RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 38, NUMBER 15 15 NOVEMBER 1988-II

Many-body effective mass and anomalous g factor in inversion layers

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(Received 24 August 1988)

We present a microscopic theory of the effects of the electron-electron interaction on the effective mass and the anomalous Landé g factor in an inversion layer. We find that the inclusion of previously neglected many-body effects, associated with charge- and spin-fluctuation-induced vertex corrections, is crucial. The present approach is based on a new self-consistent determination of the many-body local fields. Our theory has no free parameters and the results are in good agreement with the established experimental findings.

Several years have passed since the experimental work of Fang and Stiles[1] and Smith and Stiles[2] on the quasiparticle effective mass m^* and the anomalous Landé g factor g^* in Si inversion layers, but the theoretical understanding of these phenomena is still only qualitative at best. Although it is widely recognized that many-body effects are largely responsible for the observed behavior a quantitative, detailed description resting on firm theoretical ground is currently lacking.

As it turns out even a simplistic theory is at least capable of predicting the correct behavior of m^* in reasonable, albeit perhaps fortuitous, agreement with the experimental results. The situation for g^* is however far more complicated.

The basic idea was first put forward by Janak who developed an elegant theory of g^*.[3] Further work along similar lines has been also reported in references 4 and 5. All these theories suffered unfortunately from some serious problems, and, more importantly, were based on a statically screened exchange approximation to the quasiparticle self-energy which we find to be unreliable. In any case as clearly pointed out in Ref. 5, these early calculations were unable to explain the main feature of the anomalous Landé g factor, i.e. its strong dependence (a decrease) with respect to the electron density.

The most sophisticated theory to date is the one of Quinn and co-workers.[6,7] These authors used a Fermi-liquid interaction approach to evaluate the quasiparticle self-energy. Within this framework both screened-exchange and Coulomb-hole contributions to the self-energy, as well as some of the vertex corrections, were included within a simple Hubbard-type approximation. The major shortcoming of this work is, however, that a qualitative agreement with the experimental data could only be reached by arbitrarily neglecting the Hubbard corrections. In particular these authors found that inclusion of the latter leads to an anomalous g factor which strongly increases with the carrier density, in clear contrast with the observed behavior (see Fig. 2 of Ref. 6).

In this paper we report the results of a theoretical microscopic investigation of the effects of the electron-electron interaction on m^* and g^* in the quasi-two-dimensional electronic gas (2D EG) of an inversion layer. Our approach is the first attempt to properly include *both* charge- and spin-fluctuation-induced vertex corrections which will be shown to be crucial in attaining a satisfactory description of these many-body phenomena. As will be discussed below our results are in encouraging qualitative and quantitative agreement with the established experimental findings.

Our approach is based on a recently derived expression for $E(\mathbf{p})$, the (fully renormalized) quasiparticle energy in an interacting electron liquid in its normal state. As it is well known both m^* and g^* can in general be evaluated once $E(\mathbf{p})$ is known. We find that in the electric quantum limit and at zero temperature a suitable expression for $E(\mathbf{p})$ is given by [8]

$$E(\mathbf{p})=\varepsilon_{\mathbf{p}}-\sum_{\mathbf{q}}\left[n_{\mathbf{p}-\mathbf{q}}\mathrm{Re}[\Lambda_C(\mathbf{q},\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}-\mathbf{q}})+3\Lambda_S(\mathbf{q},\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}-\mathbf{q}})]+\frac{1}{\pi}\mathrm{P}\int_0^\infty d\omega\frac{|\,\mathrm{Im}[\Lambda_C(\mathbf{q},\omega)]\,|+3\,|\,\mathrm{Im}[\Lambda_S(\mathbf{q},\omega)]\,|}{\omega-\varepsilon_{\mathbf{p}}+\varepsilon_{\mathbf{p}-\mathbf{q}}}\right], \tag{1}$$

where the symbol P mandates that the principal value of the integral must be taken. Here $\varepsilon_{\mathbf{p}}$ is the unperturbed kinetic energy, $\mathbf{p}^2/2m_0$, m_0 being the appropriate value for the band mass. The second and third terms are respectively the screened- exchange and the (necessary) corresponding Coulomb-hole contribution. In Eq. (1), $\Lambda_C(\mathbf{q},\omega)$ and $\Lambda_S(\mathbf{q},\omega)$ are effective potentials defined as follows:

$$\Lambda_C(\mathbf{q},\omega)=v(\mathbf{q})+v(\mathbf{q})^2[1-G_+^{(v)}(\mathbf{q},\omega)]^2\chi_C(\mathbf{q},\omega), \tag{2}$$

and

$$\Lambda_S(\mathbf{q},\omega)=-\mu_B^{-2}v(\mathbf{q})^2[G_-^{(v)}(\mathbf{q},\omega)]^2\chi_S(\mathbf{q},\omega), \tag{3}$$

where $\chi_C(\mathbf{q},\omega)$ and $\chi_S(\mathbf{q},\omega)$ are respectively the intravalley charge and spin response functions of a 2D EG interacting via the potential $v(\mathbf{q})=2\pi e^2L(\mathbf{q})/\epsilon_s q$. Here

$L(\mathbf{q})$ is a suitable form factor which accounts for the presence of the oxide region and the metallic gate in the structure.[9] The effect of the finite thickness of the electronic inversion layer is also accounted for in $L(\mathbf{q})$ via the Stern-Howard envelope wave function.[10] It is important to emphasize that interaction effects beyond the simple random-phase approximation (RPA) are explicitly taken into account here by means of the many-body local fields $G_{\pm}^{(v)}(\mathbf{q},\omega)$,[11] which are a simple generalization to the multivalley case of the fields introduced by Niklasson.[12] These quantities are the many-body analogues in the electron liquid of the familiar Clausius-Mossotti local fields of electromagnetism. This can be seen from the fact that these quantities also determine the response functions $\chi_C(\mathbf{q},\omega)$ and $\chi_S(\mathbf{q},\omega)$ as follows:[13]

$$\chi_C(\mathbf{q},\omega)=\frac{n_v\chi_0(\mathbf{q},\omega)}{1-n_v v(\mathbf{q})[1-G_+^{(v)}(\mathbf{q},\omega)]\chi_0(\mathbf{q},\omega)}, \tag{4}$$

and

$$\chi_S(\mathbf{q},\omega)=-\mu_B^2\frac{n_v\chi_0(\mathbf{q},\omega)}{1+n_v v(\mathbf{q})G_-^{(v)}(\mathbf{q},\omega)\chi_0(\mathbf{q},\omega)}, \tag{5}$$

where n_v is the number of the relevant degenerate valleys, and $\chi_0(\mathbf{q},\omega)$ is the Lindhard susceptibility for a 2D EG.[14]

It should be stressed that the above expression for $E(\mathbf{p})$ explicitly contains all the necessary exchange and correlation corrections associated with the hitherto neglected spin fluctuations which are found to significantly contribute to both m^* and g^*.

From $E(\mathbf{p})$, m^* is then simply obtained by evaluating the quasiparticle group velocity at the Fermi energy via the well known relation

$$v_{\mathrm{qp}}=\frac{p_F}{m^*}=\left[\frac{\partial E(\mathbf{p})}{\partial p}\right]_{p_F}. \tag{6}$$

The evaluation of g^* is slightly more involved since it entails an analysis of the effects of a small magnetic field on $E(\mathbf{p})$. By a straightforward generalization of Janak's procedure[3] we have obtained the following expression for g^*:

$$\frac{g}{g^*}=1-m^*\int_0^{2\pi}d\phi\frac{1}{(2\pi)^2}\mathrm{Re}[\Lambda_C(\mathbf{p}_F-\mathbf{p}'_F,0)+3\Lambda_S(\mathbf{p}_F-\mathbf{p}'_F,0)], \tag{7}$$

where ϕ is the angle between a fixed vector $\mathbf{p}_F$ and a variable vector $\mathbf{p}'_F$ both of which lie on the Fermi surface. Equations (6) and (7) together allow a direct evaluation of the many-body enhancement of the spin susceptibility of the system so that the problem at hand acquires a self-consistent character which we have exploited (see below).

In order to perform any calculations a satisfactory and explicit expression for the many-body local fields $G_{\pm}^{(v)}$ must be assumed. In general $G_{\pm}^{(v)}$ should be taken as frequency dependent. In the present calculation however we have, as is frequently done, approximated the $G_{\pm}^{(v)}$'s with appropriate static Hubbard-type functions. In this case the presence of a multivalley structure leads however to a further complication that has to be dealt with. We find that the simplest suitable expression for $G_{\pm}^{(v)}$ is provided by[15]

$$G_{\pm}^{(v)}(\mathbf{q})=\frac{L[(\mathbf{q}^2+k_F^2)^{1/2}]}{L(\mathbf{q})}\frac{G_{\pm}^{(v)}(\infty)|\mathbf{q}|}{\{\mathbf{q}^2+[\beta_{\pm}G_{\pm}^{(v)}(\infty)k_F]^2\}^{1/2}}, \tag{8}$$

where the form factor $L(\mathbf{q})$ has been defined above and $\beta_{\pm}$ and $G_{\pm}^{(v)}(\infty)$ are functions of the electronic density to be determined. In obtaining Eq. (8) we have neglected the (small) intervalley exchange. As it turns out the $G_{\pm}^{(v)}(\infty)$ can be expressed in terms of $g(0)$, the value at the origin of the pair correlation function in a quasi-2D EG. In particular, by making use of the recently calculated exact asymptotic expressions for the many-body local fields of a 2D EG,[16] we have

$$G_+^{(v)}(\infty)=[1+(n_v^{-1}-2)g(0)], \tag{9}$$

and

$$G_-^{(v)}(\infty)=n_v^{-1}g(0). \tag{10}$$

As is well known $g(0)$ is a function of the electronic density, and its values can be taken from Jonson's work.[17]

Furthermore, and most importantly, we have determined the coefficients $\beta_{\pm}$ via the following self-consistent procedure. We first impose that, at any given density, in the $q\to 0$ limit the value of the static charge-response function $\chi_C(\mathbf{q},0)$ be consistent with the compressibility sum rule.[17,18] This establishes the value of β_+. Then, starting with a trial value for β_-, m^*, and g^* are calculated from Eqs. (6) and (7), so that a value for the long-wavelength static spin susceptibility is determined. By equating such a value to $\chi_S(\mathbf{q}\to 0,0)$, as given by Eq. (5), a new β_- is then obtained. This procedure is repeated until convergence is reached.[19] Once β_+ and β_- are determined our theory is free of arbitrary parameters.

Our results for β_+ and β_- are plotted in Fig. 1 as a function of the density parameter r_S, the average electronic distance measured in terms of the effective Bohr radius $a_B^*=\hbar^2\epsilon_{\mathrm{av}}/m_0e^2$, ϵ_{av} being the average of the dielectric constants of the semiconductor host and the oxide. These two curves, as well as the results reported below, have been obtained by making use, for the various specific parameters, of the values appropriate to a [100] surface Si inversion layer like the one studied in Ref. 1 and given in the caption of Fig. 1. Furthermore the specific values of $g(0)$ used in the present calculations were taken from Ref. 17.

We have evaluated m^* and g^* making use of Eqs. (6) and (7) and have investigated their dependence on the electronic density. We have also analyzed the effect on these quantities of both charge- and spin-fluctuation-induced vertex corrections as accounted for by means of the many-body field $G_+^{(v)}$ and $G_-^{(v)}$. The results of our

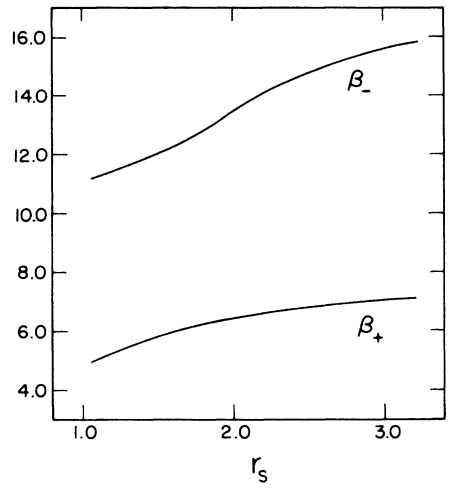

FIG. 1. Theoretical self-consistent results for the coefficients β_+ and β_-, defined in Eq. (8), versus the effective r_S, also defined in the text. We have chosen for our calculation the following parameter values: 0.19 for the band mass, 2 for the valley degeneracy, 3.8 and 11.8, respectively, for the oxide and semiconductor dielectric constants, 5330 Å for the thickness of the oxide layer. For comparison $r_S=2$ corresponds here to an areal density of 1.7×10^{12} cm^{-2}.

study are summarized in Figures 2 and 3, where we have also reproduced the corresponding original experimental data from Refs. 1 and 2, and for clarity we have plotted the two quantities as a function of the areal density n_S.[20] It is clear that the present parameter free theory for g^* leads to an unprecedented and rather encouraging agreement with the established experimental findings. Our values for the effective mass, on the other hand, deviate from the Shubnikov–de Haas data by a few percent in the small density regime, but are, however, closer to the cyclotron mass determination.[2(b)] We believe that the deviations from the actual data (as well perhaps the some-

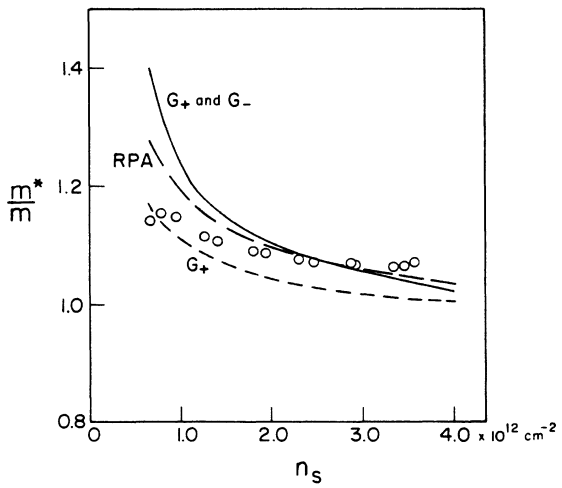

FIG. 2. Plot of the ratio m^*/m versus the electron areal density n_S. The parameters are the same as in Fig. 1. The circles are the original large-field data set of Smith and Stiles taken from Ref. 2(a). The meaning of the three curves is explained in the text. The solid curve corresponds to our full theory.

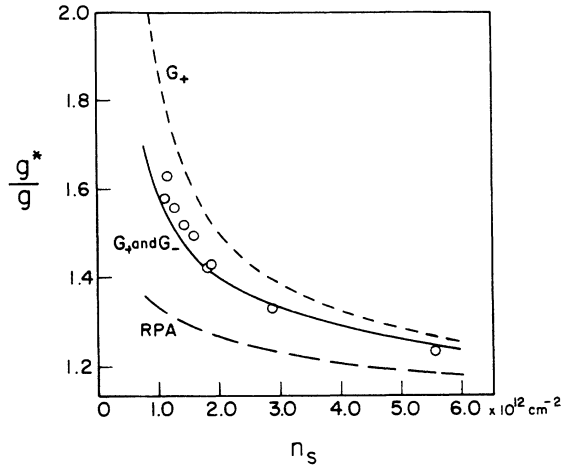

FIG. 3. Plot of the ratio g^*/g versus the electron areal density n_S. The parameters are the same as in Fig. 1. The circles are the original data set of Fang and Stiles taken from Ref. 1(a). The meaning of the three curves is explained in the text. The solid curve corresponds to our full theory.

what fortuitous perfect agreement of g^*) can be safely attributed, at least in the intermediate density range, to the lack of more specific knowledge of the functions $G_\pm^{(v)}$'s in the intermediate momentum and frequency regime. It must also be remarked that the theoretical results are also sensibly dependent on the specific values used for $g(0)$. In any case it is clear that our theory appears to be capable of describing most of the physics of the mass and g-factor renormalization and that this effect is rather sizable.

An important conclusion which can be drawn from our study is that the final values of both m^* and g^* result from a subtle balance between various competing effects and that the simple RPA, although providing a reasonable starting point, does not account for much of the many-body physics of the phenomenon at hand and is therefore unreliable. It should also be stressed however that it is not enough to go beyond the RPA just by introducing the symmetric local field $G_+^{(v)}$ while altogether neglecting the effects of the spin fluctuations; in general such a procedure tends in fact to make things worse. Both charge- and spin-fluctuation-induced vertex corrections must be included. This is particularly made clear in Figs. 2 and 3 where the different results corresponding to the three cases (i) $G_+^{(v)}=G_-^{(v)}=0$ (RPA),[13] (ii) $G_+^{(v)}\neq0$, $G_-^{(v)}=0$ (no spin fluctuations), and (iii) $G_+^{(v)}\neq0$, $G_+^{(v)}\neq0$ (full theory), are displayed.[21] A detailed account of the present analysis will be reported elsewhere.[22]

Finally we would like to point out that our study allows one to obtain an explicit microscopic derivation of some of the most relevant Landau parameters. Work on this subject is in progress.

ACKNOWLEDGMENTS

The authors acknowledge fruitful discussions with A. W. Overhauser, G. E. Santoro, and P. J. Stiles. One of the authors (G.F.G.) acknowledges the hospitality of the International School for Advanced Studies, Trieste, Italy.

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[20]It should be mentioned here that the data reported in Fig. 3 are the original ones from Ref. 1(a). This in contrast with the analysis of Ref. 4, where the same data were scaled. We thank P. J. Stiles for pointing out to us that the latter procedure is actually incorrect.

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