Surface superconductivity and the MOS system

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We solve the superconducting gap equation in the weak-coupling approximation for the electronic quasiparticles in metal-oxide-semiconductor devices, paying particular attention to the effects of the proximity of a surface on (a) the phonon-mediated and (b) screened Coulomb interactions between electrons. The frequency-dependent kernel is calculated using effective-mass-model wave functions and energies, and a microscopic description of the screening for the Si(111)-SiO_2 system, in several respects the most favorable Si system. The value of T_C over the wide range of accessible electron densities is obtained by a matrix-inversion technique applied to the gap integral equation. Values of ~ 10 mK are predicted at $r_s = 1$ ($\sim 5\times 10^{12}$ cm^{-2}) with the intervalley-phonon-mediated electron-electron interaction dominant at this density. Vertex corrections, fluctuation phenomena (crucial in this quasi-two-dimensional system), and strong-coupling corrections are considered, as are the possibilities of devices fabricated from other materials.

I. INTRODUCTION

The inversion-layer system at the Si-SiO_2 interface has proved a fruitful testing ground for ideas on many-body theory.[1,2] The electron density in the inversion layer of the MOS (metal-oxide-semiconductor) device can be altered by more than two orders of magnitude as the applied voltage is increased. This flexibility is gained at the cost of the third dimension (away from the interface); as the applied voltage bends the conduction band below the Fermi energy, the self-consistent distribution of mobile charge is confined to a layer of order 30 Å in thickness, which is comparable to an effective Bohr radius in silicon. In this system the relevant energies—Fermi energy, optical interband absorption, deformation potential shifts of the bands under applied stress, cyclotron frequencies, and even temperature—are all on the same scale of milli-electron-volts.[3] As a result, quite modest magnetic fields, stresses, temperature or gate-voltage changes produce large fractional changes in the ground-state or transport properties of an electron gas which is free in two dimensions and space quantized in the third. A rich variety of data has been collected and many-body effects seem to play a prominent role in arriving at a quantitative interpretation of transport or optical data.[2]

In this paper we set up and solve the superconducting gap equation for the MOS system, paying particular attention to the local geometry and the proximity of the Si-SiO_2 interface in the construction of the relevant electron-electron (e-e) interactions. The plasmon-mediated interaction has been considered before,[4] but we consider the phonon-mediated interaction and the electron-hole excitations for the first time. Several reasons have prompted this work. (1) The anomalous transport data (especially in terms of occupied valley degeneracy) of the Si(111)-SiO_2 system have not been convincingly explained in terms of a paramagnetic ground state, and the role of intervalley phonons as a possible source of an exchange mechanism[3] for inducing broken-symmetry states has required the detailed calculation of electron-phonon matrix elements (EPME) for the MOS system. While the phonon mechanism is too small,[5,6] of itself, to induce the charge-density-wave distortions that could account for the data, they prove sizable enough to prompt the present calculation. (2) Our results show that the phonon mechanism of superconducting pairing is dominant at high electron densities, well into the metallic regime of conduction and away from the effects induced by disorder at the interface, so that experiments should prove relatively clean. (3) While mean-field theories, such as the one presented below, are inappropriate for two-dimensional systems which are dominated by fluctuations at finite temperatures,[7] they provide estimates of the temperature regime where transport anomalies could be expected and sought experimentally. (4) The specifically surface effects have induced significant changes in the structure of the theory and the results from those derived for bulk systems at comparable electron densities. (5) The fact that all energies are on the same scale provides for unusual results as common assumptions for other systems cannot be made here.

The structure of the paper is as follows: in Sec. II we outline the theory of the MOS inversion layer, and in Sec. III we set up the gap equation for our two-dimensional system. Sections IV and V are devoted to the construction of the electron and phonon

kernels required for the gap equation. The solution of the gap equation in the weak coupling limit and the presentation and discussion of results are given in Sec. VI. Further considerations including the corrections due to strong coupling, finite temperature fluctuations, and vertex corrections, as well as the possibilities afforded by the use of other materials are discussed in Sec. VII, and the principal conclusions are summarized in Sec. VIII.

II. MOS SYSTEM

In Fig. 1 we present a schematic picture of the MOS system, including the typical dimensions and the potential of a test charge.[1-3] The self-consistent potential of the electrons in the inversion layer confines them to a region typically 30 Å thick on the Si side of the Si-SiO_2 interface, where the conduction bands of silicon are bent below the Fermi level. Space quantization in the direction normal to the interface is to be expected, and the system must be described in terms of the solution for the Schrödinger equation whose potential is integrated up from the inversion-layer charge density via the Poisson equation, and the whole system must satisfy the Bloch condition in the plane of the interface, as imposed by the Si periodicity.

While the full armory of density-functional techniques has been brought to bear on the calculation of the electronic ground state, a simple variational treatment of the Hartree total energy has been shown to yield a good qualitative and a reasonable quantitative description of the lowest occupied subband (derived from the lowest bound state in the direction normal to the interface). Electrons in the inversion layer are described by a wave function of the form[8,9]

$$\psi(\vec{r}) = \sum_{\text{valleys } v} \alpha_v F_v(\vec{r}) \phi_v(\vec{r}) \ , \tag{1}$$

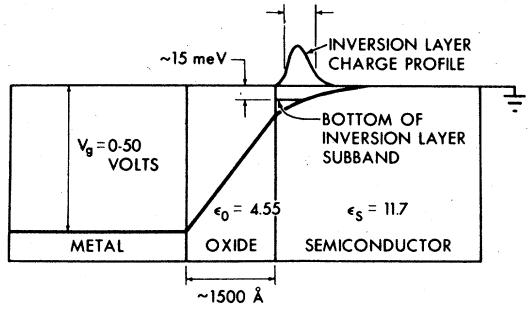

FIG. 1. The metal-oxide-semiconductor system with typical dimensions, including those of the inversion layer. The electrostatic potential energy of a test charge is included schematically.

where $\phi_v(\vec{r})$ is the full Bloch function at the conduction-band minimum in one of the ⟨100⟩ directions of the bulk Brillouin zone (so that v sums over the valleys, and the α_v are normalization constants), while the $F_v(\vec{r})$ are relatively smooth envelope functions satisfying an effective-mass Schrödinger equation of the form

$$[\epsilon_v(-i\nabla) + U(\vec{r})]F_v(\vec{r}) = eF_v(\vec{r}) \ , \tag{2}$$

where $\epsilon_v(\vec{k})$ is the second-order expansion of the conduction band about the vth minimum, and $U(\vec{r})$ is the potential set up by the inversion layer charge density (with further contributions from the depletion charges, etc., being included if necessary). A convenient variational form for $F_v(\vec{r})$ in the half space $z > 0$ is given by[3,8]

$$F_v(\vec{r}, \lambda, \vec{k}) = \frac{1}{\sqrt{A}} 2\lambda^{3/2} z e^{-\lambda z} e^{i\vec{k}\cdot\vec{r}} \tag{3}$$

and this allows one to obtain $U(\vec{r})$ in terms of the total electron density per unit area ρ, and the inverse profile thickness λ is our variational parameter. This simple form for F_v reproduces quite well the results of more accurate self-consistent solutions of the whole problem. The $\vec{k}$ refers to the (small) value of the crystal momentum (parallel to the interface) away from the center of the vth valley, and it is used to count allowed band states in the inversion layer subbands. [Higher subbands corresponding to bound states of Eq. (2) will have envelope functions orthogonalized with respect to z.] The total Hartree energy can be obtained as a function of ρ and λ and the gate voltage V_g. A simple linear capacitance relation holds between ρ and V_g, and the total energy is minimized subject to this relation, with the result that the profile parameter satisfies[3]

$$\lambda = \left(\frac{15\pi}{8a^*}\rho\right)^{1/3} \ , \tag{4}$$

where a^* is the effective Bohr radius given by $\epsilon_{Si}\hbar^2/(m_{zz}e^2)$ for this system, where m_{zz} is the effective mass in the direction normal to the interface.

At the Si(111)-SiO_2 interface,[8] all valleys project an equal mass m_{zz}, and the kinetic energy of confinement in the z direction $\hbar^2\lambda^2/2m_{zz}$ is the same for all valleys which we expect to be equally occupied in a paramagnetic ground state. In the Si(100)-SiO_2 system, two valleys present a larger m_{zz} than the other four, and only the former two are ever occupied in practice. The initial and persistent observation[10-12] of an occupied valley degeneracy of two for the Si(111)-SiO_2 system lead to a number of theoretical explanations,[3,12,13] no one of which is completely satisfactory, and some of which would not account for the recently observed sixfold degeneracy[14] in devices prepared by a novel and as yet incompletely understood set of processes. One explanation relies heavily

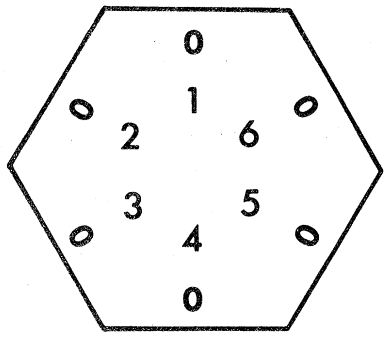

FIG. 2. The (111) surface Brillouin zone and the Fermi lines for the Si(111)-SiO_2 system.

on quantities that are calculated in Sec. V below. The surface Brillouin zone and the Fermi lines for the Si(111)-SiO_2 system are shown in Fig. 2. The in-plane dispersion is anisotropic, but we replace this by an isotropic but equal-mass dispersion in order to carry the analytic aspects of the theory one step further. The appropriate masses are accessible to cyclotron resonance studies and give ample evidence of the importance of many-body effects.[15]

The starting point of our discussion is the paramagnetic ground state in which all six valleys are equally occupied by inversion layer electrons whose normal effective mass is $m_{zz}=0.256m_e$ and whose band effective mass is $m^*=0.358m_e$. With $a^*=45.7$ a.u., the experimentally accessible electron densities range from 10^{11} to 10^{13} cm^{-2}, or equivalently, the electron spacing parameter r_s, in units of a^*, varies from ~ 7 to ~ 0.7.

III. GAP EQUATION

The possibility of superconductivity in bulk doped silicon was investigated a number of years ago by Cohen,[16] and, while the transition temperatures were extremely small, the attractive pairing was dominated by the exchange of intervalley phonons. Since then a number of improvements in the construction of the gap equation and its solution have taken place, and the formulation by Takada,[4] following Kirzhnits *et al.*[17] is particularly suited to our problem, as it has already been used to examine the plasmon mechanism of superconductivity in MOS inversion layers. In this section we summarize the important aspects, namely, the form of that gap equation, the kernels required for it, the form of the solution at T and for T_C, and the practical process of solving the equation. For further details one is referred to earlier papers.

The full Hamiltonian of our present problem contains electron, phonon, and electron-phonon parts in a completely standard manner, except for the fact that the $\vec{k}$ summation is two dimensional and we explicitly include the multivalley nature of our problem by restricting the $\vec{k}$ summation to small k and including an index i to sum over the valleys in the electronic part.[4] Thus

$$H_{\rm el}=\sum_{i=1}^{6}\sum_{\vec{k}\sigma}\epsilon_{\vec{k}\sigma}c_{i\vec{k}\sigma}^{\dagger}c_{i\vec{k}\sigma}+\frac{1}{2}\sum_{ij}\sum_{\substack{\vec{k}\vec{k}'\\ \sigma\sigma'}}\sum_{\vec{q}\neq 0}V^0(\vec{q})c_{i\vec{k}\sigma}^{\dagger}c_{j\vec{k}'\sigma}^{\dagger}c_{j\vec{k}'-\vec{q}\sigma'}c_{i\vec{k}+\vec{q}\sigma}\ ,$$

$$H_{\rm ph}=\sum_{\vec{q}\nu}\omega_\nu(\vec{q})(a_{\vec{q}\nu}^{\dagger}a_{\vec{q}\nu}+\tfrac{1}{2})\ ,\quad H_{\text{el-ph}}=\sum_{\substack{ijkk'\\ \sigma\sigma'}}g_{ikjk'\sigma'}(a_{(\vec{k}+\vec{Q}_i-\vec{k}'-\vec{Q}_j)\sigma'}+a_{-(\vec{k}+\vec{Q}_i-\vec{k}'-\vec{Q}_j)\sigma'}^{\dagger})c_{i\vec{k}\sigma}^{\dagger}c_{j\vec{k}'\sigma}\ , \tag{5}$$

where $c_{ik\sigma}$ is the annihilation operator of the electron of momentum $\vec{k}$ with respect to the bottom of valley i (centered at $\vec{Q}_i$) and spin σ, whose single-particle energy $\epsilon_{\vec{k}}$ is independent of i, and has circular dispersion so that we can define a frequency variable such that

$$\hbar\omega=\epsilon_{\vec{k}}-E_F=\frac{\hbar^2k^2}{2m^*}-E_F\ , \tag{6}$$

$V^0(\vec{q})$ is the two-dimensional Fourier transform of the Coulomb potential

$$V^0(\vec{q})=\frac{2\pi e^2}{\epsilon|\vec{q}|} \tag{7}$$

with silicon dielectric constant ϵ, $a_{q\nu}$ is the annihilation operator for a phonon of wave vector $\vec{q}$ in branch ν and with frequency $\omega_\nu(\vec{q})$, while the g's are the electron-phonon matrix elements (EPME).

In the weak coupling limit the formulation of the gap equation[17] (using the finite-temperature Green's-function formalism[18]) leads to the form

$$\Delta(\omega)=-\int_{-E_F}^{\infty}\frac{d\omega'}{2\omega'}\tanh\frac{\hbar\omega'}{2k_bT_C}K(\omega,\omega')\Delta(\omega')\ , \tag{8}$$

where the kernel K (in a two-dimensional system, with the definition $\vec{q}=\vec{k}'-\vec{k}$) is given by

$$K(\omega,\omega')=\frac{A}{4\pi^2}\frac{2m^*}{\hbar^2}\int_{|k-k'|}^{|k+k'|}\frac{qdq}{kk'\sin\theta}\left[V^0(\vec{q})+\int_0^{\infty}\frac{2}{\pi}d\Omega\frac{\mathrm{Im}\,V^R(\vec{q},\Omega)}{\Omega+|\omega|+|\omega'|}\right]\ , \tag{9}$$

where A is the area of the device, and the frequency variable defined in Eq. (6) above has been exploited. In the above equation $q = |\vec{q}|$, and V^R is the retarded irreducible $e-e$ interaction as mediated by all possible boson fields. The usual form of the BCS equation can be recovered from Eq. (8) once the sum over $\vec{k}'$ in the former is converted to a sum over $|\vec{k}'|$ (and hence the integral over ω') and a sum over the angle θ between $\vec{k}$ and $\vec{k}'$ which is incorporated into the kernel. Sections IV and V of the present paper are devoted to the construction of $V^R(q, \Omega)$.

The solution of the gap equation for T_C follows from Zubarev,[19] with the introduction of a reduced energy $x = \hbar\omega/E_F$ and a reduced gap function $\phi(x) = \Delta(x)/\Delta(0)$. The gap equation becomes

$$\phi(x) = -\int_{-1}^{\infty} \frac{dx'}{2x'} \tanh\left(\frac{E_F x'}{2k_B T_C}\right) \phi(x') K(x,x') \tag{10}$$

and, since $\phi(0) = 1$

$$1 = -\int_{-1}^{\infty} \frac{dx'}{2x'} \tanh\left(\frac{E_F x'}{2k_B T_C}\right) \phi(x') K(0,x') \ . \tag{11}$$

With the definition[4]

$$\lambda_0 = K(0,0) \tag{12}$$

we can combine the two equations as

$$\phi(x) = \frac{K(x,0)}{\lambda_0} - \int_{-1}^{\infty} \frac{dx'}{2|x'|} \phi(x') \left[K(x,x') - \frac{K(x,0)K(0,x')}{\lambda_0}\right] \ , \tag{13}$$

where the tanh factor has been replaced by unity (because the term in square brackets vanishes at $x' = 0$). This $\phi(x)$ can be rewritten into Eq. (11) and rearranged to give

$$T_C = 1.134 E_F \exp\left[\frac{1}{\lambda_0} + \int_{-1}^{\infty} \frac{dx}{2|x|} \left[\phi(x) \frac{K(0,x)}{\lambda_0} - \Theta(1-|x|)\right]\right] \ , \tag{14}$$

where the energy scale is set by E_F and the static (λ_0) and dynamic contributions to T_C are clearly separated.

Early theories involved explicit approximations to the kernels, such as replacing them by constants up to frequency cutoffs determined by the Fermi energy and Debye frequency (the two-square-well kernel[20]), which in turn resulted in simple (constant) values of $\phi(x)$ in the frequency ranges above and below those determined by E_F and ω_D. It is precisely because E_F and ω_D are of the same order of magnitude here, that we must allow greater flexibility. This can easily be seen following Takada[4] and introducing an ansatz for the structure of the kernel, namely, that it is separable in the form

$$K(x,x') = [\lambda_0 + F(x) + F(x')]\Theta(1-|x|)\Theta(1-|x'|) \ , \tag{15}$$

where $F(x)$ must satisfy only $F(0) = 0$. With the definition of an average

$$\langle F \rangle = \int_{-1}^{1} \frac{dx F(x)}{2|x|} \tag{16}$$

the condition for superconductivity becomes

$$\langle F^2 \rangle > \lambda_0 \tag{17}$$

and

$$T_C = 1.134 E_F \left[\exp \frac{-(1+\langle F \rangle)^2}{\langle F^2 \rangle - \lambda_0}\right] \ . \tag{18}$$

As Takada emphasizes, if $F(x) \sim |x|^{\alpha}$ for small x, the condition for superconductivity is that

$$[K(1,0) - K(0,0)] > 2\alpha K(0,0) \tag{19}$$

implying that the sign of λ_0 is not critical for superconductivity, but rather the slope of the kernel as a function of frequency between 0 and E_F.

Once the kernel has been set up as in the next sections, the solution of the gap equation follows a standard numerical procedure in which the kernel is regarded as piece-wise constant in its two variables, and the integral equation reverts to a matrix equation. For details, one is referred to Takada's work[4] which we have followed in constructing the spacing of the intervals for the kernel and in choosing an effective upper limit on the integral in Eq. (12).

IV. COULOMB KERNEL

In this section we calculate the dynamically screened Coulomb interaction $V^R_{\text{Coul}}(\vec{q}, \omega)$ and hence the Coulomb kernel for the gap equation, the static part $V^0(\vec{q})$ having been factored out. The Coulomb interaction we seek can be written as[21]

$$V_{\vec{k},\vec{k}'} = \int\int \psi_{\vec{k}'_{\uparrow}}(\vec{r}) \psi_{-\vec{k}_{\uparrow}}(\vec{r}) V_{\text{Coul}}(\vec{r}, \vec{r}') \times \psi_{-\vec{k}'_{\downarrow}}(\vec{r}') \psi_{\vec{k}_{\downarrow}}(\vec{r}') d\vec{r}\, d\vec{r}' \ , \tag{20}$$

where the ψ are given by Eq. (3), and the $\vec{k}$ are assumed to be associated with one valley or another. In turn the Coulomb interaction in the Fourier

representation is given by

$$V_{\text{Coul}}(\vec{r},\vec{r}') = \frac{1}{\Omega_{\parallel}} \sum_{\vec{q}} V_{\text{Coul}}(|\vec{q}|;z,z') e^{i\vec{q}\cdot(\vec{r}-\vec{r}')} , \tag{21}$$

with $\vec{r}$ being the (x,y) component of $\vec{r}$. The evaluation of the standard Coulomb interaction between two electrons with Bloch functions in different valleys requires an intervalley wave vector argument in the matrix element. The two-stage integration of effective-mass wave functions (over unit cells for the Bloch functions, assuming the envelope locally constant, and then over the larger volume with the slowly varying envelope function) produces a factor $(\lambda/q)^2$ from the second stage.[3] In practice, this factor never exceeds 10^{-2} and we can neglect intervalley matrix elements. In the case of the intravalley terms, the integration over the unit cell yields a normalizing factor, and we can write the intravalley terms using the envelope functions only. A different conclusion is reached on the relative importance of inter- and intravalley contributions to the phonon kernel in the next section.

Our matrix element can now be written in the form (with $\vec{q} = \vec{k}' - \vec{k}$)

$$V_{\vec{q}} = \Omega_{\parallel} \int\int \xi_n(z_1)\xi_m(z_1) V_{\text{Coul}}(|\vec{q}|;z_1,z_2) \times \xi_n(z_2)\xi_m(z_2) dz_1 dz_2 , \tag{22}$$

where $\xi_n(z)$ has been introduced to denote the purely z part (i.e., $2\lambda^{3/2} z e^{-\lambda z}$) of the envelope function. In fact we can now write the dynamically screened interaction as[22]

$$V_{\text{Coul}}(|\vec{q}|,\omega;z_1,z_2) = \int v(|\vec{q}|;z_1,z_3)\epsilon^{-1}(|\vec{q}|,\omega;z_3,z_2) dz_3 , \tag{23}$$

where ϵ^{-1} is the dynamical screening of the effective Coulomb interaction $v(|\vec{q}|;z_1,z_2)$ between two electrons in the inversion layer, which, taking into account the image charge, is written as

$$v(|\vec{q}|;z,z') = \frac{2\pi e^2}{\epsilon_{\text{Si}}|\vec{q}|\Omega_{\parallel}} \left[e^{-|\vec{q}|\parallel z-z'|} + \frac{\epsilon_{\text{Si}}-\epsilon_{\text{SiO}_2}}{\epsilon_{\text{Si}}+\epsilon_{\text{SiO}_2}} e^{-|\vec{q}|\parallel z+z'|} \right] . \tag{24}$$

The appropriate form for ϵ^{-1}, given the introduction of ϵ_{Si} into the expression for $v(|\vec{q}|;z,z')$ is now

$$\epsilon^{-1}(|\vec{q}|,\omega;z,z') = \delta(z-z') + \int v(|\vec{q}|;z,z'')\chi(|\vec{q}|,\omega;z',z'') dz'' , \tag{25}$$

where χ is the interacting susceptibility of the electron gas, which in turn is obtained from the bare polarization $\chi^0(|q|,\omega;z,z')$ by the solution of an integral equation of the form[22-24]

$$\chi(|\vec{q}|,\omega;z,z') = \chi^0(|\vec{q}|,\omega;z,z') + \int dz_1 \int dz_2 \chi^0(|\vec{q}|,\omega;z,z_1) v(|\vec{q}|,z_1,z_2) \chi(|\vec{q}|,\omega;z_2,z') . \tag{26}$$

In the above equations $\Omega_{\parallel}$ is the area of a surface unit cell. With the use of the envelope functions of the type derived from Eq. (3), the bare polarizability is separable in z and z',[25] and the integral equation is easily solved.[24]

We then obtain, via Eq. (22) a matrix form for $V_{\vec{q}}$ with the indices given by the subbands involved. In the present calculations, we consider two cases, one where we include only the lowest subband $(m=n=0)$ and the second where we also include the first excited subband. It is clear that the dominant contributions to the Coulomb kernel will come from the regions of (ω,q) space where ϵ^{-1} is singular. In the first calculation which retains only the lowest subband, the singular structure is that of a plasmon in the inversion layer with a $\omega \sim q^{1/2}$ dispersion. Indeed the value of χ^0 in this case is the product of the envelope functions and the standard two-dimensional susceptibility as obtained by Stern[26]

$$\chi^0(|\vec{q}|,\omega;z,z') = \xi_0^2(z)\frac{e^2}{q^2 A} \times \lim_{\alpha\to 0} \sum_{\vec{k}} \frac{f_0(E_{\vec{k}}) - f_0(E_{\vec{k}+\vec{q}})}{E_{\vec{k}+\vec{q}} - E_{\vec{k}} - h\omega - ih\alpha} \xi_0^2(z') , \tag{27}$$

where f_0 are the Fermi occupation factors. In the long-wavelength limit the plasmon (as, for example, derived by Stern) can be expected to contribute to an attractive electron-electron interaction, as has been considered by Takada[4] for a strictly two-dimensional plasmon-pole model for ϵ^{-1}. In contrast to Takada's calculation, we have not made a pole approximation but taken the intrasubband ϵ^{-1} as extracted from Eq. (27), including the "thickness" effect via the z and z' dependence. In the second calculation, additional

structure comes from the intersubband excitations,[24] which have not been considered before in the present context. We include only the first excited subband, but with the increasing energy to the higher excited subbands, we do not expect major corrections to arise from our neglect of these levels. That these levels are important at all, is a reflection of the energy scales mentioned in the Introduction.

Before completing this section, two points should be noted. (1) The Coulomb interaction is not positive definite, and at high frequencies it becomes attractive. Indeed in three dimensions (as in a doped semiconductor) a Thomas-Fermi expansion of the inverse dielectric function takes the form[27]

$$\epsilon^{-1}(\vec{q},\omega)=\left[1+\frac{\omega_p^2}{\omega^2-\omega_p^2(\vec{q})}\right] \tag{28}$$

and we see that for $\omega \lesssim \omega_p(\vec{q})$ the dielectric function changes sign. In most metals, this is irrelevant since $\hbar\omega_p \sim 10$ eV, while the relevant energy scale is ~ 1 meV, but in our system the energies are comparable. A similar comment applies to the *e-h* excitations. The Coulomb kernel is able to induce mean-field superconductivity from the lowest subband only, and this tendency is enhanced by the inclusion of *e-h* excitations. (2) It is clear that $K(0,0)$ is an important ingredient in the theory outlined in Sec. III, and the results of our calculations for the two cases considered give at $r_s=1$,

$$K_{\text{Coul}}^{\text{one subband}}(0,0)=0.138 \quad K_{\text{Coul}}^{\text{two subbands}}(0,0)=0.098 \tag{29}$$

and we see that the reduction of $K(0,0)$ in the latter case is an aid to the superconducting possibilities.

V. PHONON KERNEL

The phonon-mediated electron-electron interaction in the Bardeen-Pines[28] form is

$$V_{\text{Ph}}(\vec{q},\omega)=\sum_j \frac{\hbar\omega_j(\vec{q})|g_j(\vec{q})|^2}{[\hbar\omega_j(\vec{q})]^2-(\hbar\omega)^2}\ , \tag{30}$$

where j sums over all phonon branches and g is the electron-phonon matrix element (EPME). In this section we calculate V for a system which is an approximation to the MOS system. In bulk silicon, selection rules limit the number of modes which yield a nonzero EPME.[29] The presence of an interface with amorphous SiO_2 on the other side changes the nature of the selection rules, as well as the electron wave functions and the phonon modes, so we can expect different results. At the same time, the explicit calculation of g_j below requires in principle solving for phonon modes of the composite system, and extracting the amplitudes of the phonons in the region occupied by the inversion layer. This is inordinately difficult, and we have performed detailed and microscopic calculations on a 24-layer slab of silicon bounded by (111) surfaces to which different boundary conditions have been applied, as a crude simulation of the MOS system. The discontinuities of the conduction band wave functions on the two sides, means that free boundary conditions is not unreasonable for the electrons. We probably overestimate the changes induced by the interface on the phonon modes by using free boundary conditions for them as well, but we argue below that the overestimate is not too great.

For the EPME that measures the scattering from electrons in one Bloch function minimum to another (a to b), we calculate[6]

$$g_j(q_{ab})=\int \psi_b^*(\vec{r})\left[\int \epsilon^{-1}(\vec{r},\vec{r}')\sum_{\vec{R}}\delta\vec{R}_j\cdot\vec{\nabla}V_{\text{Ion}}(\vec{r}'-\vec{R})\,d\vec{r}'\right]\psi_a(\vec{r})\,d\vec{r}\ , \tag{31}$$

where the term in square brackets is the effective ionic potential as screened by a nonlocal dielectric function ϵ^{-1}, set up when the silicon ion potentials are shifted rigidly by amounts $\delta\vec{R}_j$ by the mode j. The ψ's are the full effective-mass wave functions, and the retention of $\vec{k}$ as a good quantum number means that a $\vec{k}$ selection rule still applies. If we were to take the amorphous silicon into account, even that selection rule is blurred.

In the slab calculation which we perform, the index j comprises both a branch index η [running from 1 to 6 to reflect the degrees of freedom in a bulk unit cell, and the fact that our electron wave functions are expanded in Eq. (36) below over bulk antibonding orbitals, so that our calculation is actually done on twelve double-layers] and q_z running from 1 to 12. In the case where we impose periodic-boundary conditions in the direction normal to the slab, q_z becomes a good quantum number, and, in the absence of the envelope function a selection rule is recovered; with any other boundary condition, it merely counts the degrees of freedom. In fact, in our detailed calculations for intervalley phonon contributions (which, just as in the case of bulk systems, we find to provide the dominant attractive pairing mechanism) the calculations performed on a slab and without the envelope function can be carried over with a minor modification. If we denote by $\delta V_j^{\text{eff}}(\vec{r})$ the term in

Eq. (31) in square brackets, and periodic-boundary conditions are applied, then the integral

$$G_p = \int_{\text{cell } ijk} \phi_b^*(\vec{r})\delta V_p^{\text{eff}}(\vec{r})\phi_a(\vec{r})\, d\vec{r} \tag{32}$$

is the same from one cell to the next, except for a phase factor and one recovers the selection rule by summing over all cells in the kth layer, and the EPME with the inversion layer wave functions can be written as

$$g_p = N_{\parallel}^{1/2} \sum_{\text{cells } k} t\,|\xi(z_k)|^2 e^{iq_z z_k} G_p \ , \tag{33}$$

where the ϕ's are normalized to a unit cell, t is the thickness of one double layer (which goes out in the conversion of the sum over k to an integral over z), and $N_{\parallel}$ is the number of unit cells in a layer. This last term and the factor $e^{iq_z z_k}$ come from the normalization and the phase factor parts of the phonon amplitude

$$\delta\vec{R}_p = \left(\frac{h}{2MN_{\parallel}N_L\omega_p(\vec{q})}\right)^{1/2} e^{i(\vec{q},q_z)\cdot\vec{R}}\vec{e}_p(\vec{q},q_z) \ , \tag{34}$$

the polarization vector of which ($\vec{e}_p$), we obtain explicitly below. Our phonon kernel is dominated by the $q_z \simeq 0$ contributions since, on the assumption that the G_p is a slowly varying function of q_z [recall $p \equiv (\eta, q_z)$], the integral in Eq. (33) is trivial and leads to

$$g_p = N_{\parallel}^{1/2} G_p \left(\frac{2\lambda}{2\lambda + iq_z}\right)^3$$

and, since λ is rather smaller than $q_{\text{intervalley}}$, only the smaller values of q_z contribute to the EPME's as they appear in the kernel in Eq. (30), with its summation over all modes. Indeed, if we consider the zero frequency value of $V_{\text{Ph}}(q,0)$ the sum over j becomes a sum over branches η and modes q_z, the latter being converted to an integral over q_z with a prefactor $N_L t/(2\pi)$, N_L being the number of layers, and t the thickness of each layer. One thus obtains

$$V_{\text{Ph}}(\vec{q},0) = -\tfrac{3}{4}\lambda N t \sum_{\eta} \frac{|G_p(q_z=0)|^2}{\hbar\omega_\eta(\vec{q})} \ . \tag{35}$$

If we choose to normalize the ϕ's in Eq. (32) to the entire system the factor N is absorbed in the normalization. Before proceeding to convert $V_{\text{Ph}}(q,0)$ into the value of $K(0,0)$, we describe the calculations for G_p in greater detail.

The ingredients of our calculation[6] include (1) an expansion of the conduction-band wave functions over a basis of antibonding orbitals as

$$\phi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{l=0}^{N_L-1} \sum_{i,m} c_i^l(k,k_z) e^{i\vec{k}\cdot\vec{R}_m} \chi_{il}(\vec{r} - \vec{R}_m^l) \ , \tag{36}$$

where l sums over the layers, $\vec{k}$ is a two-dimensional (2D) wave vector parallel to the surface, i an index ($i = 1-4$) for the antibonding orbital as specified by its axis, and $\vec{R}_m^l$ is a site in the hexagonal lattice in the lth layer, of which $\vec{R}_m$ is the 2D component. Because of the expansion over antibonding orbitals, l is strictly a double-layer index in practice. The coefficients $c_i^l(k,k_z)$ are determined by solving a secular equation resulting when interactions out to fourth-nearest neighbors (in a tight-binding sense) are included, just as in the calculation of Hanke and Sham.[30] In turn, we use their form of the antibonding orbitals

$$\chi_i = N_-[h_{\nu_i}(\vec{r} - \vec{R}) - h_{-\nu_i}(\vec{r} - \vec{R} - b\vec{\nu}_i)] \ , \tag{37}$$

where N_- is a normalizing constant, b the bond length, and ν_i the normalized vector of the antibond, while the "sp^3" hybrid orbitals are expanded as

$$h_\nu(\vec{r} - \vec{c}) = \frac{1}{4\sqrt{\pi}}[R_s(\vec{r} - \vec{c}) + \sqrt{3}\,\vec{\nu} \cdot (\vec{r} - \vec{c})R_p(\vec{r} - \vec{c})] \ , \tag{38}$$

where R_s and R_p are each expanded over Gaussians to reproduce the charge densities from more elaborate calculations, (2) a simple two-parameter force-constant model for the phonons, with a bond bending to bond stretching ratio of 0.7 (cf. Lax).[31] The resulting displacement for mode j with wave vector $\vec{q}$ and frequency $\omega_j(\vec{q})$ is precisely as given in Eq. (34), (3) a simple ionic potential of the form

$$V(r) = Qe^2\left(\frac{1}{r} - \frac{\beta}{r}e^{-\alpha r}\right) \tag{39}$$

with parameters fitted to reproduce the small-q regime of the silicon bulk pseudopotential ($Q = 4$, $\beta = 1.5$, $\alpha^{-1} = 1.71$ a.u.) and finally (4) a nonlocal dielectric formulation of the screening. In the plane of the inversion layer, we work in Fourier space and write[22]

$$\epsilon^{-1}(\vec{q}+\vec{G},\vec{q}+\vec{G}',z,z') = \delta_{\vec{G}\vec{G}'}(z-z') + \int v(|\vec{q}+\vec{G}|,|z-z''|)\chi(\vec{q}+\vec{G},\vec{q}+\vec{G}',z'',z')\,dz'' \ , \tag{40}$$

where $v(|\vec{q}|,|z|)$ is again the Fourier transform of the bare Coulomb potential, and χ the response function which, for the present calculations we take to be of the form[22,23]

$$\chi = \sum_{s,s'} A_s^\dagger(\vec{q}+\vec{G},z)[N^{-1}(\vec{q}) - V^{\text{xc}}(\vec{q})]^{-1}_{s,s'} A_{s'}(\vec{q}+\vec{G}',z') \ , \tag{41}$$

where, in turn, N^{-1} is a generalized susceptibility, V^{xc} the Coulomb interaction plus the exchange-correlation corrections, and A_s the charge-density form factors

$$A_s(\vec{q}+\vec{G},z)=e^{-i(\vec{q}+\vec{G})\cdot\vec{\sigma}_l}\int d^2\vec{r}\,\chi_i^*(\vec{r},z-z_l)e^{-i(\vec{q}+\vec{G})\cdot\vec{r}}\chi_j(\vec{r}-\vec{R}_s,z-z_{l'}) \tag{42}$$

with a composite index $s\equiv\{i,j,l,l',\vec{R}_s\}$. We consider the system in terms of hexagonal double layers, with σ_l keeping track of the registry of the different layers. The precise range of the summation over s and $\vec{R}_s$ is considered further below.

With these ingredients the calculation of the EPME of Eq. (31) follows a parallel development to that of Bar-Sagi and Hanke[32] with the result

$$g_p(\vec{k}',\vec{k})=\left(\frac{\hbar N_{\|}}{2M\omega_p(\vec{q})}\right)^{1/2}\sum_{\substack{l,l',l''\\ i,j}}c_{jl'}^*(\vec{k}')c_{il}(\vec{k})\sum_s e^{-i(\vec{k}'\cdot\vec{R}_s+\vec{q}\cdot\vec{\sigma}_l)}\vec{e}_{l''}^{\,p}(\vec{q})\cdot\vec{F}_{sl''}(\vec{q})\ , \tag{43}$$

where the force-form-factor $\vec{F}_{sl''}$ is modified from its bare form

$$\vec{f}_{sl''}(\vec{q})=\sum_{\vec{G}}\int dz\left(-i(\vec{q}+\vec{G}),\frac{\partial}{\partial z}\right)V_{\text{Ion}}(\vec{q}+\vec{G},z-z_{l''})A_s(\vec{q}+\vec{G},z)e^{i\vec{G}\cdot\vec{\sigma}_{l''}}\ , \tag{44}$$

by the matrix factor

$$\vec{F}_{sl}=(\vec{I}+\vec{V}\vec{S}^{-1})_{ss'}\vec{f}_{s'l} \tag{45}$$

involving the Coulomb matrix

$$V_{ss'}(\vec{q})=\sum_{\vec{G}}\int\int dzdz'A_s^*(\vec{q}+\vec{G},z)v(|\vec{q}+\vec{G}|,|z-z'|)A_{s'}(\vec{q}+\vec{G},z') \tag{46}$$

and the screening matrix

$$S(q)=N^{-1}(q)-V^{xc}(q)\ . \tag{47}$$

In the inversion layer problem, the factor $(\lambda/q)^2$ again arises in the evaluation of the Coulomb matrix, and again,[3] we can neglect (for the intervalley part of the screening $I+VS^{-1}\simeq I$) the correction in Eq. (45) and write $F=f$, and the calculation proceeds directly from the formulation. We first calculate the charge-density form factors including in the summation over $\vec{R}_s$ all on-site and nearest-neighbor terms, and all terms in the l,l' summation. The real-space part of the problem is slowly convergent, and this is the principal reason why the present formulation is not useful in obtaining the EPME for intravalley (i.e., small-q) phonons. The secular equations are solved for the electron and the phonon systems, and the EPME's calculated just as in Eq. (43). The imposition of periodic-boundary conditions on the secular equations is trivial. The free surfaces were assumed to have no dangling bonds, as the SiO_2 bonding would remove these away from the conduction-band minimum in a MOS system. The phonon boundary condition imposed on the free surface was as to guarantee the $\vec{k}=\vec{0}$ translational invariance, although the results are not very sensitive to this at large $\vec{q}$. In this context we argue that the discontinuity in elastic properties at the interface is not unreasonably modeled by these boundary conditions.

The results of the calculation can be summarized qualitatively as follows: the periodic-boundary conditions impose q_z as a good quantum number and restrict the number of phonons that can couple. While this restriction does not hold for the free boundary conditions, and all modes can couple, most couple weakly and using $V_{\text{Ph}}(q,0)$ as a measure, we find it enhanced by the removal of periodic-boundary conditions.

The calculations were performed on a system with force constants of order unity and thereafter normalized. Referring back to Eq. (35) the value of V_{Ph} coupling electrons associated with valleys a and b is given by

$$V_{\text{Ph}}(q_{ab},0)=-\frac{0.0701}{A}a_0^2\frac{R^{ab}}{r_s^{2/3}}\text{Ry}\ , \tag{48}$$

where A is the device area, a_0 the atomic Bohr radius, r_s the electron spacing parameter [the r_s dependence following from the factor λ in Eq. (35)], and R^{ab} the numbers (in Table I) taken directly from the calculations. One sees from the table that a 30% increase in V_{Ph} follows from the use of free boundary conditions. Calculations on a six-double layer slab provided a 100% increase (but here a different value

TABLE I. The computed phonon-mediated electron-electron interactions [normalized as in Eq. (48)].

	Periodic-boundary conditions	Free-boundary conditions
R^{12}	24.2	32.5
R^{13}	10.1	14.0
R^{14}	13.5	18.5

of k_z provided the conduction-band minima). These interactions compare with those obtained for bulk silicon by other methods, and are of themselves too small by a factor of 5–10 to induce density waves in the inversion layer that would account for the anomalous transport data on the Si(111)-SiO_2 system. The form of $V_{\rm Ph}$ given above can be introduced into Eq. (9) to yield the result that

$$K(\omega=0,\omega'=0)=-\sum_{b\neq a}\frac{0.002\,0}{r_s^{2/3}}R^{ab}\ , \tag{49}$$

which provides results of $K(0,0)=-0.22r_s^{-2/3}$ with the free boundary conditions, and $K(0,0)=-0.16r_s^{-2/3}$ with periodic-boundary conditions. A comparison of these results with those of Eq. (29) reveals that at high densities, i.e., $r_s\simeq 1$, there is a strong cancellation between the Coulomb and phonon kernels, and the resulting T_C's that we obtain rely on the enhancement of the phonon kernel near the interface.

The intravalley contribution to the phonon kernel is obtained in a continuum approximation, where we follow Vinter[33] and introduce a deformation potential into the expression for the EPME as

$$g_j(\vec{q})=i\left(\frac{h}{2MN_{\|}N_L\omega_j(\vec{q})}\right)^{1/2}\vec{q}\cdot\vec{e}_j D_{\alpha\alpha}\left(\frac{2\lambda}{2\lambda-iq_z}\right)^3 \tag{50}$$

where D is one of the principal deformation potential constants. If one inserts this into Eq. (9) the value of the kernel is

$$K(0,0)=-0.009|D|^2r_s^{-2/3}\ , \tag{51}$$

which we see to be considerably smaller than the contribution from intervalley phonons at all values of r_s, given that D, expressed in rydbergs, is always less than unity.[34] The phonon dispersion is approximated by the linear portion at small q, with an average speed of sound being employed. As in the calculations for bulk silicon, the contribution of intervalley phonons to the attractive pairing is dominant, and especially at high r_s, which is one important reason for choosing this particular system.

VI. RESULTS

We have solved the gap equation for three kernels, one which includes only the lowest subband contribution to the Coulomb kernel and with no phonon kernel, a second also includes the intersubband contribution to the Coulomb kernel as well, and finally one in which the phonon kernel is also included. The results are displayed in Fig. 3, with the electron spacing parameter as the variable. We comment on each in turn.

(a) At large r_s, we can obtain a reasonably large transition temperature because the dynamically screened Coulomb interaction is sufficiently attractive. There is a "threshold" for superconductivity at $r_s=3$, and the maximum T_C occurs for $r_s\sim 10$–20, before T_C drops. The maximum arises since T_C is the product of two factors, E_F which varies as r_s^{-2} and a negative exponential function of an interaction which increases with r_s. Our result corresponds with that of Takada,[4] except that we have incorporated the finite thickness of the inversion layer throughout. The low densitites at which the plasmon contribution is dominant correspond to threshold densities, and surface roughness and disorder in the oxide, which have been ignored in the present calculation, are likely to reduce the effectiveness of the pairing. We do not expect to be able to see the plasmon mechanism producing superconductivity on its own.

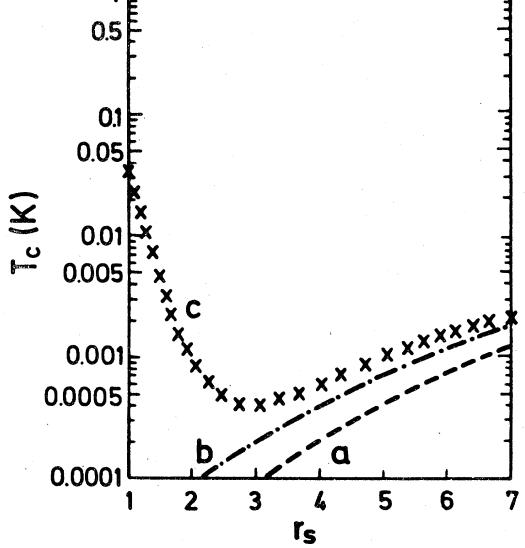

FIG. 3. Calculated values for T_C vs r_s for the Si(111)-SiO_2 system. The kernels used correspond to including (a) only intrasubband electronic excitations, (b) electron-hole excitations to the first excited subband as well as intrasubband excitations, and (c) intra- and intersubband excitations as well as the phonon-mediated interaction.

(b) The inclusion of intersubband excitations provides an additional pairing mechanism. The Coulomb matrix includes off-diagonal terms in the subband indices, and when inverted the Coulomb kernel is reduced, and T_C is enhanced by a factor of ~ 2 over the range of experimentally accessible densitites. The remaining excited states which we have ignored could be expected to further enhance the values of T_C by a factor of order 2.

(c) The phonon mechanism with its $r_s^{-2/3}$ dependence provides the dominant pairing mechanism at high densities, while at low densities it provides a modest enhancement of T_C over the values obtained with just the Coulomb kernel. The results show a qualitative similarity in the effectiveness of the mechanisms as that obtained by Cohen[16] for bulk silicon, but here a number of 2D effects play a role in raising T_C. It is the intervalley phonon mechanism that we would expect to dominate any superconducting effects in MOS devices.

While we consider a host of corrections in the next section, the following points are to be noted:

(1) The use of the smaller phonon kernel derived with the use of periodic-boundary conditions results in a significant cancellation of the Coulomb and phonon kernels at low frequencies at $r_s = 1$ [$K_{\mathrm{Ph}}(0,0) = -0.16$, $K_{\mathrm{Coul}}(0,0) = +0.095$] and a reduction by a factor of ~ 20 in T_C from that shown in Fig. 3. The correct phonon kernel should lie between the two we have calculated. In each case we have used a frequency dependence of the form such that $K(0,\omega) = K(0,0)\alpha/(\alpha+\omega)$ where α is a dominant phonon frequency, obtained by a weighted average of the contributions of the phonons. The inversion layer at high densities is of a thickness that is comparable to the slab, but in the MOS system, there is one interface, rather than two surfaces.

(2) At higher electron densities, the increase in λ brings the charge into a thin region near the interface, and the effective-mass assumption of an excess potential that is smooth on the scale of a unit cell breaks down,[35] as do corresponding approximations made in the calculation. The electon density cannot be increased without limit, as dielectric breakdown occurs.

VII. FURTHER CONSIDERATIONS

In this section we consider: (1) corrections to the mean-field theory we have presented; (2) special features of the superconductivity; (3) possibilites of other broken symmetries in the MOS system; and (4) the use of other materials than silicon.

(1) The present theory is a modification of the Kirzhnits *et al.*[17] development of the BCS theory which takes the MOS energy scales into account. A number of corrections to the BCS theory can be estimated for our system. In his consideration of the plasmon mechanism in doped silicon, Takada[36] considered the vertex corrections induced by local fields and electron correlations (in a model with approximations due to Hubbard[37] and with further corrections for short-range correlations[38]) on the kernel and T_C. The effects were small, and while the quasi-two-dimensional nature of the system may further enhance the corrections, we do not expect them to be dramatic. We have repeated the calculation with the one-subband model for $\epsilon^{-1}(\vec{q},\omega)$ and estimated the corrections due to electron-hole ladder diagrams which enter the screening ϵ^{-1} and have an important effect on the electron-electron interactions at large r_s: this correction is indispensible for obtaining the correct short-range behavior for the pair-correlation function. The corrections are modest, as are the effects of paramagnon corrections.[39] Of greater importance are the estimates of the strong coupling renormalization corrections which can be estimated in a variety of ways and result in a decrease by up to a factor of about 2 of T_C over most of the accessible range of densities.

(2) The most important aspect of the MOS system (other than the range of r_s that can be achieved) is the quasi-2D nature of the electron gas, and hence the effectiveness of finite temperatures in destroying long-range correlation in the mean-field order parameter.[7] It is clear in thin-film studies that the "excess conductivity" indicates this destruction has only a minor effect on T_c and details of the temperature-dependent resistance of the film.[40] At the same time, the analysis of Aslamov and Larkin[41] indicates that the range of temperatures over which critical fluctuations can be expected is greatly enhanced. In the MOS system, however, the precise resistance of the device near T_C will be masked by contact resistances and the external circuit. It is to be hoped that measurements as a function of r_s as well might be able to detect the "two-dimensionalness" of the system in the fluctuations as the third dimension is squeezed out [cf. Eq. (4)].

The disorder induced by amorphous SiO_2 is expected to alter the phonon kernel from the bulk equivalent in a way that differs in detail from that we have estimated in Sec. V. The appearance of good quantum oscillations at the higher densities puts an upper bound of the effects of impurities and amorphous oxide on the scattering.[1,2] The possibility of singly charged defects near the interface can be expected to have a deleterious effect on the pairing and T_C, especially at low densities. This is certainly true for the plasmon mechanism of superconductivity. This mechanism, in contrast to the phonon mechanism, introduces a long-range attraction between electrons which is particularly sensitive to defect potential fluctuations.

The coherence length in this system is dominated at high densities ($r_s \simeq 1$) by the phonon contribu-

tion, and is of order

$$\xi_0 = 0.18 v_F / T_C = 6 \times 10^4 \text{ Å } (r_s = 1)$$
$$= 8 \times 10^2 \text{ Å } (r_s = 0.73) , \quad (52)$$

which is to be contrasted with the interparticle spacing of 32 Å at $r_s = 1$. Our system is akin to that of bulk doped $SrTiO_3$ which is superconducting as mediated by the strong coupling to intervalley phonons.[42]

The effects of magnetic fields are likely to be more important than in bulk systems; since all our energy scales are small, very small critical fields will follow. As mentioned in the Introduction, the conduction-band minima can be moved with respect to each other by the application of stress.[20,43] We have examined the Si(111)-SiO_2 system since, in the absence of stress, the intervalley-phonon-mediated interaction can be most efficiently exploited. We expect stress to reduce T_C in this system. By contrast, the application of stress to the more commonly studied Si(100)-SiO_2 system enables the simultaneous occupation of two light-mass and two heavy-mass valleys, (although the quantum oscillations seem to yield an occupied valley degeneracy of two) in which case intervalley phonon coupling could again play a role, with the unusual prospect of stress-induced superconductivity, and the phase diagrams that would parallel those obtained for other broken symmetries.[44]

(3) We have alluded to the possibility of other broken symmetries. Our phonon-mediated interactions seem to be too small, by a factor of 5–10 to induce intervalley charge-density waves[3] [which would explain a whole host of otherwise anomalous transport data on the Si(111)-Si)$_2$ system] on their own. One cannot rule out the possibility that several interaction mechanisms are acting cooperatively to produce these density waves. Further, if this were the case, and the higher transition temperatures for these other broken symmetries were realizable, the superconducting state would be suppressed. At the low-density range, (for which the appropriate parameters can be further extrapolated in the electrons-on-helium-surface system[45]) the possibilites of Wigner crystallization[46] are under active investigation. In this regime we would need to treat electron correlations with much greater care than we have above, in order to test the relative instability of the paramagnetic ground state with respect to these broken symmetries.

(4) We have seen that the familiar bulk mechanism of phonon-induced electron-electron interactions can be enhanced near an interface, and the possibility exists of superconducting inversion layers at temperatures where a bulk system of comparable electron density is still normal. We have concentrated on the Si MOS devices, as these are available with high-quality interfaces. The choice of other substrate materials, with large electron-phonon interaction, such as GaP, InAs, or even $SrTiO_3$ (which can be made superconducting in bulk doped samples) would increase the range of parameters over which superconducting phenomena might be expected. At present the fabrication of interfaces that are clean on atomic scales for other than the Si-SiO_2 interfaces is exceedingly difficult, as evidenced by the poor quality of quantum oscillations from Te and Ge substrates,[47] but the possibilities of new types of phenomena to be studied might well increase the effort applied in this direction.

VIII. CONCLUSIONS

The flexibility afforded by the MOS system has been exploited in previous studies of aspects of electron gas theory. It offers the same flexibility for the study of superconductivity. While the Si(111)-SiO_2 system [or the Si(100)-SiO_2 system under stress] is the best characterized, other substrate materials might be tried on the principle that the proximity of the interface can enhance the phonon-mediated pairing mechanism.

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[1]G. Landwehr and F. Koch, Festkörperprobleme 15, 49, 79 (1975); F. Stern, Crit. Rev. Solid State Sci. 5, 499 (1974).
[2]Proceedings of the International Conference on the Electronic Properties of Two-Dimensional Systems [Surf. Sci. 58 (1976); *ibid.* 73 (1978); and *ibid.* (in press)].
[3]M. J. Kelly and L. M. Falicov, Phys. Rev. B 15, 1974, 1983 (1977).
[4]Y. Takada, J. Phys. Soc. Jpn. 45, 786 (1978).
[5]M. J. Kelly, Solid State Commun. 27, 717 (1978).
[6]M. J. Kelly and W. Hanke (unpublished).
[7]P. C. Hohenberg, Phys. Rev. 158, 383 (1967); N. D. Mermin and H. Wagner, Phys. Rev. Lett. 17, 1133 (1966); T. M. Rice, Phys. Rev. A 140, 1889 (1965).
[8]F. Stern and W. E. Howard, Phys. Rev. 163, 816 (1967).
[9]L. J. Sham and M. Nakayama, Phys. Rev. B 20, 34 (1979).
[10]A. A. Lakhani and P. J. Stiles, Phys. Lett. A 51, 117 (1975).
[11]I. Eisele, H. Gesch, and G. Dorda, Solid State Commun. 18, 743 (1976); 20, 677 (1976); 22, 185 (1977).

[12]D. Tsui and G. Kaminsky, Solid State Commun. 20, 93 (1976).
[13]B. Vinter and A. W. Overhauser, Phys. Rev. Lett. 44, 47 (1980).
[14]D. Tsui and G. Kaminsky, Phys. Rev. Lett. 42, 595 (1979).
[15]See, for example, T. K. Lee, C. S. Ting, and J. J. Quinn, Solid State Commun. 16, 1309 (1975).
[16]M. L. Cohen, Phys. Rev. 134, A511 (1964).
[17]D. A. Kirzhnits, E. G. Maksimov, and D. I. Khomskii, J. Low Temp. Phys. 10, 79 (1973).
[18]L. P. Gorkov, Sov. Phys. JETP 7, 505 (1958).
[19]D. N. Zubarev, Sov. Phys. Usp. 3, 320 (1960).
[20]P. Morel and P. W. Anderson, Phys. Rev. 125, 1263 (1962).
[21]J. R. Schreiffer, *Superconductivity* (Benjamin, New York, 1964).
[22]C. H. Wu and W. Hanke, Solid State Commun. 23, 829 (1977).
[23]W. Hanke, Adv. Phys. 27, 287 (1978).
[24]D. A. Dahl and L. J. Sham, Phys. Rev. B 16, 651 (1977).
[25]In the context of Sec. V below [Eqs. (41) and (42)], we can write $\chi_0 = \sum_{m=-1}^{\infty} A_m(z) N_m(|\vec{q}|, \omega)\, A_m^*(z')$ with $A_m(z) = \xi_0(z)\xi_m(z)$ and further we have that $\chi = \sum_m A_m(z)(N_m^{-1} - V_{\text{Coul}})^{-1} A_m^*(z')$.
[26]F. Stern, Phys. Rev. Lett. 18, 546 (1967).
[27]J. M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, Cambridge, 1969).
[28]J. Bardeen and D. Pines, Phys. Rev. 99, 1140 (1955).
[29]M. Lax and J. J. Hopfield, Phys. Rev. 124, 115 (1961); H. W. Streitwolf, Phys. Status Solidi 37, K47 (1970); M. Lax and J. L. Birman, Phys. Status Solidi B 49, K153 (1972).
[30]W. Hanke and L. J. Sham, Phys. Rev. B 21, 4656 (1980).
[31]M. Lax, *Symmetry Principles of Solid State and Molecular Physics* (Wiley, New York, 1974).
[32]J. Bar-Sagi and W. Hanke, Ferroelectrics 16, 179 (1977).
[33]B. Vinter, Phys. Rev. B 13, 4447 (1976).
[34]D is of the order of 0.7 Ry for zone-center optic and acoustic phonons, and it is unlikely that corrections from the proximity of SiO_2 will dramatically enhance this.
[35]J. M. Luttinger and W. Kohn, Phys. Rev. 97, 869 (1955).
[36]Y. Takada, Ph.D thesis (University of Tokyo, 1978) (unpublished).
[37]J. Hubbard, Proc. R. Soc. London Ser. A 243, 336 (1957).
[38]B. B. J. Hede and J. P. Carbotte, Can. J. Phys. 50, 1756 (1972); D. N. Lowy and G. E. Brown, Phys. Rev. B 12, 2135 (1975).
[39]N. F. Berk and J. R. Schreiffer, Phys. Rev. Lett. 17, 433 (1966).
[40]M. Strongin, O. F. Kammerer, J. Crow, R. S. Thompson, and H. L. Fine, Phys. Rev. Lett. 20, 922 (1968).
[41]L. G. Aslamov and A. I. Larkin, Sov. Phys. Solid State 10, 875 (1968).
[42]C. S. Koonce, M. L. Cohen, J. F. Schooley, W. R. Hosler, and E. R. Pfeiffer, Phys. Rev. 163, 380 (1967).
[43]G. Dorda, H. Gesch, and I. Eisele, Solid State Commun. 20, 429 (1976).
[44]M. J. Kelly and L. M. Falicov, J. Phys. C 10, 4735 (1977); Surf. Sci. 73, 303 (1978).
[45]C. C. Grimes, Surf. Sci. 73, 379 (1978).
[46]G. Meissner, H. Namaizawa, and M. Voss, Phys. Rev. B 13, 1370 (1976).
[47]J. Binder, K. Germanova, A. Huber, and F. Koch, Phys. Rev. B 20, 2382 (1979); R. Silberman and G. Landwehr, Solid State Commun. 16, 1055 (1975).