Emergence of heavy quasiparticles from a massless Fermi sea: Optical conductivity

Hyunyong Lee\textsuperscript{1} and S. Kettemann\textsuperscript{1, 2}\textsuperscript{*}

\textsuperscript{1}Division of Advanced Materials Science, Pohang University of Science and Technology (POSTECH), Pohang 790-784, South Korea
\textsuperscript{2}School of Engineering and Science, Jacobs University Bremen, Bremen 28759, Germany

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We study the density of states and the optical conductivity of a Kondo lattice which is immersed in a massless Dirac Fermi sea, as characterized by a linear dispersion relation. As a result of the hybridization $V$ with the $f$-electron levels, the pseudo-gap in the conduction band becomes duplicated and is shifted both into the upper and the lower quasiparticle band. We find that due to the linear dispersion of the Dirac fermions, the Kondo insulator gap is observable in the optical conductivity in contrast to the Kondo lattice system in a conventional conduction band, and the resulting gap $|\Delta_{\text{gap}}(T)|$ depends on temperature. The reason is that the Kondo insulator gap is an indirect gap in conventional Kondo lattices, while it becomes a direct gap in the Dirac Fermi Sea. We find that the optical conductivity attains two peaks and is vanishing exactly at $2b(T)V$ where $b$ depends on temperature.

\textit{Introduction.}— Recent developments in synthesis techniques have led to the discovery of many transition metals and rare earth compounds, heavy fermion materials, which have a quantum critical point separating a magnetically ordered phase from a paramagnetic phase [1]. The exotic low temperature physics of heavy fermion systems (intermetallics synthesized on the basis of $f$-electron elements), where the conduction electrons act as particles with “huge masses” comparable to that of a proton [1, 2], can be understood in terms of rescaled quasiparticles which relate the strong correlations to the properties of virtual single particles. The heavy masses directly affect the low temperature properties of materials such as the electric resistivity from electron-electron scattering and the heat capacity.

On the other hand, the low-energy excitation in graphene and topological insulators, among others, are fermionic quasiparticles described by a relativistic “massless” Dirac fermion, as characterized by a linear dispersion relation rather than usual non-relativistic Landau quasiparticles [3–8]. It is a diametrically opposed example of the heavy mass fermion. An intriguing question then arises, and deserves both theoretical and experimental studies: how does the composite quasiparticle of the massless fermion and localized $f$-electron behave?

Actually, M. Höppner \textit{et al.} have recently studied the interplay between Dirac fermions and heavy quasiparticles in the layered material EuRh$_2$Si$_2$ by means of the angle resolved photoemission (ARPES) [2]. They observed a Dirac-like conical band with an apex close to the Fermi level, which passes through an Eu 4$f^6$ final-state multiplet. They reached the conclusion that massless and heavy fermion quasiparticles may not only coexist but can also strongly interact in such solids.

The interband transition in the optical conductivity of the heavy fermion systems has been intensively studied both experimentally [10–12] and theoretically [13–15]. The interband transition takes place between one band with more $f$-electron character and another with more conduction electron character, and thus it involves an energy scale at least of the order of the Kondo temperature $T_K$ below which the local moment is screened. In a Kondo lattice there is another scale, the Fermi liquid coherence scale $T_c$ below which the composite heavy fermion develops [16]. Since the peak position of the optical conductivity could be related to $T_K$ and $T_c$, it is important to obtain detailed information about low energy excitations near the Fermi level. Optical conductivity studies have been a useful tool for this purpose and have provided much information on Kondo insulators [17–19].

In this work, we study the density of states (DOS) and the optical conductivity of the Kondo lattice system which is immersed in massless Dirac fermion bath. The pseudo-gap in the conduction band becomes duplicated and is shifted both into the upper and the lower quasiparticle band. We find that these pseudogaps are always outside the Kondo insulator gap regardless of other parameters such as $f$-electron level and bandwidth. Remarkably, we find that due to the linear dispersion of the Dirac fermions, the Kondo insulator gap is direct gap, and is therefore observable in the optical conductivity. This is in contrast to the Kondo lattice system in a conventional conduction band.

\textit{Model.}— Let us begin with the Anderson lattice model which is given by

$$H = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \varepsilon_d \sum_{i,\sigma} d_{i\sigma}^\dagger d_{i\sigma} + U \sum_{i,\sigma} n_{i\uparrow} n_{i\downarrow} + V \sum_{i,\sigma} [c_{i\sigma}^\dagger d_{i\sigma} + h.c.], \quad (1)$$

where $c_{k\sigma}$ is the annihilation operator of conduction electron with momentum $k$ and spin-index $\sigma$, $c_{i\sigma}$ ($d_{i\sigma}$) is the annihilation operator of conduction (localized $f$) electron at site $i$ and spin-index $\sigma$, $U$ is the on-site Coulomb repulsion, $V$ is the hybridization energy between the conduction and $f$-electron band, and $\varepsilon_k$ and $\varepsilon_d$ denote the
conduction band and the local energy level of $f$-electron, respectively. In order to avoid confusion between the $f$-level and Fermi level $\varepsilon_F$, we use $\varepsilon_d$, instead of $\varepsilon_f$.

Introducing a slave boson operator $b \langle b^\dagger \rangle$ and a Lagrange multiplier $\lambda_0$ to avoid a double occupancy in the limit $U \to \infty$, and diagonalizing in momentum space, the mean-field Hamiltonian takes the form \cite{20, 21},

\[ H_{\text{MFT}} = \sum_{k,\sigma,\alpha=\pm} E_k^\alpha \bar{a}_{k\sigma} a_{k\sigma}^\alpha - 2N\lambda_0, \]  

where $N$ is the number of sites in the lattice, $d_{k\sigma}^\alpha = 1 \sqrt{N} \sum_\sigma d_\sigma^\alpha e^{-ik\cdot\mathbf{r}}$, and $a_{k\sigma}^\alpha$ and $\bar{a}_{k\sigma}^\alpha$ are linear combinations of $c_{k\sigma}$ and $d_{k\sigma}$, playing the role of quasiparticle operators corresponding the momentum state eigenenergies $E_k^\pm \equiv \frac{1}{2} (\varepsilon_k + \varepsilon_d^\pm + \sqrt{2\varepsilon_d^\pm + \frac{2}{D} + 4b^2V^2})$, where $\pm$ denotes the upper and lower band, $b \equiv \langle b^\dagger \rangle$ is the order parameter of condensation of the slave bosons. It depends on temperature and vanishes in the mean field approximation at $T_K$, $\varepsilon_d^\pm = \varepsilon_d + \lambda_0$ is the renormalized $f$-level. Notice that the quasiparticle spectrum is gapped in the regime of $\omega_d^\pm < \omega < \omega_d^{\mp}$, where $\omega_d^{\mp} = \frac{1}{2} \left[ \varepsilon_d^\pm + D \pm \sqrt{(\varepsilon_d^\pm + D)^2 + 4b^2V^2} \right]$, and $D$ is the half bandwidth of conduction electrons.

Density of states.- One may calculate the density of states of the quasiparticle from its dispersion, when the conduction band has a pseudo-gap, $\rho_0(\omega) = |\omega|^{\gamma} :$

\[
\rho(\omega) = \sum_{\alpha=\pm} \frac{4 \Theta(\alpha \omega - \alpha \omega_d^{\alpha})}{1 + \alpha \omega - \omega_d^\alpha} \frac{\omega - \varepsilon_d^{\pm} + \sqrt{\frac{2}{D} + 4b^2V^2}}{\sqrt{\omega - \varepsilon_d^{\pm} + \sqrt{\frac{2}{D} + 4b^2V^2}} + b^2V^2},
\]  

where $\Theta(\omega)$ is the heavy side function. For $\gamma = 0$ (flat band) and $\gamma = 1$ (pseudo-gap), the quasiparticle DOS are plotted in Fig.1(a) and (b), respectively. As expected from previous works \cite{22, 24}, the originally flat conduction electron DOS ($\gamma = 0$) is now replaced by a “Kondo insulator gap” (also called hybridization gap), flanked by two sharp peaks which are called coherence peaks [Fig.1(a)]. Interestingly, the pseudo-gap in the conduction band is shifted to both upper and lower bands after hybridization, so that two pseudo-gaps appear in the quasiparticle DOS [Fig.1(b)] at energies $\omega_{\text{pseudo-gap}} = \frac{1}{2} \left( \varepsilon_d^\pm \pm \sqrt{\varepsilon_d^\pm + 4b^2V^2} \right)$, which depend on the renormalized $f$-level and the effective hybridization $bV$. These pseudogaps are found to be located always outside of the Kondo insulator gap: $|\omega_{\text{pseudo-gap}}| > |\omega_{\text{gap}}|$. It is very well known that the electrons on a honeycomb lattice can be described by a relativistic massless Dirac fermion model \cite{25}, which is characterized by the linear low energy dispersion relation $\varepsilon_k = \pm v_F|k|$ and $v_F$ is the Fermi velocity. S. Saremi and Patrick A. Lee have derived the dispersion of the quasiparticles of the Kondo lattice model on a honeycomb lattice, finding \cite{26}

\[ E_k^{\pm} = \frac{1}{2} \left\{ -\alpha v_F |k| + \varepsilon_d \pm \sqrt{(\alpha v_F |k| + \varepsilon_d)^2 + 4b^2V^2} \right\}, \]

where we denote $E_k^{\pm}$ for $\alpha = +$ and $E_k^{\pm}$ for $\alpha = -$ in Fig.2. When $\varepsilon_d = 0$, the pseudogaps are at two points outside the hybridization gaps [Fig.2(a)], consistent with the DOS, Fig.1(b). When $\varepsilon_d = -0.4D$, a Dirac-like cone is preserved at the Fermi level, while a heavy quasiparticle is formed around the $f$-level [Fig.2(b)]. Interestingly, similar spectra have been reported in recent ARPES measurement of EuRh$_2$Si$_2$ known as an isostructural compound of YbRh$_2$Si$_2$ \cite{9}.

Optical conductivity.- The optical conductivity in the isotropic system \cite{27} is defined by

\[ \sigma(q, i\omega) = \frac{1}{\omega} \text{Im} \Pi(q, \omega), \]

\[ \Pi(q, \omega) = -\frac{1}{d} \int_0^\beta d\tau e^{i\omega \tau} \langle T_z j(q, \tau) \cdot j(-q, 0) \rangle, \]

where $j(q) = \frac{e}{m} \sum_{k,\sigma} \langle k^+ | \frac{1}{2} q | k^\sigma - q \rangle c_{k^\sigma} c_{k^\sigma}$ is the current operator, $d$ the dimension, $e$, $m$ are the electron charge and
mass. $\Pi(q, \omega)$ is the current-current correlation function, which in the bubble approximation and long wavelength limit ($q \to 0$) is given by

$$\Pi(i\nu_n) = \frac{G_0}{\Omega} \frac{1}{\beta} \sum_{\mathbf{k}, i\omega_n} v_F^2 G_c(\mathbf{k}, i\omega_n) G_c(\mathbf{k}, i\omega_n + i\nu_n),$$

where $G_0 = 2e^2/h$ is the conductance quantum, $\Omega$ is a volume of the system, $\omega_n$ ($\nu_n$) are fermionic (bosonic) Matsubara frequencies, and $G_c(\mathbf{k}, i\omega_n)$ is the Green’s function of conduction electrons in the Kondo lattice system.

We present the optical conductivity of a Kondo lattice in a conventional uniform conduction band, in Sec. I in Suppl., comparing with Ref. [12, 23]. The threshold frequency $2bV$ is always larger than the Kondo insulator gap $\Delta_{\text{gap}}$, $2bV > \omega_{\text{gap}}^+ - \omega_{\text{gap}}^-$, as can be understood from the band structure of the quasiparticles with an indirect band gap [11, 13]. Optical absorption is only possible for direct transitions of the quasiparticle from lower band ($E_k^-$) to the upper band with same momentum ($E_k^+$) due to momentum conservation. Thus, the smallest optical excitation (threshold) energy $2bV$ is larger than the Kondo insulator gap $\Delta_{\text{gap}}$ in a conventional Kondo lattice system.

On the other hand, from the dispersion of the quasiparticles in a Dirac fermion conduction bath [Fig. 2], we may infer that the Kondo insulator gap is observable in the optical conductivity. The conduction electron Green’s function in momentum and Matsubara frequency representation is

$$G_c(\mathbf{k}, i\omega_n) = \sum_{\eta=\pm} \left\{ \frac{\alpha^{\eta}_{\mathbf{k}}}{i\omega_n - E_k^{\eta}} + \frac{\alpha^{\eta*}_{\mathbf{k}}}{i\omega_n - E_k^{\eta}} \right\},$$

where the quasiparticle eigenenergies $E_k^{\eta}$ are defined in Eq. (4) and the coherence factor is $\alpha^{\eta}_{\mathbf{k}} = \frac{E_k^{\eta} - \epsilon_0}{E_k^{\eta} - E_k^{\pm}}$.

Performing the Matsubara frequency summation in the current-current correlation function Eq. (6) for $T = 0$, $q \to 0$ and $\omega > 0$ (see section II in Suppl.), we obtain

$$\sigma(\omega) = \frac{G_0}{\omega} \sum_{k, \alpha, \beta} v_F^2 \alpha^{\alpha}_{\mathbf{k}} \alpha^{\beta}_{\mathbf{k}} \delta(\omega - E_k^{\alpha} + E_k^{\beta}),$$

where $\alpha, \beta = a$ or $b$. Note that there are 4 different kinds of interband transitions in Eq. (8), and it may be expected that the transition between the band $E_k^\alpha$ and $E_k^\beta$ [blue and green line in Fig. 2] allows us to observe the Kondo insulator gap of the quasiparticle DOS. After the momentum summation, we acquire

$$\sigma(\omega) = \frac{\sigma_0 \Theta(\omega - 2bV)}{\omega_{\pm}} \left\{ \Theta\left(\frac{\Delta_{\text{gap}}^2 + 4b^2V^2}{2\Delta_{\text{gap}}} - \omega\right) \frac{\rho(\omega_-)}{1 - \frac{\omega^2}{\omega_-^2}} + \Theta(D - \omega) \frac{(\omega/2)^4 \rho(\omega/2)}{2((\omega/2)^2 + b^2V^2)^2} \right\} + \frac{b^2V^2 \omega_-^2}{\omega^2} \left\{ \Theta\left(\frac{\Delta_{\text{gap}}^2 + 4b^2V^2}{2D} - \omega\right) \frac{\rho(\omega_+)}{1 - \frac{b^2V^2}{\omega_+^2}} + \Theta(D - \omega) \frac{(\omega/2)^4 \rho(\omega/2)}{((\omega/2)^2 + b^2V^2)^2} \right\} + \frac{\sigma_0 \Theta(\omega - \Delta_{\text{gap}}) \Theta(2bV - \omega)}{2\omega} \frac{(\omega/2)^4 \rho(\omega/2)}{((\omega/2)^2 + b^2V^2)^2},$$

where $\rho(\omega)$ is the quasiparticle DOS [Eq. (8) with $\gamma = 1$], $\omega_\pm = \frac{1}{2}\{\omega \pm \sqrt{\omega^2 - 4b^2V^2}\}$, and $D$ is the half bandwidth. Fig. 3 shows the optical conductivity Eq. (9) for $\varepsilon_d = 0, -0.4D$ for three different values of $bV$. The Kondo insulator gap $\Delta_{\text{gap}}$ is observable. The optical conductivity is found to have 2 peaks contrary to the one in the uniform ($\gamma = 0$) conduction band system. While the first peak at the Kondo insulator gap comes from the interband transition between the heavy $f$-electron character quasiparticles, the second peak at $\omega = 2bV$ originates from the transition between the Dirac-like quasiparticles around the pseudo-gaps. Notice that due to the temperature dependence of $b = b(T)$, the Kondo insulator gap depends on temperature: $\Delta_{\text{gap}} = \Delta_{\text{gap}}(T)$. We find that the optical conductivity vanishes as the frequency is approaching $\omega \to 2bV$, since there is no state which can be excited from the lower band to upper band as one can see from the energy dispersion [Fig. 2(a)]. When $\omega > 2bV$, however, there are transitions from the lower to the upper band so that the optical conductivity has a finite value as a second peak. On the other hand, when the $\varepsilon_d$ is far below the Dirac point [Fig. 3(b)], the optical conductivity changes drastically that it does not show a peak at $\Delta_{\text{gap}}$, but increases as approaching $2bV$. Even though only a single peak appears like the one in the conventional ($\gamma = 0$) conduction band system, the threshold frequency is still $\Delta_{\text{gap}}$ and the Kondo insulator gap is observable as in the case of $\varepsilon_d = 0$.

**Conclusions.** In summary, we have derived the density of states and the optical conductivity of a Kondo lattice immersed in a relativistic massless Dirac fermion conduction bath, characterized by a linear dispersion. The hybridization moves the pseudo-gap both in the upper and the lower quasiparticle band. Due to the linear dispersion of the Dirac fermions, the Kondo insulator gap is observable in the direct interband transition yielding the additional peak in the optical conductivity at $\omega \approx \Delta_{\text{gap}}$. This is in contrast, to the conven-
While the first peak at $\omega$ of the heavy fermion compounds like ter carriers.

from the Dirac-like massless conduction electron character carriers. This study was supported by the Kondo temperature and the coherence temperature. Moreover, such an experiment may allow to extract much information on the Kondo lattice systems such as the Kondo temperature and the coherence temperature.

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* hyunyong.rhee@gmail.com