Unitarity bound violation in holography and the Instability toward the Charge Density Wave

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ABSTRACT: We study the spectral function of fermions in a holographic setup with bulk Dirac mass in the regime beyond the conformal unitarity bound, and find that spectral function has the dispersion relation with tachyonic behavior, indicating an instability. Based on linearity between the density and the position of the tip of the k-gap, we suggest that this instability is toward the charge density wave (CDW) and the position of the tip can be identified as the wave vector of CDW. For the physical origin, we point out the similarity of unitarity violation in our non-Fermi Liquid theory and nesting phenomena in the Fermi liquid theory as the mechanism of CDW instability.

KEYWORDS: Gauge/Gravity duality, strong correlation
1 Introduction

Understanding the appearance of the charge density wave (CDW) in strongly interacting system attracted much attention due to its role in the under-doped cuprate and other strongly correlated systems. Since the holographic theory is developed as a strongly interacting system, it is highly desired to see how to introduce the charge density wave in such theory. The purpose of this paper is to suggest that the holographic theory of strongly interacting fermion system can encode the appearance of the CDW through the instability associated with the violation of unitarity bound.

In [1], we studied the fermion spectral function[2–6] in a holographic model [7, 8] to find a replacement of Hubbard model to describe the Mott transition. The idea was to find a model interpolating the free fermion [9, 10] and strongly interacting system with a Mott gap[11, 12] in holographic setup which is calculable. There, we restricted the bulk mass $m$ to $|m| \leq 1/2$ for the conformal unitarity and $m \geq 0$ for the normalizability of the spectral function.\(^1\) Going beyond the unitarity bound certainly causes an instability of some kind. In many cases, study of the instability gives us useful information on the nature of the instability and the fate of the vacuum. For example, Pierls instability of the 1-dimensional lattice model says that there will be a charge density wave and period doubling at a specified wave vector.

In this paper, we study fermion spectral function for $m > 1/2$ where conformal unitarity is violated. In the non-interacting system, the dispersion relation is due to the spectral function given by the a delta function. For interacting case, however, the spectral function is a smooth function, where the dispersion relation is indicated at most by the resonant peaks in Fourier space. We may call it a fuzzy dispersion relation(DR). It turns out that when the gap generating interaction is large enough, the DR is given by

$$\omega^2 - v^2 k^2 = M^2, \quad \text{with} \quad M^2 < 0,$$

\(^1\)We work in in alternative quantization for the ease of the presentation using positive $m$. Here, the relation between the conformal dimension $\Delta$ of an operator and the bulk mass of the fermion is $\Delta = \frac{d}{2} - m$. 

\[1\]
which has a \( k \)-gap instead of the usual \( \omega \)-gap with \( M^2 > 0 \). That is, the spectrum is tachyonic, indicating the instability of the vacuum. To see the fate of the vacuum, we calculated the location of the tip of the \( k \)-gap dispersion relation, \((k_c, \omega_c)\), and found that \( k_c \) was linear in the charge density for low density, which indicated that the instability is toward the charge density wave. We compared this result with experiment and found interesting agreements as well as a suggestion for future experiment.

To discuss the physical mechanism for the unitarity violation causing the \( k \)-gap and CDW, we pointed out that there is a similarity of unitarity bound violation and the nesting phenomena: in both cases one can observe the appearance of large degrees of freedom that can interact very effectively at a special momentum deliverance. We also emphasize that our discussion did not introduce explicit inhomogeneity unlike \[13\].

2 Spectral function : the setup and review

We consider the fermion action in the dual spacetime with the dipole interaction\[11, 12\]

\[
S_D = \int d^4x \sqrt{-g} i \bar{\psi} (\Gamma^M \mathcal{D}_M - m - ip \Gamma^M \mathcal{F}_M) \psi + S_{bd}, \tag{2.1}
\]

where the covariant derivative is

\[
\mathcal{D}_M = \partial_M + \frac{1}{4} \omega_{abM} \Gamma^{ab} - i q A_M. \tag{2.2}
\]

For fermions, we cannot fix the values of all the component at the boundary, and it is necessary to introduce ‘Gibbons-Hawking term’ \( S_{bd} \). The equation of motion which is defined as

\[
S_{bd} = \frac{1}{2} \int d^4x \sqrt{h} \bar{\psi} \psi = \frac{1}{2} \int d^4x \sqrt{h} (\bar{\psi}_- \psi_+ + \bar{\psi}_+ \psi_-), \tag{2.3}
\]

where \( h = -gg^{rr} \), \( \psi_\pm \) are the spin-up and down components of the bulk spinors. The former defines the standard quantization and the latter does the alternative quantization. The background solution we will use is Reisner-Nordstrom black hole in asymptotic \( AdS_4 \) spacetime,

\[
ds^2 = - \frac{r^2 f(r)}{L^2} dt^2 + \frac{L^2}{r^2 f(r)} dr^2 + \frac{r^2}{L^2} d\vec{x}^2
\]

\[f(r) = 1 + \frac{Q^2}{r^4} - \frac{M}{r^3}, \quad A = \mu \left( 1 - \frac{r_0}{r} \right), \tag{2.4}\]

where \( L \) is \( AdS \) radius, \( r_0 \) is the radius of the black hole and \( Q = r_0 \mu, \ M = r_0 (r_0^2 + \mu^2) \).

The temperature of the boundary theory is given by \( T = f'(r_0)/4\pi \) and it is related to \( r_0 \) by \( r_0 = (2\pi T + \sqrt{(2\pi T)^2 + 3\mu^2})/3 \).

Following [3], we now introduce \( \phi_\pm \) by

\[
\psi_\pm = (-gg^{rr})^{-\frac{1}{4}} \phi_\pm, \quad \phi_\pm = \begin{pmatrix} y_\pm \\ z_\pm \end{pmatrix} \tag{2.5}
\]

after Fourier transformation. Introducing the \( \xi_\pm \) by \( \xi_+ = iy_-/z_+, \) and \( \xi_- = -iz_-/y_+ \), the equations of motion can be given by

\[
\sqrt{\frac{g_{xx}}{g_{rr}}} \xi'_\pm = -2m \sqrt{g_{xx}} \xi_\pm + [u(r) - p \sqrt{g_{xx}} A'_+(r) \mp k] + [u(r) + p \sqrt{g_{xx}} A'_-(r) \pm k] \xi_\pm. \tag{2.6}
\]
and the Green functions for $m < 1/2$ can be written as

$$G^R_\pm(\omega, k) = \lim_{r \to \infty} r^{2m} \xi_\pm(r, \omega, k). \quad (2.7)$$

Notice that two components of the Green function are not independent: $G^R_-(\omega, k) = G^R_+(\omega, -k)$. Since $G_R$ for $m < 0$ case, can be also obtained by $G_R \to -1/G_R$, $\tilde{G}_R$, the Green function for the alternative quantization for $m > 0$, is the same as that for $-m$ in the standard quantization:

$$\tilde{G}^R_\pm(\omega, k; m) = -1/G^R_\pm(\omega, k; m) = G^R_\mp(\omega, k; -m). \quad (2.8)$$

In the presence of the dipole interaction, we get

$$G^R_\pm(\omega, k; m, p) = -1/G^R_\pm(\omega, -k; -m, -p). \quad (2.9)$$

The spectral function is defined as the imaginary part of the Green function. If we define $A_\pm(\omega, k) = \text{Im}[G^R_\pm(\omega, k)]$ the spectral function is sum of them:

$$A = A_+(\omega, k) + A_-(\omega, k). \quad (2.10)$$

It has been pointed out [14] that the high frequency behavior of the spectral function diverges like $\omega^{-2m}$ in alternative quantization which we take to maintain the positivity of $m$ in the interesting regime.

## 3 k-gap as an instability toward the charge density wave

For the non-interacting theory, the spectral function is a delta function which defines a dispersion relation $\omega = \epsilon_k$. For an interacting theory the spectral function is smoothed out and the dispersion relation becomes fuzzy. Numerical study of the spectral function meets very sharp peak which is not easily visible without high resolution, which cost much computational resources. Therefore we need a tool to get away: instead of looking peaks in spectral function, we look for the zero of the denominator of the Green function.

If we write the retarded Green’s function as $G_R^{-1} = C - iD$ with real $C$ and $D$, the spectral density is given by

$$A = \text{Im} G_R = D/(C^2 + D^2). \quad (3.1)$$

For finite $D$, the spectral density has its maximum at $C = 0$. Therefore, one can easily check peak of spectral density by looking zero of $C$. It depends on the value of $D$ also. When $C = 0$, the spectral density becomes $A = 1/D$, hence it is suppressed when $D$ is large. To test how useful this idea is, we calculate the zero of $C$ for $m < 1/2$ and compare with the spectral function. The comparison to the spectral density and the zero of $C$ are drawn in Figure 1, from which we can see that the two are well matched, although they do not exactly overlap. Features of Figure 1 are described below.

1. Figure (a): At $p = 0$, the peak of spectral function is same as zero of $C$. 


Figure 1. The zero of $C$ (red line) vs. the peak of spectral function. We use unsymmetrized $G_2$. (a) Here zero of $C$ overlap with the pole of the Green function. (b) The new branch of dispersion curve created by the interaction and it is not followed by the zero of $C$. (c) Decreasing of $m$ from $1/2$ deforms the original dispersion curve is and the zero of $C$ follows it, of but not the new branch.

2. Figure (b): The interaction generate new band along the maximum of $D$, Out of $C = 0$ line, $C >> D$ so that $A \sim D/C^2$.

3. Figure (c): For $m$ off $1/2$, the original linear dispersion curve deform and the zero of $C$ follow it. peaks of both band are overlapped to the zero of $C$. But there is another branch of zero of C, which is the middle band in the figure, which is not realized as the peak of the spectral function. Along this band, $D$ has maximum value and the peak is suppressed since $A \sim 1/D$.

Summarizing, $C$, the real part of the inverse of Green’s function, contains the essential information for the peak of spectral density.

3.1 Appearance of k-gap and and instability

The $m$-evolution of the spectrum can be traced by the zero of $C$. For $p < 1$, $m$-evolution of the system in $m < 1/2$ regime belongs to the gapless phase [1]. What will happen to $m > 1/2$? The results are drawn in Figure 2(a-c). Notice that there is a critical value $m_c$ such that k-gap appears for $m > m_c$ \(^2\). Figure 2(d) is drawn to show the definition of $(k_C, \omega_C)$ as the position of the tip of the hyperbola.

Now we move to the case for $p > 1$. Here it is most interesting to see the evolutions across the $m = 1/2$, which is drawn in Figure 3. Here one should notice that k-gap appears whenever $m$ is bigger than $1/2$.

Figure 4 describes the evolution of the dispersion curve as we change the $m$ for strong dipole coupling, $p = 5$. Starting from $m = 0$ which belongs to the gapped phase, it arrives at the free fermion like at $m = 1/2$, and finally it runs into the k-gapped state when $m > 1/2$. This is

\(^2\)Notice that k-gap just means that there is a window of $k$ for which there is no value of $\omega$. It does not mean that $k = 0$ is contained in this window unlike the usual $\omega$-gap.
Figure 2. (a),(b),(c) $m$-Evolution of the zero of $C$ for $p = 1/2$. We have k-gap only if $m > m_c \simeq 0.96$. (d) Definition of $(k_C, \omega_C)$ as the position of the tip of k-gapped band.

Figure 3. $m$-Evolution across the $m = 1/2$ with $p = 2$ fixed. k-gap appears for any $m > 1/2$. Red dotted line denotes IR light cone. When $m = 1/2$, spectral density coincides with IR light cone reminiscent of the figure appearing in the work of recent work of phonon dynamics\cite{15, 16} describing a transverse phonon dispersion from solid to liquids.

Figure 4. Mass evolution of spectral density at $p = 5$. Dashed line denotes free fermion dispersion, $\omega = k + \mu$.

Notice that if $\omega_C = 0$, the Fermi velocity diverges and this super-luminosity indicates the instability of the vacuum, such instability can happen spontaneously.\footnote{We should not consider the crossing of such unstable branch with the Fermi level as the Fermi surface. That is, $k_C \neq k_F$ for the $\omega_C = 0$.} Indeed, this is the kind
of the phenomena expected in the regime where the unitarity bound is violated.

3.2 Fate of the vacuum and the Charge Density Wave

To see the nature of this instability, we calculated the density dependence of the position of $k_C$ and found that there is a linear relation between them. See Figure 5(a). The strong correlation between the charge density and the wave vector at the instability indicates that the instability is associated to the charge density wave. The Figure 5(b,c) is reproduced from [17], where linear dependence of the charge density wave vector $\delta$ in the doping which is comparable to our charge density $Q$, which is related to $\mu$ by $Q = \mu r_0$ and $r_0 = (2\pi T + (2\pi T)^2 + 3\mu^2)/3$. Therefore for $\mu/T << 1$, the density and the chemical potential is also linear each other. Since the doping parameter should be interpreted as the charge density the linear dependence of wave vector in the doping parameter is consistent with our theory at least for the low doping.

For higher doping or charge density, $r_0 \sim \mu$ so that $Q \sim \mu^2$ as expected from the dimensional analysis or the non-interacting Fermi gas theory. Therefore our theory shows $k_C \sim \sqrt{Q}$. Figure 5(c) shows the a bit more recent data which shows bending of the data, which is consistent with our theory although the authors of the paper [18] tried to fit with linear plot without success. Although we do not aim to detailed match of our theory with the data, it is encouraging to see that the general trend of data vs theory is consistent. This is our main result.

Notice that the linearity of doping and the wave vector is not a character of weakly interacting system but that of a strongly interacting one. Also if we consider the charge in our theory as the 'conserved' spin, we would get the spin density wave instead of the CDW.

What would be the physical mechanism to create such unitarity bound violation? In a theory with Fermi surface(FS), CDW is associated with the nesting[19, 20], a phenomena associated with a shape of FS where a single vector $k_Q$ connects large parallel regions of a FS. In perturbation theory, it can lead to divergent scattering amplitude through $\int dk/(E_k - E_{k+q}) \cdots$
for \( q = kQ \) and \( k \in \{ \text{Nesting region} \} \). In the situation where Pauli principle is relaxed due to strong interaction so that the degrees of freedom relatively deep inside the Fermi sea can be excited, the nesting mechanism can work even in the absence of the Fermi surface. In more physical terms, such divergence can be rephrased as the appearance of large degrees of freedom that can interact effectively at a special momentum transfer \( q = kQ \), which is very similar to the unitarity violation in our theory. Therefore it is natural to identify the tip of the k-gap as the density wave vector: \( k_C = kQ \).

4 Discussion

In this paper, we calculated the spectral density of probe fermion beyond the unitarity limit and found a characteristic k-gap for most parameter regime and suggested that such spectrum leads to the instability toward the density wave. We can look for the spectrum and read off the wave number of the collective excitation by looking at the position of the tip of the k-gapped band when the tip is located at the Fermi level.

Below we discuss a few points associated with the main result. Once the new vacuum has charge density wave, what are the classification of the phases according to the gap? If we neglect the k-gapped branch of the spectral density we can read off the physics when such instability is arrived at its fate. The phase diagram for such case is drawn in Figure 6 for \( 0.5 < m < 1.0 \). Dashed line implies that these ‘phases’ are smoothly interpolated.

Another question is that for each \((p,m)\) what is the value of \( k_C \) when the tip is located at the fermi level? This is interesting since such case can be interpreted as spontaneous k-gap generation. The answer is given in figure 7(a), We expect that there is a tubular neighborhood where charge density wave is easy to be formed. \( k_C^* \) is the value of wave vector of CDW with \( \omega_C = 0 \). As a auxiliary data, the mass dependance of \( \omega_C \) for fixed \( p \) is given in Figure 7(b).

Our result indicates that in the regime \( p < 1, m < m_c \) there is a region where k-gap or ghost spectrum does not appear in spite of the unitarity violation. See the shaded region of 7(b). This

![Figure 6](image-url)
may be the fermionic analogue of the phenomena found in ref. [21] where it is shown for the scalar that there is a ghost free region in spite of the violation of the BF bound.

**Note added** After this work is uploaded to archive, we were informed that similar related idea were discussed in recent papers [22–24], where low energy scaling dimension was gravitationally calculated as a function of momentum and instability was identified as breaking its reality.

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