$	$T_{width,s}$
0.1	0.1	0.075	0.1	0.09
0.5	-0.29	0.435	-0.56	0.65
1	-0.3	0.6	-0.52	0.87

SM-V. DETAILS OF PERTURBATIVE CALCULATION.

To compute $G(\varepsilon, \omega, \mu)$, the single-electron propagator, to $O(g^2)$, we use the following procedure. We first compute $\Sigma_{el}(\omega)$, the electron-electron scattering in the absence of phonons. The resulting single-electron propagator, $G_{el}(\varepsilon, \omega, \mu_{el})$, then scatters off of the phonons, producing $\Sigma_{el,ph}(\omega)$. μ_{el} is chosen to ensure the correct number sum rule for the electrons in the absence of the phonons. The total scattering of the electron, $\Sigma(\omega)$, is given by the sum: $\Sigma(\omega) = \Sigma_{el}(\omega) + \Sigma_{el,ph}(\omega)$. $G(\varepsilon, \omega, \mu)$ is given in terms of $\Sigma(\omega)$ using the usual Dyson's equation. μ is then chosen to ensure the correct number sum rule for the electrons in the presence of the phonons. Since $\mu - \mu_{el}$ is $O(g^2)$, it is consistent to replace μ by μ_{el} in G_{el} .

Using second order perturbation theory in U , we find that

$$\begin{aligned} \rho_{\Sigma_{el}}(\omega - \mu_{el}) &= U^2 \int d\nu_1 d\nu_2 \mathcal{D}(\nu_1) \mathcal{D}(\nu_2) \mathcal{D}(\nu_1 + \nu_2 - \omega) \times \\ & [f(\nu_1 - \mu_{el}) f(\nu_2 - \mu_{el}) \bar{f}(\nu_1 + \nu_2 - \omega - \mu_{el}) + f \leftrightarrow \bar{f}] + \eta, \\ \Re \Sigma_{el}(\omega) &\equiv U \frac{n}{2} + \int d\nu \frac{\rho_{\Sigma_{el}}(\nu)}{\omega - \nu}, \end{aligned}$$

where for any dynamical object $Q(\omega)$, $\rho_Q(\omega) \equiv -\frac{1}{\pi} \Im m(Q(\omega))$, $f(\omega) \equiv \frac{1}{e^{\beta\omega} + 1}$, $\bar{f}(\omega) \equiv 1 - f(\omega)$, and $\beta \equiv \frac{1}{T}$. We find it convenient to shift the frequency by the chemical potential, since the latter grows linearly with T at high- T . $\rho_{G_{el}}(\varepsilon, \omega)$ is obtained using Dyson's equation:

$$\begin{aligned} \rho_{G_{el}}(\varepsilon, \omega - \mu_{el}) &= \rho_{\Sigma_{el}}(\omega - \mu_{el}) \times \\ & \frac{1}{(\omega - \Re \Sigma_{el}(\omega - \mu_{el}) - \varepsilon)^2 + \pi^2 (\rho_{\Sigma_{el}}(\omega - \mu_{el}))^2}. \end{aligned} \quad (\text{SM-4})$$

The chemical potential μ_{el} is fixed using the number sum rule,

$$\int d\omega A_{el}(\omega - \mu_{el}) f(\omega - \mu_{el}) = \frac{n}{2}, \quad (\text{SM-5})$$

where n is the density, and the onsite (i.e. local) spectral function

$$A_{el}(\omega - \mu_{el}) \equiv \int d\varepsilon \mathcal{D}(\varepsilon) \rho_{G_{el}}(\varepsilon, \omega - \mu_{el}). \quad (\text{SM-6})$$

The self-energy due to the electron phonon interaction is given by

$$\begin{aligned} \rho_{\Sigma_{el,ph}}(\omega - \mu_{el}) &= g^2 \sum_{\pm} A_{el}(\omega \pm \omega_0 - \mu_{el}) \times \\ & [f^{\mp}(\omega - \mu_{el} \pm \omega_0) + n_B(\omega_0)], \end{aligned} \quad (\text{SM-7})$$

$$\Re \Sigma_{el,ph}(\omega) = \int d\nu \frac{\rho_{\Sigma_{el,ph}}(\nu)}{\omega - \nu}, \quad (\text{SM-8})$$

where $f^-(\omega) \equiv f(\omega)$, $f^+(\omega) \equiv \bar{f}(\omega)$, and $n_B(\omega) \equiv \frac{1}{e^{\beta\omega} - 1}$ is the Bose distribution function. Since $\omega_0 \ll 1$, $A_{el}(\omega \pm \omega_0 - \mu_{el}) \approx A_{el}(\omega - \mu_{el})$. In addition, for $T \gtrsim \omega_0$, $\sum_{\pm} f^{\mp}(\omega - \mu_{el} \pm \omega_0) \approx 1$ and $1 + 2n_B(\omega_0) \approx \frac{2T}{\omega_0}$. Therefore, for $T \gtrsim \omega_0$, to a very good approximation,

$$\rho_{\Sigma_{el,ph}}(\omega - \mu_{el}) = \frac{\pi \lambda A_{el}(\omega - \mu_{el})}{2} \times T, \quad (\text{SM-9})$$

where λ , defined by $g^2 \equiv \frac{\pi D \lambda \omega_0}{4}$, is a dimensionless measure of the electron-phonon coupling strength.

Putting everything together, the spectral function for the electron is given by

$$\rho_G(\varepsilon, \omega - \mu_{el}) = \frac{\rho_{\Sigma}(\omega - \mu_{el})}{(R(\omega - \mu_{el}) - \varepsilon)^2 + \pi^2 (\rho_{\Sigma}(\omega - \mu_{el}))^2}, \quad (\text{SM-10})$$

where $R(\omega - \mu_{el}) \equiv \omega + \Delta\mu - \Re \Sigma(\omega - \mu_{el})$, and $\Delta\mu \equiv \mu - \mu_{el}$ tends to 0 as $T \rightarrow \infty$,

$$\begin{aligned} \Sigma(\omega) &= \Sigma_{el}(\omega) + \Sigma_{el,ph}(\omega), \quad (\text{SM-11}) \\ & \text{and } \mu \text{ is determined by the condition} \\ & (\text{SM-3}) \end{aligned}$$

$$\int d\omega f(\omega - \mu_{el}) A(\omega - \mu_{el}) = \frac{n}{2}, \quad (\text{SM-12})$$

where

$$A(\omega - \mu_{el}) = \int d\varepsilon \mathcal{D}(\varepsilon) \rho_G(\varepsilon, \omega - \mu_{el}) \quad (\text{SM-13})$$

is the LDOS.

Finally, the optical conductivity can be calculated from the spectral function via the formula:

$$\begin{aligned} \frac{\sigma(\omega)}{\sigma_{IRM}} &= 2\pi \int d\varepsilon \phi(\varepsilon) \int d\omega' \frac{[f(\omega' - \mu_{el}) - f(\omega + \omega' - \mu_{el})]}{\omega} \\ & \times \rho_G(\varepsilon, \omega' - \mu_{el}) \rho_G(\varepsilon, \omega' + \omega - \mu_{el}), \end{aligned} \quad (\text{SM-14})$$

where $\phi(\varepsilon) = \Theta(1 - \varepsilon^2) \times (1 - \varepsilon^2)^{\frac{3}{2}}$ is the transport function. In the $\omega \rightarrow 0$ limit, we recover Eqs. (5) and (6) in the MS for the dc conductivity.