Fermi surface topology in interacting anisotropic electron gas

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We investigate theoretically effects of electron-electron interactions on the shape of the Fermi surface in an anisotropic two-dimensional electron gas using the ‘GW’ self-energy approximation. We find that the interacting Fermi surface generally deviates from an ellipse, but not in an arbitrary way. We demonstrate that the interacting Fermi surface has only two qualitatively distinct shapes for most values of $r_s$. The Fermi surface undergoes two distinct transitions between the two shapes as $r_s$ increases. For larger $r_s$, the degree of the deviation from an ellipse rapidly increases, and thus the interacting topology is significantly different from the noninteracting elliptic Fermi surface although they preserve the same volume.

Introduction.— The concept of a Fermi surface is one of the great triumphs of quantum physics and is a central paradigm in solid state physics with the physics of all metallic systems being closely tied to their Fermi surface properties. In particular, the topology of a Fermi surface plays a vital role in determining low-energy physical properties (e.g. specific heat, compressibility, magnetic, transport, and optical properties) of metals. This naturally raises a question as to how the Fermi surface shape evolves under the influence of electron-electron interactions. The answer is obvious for an isotropic system because the rotational symmetry forces the Fermi surface to be a circle although the quasiparticle effective mass itself differs from the noninteracting effective mass due to many body renormalization by the Coulomb interaction. When the rotational symmetry is explicitly broken in the noninteracting system by having an elliptic Fermi surface with two different effective masses, however, the Fermi surface is not necessarily constrained to any specific shape in the corresponding interacting system. Since the Fermi surface is anisotropic for most realistic materials because of lattice-induced band structure effects, there has been interest in determining the shape of the interacting Fermi surface in an anisotropic system \cite{1-5}. In the current work, we investigate how interactions affect the low-energy properties of an anisotropic electron gas by directly calculating the self-energy including the full dynamical effects of the anisotropy. Our starting point is a noninteracting anisotropic two dimensional electron gas characterized by two unequal effective masses, as for example, in Si 110 inversion layers and other semiconductor structures \cite{6}.

The obvious way to induce anisotropy to the Fermi surface is to introduce imbalance between masses along different axes in an isotropic two-dimensional electron gas \cite{6}, i.e.,

$$\varepsilon(k) = \frac{k_x^2}{2m_H} + \frac{k_y^2}{2m_L}, \quad (1)$$

which transforms the circular Fermi surface of an isotropic electron gas to an ellipse (see black dashed line in Fig. 1). Obtaining the exact shape of the interacting Fermi surface is a formidable task because the broken rotational symmetry requires the evaluation of the self-energy at every point on the Fermi surface. In spite of the manifest conceptual and practical importance of the question (i.e. “What is the shape of the interacting Fermi surface when the noninteracting Fermi surface is an ellipse?”) in semiconductors with anisotropic band mass, there have been few attempts to address the question in spite of its importance already being obvious 50 years ago— typically, an effective isotropic approximation has invariably been used, often using the corresponding density of states effective mass, in calculating the interaction effects \cite{7-11}. A recent study approached this question by approximating the interacting Fermi surface by an ellipse (see black solid line in Fig. 1), showing that interactions reduce the anisotropy \cite{3} as also follows trivially from the use of the density of states mass in the theory. To our knowledge, however, there exists no complete study of the topology of the interacting anisotropic...
Fermi surface beyond the elliptical shape approximation, and most publications in fact make the uncontrolled drastic approximation of using the isotropic density of states effective mass in obtaining the interacting self-energy.

In this work, we investigate the deviation of the renormalized anisotropic Fermi surface from an ellipse by calculating the self-energy within the leading-order dynamically-screened Coulomb interaction (RPA) or the GW approximation [12], using the full band anisotropy in the self-energy calculation. We first show that the renormalized effective masses \(m^*_x\) and \(m^*_y\) vary as a function of the location on the Fermi surface (and hence, the interacting Fermi surface is no longer elliptic), and analyze their behaviors in several regimes of the dimensionless Coulomb interaction strength parameter \(r_s\) [13]. We then demonstrate the evolution of the Fermi surface by using the obtained results for the effective mass. We find that there are two typical shapes for the interacting Fermi surface defined by the effective mass, and the degree of the deviation from the noninteracting bare elliptic shape becomes significant for strongly interacting systems at larger \(r_s\) (although the interacting Fermi surface is nonelliptic for all \(r_s\)). We focus on two-dimensional electron systems, but our qualitative conclusions apply to 3D systems as well.

**Formula for GW approximation.**— The self-energy for an anisotropic electron gas within the GW approximation is given by [Fig. 2(a)],

\[
\Sigma(k, i\omega_n) = -\int \frac{d^2q}{(2\pi)^2} \frac{1}{\beta} \sum_{i\Omega_n} W(q, i\Omega_n) \times G_0(k + q, i\omega_n + i\Omega_n),
\]

where \(G_0 = (i\omega_n + i\Omega_n - \xi_{k+q})^{-1}\) is the bare Green’s function, \(\xi_k = \epsilon_k - \mu\), and \(\mu\) is the chemical potential. Here \(W(q, i\Omega_n) = v_c(q)/\epsilon(q, i\Omega_n)\) is the dynamically screened Coulomb interaction where \(v_c(q) = 2ne^2/|q|\) is the 2D bare Coulomb interaction and \(\epsilon(q, i\Omega_n) = 1 - v_c(q)\Pi_0(q, i\Omega_n)\) is the two-dimensional dielectric function obtained within RPA [Fig. 2(b)] with \(\Pi_0(q, \omega)\) being the noninteracting polarization function for an anisotropic two-dimensional electron gas. \(\Pi_0(q, \omega)\) can be obtained exactly from the existing result [14] for an ideal isotropic gas by rescaling \(m_e \rightarrow m_{DOS}\), \(k_x \rightarrow \sqrt{m_{DOS}/m_x}k_x\), and \(k_y \rightarrow \sqrt{m_{DOS}/m_y}k_y\), where \(m_e\) refers to the bare electron mass, and \(m_{DOS} = (m_{1D}m_L)^{1/2}\) as arising in the definition of the density of states for the noninteracting system.

It is useful to divide the GW self-energy into the exchange and correlation parts: \(\Sigma = \Sigma^{ex} + \Sigma^{corr}\). The exchange part corresponds to the self-energy with bare Coulomb interaction, given by

\[
\Sigma^{ex}(k) = -\int \frac{d^2q}{(2\pi)^2} \Theta(-\xi_{k+q})v_c(q).
\]

The correlation part contains all contributions beyond bare exchange interaction. After performing a standard procedure of analytical continuation \(i\omega_n \rightarrow \omega + i\eta\), the retarded correlation-self energy is decomposed into

\[
\Sigma^{corr} = \Sigma^{line} + \Sigma^{res}
\]

where

\[
\Sigma^{line}(k, \omega) = -\int \frac{d^2q}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{d\Omega}{2\pi} \frac{v_c(q)}{\xi_{k+q} - \omega - i\Omega}
\]

\[
\times \left[ \frac{1}{\epsilon(q, i\Omega) - 1} \right],
\]

and

\[
\Sigma^{res}(k, \omega) = \int \frac{d^2q}{(2\pi)^2} \left[ \Theta(\omega - \xi_{k+q}) - \Theta(-\xi_{k+q}) \right]
\]

\[
\times v_c(q) \left[ \frac{1}{\epsilon(q, \xi_{k+q} - \omega) - 1} \right].
\]

**Effective Mass.**— Once we know the self-energy, we can calculate the renormalized single particle energies by solving the Dyson’s equation

\[
E(k) = \epsilon(k) + \text{Re} \left[ \Sigma(k, \omega) \right]_{\omega = E(k) - \mu}.
\]

Within the on-shell approximation which in this context is the first iteration of Dyson’s equation, the self-energy is evaluated only at \(\omega = \epsilon(k) - \mu\), yielding

\[
E(k) = \epsilon(k) + \text{Re} \left[ \Sigma(k, \epsilon(k) - \mu) \right].
\]

We assume that the renormalized energy dispersion is written in a form as

\[
E(k) = E(0) + \frac{k_x^2}{2m_x^*(k)} + \frac{k_y^2}{2m_y^*(k)},
\]

where the momentum-dependent masses \(m_x^*(k)\) and \(m_y^*(k)\) absorb any terms that distort the Fermi surface from an ellipse (The neglect of the momentum dependence in the effective mass corresponds to the elliptic approximation being avoided in the current work). Note that the momentum dependence disappears in the limit where the renormalized Fermi surface is a perfect ellipse. Assuming that \(m_y^*(k)\) varies slower than \(k_y^2\) on the Fermi surface, where \(i = x, y\), the renormalized energy dispersion expanded around the Fermi surface is given by

\[
E(k) \approx \mu^* + (k_x - k_{F_x}) \frac{k_F x}{m_x^*(k_F)} + (k_y - k_{F_y}) \frac{k_F y}{m_y^*(k_F)}.
\]

![FIG. 2. (a) Feynman-Diagram representing the self-energy within GW–RPA approximation, where \(W\) refers to a dynamically screened Coulomb interactions within the RPA. (b) Series of diagrams corresponding to RPA. The wiggly line represents the Coulomb interaction and \(\Pi_0\) the bare polarizability](image)
where $\mu^*$ is the renormalized Fermi energy. Using Eq. 9, we can find an expression for the renormalized effective mass dependent on the location on the Fermi surface:

$$\frac{m^*_e(k_F)}{m_i} = \frac{1}{\frac{m_i}{k_i}} \frac{\partial}{\partial k_i} \left| \sum_{\ell} \frac{(\sum_{\ell} |\Xi(k, \xi_k)|} {k = k_F} \right| \left| \frac{k_F}{k_i} \right|^{-1}$$

which is a generalization of the standard definition of the effective mass that takes into account its momentum-dependent nature. Our interacting Fermi surface is defined by Eq. (10). By taking the derivative of Eq. (7), we obtain the renormalized effective mass to be

$$\frac{m^*_e(k_F)}{m_i} = \left\{ 1 + \frac{m_i}{k_i} \frac{\partial}{\partial k_i} \left| \sum_{\ell} \frac{\xi(k, \xi_k)}{k = k_F} \right| \right\}^{-1} \left\{ \frac{\partial E}{\partial k} \right\}$$

In the following, we present results of the calculated effective mass for an anisotropic 2D electron gas. Throughout the paper, we set $m_x \rightarrow m_H = 10m_e$ and $m_y \rightarrow m_L = m_e$.

**FIG. 3.** (a),(b) Numerically calculated effective mass as a function of $r_s$ at $\theta = 0$, $\pi/4$, and $\pi/2$, where $\theta$ is the angle from the semi-major axis [see the inset in (a)]. Black-dotted boxes indicate regions where the effective mass curves cross each other. (c),(d) Plots of the effective mass as a function of $\theta$ at $r_s = 0.02$, 0.2 and 0.5. Each plot is normalized by $m^*(\theta = 0)$ which refers to the effective mass at $\theta = 0$.

Figure 3(a) and (b) present calculated $m_H(r_s)$ and $m_L(r_s)$ for small $r_s$ at $\theta = 0$, $\pi/4$ and $\pi/2$. It should be noted that $r_s^{\text{min}}(\theta)$, which we define as the value of $r_s$ where the effective mass at an angle of $\theta$ is minimum, is shifted to the right with increasing $\theta$. This leads to a crossover of effective mass curves [see black-dotted box in Fig. 3(a) and (b)], having a direct consequence on the angular behavior of the effective mass. Fig. 3(c) and (d) show the effective mass as a function of $\theta$ for a fixed $r_s$. Before the crossover occurs, the effective mass monotonically increases with increasing $\theta$ [at $r_s = 0.02$ in Fig. 3(c) and (d)]. As $r_s$ increases up to the crossover regime, the effective mass at small $\theta$ starts decreasing but it keeps its increasing behavior at large $\theta$, resulting in a local minimum at an arbitrary $\theta$ off the symmetry axes [$r_s = 0.2$ and 0.1 in Fig. 3(c) and (d), respectively]. As $r_s$ increases further, the local minimum is shifted to a larger $\theta$ expanding the region where the effective mass decreases. When $r_s$ is large enough to be out of the crossover regime, the local minimum disappears and the effective mass shows a decreasing behavior over the whole range of $\theta$ [$r_s = 0.5$ in Fig. 3(c) and (d)]. The results of Fig. 3 are restricted to $r_s < 1$, where our RPA theory is essentially exact because of the weak-coupling nature of the system, but the qualitative distortion of the interacting Fermi surface topology is already apparent.

**FIG. 4.** (a),(b) Numerically calculated effective mass as a function of $r_s$ at $\theta = 0$, $\pi/4$, and $\pi/2$. Here each plot is normalized by the result at $\theta = 0$, i.e., $m^*(\theta = 0)$. The inset in (b) shows results for larger $r_s > 12$, where the effective mass increases more rapidly. The black-dotted box in (b) indicates the region where the effective mass curves pass each other. (c),(d) Plots of the effective mass as a function of $\theta$ for $r_s = 5.0$, 7.0, 10.0 and (e),(f) for still larger $r_s$.

In Fig. 4(a) and (b), we present the calculated effective mass for large $r_s > 2$ at $\theta = 0$, $\pi/4$ and $\pi/2$. Here each plot is normalized by the result at $\theta = 0$, i.e., $m^*(\theta = 0)$. The inset in (b) shows results for larger $r_s > 12$, where the effective mass increases more rapidly. The black-dotted box in (b) indicates the region where the effective mass curves pass each other. (c),(d) Plots of the effective mass as a function of $\theta$ for $r_s = 5.0$, 7.0, 10.0 and (e),(f) for still larger $r_s$. Note that in Fig. 4(a) the difference between the effective mass curves for different angles becomes smaller as $r_s$ increases, but their sequence is not reversed [Fig. 4(a)]. Thus the de-
creasing behavior of $m^*_H(\theta)$ observed at small $r_s < 2$ persists with increasing $r_s$ beyond $r_s = 2$ as explicitly shown in Fig. 4(c). For $m^*_s$, however, the effective mass curves cross each other around $r_s \approx 7$, completely reversing their sequence at $r_s > 8$ as compared to the case for $r_s < 6$. This leads $m^*_L(\theta)$ to have qualitatively different behaviors from $m^*_H$ as shown in Fig. 4(d). The effective mass $m^*_s(\theta)$ shows a decreasing behavior before the crossover occurs $|r_s| = 5.0$ in Fig. 4(d). When one enters the crossover regime ($r_s = 7.0$), the effective mass at small $\theta$ starts increasing, yielding a local maximum off the symmetry axes. The local maximum is shifted to the right with increasing $r_s$, expanding the region where the effective mass increases. For $r_s$ beyond the crossover regime, the effective mass monotonically increases over the whole range of $\theta$ ($r_s = 10.0$). Note that for these larger values of $r_s$ used in Fig. 4 the RPA $GW$ theory becomes progressively quantitatively worse, but it is known that even for metals with $r_s \sim 6$, the $GW$ theory provides reasonable results although the perturbation expansion of Fig. 2 is no longer valid for large $r_s$ [12–15]. This could be because the effective expansion parameter at large $r_s$ may be renormalized to an effectively much smaller value as has been argued theoretically [16, 17].

**Fermi Surface.**— Using Eq. (8), we can obtain the renormalized Fermi surface by solving

$$
\mu^* = \frac{k_{Fx}^2}{2m^*_H(k_F)} + \frac{k_{Fy}^2}{2m^*_L(k_F)},
$$

(12)

where $\mu^*$ is the renormalized Fermi energy. Assuming that $m^*_H(k)$ and $m^*_L(k)$ vary slower than $k_{Fx}^2$ and $k_{Fy}^2$ near the Fermi surface, respectively, we obtain

$$
k_F(\theta) = \frac{\sqrt{2\mu^* \sqrt{m^*_H(\theta)m^*_L(\theta)}}}{\sqrt{m^*_H(\theta)\sin^2 \theta + m^*_L(\theta)\cos^2 \theta}},
$$

(13)

where we parameterize the Fermi surface by $k_F = k_F(\theta)\tilde{k}_F$. Here $\theta$ is the angle from the axis corresponding to the high mass direction. To describe the deviation of the Fermi surface from an ellipse, we define

$$
\eta(\theta) = \frac{k_F(\theta)}{k_F(\theta)},
$$

(14)

where $k_F(\theta)$ represents the Fermi surface approximated as an ellipse, and thus is given by the standard equation of an ellipse with $k_F(\theta = 0)$ and $k_F(\theta = \pi/2)$ being the semi-major and semi-minor axes, respectively:

$$
\tilde{k}_F(\theta) = \frac{\sqrt{2\mu^* \sqrt{m^*_H(0)m^*_L(\theta)}}}{\sqrt{m^*_H(0)\sin^2 \theta + m^*_L(\theta)\cos^2 \theta}}.
$$

(15)

Note that $\mu^*$ drops out of Eq. (14), and thus we need only the effective mass to describe the deviation of the Fermi surface from an ellipse.

For exact results, Eq. (13) should be solved in a self-consistent manner because the effective mass is evaluated at the renormalized Fermi surface. This requires obtaining the effective mass from the self-consistent Dyson equation [Eq. (6)], i.e., within the off-shell approximation. It is clear that the off-shell approximation is exact if we work with the full self-energy. But it has been argued that because of vertex corrections, the on-shell approximation is the appropriate approximation to be used in the $GW$ theory so that different perturbative orders are not mixed in the results [15–21]. Thus we use our on-shell effective mass results presented in the previous section for the calculation of the Fermi surface.

![FIG. 5. Plots of $\eta(\theta)$ in (a), (b) crossover regimes and (c) for larger $r_s$. (d) The shape of Fermi surfaces corresponding to a convex (type I) and concave (type II) shape of $\eta(\theta)$ along with the ellipse that approximates the renormalized Fermi surfaces](image-url)

In the previous section, we have shown that there are two crossover regimes (one around $r_s \sim 0.1$ and the other $r_s \sim 8$) where $m^*(\theta)$ changes its behavior qualitatively. In the following we investigate its consequence on the Fermi surface. Figure 5(a) presents $\eta(\theta)$ in the first crossover regime around $r_s \sim 0.1$. At very small $r_s = 0.02$, $\eta(\theta)$ exhibits a convex shape, for which the corresponding Fermi surface shape is schematically shown in Fig. 5(d) as type I. When $r_s$ increases to 0.1, $\eta(\theta)$ becomes almost flat, and the corresponding Fermi surface is close to an ideal ellipse. As we increase $r_s$ further, $\eta(\theta)$ becomes concave, and the corresponding Fermi surface becomes type II in Fig. 5(d). Thus, the Fermi surface qualitatively changes its shape from type I to type II in the first crossover regime. Until $r_s$ increases up to the second crossover regime, the shape of the Fermi surface does not qualitatively change because there is no qualitative change in the angular behavior of the effective mass. In the second crossover regime, a similar but opposite behavior is observed: $\eta(\theta)$ undergoes a concave to con-
vex transition [see Fig. 5(b)], and thus the Fermi surface changes its shape from type II to type I.

After the second (last) crossover regime, the Fermi surface maintains its type I shape as \( r_s \) increases further. We show in Fig. 5(c) plots of \( \eta(\theta) \) for still larger \( r_s \). Since the effective mass increases more rapidly at larger \( r_s \) [see the inset in Fig. 5(b)], even a small increase of \( r_s \) for large \( r_s \) leads to a substantial change of \( \eta(\theta) \). Whether this interesting interaction-driven qualitative topology change in the Fermi surface at large \( r_s \) is real or an artifact of our RPA approximation is unknown at this time and should be experimentally investigated in gated 2D systems by varying electron density so as to change \( r_s \).

Summary.— Within the highly successful leading order dynamically screened RPA theory, we have studied the distortion of the Fermi surface by Coulomb interactions in an anisotropic two-dimensional electron gas by calculating for the first time the full frequency and momentum dependent self-energy in the presence of mass anisotropy. We show that the renormalized interacting effective mass exhibits an emergent angular dependence, leading the Fermi surface to deviate from an ideal ellipse. Thus, in general, one cannot define a density of states effective mass for the interacting system. By analyzing the angular behavior of the effective mass, we show that the deviation does not occur in an arbitrary way: For most values of \( r_s \), the Fermi surface has only two qualitatively distinct shapes, which we classify as type I and type II. A transition between the two shapes can occur as \( r_s \) varies, but only in a limited range of \( r_s \). Our predictions on the topology of the interacting 2D Fermi surface can be experimentally tested in gated 2D semiconductor structures by varying \( r_s \) through varying carrier density.

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