Reply to "Comment on 'Magnetotransport signatures of a single nodal electron pocket constructed from Fermi arcs' "

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We provide arguments relating to those recently made in a comment by Chakravarty and Wang, who question the validity of our proposed charge-density wave Fermi surface reconstruction model and its relation to sign changes in the Hall effect. First, we show that the form of rounding of the vertices (i.e. sharp corners) of the reconstructed electron pocket, as used in our model calculations of the Hall coefficient, is consistent with Bragg reflection from the periodic potential of a charge-density wave, rather than being arbitrarily chosen. Second, we provide further justifications for why an oscillatory transport scattering time provides a useful means for modeling Shubnikov–de Haas oscillations in the Hall effect, in the situation where a Fermi surface pocket departs from the ideal circular form. Third, we discuss recent experimental evidence gathered from two different families of underdoped cuprates supporting the existence of a single electron pocket produced by biaxial charge-density wave order as a universal phenomena.

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In a recent paper [1], we showed how an electron pocket in the shape of a diamond with concave sides [see, for example, Fig. 1(a)] could potentially explain changes in sign of the Hall coefficient R_{H} in the underdoped high-T_{c} cuprates as a function of magnetic field and temperature. For simplicity, this Fermi surface is assumed to be constructed from arcs of a circle connected at vertices [see Fig. 1(b)], which is an idea borrowed from Banik and Overhauser [2]. Such a diamond-shaped pocket is proposed to be the product of biaxial charge-density wave order [3], which was subsequently supported by x-ray scattering experiments [4,5]. Since those x-ray scattering experiments were performed, the biaxial Fermi surface reconstruction scheme has garnered widespread support in the scientific literature [6–8]. It has been shown to account for the cross section of the Fermi surface pocket observed in quantum oscillation measurements [9–11], the sign and behavior of the Hall coefficient [1,12], the size of the high magnetic field electronic contribution to the heat capacity [13], and more recently the form of the angle-dependent magnetoresistance [14]. The measured charge-density wave correlation length is comparable to the mean free path obtained from quantum oscillations [10], indicating it may be reasonably expected to yield Fermi surface reconstruction.

In their comment [15], Chakravarty and Wang raise several important questions relating to the validity of the Hall coefficient we calculated for such a diamond-shaped Fermi surface pocket. These questions concern specifically (1) whether a change in sign of the Hall coefficient R_{H} with magnetic field and temperature is dependent on a "special" form for the rounding of the vertices in Fig. 1(a), (2) whether a pocket of such a geometry can produce quantum oscillations in R_{H} in the absence of other Fermi surface sections, and (3) whether a reconstructed Fermi surface consisting of a single pocket is less "natural" than one consisting of multiple pockets. Below we consider each of these in turn.

1. Rounding of the diamond vertices. Bragg reflection, similar to that occurring with regard to the crystalline lattice in conventional metals [2], is likely to be a crucial factor in determining the form of the Hall coefficient in underdoped cuprates. Bragg reflection, in which quasiparticles scatter elastically from a periodic potential, is consistent with the findings of a static charge-density wave in both x-ray scattering [4,5] and quantum oscillation [9–11] experiments. In such a case, we can consider the sharp corners of the Fermi surface in Fig. 1(a) to be the product of mixing between states $\varepsilon_{\mathbf{k},1}$ and $\varepsilon_{\mathbf{k},2} = \varepsilon_{\mathbf{k+Q},1}$ (where $\mathbf{Q}$ is the charge-density wave ordering vector), whose Fermi velocities before ($\mathbf{v}_{\mathbf{k},1}$) and after ($\mathbf{v}_{\mathbf{k},2}$) reflection point in different directions [see Fig. 2(a)]. Irrespective of the magnitude Δ of the periodic charge-density wave potential, the y component of the Fermi velocity $v_{\mathbf{k},y}$ tangential to the Bragg plane illustrated in Fig. 2(b) is unchanged by the Bragg reflection process. The x component of the velocity $v_{\mathbf{k},x}$ normal to the Bragg plane, by contrast, passes through zero and undergoes a change sign. The vanishing of $v_{\mathbf{k},x}$ at the point of intersection between $\varepsilon_{\mathbf{k},1}$ and $\varepsilon_{\mathbf{k},2}$ upon mixing the two bands implies that the magnitude $v_{\mathbf{k}} = \sqrt{v_{\mathbf{k},x}^2 + v_{\mathbf{k},y}^2}$ of the Fermi velocity is reduced at the vertices relative to the magnitudes of $\mathbf{v}_{\mathbf{k},1}$ and $\mathbf{v}_{\mathbf{k},2}$. It is this local reduction in the magnitude of the velocity at the vertices that is fundamentally responsible for the change in sign of the Hall coefficient with magnetic field, as originally reported by Banik and Overhauser [2].

When one neglects the rounding of the vertices, the effect of Bragg reflection is implicitly included in the calculation of the Hall coefficient using the Shockley-Chambers tube integral method [17,18] by virtue of the fact that $v_{\mathbf{k},x}$ (normal to the reflection plane) changes sign at the vertex while $v_{\mathbf{k},y}$ (tangential to the reflection plane) remains unchanged. In modeling the Hall coefficient using the Jones-Zener method [16], by contrast, the velocity reduction associated with Bragg reflection needs to be carefully inserted by hand [1]. Only when one correctly accounts for the reduction in the magnitude of the Fermi velocity at the vertices does one obtain consistency of the Jones-Zener [16] method with Shockley-Chambers tube integral [17,18] method.

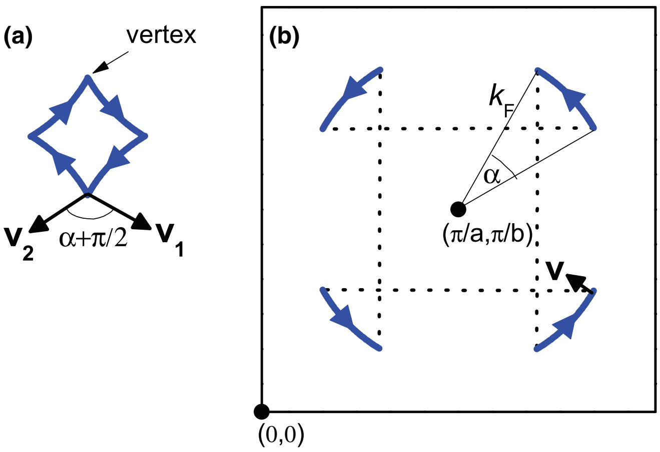

FIG. 1. (a) Schematic diamond-shaped electron pocket from Ref. [1], with blue arrows indicating the direction of cyclotron motion and $\mathbf{v}_1$ and $\mathbf{v}_2$ indicating the Fermi velocity direction. (b) Schematic showing how the electron pocket is produced by connecting arcs of a larger hole Fermi surface, with α being the angle subtended by the arc and the dotted lines indicating how they are connected.

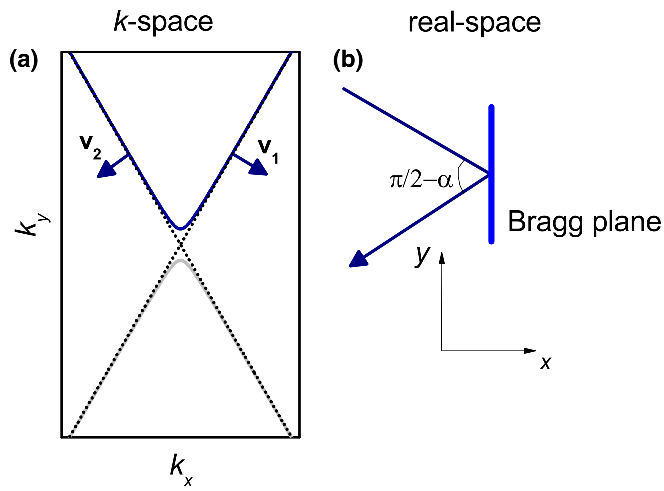

FIG. 2. (a) Solid lines showing the reconstructed Fermi surface in the vicinity of a vertex produced by Bragg reflection. Dotted lines indicate the Fermi surface in the absence of hybridization. $\mathbf{v}_1$ and $\mathbf{v}_2$ are velocities before and after a quasiparticle traverses the vertex. (b) Schematic of the Bragg reflection in real space assumed to be responsible for the sharp corner.

An important question in the cuprates is whether there exists an alternative *inelastic* mechanism that can lead to a different form for the rounding of the vertices of the diamond-shaped pocket in Fig. 1(a). Chakravarty and Wang [15] refer to a scenario postulated in Ref. [19] in which the magnitude $|\mathbf{l}_\mathbf{k}|$ of the mean free path vector $\mathbf{l}_\mathbf{k} = \mathbf{v}_\mathbf{k}\tau_\mathbf{k}$ is invariant over the Fermi surface, leading to a situation in which the sign of R_H no longer changes with magnetic field. We note that a constant $|\mathbf{l}_\mathbf{k}|$ runs into compatibility problems with Bragg reflection. For example, in order to maintain a constant $|\mathbf{l}_\mathbf{k}|$ while traversing the vertices, either of two unlikely situations would need to apply. In one, the scattering rate would need to be locally suppressed at the vertices to compensate for the momentarily reduced magnitude of the velocity at the vertices. In the other, the y component of quasiparticle velocity would need to momentarily accelerate at the vertices in order to maintain both $\mathbf{v}_\mathbf{k}$ and $\tau_\mathbf{k}$ constant. Neither of these scenarios appear to be more realistic than the standard Bragg reflection scenario considered above and in Ref. [1].

When interactions do accompany Bragg reflection, as in the case of "hot spots," it is more likely that these will suppress the contribution to R_H from the vertices, causing a sign change in R_H to become more pronounced or to occur for smaller values of the parameter α in Fig. 1. Possibilities include a local increase in the effective mass at the hot spots [20] or an increase in the quasiparticle scattering rate [21].

2. Oscillations in the Hall coefficient. The comment of Chakravarty and Wang [15] focuses on the Drude treatment of a multiband metal and does not, we believe, adequately consider the nongeometric nature of the Hall coefficient R_H in a bulk metal in the intermediate regime regime in which $\hbar\omega_\mathrm{c}$ is neither in the limit $\omega_\mathrm{c}\tau \to 0$ nor $\omega_\mathrm{c}\tau \to \infty$.

It is well known that for a multiband metal consisting of pockets with different mobilities, or different values of the product $\omega_\mathrm{c}\tau$, R_H is a function of $\omega_\mathrm{c}\tau$, causing it to vary with the strength of a magnetic field. Only in limits $\omega_\mathrm{c}\tau \to 0$ and $\omega_\mathrm{c}\tau \to \infty$ does R_H become a truly geometric quantity and approach constant low and high magnetic field values. Since $\sigma_{xx,yy}/\sigma_{xy} \approx \omega_\mathrm{c}\tau$ for a given section of Fermi surface and Shubnikov–de Haas oscillations occur only in $\sigma_{xx,yy}$, oscillations in the quasiparticle scattering rate τ^{-1} provide a natural means for modeling the Shubnikov–de Haas effect in metals. Such a method also reproduces the correct behavior for various different limits. For example, in the case of a single band metal, it correctly predicts that there are no oscillations in R_H [22,23]. Meanwhile, for a multiband metal, it correctly predicts that oscillations are present in R_H [24], yet vanish in the limits $\omega_\mathrm{c}\tau \to 0$ and $\omega_\mathrm{c}\tau \to \infty$. The justification for considering the oscillations to occur in τ^{-1} is provided by Fermi's golden rule, which states that the transport scattering rate that enters into the electrical resistivity is approximately proportional to the number of states available for scattering [25]—in other words, the electronic density of states. The oscillatory $\tilde{\tau}^{-1}$ is therefore expected to be approximately proportional to the oscillatory density of states, which is precisely what we assume for our calculations in Ref. [1]. A more rigorous model for quantum oscillations in the Hall coefficient of the underdoped cuprates could be developed by a fully quantum mechanical derivation for a diamond-shaped pocket, which we look forward to.

Banik and Overhauser showed that, in a manner similar to that for a multiband metal, the Hall conductivity of a diamond-shaped pocket is a function of $\omega_\mathrm{c}\tau$ [2]. Therefore, in a manner like that for a multiband metal, R_H of a diamond-shaped pocket varies with the strength of a magnetic field. In a manner similar to that for a multiband metal, R_H also becomes constant (i.e., nonoscillatory) in the limits $\omega_\mathrm{c}\tau \to 0$ and $\omega_\mathrm{c}\tau \to \infty$. The quantum oscillations in the underdoped cuprates are observed in the intermediate regime in which $\omega_\mathrm{c}\tau \sim 1$ for which R_H does not have a simple geometric representation and for which oscillations in R_H cannot therefore be excluded.

3. Single versus multiple pockets. The occurrence of multiple pockets in the majority of Fermi surface reconstruction scenarios [6,7,26–28] does not make these scenarios more likely, as argued by Chakravarty and Wang [15]. Other considerations such as the small value of the electronic heat capacity at high magnetic field in fact point to a single pocket per CuO_2 plane [29], making such multiple-pocket scenarios less likely. We note that while low-frequency oscillations have been detected in underdoped $YBa_2Cu_3O_{6+x}$ [30] (displayed in one of the supplementary figures), the weight of the experimental evidence points to their origin from a Stark quantum interference effect [1,31] rather than additional small pockets [9].

There are at least two other materials [32,33] in which Fermi surface reconstruction by incommensurate spin- and or charge-density wave order has been shown experimentally to yield only a single reconstructed pocket. In the case of the underdoped cuprates as well, two Fermi surface reconstruction scenarios based on biaxial charge-density wave order [11,34] have been shown to be capable of producing a reconstructed Fermi surface consisting of only a single electron pocket. In addition to the biaxial charge-density wave $YBa_2Cu_3O_{6+x}$, which is associated with the electron pocket [35], a uniaxial charge-density wave with longer correlation lengths is found to onset at lower temperatures [35,36]. The lower integrated spectral weight of the uniaxial charge-density wave compared to the biaxial charge-density wave indicates the role of the uniaxial charge-density wave in Fermi surface reconstruction to be secondary.

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