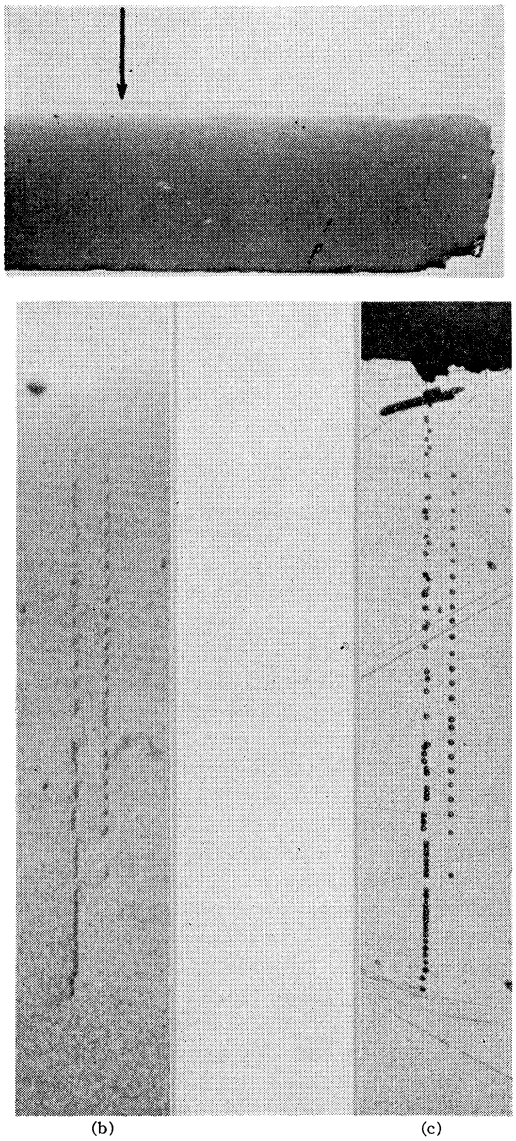

FIG. 3. A B-B photograph of the repolished $(11\bar{2})$ surface shows two rows of spots which correspond with pits on the formerly etched surface. (a) B-B image optically magnified twenty times; (b) B-B image optically magnified 115 times; (c) Light micrograph of the etched $(11\bar{2})$ surface corresponding to the area in Fig. 3(b). Magnification 100×.

on a high resolution spectrographic plate. The B-B photograph is shown at two magnifications in Fig. 3(a), (b). A light micrograph of the etched area corresponding to Fig. 3(b) is given in Fig. 3(c). The correspondence of B-B spots and etch pits is evident.

The extra diffracted intensity which renders visible the dislocations in the B-B image is probably due to a reduction in x-ray extinction induced by the perturbation of lattice periodicity normal to the reflection planes at dislocation sites.[6] Experimental conditions were chosen so as to maximize the effect of lattice distortion, due to the dislocations, upon the B-B image. Since the leg of the dislocation loop which emerges from the $(11\bar{2})$ surface is largely made up of screw dislocations with $[01\bar{1}]$ Burgers vectors, the loss of lattice periodicity at the dislocation sites would be expected to be high in the $[01\bar{1}]$ direction. The extinction effect is, therefore, expected to be large for the $(02\bar{2})$ reflection.

As a test for this hypothesis the specimen was mechanically polished on the $(1\bar{1}0)$ surface and a B-B photograph was made (from that surface) using the $(2\bar{2}0)$ reflection. It was found that spots, corresponding to surface pits which developed on subsequent etching, did appear on the B-B photograph but were much less distinct than those observed in the $(02\bar{2})$ reflection from the $(11\bar{2})$ surface. This result is consistent with the idea that the dislocations in the leg emerging from the $(1\bar{1}0)$ surface have a small $[2\bar{2}0]$ component of Burgers vector.

Conclusion.—By means of x-ray reflection microscopy, emergent screw dislocations can be seen on the polished surface of a single crystal of silicon. Since the method depends upon x-ray extinction, the best contrast is obtained when a reflection is used which has a large component of the dislocation Burgers vector normal to the reflecting planes.

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Variation Theorem for Excited States*

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THE variation theorem[1] has proved of utmost practical importance in its application to the lowest state of each symmetry type in a given system. In addition, it has had limited applicability to excited states because of a theorem first proved by Hylleraas and Undheim[2] and later by MacDonald,[3] that if the roots of the secular equation, J_i, are ordered such that $J_0 \leqslant J_1 \leqslant \cdots \leqslant J_n$, then each such root is an upper bound to the corresponding exact eigenvalue: $J_i \geqslant E_i$. Eckart[1] has analyzed the mean square deviation of the lowest eigenvector ϕ_0 from the true eigenfunction, ψ_0,

and has shown that

$$\int|\phi_0-\psi_0|^2d\tau=\alpha^2\leqslant(J_0-E_0)/(E_1-E_0). \quad (1)$$

A similar analysis has not seemed possible for excited states, however, and it has been generally believed that in order to obtain a good excited state function, one must explicitly require it to be orthogonal to the exact ground state function.

In this Letter we analyze the error in a nondegenerate first excited state, but as we shall show in a subsequent publication the results are easily generalized. We conclude that such an explicit orthogonalization is not at all necessary. Let ϕ_0 and ϕ_1 be the two lowest normalized eigenvectors of a linear variation problem. Then

$$\int\phi_0\phi_1d\tau=0 \quad \text{and} \quad \int\phi_0H\phi_1d\tau=0.$$

By the usual expansion theorem, $\phi_0=\sum_i a_{0i}\psi_i$; $\phi_1=\sum_i a_{1i}\psi_i$. Following precisely the Eckart development for the ground state, one arrives at the error expression for the first excited state:

$$\int|\phi_1-\psi_1|^2d\tau=\beta^2\leqslant[(J_1-E_1)+a_{10}^2(E_2-E_0)]/(E_2-E_1). \quad (2)$$

To find a limit on a_{10}, we form a new normalized function $\Phi=\mu_0\phi_0+\mu_1\phi_1$ with μ_0 and μ_1 arbitrary multipliers subject to the constraint $\mu_0^2+\mu_1^2=1$. It is straightforward to show[4] that

$$\int\Phi H\Phi d\tau=\mu_0^2J_0+\mu_1^2J_1=\sum_k c_k^2E_k,$$

where $c_k=\mu_0a_{0k}+\mu_1a_{1k}$. Now we choose $\mu_0=a_{10}/(a_{00}^2+a_{10}^2)^{\frac{1}{2}}$, $\mu_1=-a_{00}/(a_{00}^2+a_{10}^2)^{\frac{1}{2}}$, so as to make c_0 vanish. We then have that

$$\mu_0^2J_0+\mu_1^2J_1=\sum_{k\geqslant1}c_k^2E_k\geqslant E_1.$$

Substituting the chosen values for μ_0 and μ_1, and rearranging the equation, we find[5] that

$$a_{10}^2\leqslant a_{00}^2(J_1-E_1)/(E_1-J_0)\leqslant(J_1-E_1)/(E_1-J_0).$$

We finally have from (2),

$$\beta^2\leqslant\{(J_1-E_1)/(E_2-E_1)\}\{1+(E_2-E_0)/(E_1-J_0)\}. \quad (3)$$

Since β^2 is in the limit proportional to (J_1-E_1), one can make β^2 as small as one pleases by making J_1 sufficiently close to E_1 without simultaneously requiring that $J_0=E_0$.

As an example, we can compare results we have obtained for helium using 20 base functions with a single orbital exponent of 2.2 (set A), and 1.05 (set B),[6] with those of Green *et al.*,[7] using 4 base functions composed from hydrogenlike functions with $Z=2$ (set C). Using $E_0=-2.90372$, $E_1=-2.14600$, and $E_2=-2.06130$, we find the results summarized in Table I.

TABLE I. Illustrative comparison of wave-function accuracy.

	Set A	Set B	Set C
J_0	−2.90123	−2.88245	−2.84139
J_1	−1.81045	−2.13392	−2.13690
α^2 [Eq. (1)]$\leqslant$	0.0033	0.0281	0.0823
β^2 [Eq. (3)]$\leqslant$	8.380[a]	0.306	0.238

[a] This meaningless figure from Eq. (3) arises because $J_1\gg E_2$. From other considerations, $0\leqslant\beta^2\leqslant2$.

Although the excited state wave functions are considerably more in error than the ground state functions in these particular calculations, largely because (E_2-E_1) is so small, the results clearly demonstrate (1) the desirability of using different sets for different states and (2) the practicability of obtaining good excited state wave functions without using unduly large secular equations.

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Resonant Absorption of Sound in Metals

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ULTRASONIC attenuation in metals at low temperatures may oscillate with the strength of an applied magnetic field.[1–3] Although it has been generally considered that this phenomenon might arise from a spatial coherence of the electron orbits with the periodic fields associated with the acoustic wave, the mechanism has remained obscure. The purpose of this note is to point out that, in ideal metals, magnetic oscillations arise from resonance of the electronic momentum current with the (negative) acoustic velocity gradient, and to deduce from this principle the elementary resonance rules observed by Morse, Bohm,