Valley dependent many-body effects in 2D semiconductors

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(Dated: April 17, 2009)

We calculate the valley degeneracy \( g_v \) dependence of the many-body renormalization of quasiparticle properties in multivalley 2D semiconductor structures due to the Coulomb interaction between the carriers. Quite unexpectedly, the \( g_v \) dependence of many-body effects is nontrivial and non-generic, and depends qualitatively on the specific Fermi liquid property under consideration. While the interacting 2D compressibility manifests monotonically increasing many-body renormalization with increasing \( g_v \), the 2D spin susceptibility exhibits an interesting non-monotonic \( g_v \) dependence with the susceptibility increasing (decreasing) with \( g_v \) for smaller (larger) values of \( g_v \) with the renormalization effect peaking around \( g_v \sim 1 - 2 \). Our theoretical results provide a clear conceptual understanding of recent valley-dependent 2D susceptibility measurements in AlAs quantum wells.

PACS numbers: 71.10.Ca,73.20.Mf

Two dimensional (2D) electron (or hole) systems based on semiconductors, e.g. inversion layers, FETs, quantum wells, and heterostructures, have served as useful laboratory systems for studying electron-electron interaction induced many-body effects for almost forty years [1]. The reason is the ease with which the 2D carrier density \( n \) can be tuned in these systems, thus effectively changing the 2D electron gas (2DEG) from being a weakly interacting system at large \( n \) to a strongly interacting system at low \( n \). Such a variation in carrier density can not be achieved in 3D metals where only a modest tuning of the electron-electron interaction effect is possible by going from one metal to another with the concomitant complication of a varying background lattice structure [2]. The electron interaction strength in a many-body Coulomb quantum system is characterized [2] by the dimensionless \( r_s \) parameter which measures the average inter-particle separation in units of the effective Bohr radius. For the 2DEG, \( r_s \equiv (\pi n)^{-1/2}/(\kappa \epsilon_0 m^2) \), where \( n, m, \) and \( \kappa \) are respectively the 2D electron density, the electron effective mass, and the background lattice dielectric constant. Often \( r_s \) is considered to be the ratio of the average Coulomb potential energy, \( e^2/(\kappa \epsilon_0) \) where \( r_0 = (\pi n)^{-1/2} \) is the average inter-particle separation, to the average kinetic energy \( E_F = n\pi \hbar^2/m \) for a 2DEG (including the spin degeneracy). Although the appropriate definition of \( r_s \), also called the Wigner-Seitz radius, is in terms of a dimensionless length, the definition in terms of the dimensionless interaction energy is physically more appealing since \( r_s > 1 \) (or \( r_s < 1 \)) region may be considered as the dilute strongly interacting (or the dense weakly interacting) regime. Varying the carrier density one can increase \( r_s \), thus accessing the strongly interacting dilute regime where the quasi-particle renormalization correction due to many-body effects would be large. In practice, the very strongly correlated regime of \( r_s \approx 10 \sim 30 \) [3] can be achieved in 2DEG whereas in 3D metals [2], \( r_s \approx 2 \sim 5 \). It is, therefore, not surprising that 2D semiconductor systems have long served as the laboratory test-bed for studying \( r_s \) dependent interaction effects. In general, the quasi-particle many-body renormalization is enhanced with increasing \( r_s \), and in principle, there could be quantum phase transitions (e.g Wigner crystallization, ferromagnetic instability, dispersion instability, etc.) in the strong-coupling \( r_s \gg 1 \) regime.

Although electron interaction effects at \( T = 0 \) are completely characterized by the single dimensionless density parameter \( r_s \) in a single-valley system (e.g. GaAs), a multi-valley semiconductor (e.g. Si, Ge, AlAs) is far more complex since the valley degeneracy \( (g_v) \), i.e the number of the equivalent valleys the electrons occupy in the ground state due to the semiconductor band structure, becomes an additional relevant parameter characterizing the electron-electron interaction strength. (We consider only equal valley population of all \( g_v \) valleys and equal spin population of spin up-down levels at \( T = 0 \) in this work, i.e. we consider only a paramagnetic ground state in both valley and spin quantum numbers.) It is obvious that in the presence of a valley degeneracy (i.e. an arbitrary value of \( g_v \geq 1 \)), both \( r_s \) and \( g_v \) will determine the many-body renormalization effects, but a careful investigation of how \( g_v \) itself affects the quantum many-body effects in 2DEG has not yet been carried out in the theoretical literature [4]. This is precisely what we report in this Letter, concentrating on the interacting 2D spin susceptibility and 2D compressibility and calculating their many-body renormalizations as functions of both \( g_v \) and \( r_s \).

A relatively straightforward interpretation of the \( r_s \) parameter as a dimensionless coupling energy, i.e. the Coulomb energy divided by the Fermi energy, gives \( r_e \equiv \text{Coulomb energy}/E_F \equiv (e^2/(\kappa \epsilon_0))/(\pi \hbar^2/n/g_v m) \equiv r_s g_v. \) As stated before, \( r_s \equiv r_e \) for \( g_v = 1 \), but for \( g_v > 1 \), \( r_e > r_s \), implying that the interpretation of the quantum Coulomb coupling as a dimensionless energy would imply that increasing \( g_v \) automatically involves a linear increase...
It was emphasized in these experimental papers [6] that the susceptibility of AlAs quantum wells depends on the spin susceptibility, which has often been emphasized in the literature in order to claim that a multi-valley (i.e. $g_v > 1$) system is more strongly interacting than a single-valley system at the same total electron density (i.e. fixed $r_s$). We assert that the many-body problem for the multi-valley situation is necessarily a two-parameter problem (i.e. $r_s$ and $g_v$) which can not be described in any situation by a single effective parameter such as $r_s \equiv g_v r_s$ or $r_s \equiv g_v r_s$ or any other combination of $r_s$ and $g_v$. The non-trivial dependence of the interaction-induced many-body effects on the two independent parameters $r_s$ and $g_v$, in particular, how even the qualitative nature of the quasiparticle renormalization as a function of $r_s$ and $g_v$ manifests itself completely differently in different properties of the multivalley 2D EG (e.g. compressibility versus susceptibility), is the central theme of this work. Specifically, we show that many-body effects could either be enhanced or suppressed with increasing $g_v$.

Although the main motivation of our work is theoretical, a part of our motivation comes from the extensive recent experimental work on the multivalley AlAs 2D quantum wells carried out at Princeton University [4]. These experiments demonstrate that the measured 2D spin susceptibility of AlAs quantum wells depends on $g_v$ (as well as $r_s$), and in general the susceptibility is smaller for larger values of $g_v$, with the difference between $g_v = 1$ and 2 decreasing with decreasing $r_s$ (i.e. increasing density). It was emphasized in these experimental papers [6] that such a higher value of susceptibility for $g_v = 1$ compared with $g_v = 2$ is contrary to the popular wisdom, based on considerations which claim $r_s \equiv g_v r_s$ or $r_s \equiv g_v r_s$ to be the appropriate interaction parameter, which would imply an increasing many-body renormalization with increasing $g_v$. In the current work, we resolve this puzzle by showing that the many-body enhancement of the 2D spin susceptibility decreases with increasing $g_v$ (between 1 and 2) except at very small values of $r_s$. We also make the predication that an increasing $g_v$ will always increase the many-body renormalization effect of the compressibility (for all values of $r_s$ and $g_v$) in a sharp contrast with the susceptibility.

We employ the one-loop self-energy calculation as our basic underlying theory to calculate the $T = 0$ susceptibility and compressibility as a function of $r_s$ and $g_v$. The self energy is being calculated in the leading order expansion in the dynamically screened Coulomb interaction because of the well-known long distance (i.e. $q \to 0$) divergence of the bare Coulomb interaction. This is equivalent to calculating the thermodynamic grand potential in the infinite ring or bubble diagram expansion and then obtaining the spin susceptibility and the compressibility by taking the appropriate derivatives with respect to the magnetic field and the volume respectively. The important thing to remember is that each bubble diagram carries a factor of $g_v$ due to the valley degeneracy (in addition to the factor of 2 due to the spin degeneracy), and the Fermi wave vector $k_F$ and the Fermi energy $E_F$ (i.e. the non-interacting chemical potential) are both suppressed by the valley degeneracy:

$$k_F = (2\pi n/g_v)^{1/2}; E_F = \pi \hbar^2 n/(mg_v)$$

where $n$ is the 2D carrier density and $m$ is the bare effective mass. The basic 2D non-interacting polarizability function, i.e. the bubble diagram, is given by,

$$\Pi(q, \omega) = -2g_v \int \frac{d^2k}{(2\pi)^2} \frac{f_{k+q} - f_{k}}{\hbar^2 - \varepsilon_{k+q} - \varepsilon_k + i\delta}$$

where $\varepsilon_k = \hbar^2 k^2/2m$, and $f_k$ is the Fermi distribution function corresponding to the energy $E(k)$. We note that the $q \to 0$, $\omega \to 0$ limit of the bubble diagram gives the 2D non-interacting density of states, $D(E) = g_v n/\pi \hbar^2$, which is enhanced by $g_v > 1$. Eqs. (1) and (2) show how $g_v$ enters the theory: (1) By decreasing $E_F$ (Eq. (1)), $g_v$ tends to enhance interaction effects; (2) By increasing screening through Eq. (2), i.e. by enhancing the density of states, $g_v$ tends to suppress the interaction effects. Depending on which of these effects is more important in determining a particular property, the many-body renormalization may increase, decrease, or show a non-monotonic behavior with increasing $g_v$.

We skip the technical details of the single-loop self-energy calculation, and provide below the final formula we use for calculating the interacting susceptibility ($\chi$) and compressibility ($K$) in terms of $r_s$ and $g_v$,

$$\frac{\chi_0}{\chi} = 1 + \frac{\alpha r_s}{\sqrt{2\pi}} \int dq \int \frac{du}{q} \frac{1}{\epsilon(q, iuq)} \times \left( \frac{d}{dk} \frac{\sqrt{\alpha + \sqrt{a^2 + b^2}}}{\sqrt{a^2 + b^2}} \right) |_{k=1}$$

$$K_0 = \frac{K}{k_F} = \frac{1}{k_F} \frac{d(k_F^2/2 + Re[\Sigma(k_F, E_F)])}{dk_F}$$

In Eqs. (3) and (4), $\chi_0$ and $K_0$ refer to the corresponding non-interacting quantities. $a = \alpha^2 + k^2 - q^2/4$, $b = uq$, and $\epsilon(q, iuq) = 1 - v_0 \Pi(q, iuq)$ is the dynamical RPA dielectric function, and $\Sigma(k_F, E_F)$ is the one-loop self energy calculated at the Fermi surface, and $\alpha = \sqrt{g_v}/2$ and $k_F = 1/(\alpha r_s)$. We note that the final equations are sufficiently complex that it is not possible to read off the $(r_s, g_v)$ dependence for arbitrary values of $r_s$ and $g_v$. Clearly, the results depend on both $r_s$ and $g_v$ independently. We have, therefore, numerically calculated the $(r_s, g_v)$ dependence of the susceptibility and the compressibility for arbitrary $r_s$ and $g_v$ values.
First, we present our susceptibility results in Fig. 1 and 2. In Fig. 1, we show $\chi/\chi_0$ as a function of $r_s$ (for $g_v = 1, 2, 4, 6$) in the small $r_s$ regime ($r_s = 0 - 0.2$) in Fig. 1(a) and in the large $r_s$ regime ($r_s = 1 - 7$) in Fig. 1(b). It is clear that the situation is qualitatively different between the small ($r_s < 1$) and the large ($r_s > 1$) $r_s$ regime. For small $r_s$, the many-body effects are enhanced by increasing $g_v$ in accordance with one’s naive expectation based on the suppression of $E_F$ by $g_v$. For large $r_s$ values, on the other hand, the many-body renormalization of $\chi$ decreases with increasing $g_v$, in complete agreement with the recent experimental measurements which were carried out in the $r_s > 1$ regime. One of our predications is, therefore, that a measurement of the 2D susceptibility at high densities ($r_s < 1$) would manifest a non-monotonic crossover in the $g_v$ dependence of the many-body effects as can be seen in the inset of Fig.1(a). In Fig.1(a), we show by the dotted line our analytic formula valid in the $r_s \ll 1$ regime which can be derived to be

$$\frac{\chi}{\chi_0} = 1 + \sqrt{2g_v r_s^2} \frac{g_v}{\pi} + \frac{g_v r_s^2}{2\pi^2} - 2.22 \frac{r_s g_v^2}{2\sqrt{2\pi}}. \quad (5)$$

We can see from Eq. (5) that $\chi$ can not be written, even in the $r_s \ll 1$ limit, as a single-parameter function.

In Fig. 2, we show the $g_v$ dependence of the interacting susceptibility, both for small and large $g_v$. The non-monotonic behavior of the susceptibility as a function of $g_v$ for smaller $r_s$ values is obvious in Fig. 2, and the decrease of $\chi$ with increasing $g_v$, eventually reaching a constant for unphysically large $g_v$ (all $g_v > 6$ is unphysical since no known multivalley 2D semiconductor system has more than six valleys). For $r_s < 1$, the maximum in $\chi/\chi_0$ occurs between $g_v = 1$ and $2$, and should therefore be experimentally accessible as a matter of principle. For $r_s > 1$, however, the maximum in Fig. 2 moves to the $g_v < 1$ regime which is unphysical. The very large $g_v \gg 6$ regime (Fig. 2b) is of theoretical interest only. We obtain the following asymptotic analytic formula for

![FIG. 1: (a) Susceptibility vs $r_s$ for different valley degeneracy. The solid line is for the numerical data, dash-dotted line for the asymptotic formula shown as Eq. (5). Inset gives the inverse spin susceptibility vs $r_s \leq 1$ showing non-monotonicity. (b) Susceptibility vs $r_s \geq 1$ for different valley degeneracy.](image1)

![FIG. 2: (a) Susceptibility vs $g_v$ for different electron density $r_s$. For small values, the non-monotonicity can be seen in the inset. (b) Inverse susceptibility vs $1/g_v$ for different $r_s$. Inset shows the constant $\chi$ for $g_v \gg 1$.](image2)
FIG. 3: (a) Compressibility vs $r_g$ for different valley degeneracy. (b) Compressibility vs $g_v$. Dotted lines are HF results. Inset shows the compressibility vs $g_v$ for large $g_v$.

$g_v \gg 1$:

$$\frac{K_0}{K} \approx 1 + \frac{r_s^{2/3}}{4 \times 2^{5/6}} + \frac{1.4}{g_v} \approx 1 + 0.14 r_s^{2/3} + \frac{1.4}{g_v},$$

(6)

up to logarithmic corrections in $r_s$ and $g_v$. Our $g_v \to \infty$ formula (Eq. 6) agrees well with our numerical results for $g_v \gg 100$. The small $g_v$ (and the small $r_s$) regime shown in Fig. 2 agrees with the analytic Eq. 5 derived for the small $r_s$ regime, where the non-monotonicity with respect to $g_v$ can be seen to be arising from the negative sign in the last term. We see that Eq. 5 implies a maximum in $\chi$ at $g_v^{\text{max}} \approx 1.07$ (for $r_s = 1$) and 1.78 ($r_s = 0.5$), which is consistent with the numerical result of Fig. 2.

In Fig. 3, we show our calculated $r_s$ and $g_v$ dependence of the 2D interacting (inverse) compressibility. It is clear that, in contrast to the interacting susceptibility, the interacting compressibility manifests monotonically stronger many-body effects with increasing valley degeneracy $g_v$ in all regimes of $r_s$ and $g_v$. There is, in fact, no non-monotonicity at all in the interacting compressibility which decrease continuously with increasing $r_s$ or $g_v$, eventually becoming negative for $r_s \lesssim 2.5$ in a 2DEG [7]. We can analytically calculate the small $r_s$ dependence of the interacting compressibility, obtaining:

$$\frac{K_0}{K(r_s \ll 1)} \approx 1 - 0.45 r_s g_v^{1/2} + 0.022 (r_s g_v)^{3/2} \log(r_s g_v^{3/2}),$$

(7)

where we note that the first two terms of the expansion (i.e. the Hartree-Fock result with just the exchange self-energy correction) are identical to the corresponding first two terms (i.e. the Hartree-Fock result) for $\chi_0/\chi$ in Eq. 5. We mention that the leading-order correlation correction, the third term in Eq. 7, has an $r_s^2 g_v$ dependence in the compressibility (in contrast to the $r_s^2 g_v^2$ dependence in Eq. 6 for the susceptibility). Consequently the correlation correction to the compressibility is very weak [7] for small $r_s$ values. In Fig. 3(b), we compare the Hartree-Fock result with our numerical results, and for small $r_s$, the agreement is excellent. For large $g_v$, $K_0/K$ decreases monotonically linearly in $g_v$ (neglecting logarithmic corrections).

In discussing the significance of our results, we emphasize that we have provided a complete qualitative resolution of the puzzle raised by the experimental observations of ref. [6], where the 2D interacting susceptibility was found to be smaller for the larger valley degeneracy system. In addition, we make a clear prediction that if the experiments are carried out in higher-density (i.e. lower $r_s$) samples than used so far, the susceptibility will be larger in the higher valley degeneracy system. We also predict that the many-body effects in the 2D compressibility, in sharp contrast to the 2D susceptibility, would be enhanced monotonically with increasing $g_v$ for all $r_s$ values. We mention that in our theory the valley ($g_v$) and the spin ($g_s$) degeneracy are equivalent, and therefore a measurement of valley susceptibility [8] in the presence of a variable spin degeneracy (e.g. $g_s = 2$ or 1) would manifest exactly the same qualitative trend as seen in Figs. 1 and 2 with the roles of valley and spin being interchanged. Similarly we predict a suppression of the compressibility with decreasing spin degeneracy from $g_s = 2$ to 1 by applying an external parallel magnetic field at fixed value of $g_v$. We believe that an experimental confirmation of our qualitative predictions would be compelling evidence of the Fermi liquid nature of 2D interacting systems even at large $r_s$ and $g_v$ values.

This work is supported by DOE Sandia national Labs and by LPS-CMTC.

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