Response to Comment on “The role of electron-electron interactions in two-dimensional Dirac fermions”

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Hesselmann et al. question one of our conclusions: the suppression of Fermi velocity at the Gross-Neveu critical point for the specific case of vanishing long-range interactions and at zero energy. The possibility they raise could occur in any finite-size extrapolation of numerical data. Although we cannot definitively rule out this possibility, we provide mathematical bounds on its likelihood.

Our procedure to extract the interaction correction to Fermi velocity \( \Delta v_F(k) \) from quantum Monte Carlo (QMC) simulations for on-site Coulomb interactions \( (\gamma = 0) \) and very close to criticality \( (U \rightarrow U_c) \) has been questioned \((1)\). To put this in context, our figure 2 in \((2)\) comprises about 120 data points for on-site interactions ranging from weak to strong coupling, and with varying long-range interaction. The critique concerns at most three of these data points. Additionally, our data can be thought of as momentum slices of figure 2, for which we use 16 such slices. Their criticism is only close to the Dirac point \( (\Delta k \rightarrow 0) \), and as such, it concerns only these three data points out of the ~2000 projected datasets, and therefore no more than 0.2% of the QMC data in \((2)\).

Most of our core findings and conclusions are unaffected. Here, we defend our claim of a Fermi velocity suppression for \( \gamma = 0, U \rightarrow U_c, \) and \( \Delta k \rightarrow 0. \) We consistently use the following estimator for \( \Delta v_F: \)

\[
\Delta v_F^{\text{Tang}}(k) = \lim_{L \to \infty} \frac{\Delta E(k, L) - \Delta E(0, L)}{k}
\]

(1)

where \( \Delta E(k, L) \) is obtained from QMC data for system size \( L. \) We evaluate our estimator at the smallest momentum accessible to QMC, \( k_{\min} = 4\pi / \left(\sqrt{3L_{\max}}\right). \) \( \Delta E(k_{\min}, L) \) is obtained for \( L < L_{\max} \) from \( \Delta E(k_L, L) \) and \( \Delta E(0, L) \) by linear interpolation (see Fig. 1). Here \( k_L = 4\pi / \left(\sqrt{5L}\right). \) Note that if we could simulate infinite lattices, our estimator would be identical to the mathematical definition of \( \Delta v_F(k \to 0), \)

\[
\Delta v_F^{\text{Tang}}(k \to 0) = \lim_{k_{\min} \to 0} \lim_{L \to \infty} \frac{\Delta E(k_{\min}, L) - \Delta E(0, L)}{k_{\min}}
\]

(2)

Hesselmann et al. observe from our numerical data that close to criticality, the Dirac point energy is more strongly affected by finite lattice size than neighboring momenta. To correct for this, they outline an alternate procedure: (i) Set the Dirac point energy to zero (throwing away all information that the QMC provides about the Dirac point), and (ii) use an estimator obtained from a single system size,

\[
\Delta v_F^{\text{Hesselmann}} = \frac{\Delta E\left(\frac{4\pi}{\sqrt{3L_{\max}}}, L_{\max}\right)}{4\pi / \left(\sqrt{5L_{\max}}\right)}
\]

(3)

This estimator ignores any finite-size scaling information. Figure 1 shows that the two estimators give different results when applied to our QMC data. This can be understood by first noting that in the thermodynamic limit, the Hesselmann et al. estimator is different from the mathematical definition of the Fermi velocity,

\[
\Delta v_F^{\text{Hesselmann}} = \lim_{k_{\min} \to 0} \frac{\Delta E\left(\frac{4\pi}{\sqrt{3k_{\min}}}, k_{\min}\right)}{k_{\min}} = \Delta v_F^{\text{Tang}}(k \to 0)
\]

(4)
This is illustrated graphically in Fig. 1B. \( \Delta v_F^H \) is taken along the black diagonal arrow, whereas \( \Delta v_F^{Tang}(k \to 0) \) is taken along the red horizontal arrow. We note that if in the thermodynamic limit the two estimators disagree, then ours is always correct. However, at issue here is not the thermodynamic limit, but the finite lattice sizes achievable using QMC. Although we cannot make a priori assumptions about the functional form of \( \Delta E(k, L) \) at the critical point (because we have a strongly correlated many-body state), we can still construct hypothetical functions \( \Delta E(k, L) \) to illustrate when and why \( \Delta v_F^{Tang}(k_{\text{min}}) \) and \( \Delta v_F^H \) disagree.

First consider \( \Delta E_s(k, L) = \Delta v_F^{Tmac}(k) + \left[ a(k)/L \right] \), where \( \Delta v_F^{Tmac}(k) = \Delta v_F + \Delta v_F k \) and \( a(k) = a_0 + a_k \) \( (\Delta v_0 = -0.3, \Delta v_1 = 0.1, a_0 = 2, \text{ and } a_1 = 1 \) are all chosen to be consistent with QMC data). For \( L = 24 \), this gives \( \Delta v_F^H \approx 0 \) and \( \Delta v_F^{Tang}(k_{\text{min}}) \approx \Delta v_F^{Tmac} = -30\% \). This simple and reasonable construction shows how it is possible for the Hesselmann et al. estimator to find no Fermi velocity renormalization, despite there being a strong suppression correctly captured by our estimator (see Fig. 1B).

Now consider \( \Delta E_s(k, L) = \left[ a_0 \delta(k)/L \right] + \Delta v_F^{Ttrue} k \), where \( \delta(k) \) is the Dirac delta function. This is an extreme example of Hesselmann et al.’s concern: Only the Dirac point has finite-size effects, but no other momenta. We emphasize that this functional form is inconsistent with our numerical data. Nonetheless, for this hypothetical worst-case scenario, \( \Delta v_F^H = \Delta v_F^{Ttrue} \), and \( \Delta v_F^{Tang}(k_{\text{min}}) = \Delta v_F^{Ttrue} - \left( \sqrt{5}a_0/4\pi \right) \). Taking \( \Delta v_F^{Ttrue} = 0 \) and \( a_0 \) as above, we would underestimate \( v_F \) by at most 28%.

Hesselmann et al.’s core claim is that “the strong suppression of the Fermi velocity near the Gross-Neveu QCP [quantum critical point] merely reflects the enhanced finite-size effects ... at the Dirac point, but not the renormalization of the actual low-energy dispersion.” Because Hesselmann et al. cannot exclude \( \Delta E(k, L) \) as a possible energy function, their claim is unsubstantiated. Moreover, even in the hypothetical worst-case scenario \( \Delta E_s(k, L) \), for the data in Fig. 1, it would require that \( a_0 > 2.79 \) for their claim to be correct. As seen in Fig. 1C, our QMC data lie outside the shaded region, and therefore, for this case, their claim is false. In addition, the finite-size scaling at nonzero momenta (e.g., Fig. 1D) and the observation that all the data points for \( L < 24 \) lie below \( \Delta v_F^H \) provides convincing evidence that a functional form such as \( E_s(k, L) \) is more likely than \( E_s(k, L) \).

Some further remarks are in order:

1) The positive \( \Delta v_F^H \) is physically counterintuitive, as the fermions will scatter off paramagnons and thereby slow down. This interaction with a bosonic mode is analogous to graphene interacting with phonons for which \( v_F(k) \) is suppressed close to the Dirac point and enhanced for energies larger than the Debye energy [e.g., figure 2 of (3)]. This framework allows us to understand how a functional form such as \( \Delta E_s(k, L) \) arises physically, and why \( \Delta v_F^H \) incorrectly gets an enhanced Fermi velocity.

2) The renormalization group flows in (2) were most strongly influenced by the logarithmic divergence (at finite \( \gamma \)) of \( \alpha \) values \( (k \to 0) \) at large momenta, and as such, the numerical value of \( \alpha \) at \( \gamma = 0, U = U_c \), and \( k \to 0 \) is not germane to our paper. Nor did we claim to be the first to calculate it. Figure 14 of (4) shows a 38% suppression of \( \alpha \) (in our case, the prefactor of the density-density correlation function (in the Brinkman-Rice metal-insulator transition, both \( v_F \) and \( \alpha \) vanish at the transition). Moreover, the Fermi velocity renormalization can be obtained from the specific heat \( (c_v \sim T^2/v_F^3) \), for which figure 13 of (5) calculates a ~30% enhancement of \( c_v \) at \( U = U_c \). Both of these works (and ours) support a velocity suppression.

3) Another indication that \( E_s(k, L) \) is more likely than \( E_s(k, L) \) is the relative stability of the two estimators. We could use \( \Delta v_F^H \) for our QMC data, and our main conclusions would not change except at \( U \to U_c \) (away from criticality, \( \Delta v_F^{Tang} = \Delta v_F^H \) in the thermodynamic limit). However, (i) \( \Delta v_F^H \) is inconsistent with the actual QMC data, (ii) we would need different fitting procedures for different parts of our phase diagram, and (iii) \( \Delta v_F^H \) is unstable with changing \( L \). Going from \( L = 15 \) to \( L = 24 \), \( \Delta v_F^H \) changes from -1.17% to +2.94%, whereas \( \Delta v_F^{Tang} \) only changes from -31.4% to -30.5%.

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Fig. 1. Change in energy for Dirac fermions stemming from electron-electron interactions. The data were obtained using the projective quantum Monte Carlo method developed in (2). (A) Open data points are for lattice sizes $L \times L$, where $L = 6, 9, 12, 15, 18, 24$. The solid red line is our estimator $\Delta v_F \mathrm{Tang}$ (Eq. 1), and the black line is the alternate estimator $\Delta v_F \mathrm{H}$ (Eq. 3). The two estimators disagree at $k_{\text{min}}$: $\Delta v_F \mathrm{Tang}(k_{\text{min}}) = -30.5\%$ while $\Delta v_F \mathrm{H} = +2.94\%$. (B) Our estimator is always correct in the thermodynamic limit (see text). (C) Finite-size scaling of the Dirac point. Because the QMC data are outside the shaded region, even in the hypothetical worst case for our estimator, our numerical data are inconsistent with an unrenormalized Fermi velocity. (D and E) Finite-size scaling of $v_F(k)$ at nonzero momenta provides clear evidence that $E_1(k, L)$ (the best case for our estimator) is more likely than $E_2(k, L)$ (the worst case for our estimator).