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Effective Mass and g Factor of Interacting Electrons in the Surface Inversion Layer of Silicon*

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The effective mass and the g factor of quasiparticles near the Fermi surface of a two-dimensional electron gas are calculated in the random-phase approximation and in the Hubbard approximation, and are compared with the experimental results for an inversion layer on a (100) surface of silicon.

When a sufficiently strong electric field is applied normal to the surface, the electrons in the inversion layer of a metal-insulator-semiconductor (MIS) structure form an essentially two-dimensional interacting electron gas.[1] Because the electron concentration can be experimentally varied over a wide range, this system is a useful testing ground for approximate methods of calculating the effect of many-body correlations on measurable properties of the system. The g factor and the effective mass m^* of quasiparticles near the Fermi surface are two such properties. They have been measured over a wide range of concentrations for a (100) surface inversion layer of silicon by Fang and Stiles,[1] and by Smith and Stiles.[2] The measured values of both quantities are considerably larger than their counterparts in intrinsic bulk silicon, and they increase as the electron density is lowered. Janak,[3] and later Suzuki and Kawamoto,[4] evaluated the enhancement of the g value and of the effective mass caused by electron correlations within the framework of a static approximation which neglects the frequency dependence of the dielectric function. Chaplik[5] has calculated the effective mass by using an approximate dielectric function. Though some of the results obtained by these authors are in qualitative agreement with experiment, the many-body approximations employed are equivalent to the simplest approximations in three-dimensional systems.[6] Since such approximations are incapable of yielding quantitative results, these calculations cannot be used as a test of the most refined many-body approximations, nor of the assumption built into the two-dimensional model of a semiconducting inversion layer. In the present paper we calculate m^* and g^* by using the dynamic random-phase approximation (RPA) and the Hubbard approximation (HA). The HA and slight modifications of it are considered the most accurate many-body approximations for a three-dimensional electron gas. Both the RPA and the HA are discussed clearly by Rice,[7] and the reader is referred to his paper for general background.

The total energy of the interacting electron

system can be written[7,8]

$$E = E^{(0)} - \sum_{\vec{q}} \int_0^{e^2} (d\lambda/\lambda)\{\mathrm{Im}\int_0^\infty (d\omega/2\pi)[\epsilon(q,\omega)]^{-1} + N\pi\lambda/q\}. \tag{1}$$

In the HA the dielectric function is given by[8]

$$\epsilon(q,\omega) = 1 + \sum_{v\sigma} 4\pi A_{v\sigma}(q,\omega)[1 - 8\pi g(q) A_{v\sigma}(q,\omega)]^{-1}, \tag{2}$$

where

$$A_{v\sigma}(q,\omega) = -(\lambda/2q)\sum_{\vec{k}} \int_{-\infty}^{\infty} (d\omega'/2\pi i) G^{v\sigma}(\vec{k},\omega') G^{v\sigma}(\vec{k}+\vec{q},\omega'+\omega) \tag{3}$$

is the contribution from electrons in valley v with spin σ to the polarizability of a noninteracting electron gas $A(q,\omega)$. Throughout this paper we neglect intervalley scattering.[4] The effective charge e is equal to the free-electron charge divided by the square root of the background dielectric constant ϵ_0 of the surrounding medium. The Hubbard modification factor[8] $g(q)$ is assumed to be given for the two-dimensional system by $g(q) = \frac{1}{2} q[q^2 + \beta k_F^2]^{-1/2}$, where k_F is the Fermi momentum and β is a parameter of the order of unity.[9] The single-particle Green's function $G^{v\sigma}(\vec{k},\omega)$ for an electron in valley v with spin σ is given by

$$G^{v\sigma}(\vec{k},\omega) = \frac{n^{v\sigma}(k)}{\omega - \omega_\sigma(k) - i\delta} + \frac{1 - n^{v\sigma}(k)}{\omega - \omega_\sigma(k) + i\delta}. \tag{4}$$

Here $n^{v\sigma}(k)$ is the Fermi distribution function and $\omega_\sigma(k) = \omega(k) + \sigma g\mu_B H/2$, where $\omega(k) = k^2/2m$, μ_B is the Bohr magneton, and H is the strength of the applied magnetic field. The single-particle energy $\epsilon_{v\sigma}(p)$ can be obtained from Eq. (1) by taking the functional derivative with respect to $n^{v\sigma}(p)$:

$$\epsilon^{v\sigma}(\vec{p}) = \omega(\vec{p}) + \tfrac{1}{2}\sigma g\mu_B H - \sum_{\vec{q}} \int_0^{e^2} \frac{d\lambda}{\lambda} \mathrm{Im}\int_\infty^\infty \frac{d\omega}{2\pi} \frac{2\pi\alpha G^{v\sigma}(\vec{p}+\vec{q},\omega_\sigma(p)+\omega)}{q\epsilon^2(q,\omega)[1 - 8\pi g(q) A_{v\sigma}(q,\omega)]^2}. \tag{5}$$

This is the basic starting equation for calculation of the effective mass m^*. The effective mass is defined by $m^* = [(p^{-1} d\epsilon_{v\sigma}/dp)^{-1}]_{p=k_F, H=0}$. In the absence of an applied magnetic field $\epsilon^{v\sigma}(p)$ can be determined by dropping the spin index σ and valley index v and integrating over the coupling constant λ:

$$\epsilon(\vec{p}) = \omega(\vec{p}) - \sum_{\vec{q}} \int (d\omega/2\pi i)[2e^2/q\epsilon_S(q,\omega)] G(\vec{p}+\vec{q}, \omega+\omega(p)). \tag{6}$$

In this equation the "dielectric function" ϵ_S is given by $\epsilon_S(q,\omega) = 1 + 2[n_v - g(q)]4\pi A(q,\omega)$, where n_v is the valley degeneracy. $\epsilon_S(\vec{q},\omega)$ is analytic in the upper and lower halves of the ω plane, but has zeros along the real axis. In order to carry out the ω integration in Eq. (6), the singularities arising from $\epsilon_S(\vec{q},\omega)$ have to be avoided. This difficulty can be solved by transforming the integration[6,7] along the real ω axis to the imaginary ω axis. The resulting expression for m^* takes the form $m/m^* = 1 + I^{\mathrm{line}} + I^{\mathrm{res}}$, where I^{line} is the contribution from the integration along the imaginary ω axis, and I^{res} is the contribution from the poles of the Green's function. If we make the variable transformation $z = q/2k_F$, $\omega/\omega(k_F) = 2zu$, then I^{line} and I^{res} can be shown to have the form

$$I^{\mathrm{line}} = -2\alpha r_S/\pi + (4\sqrt{2}\,\alpha r_S/\pi)\int_0^\infty dz \int_0^\infty du\,[1/\epsilon_S(z,iu) - 1][C(z,u)]^{-5/2} \times\{D(z,u)[1 + D(z,u)/C(z,u)]^{1/2} - B(z,u)[1 - D(z,u)/C(z,u)]^{1/2}\}, \tag{7}$$

$$I^{\mathrm{res}} = (\alpha r_S/\pi)\int_0^1 dz/z(1 - z^2)^{1/2}\epsilon_S(z,0). \tag{8}$$

The functions D, B, and C are given by $D(z,u) = 4z^2 - u^2 - 4$, $B(z,u) = 4zu$, and $C(z,u) = [D^2(z,u) + B^2(z,u)]^{1/2}$. α equals $(n_v/2)^{1/2}$ and $r_S = (\pi a_B^2 N_{\mathrm{inv}})^{-1/2}$ is the ratio of the mean radius per particle in the layer to the Bohr radius a_B in bulk silicon. $\epsilon_S(q,\omega)$ has been calculated by Stern[10] for real values of ω. For imaginary ω, it can be evaluated by using the fact that the polarizability $A(z,iu)$ can be written as $A(z,iu) = \alpha r_S(16\pi z^2)^{-1}\{2z - [\frac{1}{2}C(z,u) + \frac{1}{2}D(z,u)]^{1/2}\}$.

To obtain the g value, we use Landau's Fermi-liquid theory.[11] A Landau interaction function $f_{v\sigma,v'\sigma'}(\vec{p},$

$\vec{p}'$) can be obtained by taking the variational derivative of Eq. (5) with respect to $n_{v'\sigma'}(\vec{p}')$:

$$f_{v\sigma,v'\sigma'}(\vec{p},\vec{p}') = -\frac{\delta_{\sigma\sigma'}\delta_{vv'}2\pi e^2}{|\vec{p}-\vec{p}'|\epsilon_S(\vec{p}-\vec{p}',0)} + \int_0^{e^2}\frac{d\lambda}{\lambda}\int d^2q\,\mathrm{Re}\int_\infty^\infty \frac{d\omega}{2\pi i}\left(\frac{\lambda}{q}\right)^2 \frac{G^{v\sigma}(\vec{p}+\vec{p},\xi_p+\omega)\,[G^{v'\sigma'}(\vec{p}'+\vec{q},\xi_{p'}+\omega)+G^{v'\sigma'}(\vec{p}'-\vec{q},\xi_{p'}-\omega)]}{\epsilon^2(q,\omega)\,[1-8\pi g(q)A_{v\sigma}(q,\omega)]^2} \times\left(\frac{\delta_{\sigma\sigma'}\delta_{vv'}4g(q)}{1-8\pi g(q)A_{v\sigma}(q,\omega)} - \frac{2}{\epsilon(q,\omega)\,[1-8\pi g(q)A_{v'\sigma'}(q,\omega)]^2}\right). \quad (9)$$

This function represents the interaction between a quasiparticle of momentum $\vec{p}$ and spin σ in valley v with one of momentum $\vec{p}'$ and spin σ' in valley v'. The quantity ξ_p is the energy $\omega(p)$ measured relative to the Fermi energy. We sum Eq. (9) over v', and, following Landau, define $f_S(\vec{p},\vec{p}')$ and $f_a(p,p')$ by the relation $\sum_{v'} f_{\sigma v,\sigma' v'}(\vec{p},\vec{p}') = f_s(\vec{p},\vec{p}') + \vec{\sigma}\cdot\vec{\sigma}' f_a(\vec{p},\vec{p}')$. To obtain the g factor for the quasiparticles we use the result[12]

$$g/g^* = 1 + (m^*/\pi)\int_0^{2\pi}(d\varphi/2\pi) f_a(\varphi), \quad (10)$$

where $\vec{p}\cdot\vec{p}' = k_F^2\cos\varphi$. This expression can be transformed to $g/g^* = 1 + I_1 + I_2$, where

$$I_1 = -\frac{\alpha r_S}{2\pi}\frac{m^*}{m}\int_0^{2\pi}\frac{d\varphi}{2\sin(\frac{1}{2}\varphi)\epsilon_S(2\sin(\frac{1}{2}\varphi),0)}, \quad (11)$$

$$I_2 = \frac{4(\alpha r_S)^2}{\pi}\frac{m^*}{m}\int_0^\infty dz\frac{g(z)}{z^2}\int_0^\infty d\omega\frac{F(z,u)}{C(z,u)}\left(1+\frac{D(z,u)}{C(z,u)}\right). \quad (12)$$

The function $F(q,\omega)$ is defined by

$$F(z,u) = [8\pi n_v A(z,iu)]^{-2}\left[\frac{-8\pi n_v A(z,iu)}{\epsilon_S(z,iu)} + \ln\left(\frac{\epsilon_S(z,iu)}{\epsilon_S(z,iu)-8\pi n_v A(z,iu)}\right)\right]. \quad (13)$$

With neglect of I_2, our expression for g/g^* should reduce to the results of the static approximation.[3,4] However, a careful examination shows that our result for I_1 differs from that of Janak[3] by a factor n_v when the Hubbard factor $g(q)=0$, and our $g(q)$ differs from that of Suzuki and Kawamoto[4] by a factor n_v. This is due to the fact that the contribution from valley degeneracy has not been properly accounted for in these references. The integrals appearing in Eqs. (7), (8), (11), and (12) can be done numerically. By using $n_v=2$, $\epsilon_0=11.8$, and $m=0.19m_e$ for the mass of electrons on the (100) plane of the intrinsic silicon, we obtain the results for m^*/m as a function of r_S shown in Fig. 1, and for g^*/g as a function of electron concentration shown in Fig. 2. The curves labeled HA correspond to the Hubbard approximation with $\beta=1$[9]; the curves labeled RPA correspond to setting the modification factor $g(q)$ equal to 0. The open circular dots are obtained from experiment.[1,2] For m^* both the HA and RPA give reasonable agreement with experiment.[13] Quite surprisingly for g^* the RPA gives much better agreement with experiment than the HA. The decrease of g^* for small values of the electron concentration (or large r_S) in the HA is in qualitative agreement with the calculated results in three dimensions,[7] but the physical reason for the disagreement with experiment is not known.[14]

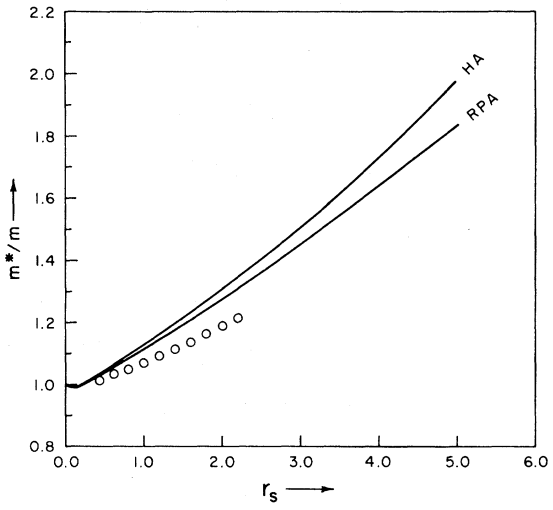

FIG. 1. m^*/m as a function of r_S. Our result in Hubbard approximation is shown by the curve HA. The result with $g(q)=0$ is shown by the curve RPA. The experimental curve of Ref. 2 is shown by open circles.

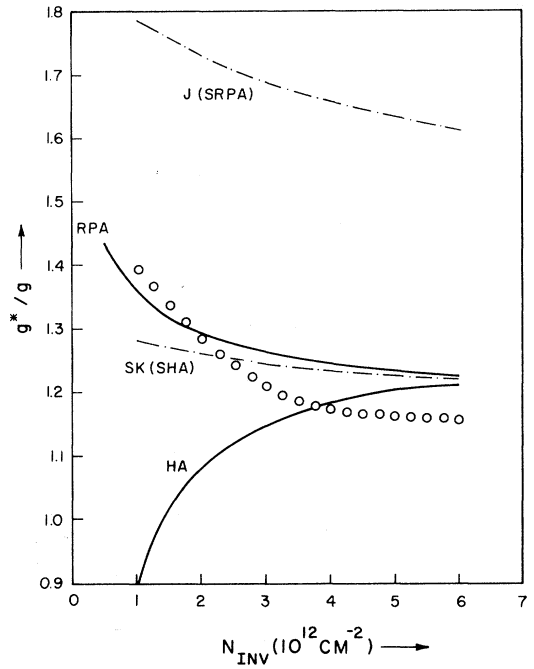

FIG. 2. g^*/g as a function of N_{inv}. J (SRPA) and SK (SHA) represent curves obtained in Refs. 3 and 4 for static RPA and static HA, respectively. The curve with open circles was obtained experimentally in Ref. 1 and corrected with effective mass in Ref. 4.

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Note added.—Since submitting this paper we have investigated the modification of the Coulomb interaction between inversion-layer electrons caused by the presence of the insulator and metallic gate electrode and by the finite extent of the electron wave function normal to the surface. When this effect is accounted for, the problem of which dielectric constant (that of silicon or the average of silicon and its oxide) enters the effective interaction disappears. The results for m^* and g^* obtained with the modified interaction are in much better agreement with experiment.[15] The effective mass has been evaluated by Vinter[16] in the plasmon-pole approximation starting from Dyson's equation. Dyson's equation differs from our Eq. (5) because the quasiparticle energy $\epsilon^{\nu\sigma}(p)$ instead of the bare-particle energy $\omega_\sigma(p)$ enters the Green's function appearing on the right-hand side. We believe that Eq. (5) is more reliable if the electron self-energy is evaluated only to the lowest order in the effective interaction.[7] We thank Dr. L. Sham, Dr. F. Stern, and Dr. B. Vinter for bringing this to our attention.

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[13]The small overestimate of m^* in our calculations might be understood as follows: It is well known that the effective mass of an electron in an intrinsic semiconductor can be enhanced considerably by electron-phonon (e-p) interaction [see, e.g., D. Pines, in *Polarons and Excitons*, edited by C. Kuper and G. Whitfield (Plenum, New York, 1962), p. 33]. The strength of the e-p interaction in the two-dimensional electron gas should be reduced because of the screening effect of the electrons. Consequently, the effective mass will be overestimated if screening of the interaction is not considered. By properly including e-p interaction our

result should be brought into better agreement with experiment.

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Photoemission Measurements of Step-Dependent Surface States on Cleaved Silicon (111)

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Ultraviolet photoemission spectroscopy has been used to measure surface states on cleaved silicon with varying step-atom densities determined by low-energy-electron diffraction. For high step densities (~ 10%) a new surface-state peak is found at an energy 0.4 eV higher than the main surface-state peak. These measurements are the first demonstration that surface-state photoemission spectra depend strongly on cleavage steps.

Intrinsic surface states have been observed in several laboratories by ultraviolet photoelectron spectroscopy (UPS) for cleaved silicon, germanium, and gallium arsenide as well as for annealed silicon and germanium surfaces.[1-5] It is somewhat surprising that most results on the same surface obtained by different workers tend to agree since the surface morphology may not be reproduced.[4-7] An exception to this rule are UPS experiments[2] on cleaved gallium arsenide (110) where it has been suggested that surface steps on poor-quality cleavages may play an important role in determining the surface-state distribution.[4,5] We report in this paper the first experimental correlation of surface steps observed by low-energy-electron diffraction (LEED) and UPS measurements of surface-state energy distributions. The present measurements are restricted to the (111) cleavage faces of silicon but qualitatively similar results should be obtained on other cleaved semiconductor surfaces.[6-8]

The importance of surface steps on semiconductor surfaces has been recognized by a number of authors. Henzler has discussed LEED techniques for determining step heights and terrace widths.[6-8] Ibach and co-workers have determined the step dependence of oxygen chemisorption on cleaved silicon surfaces.[9] Since detailed studies of surface states[1-3] have been made on both annealed and cleaved silicon surfaces, this material seems to be most appropriate for studying the correlation of surface states and surface steps. We find that both dangling-bond surface states and back-bond surface states depend on the step density. Some additional features of dangling-bond states near the band gap of high-step-density cleaved surfaces are found to be similar to previous results on annealed (111) surfaces.[3]

Single crystals of boron-doped Si were used with carrier concentrations in the range 10^{14}–10^{15} cm^{-3}. The samples were oriented with (111) surfaces parallel to notches cut in a bar of $5 \times 15 \times 70$ mm^3 dimensions which allowed multiple cleavages. Experiments were performed in a stainless-steel ultrahigh-vacuum chamber with a base pressure of $\sim 5 \times 10^{-11}$ Torr. Hydrogen could be introduced from a high-purity flask by a standard leak valve. A polycrystalline tungsten ribbon of dimensions $6 \times 20 \times 0.2$ mm^3 was heated to ~ 2000°K to dissociate the H_2 gas into H atoms. This proved to be a factor of $\sim 10^2$ more efficient than the shielded filament of an ion gun used in previous UPS studies of hydrogen adsorption on silicon surfaces.[10] A PHI 15-250 double-pass cylindrical-mirror electron-energy analyzer[11] was used with a He resonance lamp for UPS measurements. Other details of the multiple-technique apparatus have been previously described.[12]

Typical experimental LEED observations are shown in Fig. 1 for (a) low-step-density and (b) high-step-density surfaces at 40-eV primary energy. Using the methods discussed by Henzler[6,8] we verified that the average step height is one double layer (3.14 Å) and that the fractional density of step-edge atoms is (3 ± 2)% for the low-step-density surface [Fig. 1(a)] and (10 ± 2)% for the high-step-density surface [Fig. 1(b)]. The low-step-density surface has two domain