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## Two-particle excitations under coexisting electron interaction and disorder C. E. Ekuma Phys. Rev. B **98**, 085129 — Published 17 August 2018 DOI: 10.1103/PhysRevB.98.085129

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## Two-particle excitations under coexisting electron interaction and disorder

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(Dated: August 3, 2018)

We study the combined impact of random disorder, electron-electron, and electron-hole interactions on the absorption spectra of a three-dimensional Hubbard Hamiltonian. We determine the singleparticle Green function within the typical medium dynamical cluster approximation. We solve the Bethe-Salpeter equation (BSE) to obtain the dynamical conductivity. Our results show that increasing disorder strength at a given interaction strength leads to decreased absorption with the dynamical conductivity, systematically going to zero at all frequencies, a fingerprint of a correlationmediated electron localization. Surprisingly, our data reveal that taking into account the effects of electron-hole interactions through the BSE significantly changes the oscillator strength with a concomitant reduction in the critical disorder strengths  $W_c^U$ . We attribute this behavior to enhanced quantum correction induced by electron-hole interactions.

PACS numbers: 71.35.-y, 64.70.Tg, 31.15.V-, 71.35.Cc

Introduction.- Recent experiments have shown that 54 16 most correlated materials contain a significant amount 55 17 of defects, which appear to be intrinsic [1-7]. These 56 18 inhomogeneities could significantly affect device perfor- 57 19 mance. Most of the experimental transport data on dis- 58 20 ordered materials have defied explanation by the con- 59 21 ventional transport theory. For instance, the phase dia-60 22 gram of the binary mixture of the correlated ferromag-61 23 netic metal SrRuO<sub>3</sub> (T<sub>C</sub>  $\approx 160$  K) [8] and the band in- 62 24 sulator SrTiO<sub>3</sub> (band gap  $\approx 3.2$ ) [9] is still under active <sup>63</sup> 25 research. One suggestion is that there is an Anderson 64 26 insulator around  $x \gtrapprox 0.5$  and a disordered correlated in-  ${}_{\rm 65}$ 27 sulator at  $\sim 0.2$  [7]. Other potential candidates where the 66 28 coexistence of defects, electron-electron and electron-hole 67 29 interactions could play a crucial role are the perovskite 68 30 transition metal oxides, e.g.,  $A_{1-x}BA'_xO_3$ . Understand- 69 31 ing the defect morphology could greatly improve better 70 32 characterization of their properties and that of materials 71 33 in general. 72 34

There is a decade's history of theoretical research in- $\frac{1}{74}$ 35 quiry into electron localization. Majority of these com-  $\frac{1}{75}$ 36 putational/theoretical works focus on localization due 37 to disorder or electron-electron interactions [2, 10–19]. 38 These two limiting cases were pioneered by P. Ander-77 39 son [20, 21] and N. F. Mott [22, 23], now known as An-78 40 derson and Mott localization, respectively. As explained 79 41 above, defects and electron-electron interactions coexist 80 42 in many physical systems and they can both be substan-81 43 tial. Also, in some cases, due to dynamical screening in 82 44 the local environment of the system, the transport is no 83 45 more driven by electron or hole carriers but dominated by 84 46 bound electron-hole pairs known as excitons. One conse- 85 47 quence of this is the emergence of nontrivial many-body 86 48 effects, e.g., spectral weight redistribution, multiferroic- 87 49 ity [24–27] not observed in conventional systems. The in- \*\* 50 cipient of electron localization in an otherwise "strongly" 89 51 correlated system is generally difficult to model due to 90 52 the competing energy scales that abound in this regime. 91 53

Based on model-coupling theory, Götze [11, 28] develop a self-consistent localization formalism, which has been used by many authors, e.g., Prelovšek [19] to calculate the conductivity of the noninteracting electron system. An approach based on the potential well analogy of the coherent potential approximation was formulated and used to calculate the conductivity of various disorder distributions [3, 15–18, 29]. The diagrammatic, selfconsistent approach of Vollhardt and Wöfle [10] was used to calculate conductivity for the Anderson model [30-33], and various other models [15, 17, 34, 35]. Aguair et al [7] used the inverse of the typical density of states as an approximation to the resistivity and showed that the resistivity curves as a function of temperature are reminiscent of the Mooij correlations originally observed in disordered transition metal alloys [36]. Girvin and Jonson [37] introduced an approximate scheme for calculating conductivity that becomes accurate only close to the localization transition. This method was further used by Dobrosavljević et al [38] in their study using Bethe lattice. Zhang et al [39] proposed a two-particle formalism and calculated the dc-conductivity within the typical medium theory for the noninteracting fermionic system.

In this paper, we present and explore the absorption properties of a disordered Hubbard model at experimentally relevant Hubbard interactions using the typical medium dynamical cluster approximation [40–46]. Herein, we focus on the limit where the disorder and the kinetic term is far greater than the interaction strength (i.e., the interaction strength is far smaller than the noninteracting bandwidth). Also, we will explore the regime where disorder and interaction strength are both substantial (i.e., the interaction strength is large but still significantly smaller than the noninteracting bandwidth). The former is reminiscent of a correlated and strongly disordered semiconductor, e.g., Si:B [47] and the latter could be compared to the perovskite compounds, e.g., (Ca,Sr)VO<sub>3</sub>. We will, however, not explore the

Mott physics, which is in the regime where the interac-144 92 tion strength is far greater than the effective bandwidth.145 93 This regime has been extensively studied in the litera-146 94 ture (see, e.g., Refs [48–53]). The main findings of this<sub>147</sub> 95 work is that electron-hole interactions significantly alters<sub>148</sub> 96 the critical behavior of a disordered, three-dimensional<sub>149</sub> 97 Hubbard Hamiltonian. Our calculations reveal that the150 98 critical disorder strengths are reduced by more than 10%<sub>151</sub> 99 due to electron-hole interaction effects. 152 100

It is worthwhile to contrast the method presented<sup>153</sup> 101 herein from other approaches of calculating absorption<sup>154</sup> 102 spectra [2, 10–14]. The single-particle Green functions<sup>155</sup> 103 used in our two-particle calculations are obtained self-156 104 consistently from a mean-field approach with an intrinsic<sup>157</sup> 105 order parameter for characterizing electron localization<sup>158</sup> 106 even in the proximity of a localization transition [40–159 107 42]. Our approach also takes into account resonance ef-160 108 fects, which systematically incorporate longer-range spa-161 109 tial fluctuations up to the system (cluster) size. This<sup>162</sup> 110 resonance effect is due to having more than one lattice<sup>163</sup> 111 sites in the system as against just one impurity site, e.g.,<sup>164</sup> 112 as in the coherent potential approximation. The carriers<sup>165</sup> 113 now collide with each other as well as scatter off multiple<sup>166</sup> 114 lattice sites. One consequence of this inter-site correla-167 115 tion effect is coherent backscattering, which is a precur-168 116 sor to Anderson localization in a disordered system. We<sub>169</sub> 117 further take into account vertex corrections within the<sub>170</sub> 118 cluster. The vertex correction accounts for the polariza-171 119 tion effects in the effective medium beyond the leading<sub>172</sub> 120 order of the perturbation theory (see, e.g., Refs. [54–57].173 121 The typical medium, inter-site correlations, and the ver-174 122 tex corrections ensure the proper characterization of the<sub>175</sub> 123 large fluctuations in the local Green function that could<sub>176</sub> 124 lead to its *typical value* being far removed from the av-177 125 erage one [43, 58]. Unless otherwise stated, all the re- $_{178}$ 126 sults presented herein are for the three-dimensional cu-179 127 bic lattice of size  $3 \times 3 \times 3$  corresponding to a cluster size<sub>180</sub> 128  $N_c = 27$ . We will focus on the paramagnetic phase, i.e,<sub>181</sub> 129 we do not allow for the formation of any local moments.<sub>182</sub> 130 All the reported results are obtained at zero tempera-183 131 ture. We used a broadening parameter of  $10^{-4}$  and  $a_{184}$ 132 computational accuracy (numerical uncertainty) of up to 133  $\sim \pm 0.1$  in our calculations. 134

Method.- We consider the Hubbard Hamiltonian of in teracting electrons subjected to quenched random disor ders

$$H = -\sum_{\langle ij \rangle \sigma} t_{ij} (c_{i\sigma}^{\dagger} c_{j\sigma} + h.c.) + \sum_{i} U_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} V_{i} n_{i\sigma}, \frac{1}{186} (1)_{186}$$

where the first term describes the hopping of electrons<sub>190</sub> on the lattice, the second term describes the energy cost of having two electrons with opposite spin sitting on the same lattice site, and the last term depicts the disorder potential.  $c_i^{\dagger}(c_i)$  is the creation (annihilation) operator of an electron on site *i* with spin  $\sigma$ ,  $n_i = c_i^{\dagger}c_i$  is the number operator,  $t_{ij} = t$  is the hopping matrix element between nearest-neighbor sites, and  $U_i = U$  is the electron-electron interactions strength parameterized by the Hubbard onsite energy. The disorder is represented by a spatially, uncorrelated, spin-independent random potential  $V_i$  distributed according to a probability distribution function  $P(V_i) = \frac{1}{2W}\Theta(W - |V_i|)$ , where  $\Theta(x)$ is the Heaviside step function and W is the width of the box, which parametrizes the strength of the disorder. We set the energy unit to 4t.

To calculate the two-particle Green function, we need the single-particle counterpart. To obtain the singleparticle Green function  $G(\vec{k}, E)$  in the presence of electron-electron interactions and random disorder, we solved the typical medium dynamical cluster approximation (TMDCA) self-consistency equations. The TMDCA maps the lattice problem (1) onto a periodically repeated cluster of size  $N_c$  primitive cells embedded in a typical medium. This typical medium is characterized by a self-consistently determined non-local, hybridization function  $\Delta(k, E)$  [40–46, 59–63]. The mapping is accomplished by dividing the first Brillouin zone of the original lattice into  $N_c$  non-overlapping equal cells. As one increases  $N_c$ , longer-range spatial fluctuations are systematically accounted for up to  $\leq N_c^{1/d}$ , where d is the spatial dimension. The TMDCA self-consistency could be summarized as follows. We make an initial guess of hybridization function;  $\Delta(\vec{k}, E)$  describes how the cluster sites couple to the typical medium. Using  $\Delta(\vec{k}, E)$ , we calculate the fully dressed cluster Green function  $G^{c}(E) = (\mathcal{G}^{-1} - V - \Sigma^{\text{Int}})^{-1}$ , where  $\mathcal{G}$  is the clusterexcluded Green function, V is the disorder potential, and  $\Sigma^{\text{Int}}$  is the electron-electron interactions, which is included up to its second-order perturbation expansion. We note that the disorder is accounted for exactly within the cluster and  $\Sigma^{\text{Int}}$  is obtained self-consistently within the cluster solver using second-order perturbation theory. The cluster density of states  $\rho^c = -\frac{1}{\pi} \Im \mathfrak{m} G^c$  is then calculated by averaging over a large number of configurations to obtain the momentum dependent, non-self-averaged typical density of states [41, 42, 42]

$$\rho_t^c(\mathbf{K}) = \langle \rho_i^c \rangle_{\text{geom}} \left\langle \frac{\rho^c(\mathbf{K})}{\frac{1}{N_c} \sum_i \rho_i^c} \right\rangle_{\text{arit}}, \qquad (2)$$

where  $\langle \rho_i^c \rangle_{\text{geom}} = \exp \langle \ln \rho_i \rangle_{\text{arit}}$  is the diagonal elements of  $\rho^c$  and the second factor ensures that non-local fluctuations up to  $\lesssim N_c^{1/d}$  is captured withing the typical environment. Using Hilbert transformation, we obtain the cluster typical Green function  $G_t^c(\mathbf{K})$  from  $\rho_t^c(\mathbf{K})$  and then calculate the coarse-grained Green function

$$\bar{G}(\mathbf{K}) = \frac{N_c}{N} \sum_{\tilde{\mathbf{k}}} \left[ G_t^c(\mathbf{K})^{-1} + \Delta(\mathbf{K}) - \epsilon(\mathbf{k}) + \bar{\epsilon}(\mathbf{K}) + \mu \right]^{-1},$$
(3)

where the overbar depicts cluster coarse-graining and  $\mu_{215}$ is the chemical potential. The TMDCA loop is closed by<sub>216</sub> calculating a new hybridization function

$$\Delta_{\rm n}(\mathbf{K}) = (1 - \varsigma) \Delta_{\rm o}(\mathbf{K}) + \xi \left[ (G^c)^{-1} - \bar{G}^{-1} \right], \qquad (4)_{219}^{218}$$

where  $\Delta_n$  ( $\Delta_o$ ) refers to the new (old) hybridization<sub>221</sub> function and  $\xi$  is a mixing parameter. Convergence<sub>222</sub> is achieved when  $G_t^c \approx \bar{G}$ , which also coincides with<sub>223</sub>  $\Delta_n \approx \Delta_o$ .

To determine the two-particle properties of the many-198 body Hamiltonian above, we solve the Bethe-Salpeter 199 equation using the converged, single-particle Green func-200 tion obtained from the above TMDCA self-consistency 201 equations as input. Herein, we focus on the particle-225 202 hole channel and calculate the dynamical, conductivity<sub>226</sub> 203 with and without electron-hole interactions. We obtain<sub>227</sub> 204 the full lattice, dynamical conductivity by solving the<sub>228</sub> 205 Bethe-Salpeter equations as outlined below. 206 229

230 1. The TMDCA self-consistency equations is solved<sub>231</sub> 207 to obtain the single-particle Green functions used<sub>232</sub> 208 in the two particle calculations. This requires, 209 both the single particle retarded  $G^R(\vec{k}, E)$  and  $\operatorname{ad-}_{24}$ 210 vanced  $G^A(\vec{k}, E)$  Green functions. However, since 211  $A(\vec{k}, E)A(\vec{k}, E) = \frac{1}{2\pi i} [\vartheta] \times \frac{1}{2\pi i} [\vartheta], \text{ where } \vartheta =_{236}^{235} G^A(\vec{k}, E) - G^R(\vec{k}, E) \text{ and } A(\vec{k}, E) = -\frac{1}{\pi} \Im \mathfrak{m} G(\vec{k}, E)_{237}$ 212 213 is the spectral function, we only require to know<sub>238</sub> 214

the retarded Green function. In calculating the two-particle Green function, we have used the averaged lattice and cluster Green functions obtained within the typical medium. This is important as the underlying dynamics present in the system are encoded in these average quantities. Further and most importantly, these averaged quantities are the only ones that represent the physical Green functions of the material. In Matsubara frequency, the bare dynamic charge susceptibility  $\chi_0(\vec{q}, i\omega)$  is

$$\chi_0(\vec{q}, i\omega) = \frac{1}{\beta N} \sum_{\vec{k}, iE} G(\vec{k} + \vec{q}, iE + i\hbar\omega) G(\vec{k}, iE) \quad (5)$$

where  $\beta$  is the inverse temperature [56, 57]. Generally, one needs to carryout analytic continuation of Eq. 5 in order to calculate any observable. This process especially for disordered systems could miss important features in the spectra if not done carefully. However, since our cluster problem is solved in real space, we can avoid the analytic continuation by converting the Matsubara sums to real frequency integrals using spectra representation:  $G(\vec{q}, i\omega) = \int d\epsilon A[G](\epsilon)/(i\omega - \epsilon)$ , where  $A(\vec{k}, E) = -\frac{1}{\pi} \Im \mathfrak{m} G(\vec{k}, E)$  is the spectral function. Using the spectral representation, the Matsubara sum in Eq. 5 could be converted to real frequency integrals as [64]

$$\Im\mathfrak{m}\,\chi_0(\vec{q},\omega) = -\frac{2\pi}{N_c} \sum_{\vec{k}} \int_{-\infty}^{+\infty} [f(E) - f(E + \hbar\omega)] \,A(\vec{k} + \vec{q}, E + \hbar\omega) \,A(\vec{k}, E) \,\mathrm{d}E,\tag{6a}$$

$$\mathfrak{Re}\chi_0(\vec{q},\omega) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{+\infty} \frac{\mathfrak{Im}\,\chi_0(\vec{q},\omega)\mathrm{d}\omega'}{\omega'-\omega},\tag{6b}$$

where  $\mathcal{P}$  denotes the principal value and f(E) is<sub>250</sub> the Fermi function. 251

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2. The bare charge susceptibility for both the cluster
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(c) and the lattice (l) is then obtained as the renor243
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$$\tilde{\chi}_{0}^{c/l}(\vec{q},\omega) = \chi_{0}^{c/l}(\vec{q},\omega) \left[\mathbb{1} - U\chi_{0}^{c/l}(\vec{q},\omega)\right]^{-1} \qquad (7)_{_{256}}^{^{257}}$$

- where 1 is the identity matrix.
- 246 3. The lattice irreducible vertex is approximated with 247 the cluster counterpart, i.e.,  $\Gamma^l \approx \Gamma^c \equiv \Gamma$  [59–63]. 248 The full lattice vertex function is then calculated 249 using  $\Gamma(\vec{q}, \omega)$  as

$$\mathbf{F}(\vec{q},\omega) = \Gamma(\vec{q},\omega) [\mathbb{1} - \tilde{\chi}_0(\vec{q},\omega)\Gamma(\vec{q},\omega)]^{-1}$$
(8)

The full vertex function  $\mathbf{F}$  includes all the possible scattering events between any two propagating particles. Diagrammatically,  $\mathbf{F}$  consists of all the fully connected two-particle diagrams to infinite orders as such, reducible. On the other hand, the irreducible vertex function  $\Gamma$  is a subclass of the two-particle diagram in  $\mathbf{F}$  that cannot be separated into two distinct parts by cutting two internal Green function lines in any given channel [59–61].

4. With the full lattice vertex function and the renormalized dynamical charge susceptibility calculated, the full, dynamical lattice susceptibility is obtained

$$\langle \vec{k} | \chi | \vec{k}' \rangle = \langle \vec{k} | \tilde{\chi}_0 | \vec{k} \rangle + \sum_{\vec{k}''} \langle \vec{k} | \tilde{\chi}_0 | \vec{k} \rangle \langle \vec{k} | \mathbf{F} | \vec{k}'' \rangle \langle \vec{k}'' | \chi | \vec{k}' \rangle.$$
(9)

ton) effects  $\sigma_{eh}(\omega)$  is then obtained from Eq. 9 as

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$$\sigma_{eh}(\omega) = \lim_{\vec{q} \to 0} \frac{1}{\omega} \Im \mathfrak{m} \chi(\vec{q}, \omega)$$
(10)

*Results.*– We start the discussion of our results by pre-262 senting in Fig 1 the single-particle quantity as manifested 263 in the imaginary part of the integrated hybridization 264 function  $\Im \mathfrak{m} \int \Delta(\mathbf{K}, \omega) d\mathbf{K} d\omega$  for various disorder and in-265 teraction strengths, respectively. The hybridization func-266 tion is a natural order parameter for characterizing disor-267 dered systems as it measures the probability of how the 268 electrons move between the cluster and the host (escape 269 rate) [43]. In the dilute limit, i.e., small disorder strength 270 up to  $W \approx 0.5$ , the hybridization function is practical the 271 same for all the interaction strengths studied. However, 272 as the strength of the disorder increases and in the limit 273 where the interaction strength is far smaller than the 274 noninteracting bandwidth of 3 (in unit of 4t), the spec-275 tra starts to deviate from each other with the critical dis-276 order strength  $W_c^U$  systematically moving to higher val-277 ues (as indicated by the arrow) for increasing interaction 278 strength. Observe also that as both W and U becomes 279 substantial and comparable to each other, the delocaliza-280



FIG. 1. The semi-log plot of the integrated, imaginary part of the hybridization function for a  $3 \times 3 \times 3$  cubic lattice sites<sup>296</sup> at various interaction strengths,  $U = 0.0, 0.4, 1.0, \text{ and } 2.0 \text{ in}^{297}$ the unit of 4t. The arrow indicates the systematic increase<sub>298</sub> of the critical disorder strengths  $W_c^U$  due to interaction in-<sup>299</sup> duced delocalization (disorder screening). The obtained  $W_c^U$ are 2.13, 2.21, 2.51, and 2.49 for the  $3 \times 3 \times 3$  cubic lattice sites. Inset is the typical density of states for U = 0.0, 0.4,<sup>301</sup> 1.0, and 2.0 at W = 2.0, which is close to the  $W_c^{U=0.0}$ . An<sup>302</sup> unconventional soft-pseudogap develops at the Fermi level for<sup>303</sup> small interaction  $U \ll W$ , which systematically evolves into<sup>304</sup> a conventional hard-gap at large U. The former gap is linear<sup>305</sup> in E while the latter shows  $E^2$ -dependent. Observe that this<sup>306</sup> gap is absent for U = 0.



FIG. 2. The dynamical conductivity obtained with the effects of electron-hole interactions included for a disordered Hubbard model as a function of the excitation energy  $\hbar\omega$  obtained using Eq. 9. Electron-hole interactions effect are included using the Bethe-Salpeter equations. The disorder strengths are 0.5, 1.0, 1.5, and 2.0, respectively for the various Hubbard interaction strengths U = 0.0, 0.4, 1.0, and 1.0, respectively in the unit of 4t.

tion of the states rather increases. This is different from the monotonic decrease in the magnitude of the spectra for increasing disorder strength observed in the noninteracting systems [41, 43, 65–72]. The renormalization of the spectra and the increase in  $W_c^U$  could be attributed to delocalization induced by U, which injects mobile carriers into the system. This is in agreement with the conclusions reached using the typical density of states as an order parameter [42] and has been interpreted by various authors to be due to disorder screening [42, 73–75]. Our calculations for the various interaction strengths 0.0, 0.4, 1.0, and 2.0 also led to  $W_c^U$  of 2.13, 2.21, 2.51, and 2.49. The critical disorder strength of 2.13 for the noninteracting limit is in good agreement with that obtained using the typical density of states within the typical medium dynamical cluster approximation [41, 42, 42] and with numerical exact value  $W_c \approx 2.10$  [65–72].

The insert in Fig 1 is the typical density of states obtained at W = 2.0 for various interaction strengths. This disorder strength is close to the  $W_c^{U=0.0}$  and could be said to depict a strongly disordered system. Observe that at U = 0.0, there is no gap in the spectra. However, for finite U, a gap (which is independent of filling) opens at the Fermi level. For small U, this gap is an unconventional soft-pseudogap, which is almost linear in energy E. We have recently demonstrated that this softpseudogap emerges due to the reduction in phase space

for scattering by U and it is linear instead of the nor-360 308 mal  $E^2$ -dependence due to the loss of momentum con-361 309 servation [42]. Hence, a strongly disordered, correlated<sub>362</sub> 310 system  $(W \gg U)$  could be said to exhibit a non-Fermi<sub>363</sub> 311 liquid behavior since a well-defined quasiparticle could<sub>364</sub> 312 be said to no longer exist [76]. The deviation from the<sub>365</sub> 313 usual  $E^2$  behavior in the vicinity of electron localization<sub>366</sub> 314 have been experimentally observed in some perovskite<sub>367</sub> 315 materials, e.g.,  $A_{1-x}BA'_{x}O_{3}$  [77–79]. For example, the<sub>368</sub> 316 photoemission spectra of  $SrRu_{1-x}Ti_xO_3$  exhibit a soft<sub>369</sub> 317 pseudogap gap at x = 0.5 and a hard gap at higher val-370 318 ues of x [79]. Observe further from the inset that the<sub>371</sub> 319 soft-pseudogap systematically evolves into a hard-gap at<sub>372</sub> 320 large U with the usual  $E^2$ -dependence behavior restored<sup>373</sup> 321 and inelastic scattering now vanishes as  $E \rightarrow 0$  reminis-374 322 cent of a Fermi liquid. This latter observation suggests<sup>375</sup> 323 that a strongly correlated and disordered system could be<sub>376</sub> 324 described using the Fermi liquid physics but the contrary<sub>277</sub> 325 may not be the case especially in the regime of strong dis- $_{378}$ 326 order and weak interaction strength as observed herein. 327 Next, we consider the two-particle quantities for a dis- $_{380}$ 328 ordered Hubbard model. We show in Fig. 2 the calcu-329 lated dynamical conductivity  $\sigma_{eh}(\omega)$ , which accounts for<sub>382</sub> 330 the effects of electron-hole interactions obtained  $using_{383}$ 331 Eq. 10 for the same parameters as in Fig. 1. This spec-332 trum also included vertex corrections. The vertex  $cor^{-384}$ 333 rection effects renormalized the spectra, which is more<sup>385</sup> 334 significant at low-energy  $\omega < 1.0$ . While the vertex cor-<sup>386</sup> 335 rections have subtle effects, i.e., it increases the mag-<sup>387</sup> 336 nitude of the low-energy of the absorption spectra (not  $^{\scriptscriptstyle 388}$ 337 shown), our calculations show that non-local corrections<sup>389</sup> 338 are more important for the proper description of the ab-<sup>390</sup> 339 sorption spectra of correlated, disordered systems. We<sup>391</sup> 340 note that the former effect could become significant, e.g.,<sup>392</sup> 341 for the description of transport phenomena in Kondo sys-<sup>393</sup> 342 tems [80]. 343

Our data show different behavior at different energy.<sup>395</sup> 344 At high-energy  $\omega > 1.0$ , we observed Lifshitz tails and<sup>396</sup> 345 the suppression of the spectra with significant broaden-<sup>397</sup> 346 ing and a reduction in the oscillator strength. The latter  $^{\rm 398}$ 347 measures the absorption probability. In the low-energy  $^{\rm 399}$ 348 regime  $\omega < 1.0$ , observe that the Drude-like behavior<sup>400</sup> 349 normally observed at zero or small disorder strength (as  $^{\scriptscriptstyle 401}$ 350 could be seen in Fig. 3) is absent. This could be un-402 351 derstood since the transport is now dominated by the<sup>403</sup> 352 electron-hole pairs. The maximum of the spectra oc-404 353 curs at  $\sim 1.0$  and it is systematically blue-shifted as the<sup>405</sup> 354 strength of the disorder and interaction is increased. Our<sup>406</sup> 355 data further reveal that the initial delocalization effects<sub>407</sub> 356 are significantly higher at small W and U. For exam-408 357 ple, the highest magnitude of the spectra occurs for the<sub>409</sub> 358 parameters W = 0.5 and U = 0.4. However, in the in-410 359

termediate and strong disorder limit  $1.5 \leq W = 2.0$ , the delocalization effects systematically increases as U is increased. We explain this observation as follows: when the disorder strength is small and the interaction is finite but also smaller, more free electron-hole pairs are generated leading to the observed increase in conductivity. Still, even in the small disorder limit, if the interaction strength is significantly larger than W, "strongly correlated" physics could dominate. The system adopts a Mott-like behavior preferring to open a gap at the Fermi level due to less generation of free electron-hole pairs (see the inset of Fig. 1 where increasing U induces the opening of a gap at the Fermi level). On the other hand, when the interaction strength is large and the disorder strength is close to the noninteracting critical disorder limit, the system could become a correlated dirty metal leading to the observed delocalized in this regime.

Generally, the single- and two-particle behavior is qualitatively similar since they both systematically go to zero as the strength of the disorder is increased. But quantitatively, significant differences exist in their critical behavior. For instance, the two-particle calculations led to critical disorder strengths that are far smaller than their single-particle counterparts.

We can further gain some insights on how the critical quantities, e.g., the critical disorder strengths change in the two-particle picture by exploring the dc-conductivity, which could be obtained from the dynamical conductivity by taking the zero limit of the excitation energy as  $\sigma_{eh}(\omega \to 0)$ . In our analysis, we instead adopt the maximum value  $\sigma_{eh}(\omega \to \omega_{max})$  to avoid any ambiguity due to the nature of the excitation spectra, e.g., Lifshitz tails [81]. The extracted  $\sigma_{eh}(\omega \to \omega_{max})$  values were further interpolate to a finer grid. The associated contour plot is shown in Fig. 3. The essence of this plot is to show more clearly, the overall evolution of the dynamical conductivity in the disorder-interaction parameter space. From Fig. 3, up to  $W \approx 0.25$  for all U-values, we observed a 'pure' metallic-like behavior. Then a weakly interacting metallic character up to  $W \approx 0.75$ , followed by some intermediate states, and then a correlated 'dirty' metal before the system goes into the strongly correlated Anderson insulator regime. The  $W_c^U$  obtained from our data are: 1.93, 2.04, 2.11, and 1.98 for U = 0.0, 0.4, 1.0, and2.0 in that order. This shows a reduction of more than 10%, e.g.,  $W_c^{U=0.0}$  is reduced by  $\approx 0.2$  when compared to the single-particle equivalent.

To explore the origin of this discrepancy, we further calculated the dynamical conductivity (without the effects of electron-hole interactions) using the Kubo-Greenwood formula [82, 83]

$$\sigma(\omega) = \frac{\sigma_0}{2\pi^2} \Re \mathfrak{e} \int_{-\infty}^{\infty} \mathrm{d}E \, \frac{[f(E) - f(E+\omega)]}{\omega} \, \left[ \frac{G^*(E) - G(E+\omega)}{\gamma(E+\omega) - \gamma^*(E)} - \frac{G(E) - G(E+\omega)}{\gamma(E+\omega) - \gamma(E)} \right],\tag{11}$$

where  $\gamma(\omega) = \omega - \mu - \Sigma(\omega)$  and  $\sigma_0$  is the zero frequency 411 value. We show in Fig. 4 the plot of the dynamical con-412 ductivity obtained using Eq. 11 in unit of  $\sigma_0$  for the 413 same parameters as in Fig. 2. Our results show a Drude-414 like behavior at the low-energy regime when the disorder 415 strength is still small. However, for a given interaction, 416 as the strength of the disorder increases, the conductivity 417 is suppressed especially in the low-energy regime, which 418 becomes non-Drude-like. At high-energy, the delocaliza-419 tion by interaction and the suppression of the spectra 420 as W increases are seen both in the single-particle hy-421 bridization function and the two-particle spectra data. 422 We interpret this behavior to be due to quantum correc-423 tions to the Drude conductivity by both weak localization 424 effects and the disorder-modified electron-electron inter-425 actions [84]. 426

As can be inferred from Fig. 4, the  $\sigma(\omega \rightarrow 0)$  or 427  $\sigma(\omega \rightarrow \omega_{max})$  is still significant at the disorder and 428 interaction strengths where their two-particle counter-429 part that included the electron-hole interaction effects 430 are already localized. For example, at U = 0.0 and 431 W = 2.0, the calculated dynamical conductivity with-432 out the electron-hole interactions is still finite while the 433 counterpart obtained from the BSE is already practical 434 zero. The overall trend of the critical parameters, e.g., 435  $W_c^U$ -values obtained in the absence of electron-hole in-436 teractions is in agreement with the ones calculated from 437 the single-particle quantity. Since the critical behavior of 438 the dynamical conductivity calculated without electron-440 439



FIG. 3. The contour plot of disorder-interaction phase diagram of the dynamical conductivity obtained with the effects<sup>461</sup> of electron-hole interactions included in the unit of 4t. Data<sup>462</sup> is obtained from Fig. 2 by interpolating the maximum for<sup>463</sup> each data set to finer grid. The dashed-white line is intended<sup>464</sup> to give a rough estimate of the location of the critical disorder<sup>465</sup> strengths in the parameter space. The trend of the W<sup>U</sup><sub>c</sub> is in<sup>466</sup> agreement with previous studies [85, 86].



FIG. 4. The dynamical conductivity obtained without the effects of electron-hole interactions ((normalized to its zero frequency value  $\sigma_0$ ) at various interactions and disorder strength for the same system size as in Fig. 1 obtained using Eq. 11 in the unit of 4t. Observe the systematic evolution from a Drude-like to non-Drude-like behavior and also decrease in the oscillator strength at the low-energy regime as the strength of the disorder increases.

hole interactions (Eq. 11) is in basic agreement with the single-particle behavior of the critical quantities, we attribute the reduction in the critical disorder strengths in the presence of electron-hole interactions to enhanced multiscattering processes induced by the disorder, which breaks up the extended states within the system, leading to less generation of free electron-hole pairs.

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While we cannot directly verify with our data, the exciton states induce changes in the oscillator strengths, i.e., the relative heights/positions of the absorption spectra thereby lowering  $W_c^U$ . This is similar to what is observed in some materials where an electron-hole pair has a binding energy that causes the quasiparticle gap to be higher than the fundamental gap obtained from conventional methods or measured via photoemission spectroscopy. Several experiments have shown that exciton effects drastically change the spectra of materials. The data of Varley and Schleife [87] for some transparent conducting oxides showed that the absorption spectra is strongly modified by the inclusion of electron-hole interactions especially the lower photon-energy behavior which, was red-shifted. The redistribution of the spectral weight at low photon-energy due to excitonic effects were also reported in several oxides [88–90]. The electron-hole interactions have also been demonstrated to be important in describing the properties of nanostructure materials, e.g., monolayer  $MoS_2$  where it is vital for the proper interpretation of the low-energy absorption spectra [91] es-

pecially the position of the principal exciton peaks. Thes23 468 impact of electron-hole interactions could even be greater<sup>524</sup> 469 in disordered and/or interacting physical systems where<sup>525</sup> 470 the disorder degrees of freedom could couple nontrivially  $^{\scriptscriptstyle 526}$ 471 to the electron-electron interactions and/or the electron- $\frac{527}{528}$ 472 hole interactions. Hence, the approach and the results 473 presented herein could be of great importance in under-530 474 standing and interpretation of transport data of disor-531 475 dered and/or interacting systems where conventional ap-532 476 533 proaches may not be adequate. 477 534 Summary.– We have presented and explored the role of  $_{535}$ 478

electron-hole interactions in disordered Hubbard model536 479 for a random disorder potential distributed according to a<sup>537</sup> 480 box probability distribution function in three dimensions<sup>538</sup> 481 using the typical medium approach. Our calculations  $^{\scriptscriptstyle 539}$ 482 reveal heretofore, a significant reduction in the critical  $_{541}^{540}$ 483 disorder strengths when compared to the single-particle  $\frac{3}{542}$ 484 values. We attribute this reduction in  $W_c^U$  to enhanced<sub>543</sub> 485 coherent backscattering processes (cooperon correction)544 486 due to the inclusion of electron-hole interactions. 487 546

Acknowledgment.- Research was sponsored by the 488 Army Research Laboratory and was accomplished under<sub>548</sub> 489 the Cooperative Agreement Number W911NF-11-2-0030549 490 as an ARL Research [George F. Adams] Fellow. This<sup>550</sup> 491 work was supported in part by a grant of computer time<sup>551</sup> 492 from the DOD High Performance Computing Moderniza-  $^{\rm 552}$ 493 553 tion Program at the Army Engineer Research and Devel- $\frac{1}{554}$ 494 opment Center, Vicksburg, MS. 495 555

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