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Atomic physics of channeled particles*

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The problem of the modification of the atomic structure of a hydrogenlike atom or ion as it is channeled through a thin single crystal is formulated. For high-velocity channeling there is an approximate decoupling of the internal atomic motion and the solid state. This allows a single-particle equation to be written for the modified hydrogen atom. The effective potential in the equation is absorptive because of the ionization of the atom due to collisions with the solid. Effects of both single-particle and collective excitations are discussed. An approximate Schrödinger equation is derived for the atom, and solved approximately for the distorted states.

I. INTRODUCTION

The channeling of atomic particles in single crystals was predicted[1] and discovered[2] some time ago. Since then it has been explored and used as a tool for various kinds of physical applications.[3] However, in each of these emphasis has been placed upon the channeled motion of the atomic particle as a whole. As far as we know, there has been no investigation of the motion of the internal degrees of freedom (if any) of the channeled particle (c.p.). This is the problem we wish to turn to here.

Clearly, this is an extremely complicated many-body problem since the c.p. can be considered an imbedded impurity in the crystal, and then the full complexity of the solid-state many-body problem enters. There are, however, two free parameters which allow us to approximately decouple the internal motion of the c.p. from the rest of the solid and thereby reduce the problem of the motion of the internal degrees of freedom to that of an atom in an external potential.

The first parameter is v, the velocity of the c.p. as it moves through the solid. As this gets sufficiently large, the interaction of the rapidly translating electrons on the c.p. with the solid goes down and may be treated as a small perturbation on the usual atomic motion. The second parameter is the nuclear charge of the c.p. For simplicity we shall deal only with hydrogenlike c.p.'s with a nucleus of charge Ze. As Z gets larger the structure of the c.p. becomes more compact with a greater binding energy which, in effect, makes the coupling of the internal degrees of freedom of the c.p. to the solid smaller. Again, for sufficiently large Z the effect of the solid can be treated as a small perturbation on the motion of the internal degrees of freedom of the c.p.

There are other parameters which could also be exploited to this end: for example, the type of solid and the channeling direction of the c.p. These both have the effect of controlling the size of the channel through which the particle moves. We shall not discuss them here, since the freedom in Z already gives us sufficient control over the size of the atom. This parameter is in effect a scaling of the size of the channel.

We seek a decoupling of the c.p. and the solid which will allow all the solid effects to be subsumed in an effective potential for the atom. This potential must have an absorptive part to account for the decay of the atom due to ionizing collisions with the solid. It must also be time dependent to allow for the oscillations of the c.p. as it moves down the channel and to allow for the rapid variation in potential by the individual atoms in the solid as the c.p. moves.

We shall neglect this second effect of time dependence, since its frequency $\sim v/d$, where d is the atomic spacing in the channeling direction, will be high for large v. For sufficiently large v this will be a frequency higher than the atomic one, so that the oscillation of the potential will couple only weakly to the internal motion of the c.p. In addition, the amplitude of the oscillation will be small compared to other potentials, so the effect will be doubly weak. This neglect is just the replacement of the "beaded necklace" of atoms in the channeling direction by a continuous "string."

The other introduction of time dependence comes from the oscillatory motion of the c.p. in the channel. The dynamics of the nucleus of the c.p., henceforth referred to as the proton, are essentially classical. That is, the proton's de Broglie wavelength is so small that the variation of the effective potential over its wave packet is negligible and therefore its motion may be treated classically.

In addition, we shall treat it as a prescribed motion, since the effect of the internal degrees of freedom on the motion of this heavy particle is negligible and the dynamics of heavy-particle channeling is well understood.

We further restrict our attention to "proper channeling," the case where the c.p. remains trapped between a given group of strings in its passage through the crystal. In that case the c.p. moves down the channel while performing transverse oscillations within the channel. The frequency of these oscillations is of the order

$$\omega_T \sim (8V/Md^2)^{1/2},$$

where M is the proton mass, d the channel spacing, and V the potential which traps the c.p. in the channel. Typically, V is of the order of a few volts and ω_T is low compared to the frequency of the internal motion of the c.p. This motion can therefore be treated adiabatically. That is, we could solve for the internal motion in the c.p. for various transverse positions of the proton in the channel and then correct for the small effect of the transverse motion of the proton by standard adiabatic theory. We expect no startling effects from this motion, so for the first calculation of this phenomenon we shall neglect the transverse oscillation of the proton and consider only the case of a proton moving in a straight line down the exact midpoint of a channel.

With these approximations we expect that the effective potential of the solid on the c.p. is time independent.

II. THEORY

Consider a fast hydrogenlike c.p. moving through an otherwise cold single crystal. The fast electron of the c.p. will scatter off the slow particles of the solid via the Coulomb interaction which favors small momentum- (or energy-) transfer collisions. These collisions can occur coherently and many of them will distort the internal state of the c.p. Each of these weak collisions will have associated with it a recoiling solid electron which will have only a low-lying excitation above its original state. Occasionally the fast electron will undergo a hard collision with the solid, transfering a momentum (or energy) to the solid which is larger than the typical momenta (or energy) in its bound state. This will result in an ionization of the c.p.

From this discussion we see that it is reasonable (but not rigorous) to associate a group of low-lying excitations of the solid with channeling of the bound structure of the c.p. We call these states the channeling subspace of the solid. They are defined (in a single-particle sense) so that no one of them has an excitation with an energy or momentum greater than some value. The value will depend upon the details of the bound state of the c.p., which are not yet known, so the procedure is a self-consistent one.

If the c.p. electron suffers a strong collision and is removed from the fast proton, the proton will proceed down the channel and may collide with another electron of the solid and capture it, thereby reforming the bound state. It might be thought that this regenerative process would be reflected in an anti-absorptive term in the effective potential. This is not the case, since the process requires first a hard collision to ionize and then a very hard collision to recapture. The latter is very hard since it takes an essentially stationary electron and raises it to the (high) speed of the proton. The process yields a beam of c.p.'s which is incoherent with the original one, so that it is a regeneration of the beam probability—not of the state amplitude—which occurs. The mathematics described below has no such anti-absorptive terms in the effective potential.

Finally, we neglect the Pauli principle between the electron of the c.p. and the electrons of the solid. This is a good approximation because of the high momentum (mv) of the fast electron in the direction of the channel and its low momentum in the perpendicular directions. Its wave function is therefore effectively orthogonal to the electrons of the solid.

Our starting point is the equation

$$\left(i\frac{\partial}{\partial t} - H(A,S)\right)\Psi(A,S,t)=0\,, \tag{2.1}$$

where A and S are atomic and solid coordinates, respectively, and $H(A,S)$ is the full Hamiltonian of the atom and solid, except that the proton's motion is prescribed to be an unaccelerated motion with velocity v down the middle of the channel. The next step is the splitting of the Hilbert space of the solid into the channeling subspace described above and the remainder. If we define a projection operator onto the channeling subspace C,

$$P' = \sum_{n\in C} U_n(S)U_n^*(S')\,, \tag{2.2}$$

where the U_n are wave functions of the solid, then we obtain

$$P'\Psi = \sum_{n\in C} \psi_n(A,t)U_n(S) \tag{2.3}$$

and a set of coupled equations for the $\psi_n(A,t)$. This implies that we can distinguish between different solid states (in C) and their different effects upon the atom. This is in principle true, but since the states of the solid are dense on the scale set by the energy levels of the atom, it is not a bad approximation to say that that atom takes on some average state within C and that the individual states of (2.3) are indistinguishable. This may be further justified by noting that the quasielastic scatterings represented by the different channels in Eq. (2.3) are not necessarily incoherent with each other, so that amplitudes may be added. The condition for this is derived as follows: Suppose that the fast electron collides with the solid and loses an energy $\Delta\epsilon$ and then suffers a second collision a time d/v later. If the condition

$$\Delta\epsilon < \hbar v/d$$

is satisfied then the uncertainty in the phases of the different channels in Eq. (2.3) overlaps and the amplitudes can be added directly. We then replace (2.3) by

$$P\Psi = N_C^{-1/2}\psi(A,t)\sum_{n\in C} U_n(S)\,, \tag{2.4}$$

which implies

$$P = N_C^{-1}\sum_{n,m\in C} U_n(S)U_m^*(S')\,, \tag{2.5}$$

where N_C is the number of states in C. This average state approximation is a familiar one in the theory of the nuclear optical model.[4]

Having chosen P the procedure for isolating $\psi(A,t)$ is a familiar one from scattering theory. The resulting equation is

$$\left(i\frac{\partial}{\partial t} - \mathcal{H}\right)\psi = 0\,, \tag{2.6}$$

where

$$\mathcal{H} = PHP + PHQG_{QQ}(t,t')QHP\,, \tag{2.7}$$

where

$$Q = 1 - P \tag{2.8}$$

and the intermediate Green's function is defined by

$$\left(i\frac{\partial}{\partial t} - QHQ\right)G_{QQ}(t,t') = \delta(t-t') \tag{2.9}$$

and causal boundary conditions. We may conveniently introduce the transform of ψ by

$$\psi(A,E) = \frac{1}{2\pi}\int_0^\infty dt\, e^{+iEt}\psi(A,t) \tag{2.10}$$

with the initial condition

$$\psi(A,t)\big|_{t=0} = \psi_0(A)\,, \tag{2.11}$$

which satisfies

$$P\left(E - H - H\frac{Q}{E + i\eta - QHQH}\right)P\psi(A,E) = \frac{i}{2\pi}\psi_0\,. \tag{2.12}$$

If we now define

$$H = H(A) + H(S) + V(A,S)\,, \tag{2.13}$$

where the successive terms are the Hamiltonian of the isolated atom, of the isolated solid, and the interaction between the two, then we may write

$$PHP = \left(H(A) + N_C^{-1}\sum_{n\in C}\nu_n + N_C^{-1}\sum_{n,m\in C} V_{nm}(A)\right)P \tag{2.14}$$

and the ν_m are the energy levels of the solid and

$$V_{nm}(A) = \langle n|\,V(A,S)\,|m\rangle\,. \tag{2.15}$$

If we define

$$W = E - N_C^{-1}\sum_{n\in C}\nu_n \tag{2.16}$$

then W will be the energy of the channeled pair, i.e., the total energy minus the average energy of the solid in the channeling space.

The equation may now be written

$$[W - h(A)]\,\psi = \frac{i}{2\pi}\psi_0\,, \tag{2.17}$$

where

$$h(A) = H(A) + N_C^{-1}\sum_{n,m\in C} V_{nm}(A) + \mathcal{V}\,, \tag{2.18}$$

where

$$\mathcal{V} = N_C^{-1}\sum_{n,m\in C}\langle n|\,V\frac{Q}{E + i\eta - QHQ}V\,|m\rangle\,. \tag{2.19}$$

This term contains the dynamics of the virtual ionization of the c.p. and the absorptive part of the potential. That it is absorptive, i.e., that $(\mathcal{V} - \mathcal{V}^\dagger) = -iX$, where X is a non-negative definite operator, may easily be shown by expanding the intermediate part of (2.19) in eigenfunctions of QHQ.

Equation (2.17) may be formally solved as

$$\psi(E) = \frac{i}{2\pi}(W - h)^{-1}\psi_0 \tag{2.20}$$

and then transformed back to the time argument by the inverse of (2.10). It is clear then that for large values of time the eigenfunctions of h whose eigenvalues lie closest to the real axis in W space will be dominant in ψ. We are therefore led to examine the eigenfunctions and eigenvalues of h.

III. CONSTRUCTION OF h

The effective single-particle Hamiltonian in the channeling space is given by (2.18), which we repeat here:

$$h(A) = H(A) + N_C^{-1}\sum_{n,m\in C} V_{nm}(A) + \mathcal{V}\,. \tag{3.1}$$

In the frame of reference of the unaccelerated proton the first term is

$$H(A) = -\frac{1}{2m}\nabla_r^2 - \frac{Ze^2}{r}. \tag{3.2}$$

The second term in (3.1) is the potential due to the solid when it is frozen into some average state in the channeling subspace. This average state is defined by (2.4):

$$U_{\text{AVE}}(s) = N_C^{-1/2} \sum_{n \subset C} U_n(S). \tag{3.3}$$

Viewed this way, this potential is a simple generalization of the static potential which occurs in scattering problems. We have made formal calculations of this potential with the result that for a Slater-determinant approximation for the solid wave functions the off-diagonal elements vanish in the limit where the number of solid particles becomes large and the potential can be written

$$V_S(r) = e^2 \int d^3x\, n(x) |\vec{r} - \vec{x}|^{-1} + \sum_l Z_2 e^2 |\vec{r} - \vec{R}|^{-1}, \tag{3.4}$$

where $n(x)$ is an average electron density in the channeling subspace and the second term represents the potential due to the fixed nuclei of the solid. One could attempt a further evaluation of (3.4) in terms of localized orbitals and Bloch states for the electron, but we will not do so since that problem is outside the scope of this work and the result, if we had it, would be too complicated to use in our subsequent numerical work. We shall therefore approximate V_S by as reasonable a phenomenological potential as we can handle in our calculations.

The potential $\mathcal{V}$ given in (2.19) is

$$\mathcal{V} = N_C^{-1} \sum_{n, m \in C} \langle n | V \frac{Q}{E + i\eta - QHQ} V | m \rangle . \tag{3.5}$$

It represents the coupling of the channeling space to the remaining part of the Hilbert space of the solid, Q. It is absorptive due to the fact that the Q subspace is energetically accessible, i.e., that ionization of the c.p. is possible. Calculation of $\mathcal{V}$ from first principles is a truly formidable task which we will not attempt here. Its Hermitian part will be lumped with V_S, which is also Hermitian and treated phenomenologically. Its absorptive part can be related to the ionization cross section of the c.p. as follows.

The absorptive part of $\mathcal{V}$ ($\mathcal{V}_I$) is related to the change in density of the c.p. through flux conservation with the result

$$\frac{\partial}{\partial t} \int |\psi|^2 d^3r = -2 \int \psi^* \mathcal{V}_I \psi \, d^3r = -\Gamma \int |\psi|^2 d^3r, \tag{3.6}$$

where Γ is the width of the state.

The loss of the c.p. flux takes place only through ionization, since we assume only a single bound state of the c.p. This is expressed by

$$\frac{\partial}{\partial t} \int |\psi|^2 d^3r = -n_e \sigma_I v \simeq -\Gamma, \tag{3.7}$$

where n_e is the electron density of the solid, σ_I is the ionization cross section of the c.p. due to scattering off the electrons in n_e, and v is the velocity of the electron of the c.p. relative to the colliding electron in n_e. In the limit of high energy channeling v is just the velocity of the c.p. and σ_I can be obtained by an impulse approximation. Combining (3.6) and (3.7) we get

$$\int \psi^* \mathcal{V}_I \psi = n_e \sigma_I v . \tag{3.8}$$

If σ_I were known this would be a constraint on $\mathcal{V}_I$ in terms of the bound-state wave function ψ. Since all potentials are treated phenomenologically one could think of postulating a local $\mathcal{V}_I$ proportional to n_e with a coefficient determined by (3.8). This coefficient would depend upon the bound-state wave function which would have to be determined self-consistently with Eq. (2.12). This procedure will not be followed here. Instead we shall treat $\mathcal{V}_I$ as a perturbation on the rest of the equation. This is reasonable since we are interested in thin single crystals in which the probability of survival of the bound c.p. is high. In addition we can think of the nuclear charge of the c.p., Z, as a parameter and it is evident that for large Z the effect of $\mathcal{V}_I$ will be small. Then in lowest-order perturbation theory the only matrix element of $\mathcal{V}_I$ which will enter is the one appearing in (3.8) so that the calculation of $\mathcal{V}_I$ is replaced by a calculation of σ_I.

There are many techniques for the calculation of the ionization of complex bound states by fast electrons. One of the simpler and more accurate ones is the classical impulse approximation of Gryzinski.[5] At high impact velocities the result is[6]

$$\sigma_I = \frac{2\pi e^2}{m v^2}\left(I_0^{-1} - E_0^{-1}\right) \quad \text{for } E_0 \geq I_0$$

$$= 0 \qquad \text{for } E_0 < I_0, \tag{3.9}$$

where I_0 is the binding energy of the c.p. and E_0 is the kinetic energy of one of the solid electrons in the rest frame of the c.p.

The binding energy I_0 is not yet known, so we are faced with the self-consistent problem of solving the equation of motion to determine I_0 while $\mathcal{V}_I$ depends upon I_0 through (3.8) and (3.9).

Returning to (3.7) for a moment, we have inserted only σ_I, the ionization cross section, as the mechanism for extracting flux from the bound state of the c.p. If there is more than one bound state of the c.p. then ψ occurring in the equation of this section should be interpreted as the ground state of the c.p. and the flux loss in (3.7) should also include the excitation cross section as well as σ_I. In principle this would require the solution of the equations for all bound states self-consistently, the coupling coming from the excitation cross section which will depend upon the details of the various bound states. If we had to resort to this it would probably be simpler to attempt a direct construction of $\mathcal{V}$ from (3.5). We may, however, incorporate these effects within the spirit of the calculation described above by simply modifying σ_I in (3.9) so that I_0 is now interpreted as the excitation energy of the c.p. rather than the ionization energy.

So far we have been concerned only with single-particle excitations of the solid. However, the fast c.p. can also excite collective modes of the solid which participate in the P- and Q-space part of the discussion just as the single-particle excitations do. We shall use electron-plasma wave collective excitations as an example. Each member of the fast pair moving through the plasma leaves behind a wake since they are moving supersonically. This will cause a change in the interparticle potential due to the presence of the polarized medium, a kind of screening. If the motion were slow compared to the plasma relaxation time this would yield the usual exponentially screened potential for the pair interaction, which might eliminate the binding of the pair. However, since the translational motion of the pair is fast the c.p. outruns the screening and leaves a Cherenkov wave.

We shall illustrate this with a calculation which treats the plasma semiclassically. The quantum case is slightly more complicated and illustrates no new effects. We follow the original calculation of Neufeld and Ritchie,[7] neglecting relativistic effects in the plasma.

The plasma is treated by a linearized Vlasov equation[8]

$$\left(\frac{\partial}{\partial t}+\vec{u}\cdot\nabla\right)f_1=-\frac{e}{m}\nabla\phi\cdot\nabla_u f_0(u)\,, \tag{3.10}$$

where the electric potential is obtained from the Poisson equation

$$\nabla^2\phi=-4\pi(\rho_{\rm ex}+\rho_{\rm in})\,, \tag{3.11}$$

where

$$\rho_{\rm in}=-e\int d^3u\, f_1 \tag{3.12}$$

and $\rho_{\rm ex}$ is the charge density of the c.p.,

$$\rho_{\rm ex}=e[Z\delta(\vec{x}-\vec{v}t)-\delta(\vec{x}-\vec{r}(t)-\vec{v}t)]\,, \tag{3.13}$$

where $\vec{r}(t)$ is the coordinate of the electron relative to the proton in the Heisenberg representation. Solution of this set is most easily accomplished by first Fourier transforming all unknowns and then solving algebraically.[7,8] The result is

$$\phi(\vec{x},t)=4\pi\int\frac{d^3k}{k^2}d\omega\,\epsilon^{-1}(\vec{k},\omega)e^{i(\vec{k}\cdot\vec{x}-\omega t)}\tilde{\rho}_{\rm ex}(\vec{k},\omega)\,, \tag{3.14}$$

where

$$\tilde{\rho}_{\rm ex}(\vec{k},\omega)=\int\frac{d^3x\,dt}{(2\pi)^4}\,e^{-i(\vec{k}\cdot\vec{x}-\omega t)}\rho_{\rm ex}(\vec{x},t) \tag{3.15}$$

and $\epsilon(\vec{k},\omega)$ is the dielectric function of the plasma

$$\epsilon(\vec{k},\omega)=1-\frac{\omega_p^2}{k^2}\int d^3u\,\frac{\vec{k}\cdot\nabla_u f_0(u)}{\vec{k}\cdot\vec{u}-\omega-i\nu}\,, \tag{3.16}$$

where ω_p^2 is the plasma frequency.

The (uniform) zero-order distribution function is normalized so that

$$\int d^3u\, f_0(u)=1\,. \tag{3.17}$$

Inserting (3.13) into (3.14) and (3.15) yields

$$\begin{aligned}\phi(\vec{x},t)=&\frac{eZ}{2\pi^2}\int\frac{d^3k}{k^2}\,\epsilon^{-1}(\vec{k},\vec{k}\cdot\vec{v})\exp[i\vec{k}\cdot(\vec{x}-\vec{v}t)]\\&-\frac{e}{4\pi^3}\int\frac{d^3k}{k^2}\,d\omega\,dt'\,\epsilon^{-1}(\vec{k},\omega)\\&\times\exp\{i\vec{k}\cdot[\vec{x}-\vec{r}(t')-\vec{v}t']+i\omega(t-t')\}\end{aligned} \tag{3.18}$$

where the first term arises from the proton and the second from the electron. We shall need $\phi(\vec{r},t)$, which is the potential at the electron's location. The second term has a self-energy term due to the electron's interaction with itself which must be subtracted away. This is accomplished by simply subtracting away the *vacuum* self-energy, $\epsilon=1$, so that the second term in (3.18) must be modified by the replacement[9]

$$\epsilon^{-1}(\vec{k},\omega)\rightarrow\epsilon^{-1}(\vec{k},\omega)-1\,. \tag{3.19}$$

One can calculate the force on the electron in the frame of the proton from

$$F=e\nabla\phi|_{\vec{x}=\vec{r}+\vec{v}t}\,, \tag{3.20}$$

which yields

$$\vec{F}=\frac{ie^2Z}{2\pi^2}\int\frac{d^3k}{k^2}\vec{k}\epsilon^{-1}(\vec{k},\vec{k}\cdot\vec{v})e^{i\vec{k}\cdot\vec{r}}$$

$$-\frac{ie^2}{4\pi^3}\int\frac{d^3k}{k^2}d\omega\,dt'\vec{k}(\epsilon^{-1}-1)$$

$$\exp[i\vec{k}\cdot(\vec{r}(t)-\vec{r}(t')+\vec{v}(t-t'))]+i\omega(t-t')]. \tag{3.21}$$

If the period associated with the internal motion of the c.p. is larger than the response time of the plasma then one can expand $r(t')$ in the second term

$$r(t')=r(t)+(t'-t)\hat{r}(t)+\ldots \tag{3.22}$$

and perform the t' and ω integrals with the result

$$\vec{F}=\frac{ie^2Z}{2\pi^2}\int\frac{d^3k}{k^2}\vec{k}\epsilon^{-1}e^{i\vec{k}\cdot\vec{r}}-\frac{ie^2}{2\pi^2}\int\frac{d^3k}{k^2}\vec{k}[\epsilon^{-1}(\vec{k},\vec{k}\cdot\vec{v})-1], \tag{3.23}$$

where we have used the fact that the internal motion is much slower than the translational motion of the c.p. If we use the well-known property of the dielectric function

$$\epsilon(\vec{k},\omega)=\epsilon^*(\vec{k},-\omega), \tag{3.24}$$

the force can be shown to be real.

The last term in (3.23) is logarithmically divergent since the integrand behaves as k^{-1} for large k. The inclusion of k greater than the interparticle spacing is unphysical and should be excluded. Therefore the integrals will be cut off at a maximum value $k \sim d^{-1}$.

For the purposes of our equation (3.1) we need a potential energy from which $\vec{F}$ can be derived:

$$\vec{F}=-\nabla V_{Pl}$$

or

$$V_{Pl}=-\frac{e^2Z}{2\pi^2}\int'\frac{d^3k}{k^2}\epsilon^{-1}(\vec{k},\vec{k}\cdot\vec{v})(e^{i\vec{k}\cdot\vec{r}}-1)$$

$$+\frac{ie^2}{2\pi^2}\int'\frac{d^3k}{k^2}\vec{k}\cdot\vec{r}(\epsilon^{-1}-1), \tag{3.25}$$

which is the result we sought. (The primes on the integrals indicate the cutoff.) It should be pointed out that the expansion (3.22) was necessary in order to get (3.25). Otherwise the "potential" would depend on the history of the motion.

Note that the last term in (3.25) acts as a dc electric field which vanishes when $\operatorname{Im}\epsilon=0$, i.e., when there is no absorption. For large v it is of order v^{-2} and so small. The first term contains the unshielded electron-proton interaction and its modification due to the interaction of the electron with the proton wake. We are interested in the potential only for small r, of the order of the size of the c.p. bound state. In that case the new terms, obtained earlier by Neufeld and Ritchie,[7] are of order v^{-1} or smaller. As a first approximation these may then be dropped.

It might be thought that part of the force (3.23) acts to retard the center of mass motion of the c.p. and the remaining part on the internal degrees of freedom. This can be checked by repeating the above calculation with both electron and proton treated dynamically. That is, the proton's motion is not prescribed. In that case (with the approximation $m/M\simeq 0$) we still get (3.23) and (3.25), but in addition we get the force acting on the c.p. as a whole:

$$F_{cm}=-\frac{2ie^2}{\pi^2}\int\frac{d^3k}{k^2}\vec{k}\epsilon^{-1}(\vec{k},\vec{k}\cdot\vec{v})\sin^2\left(\frac{\vec{k}\cdot\vec{r}}{2}\right). \tag{3.26}$$

The force acting on the center of mass of the c.p. depends on the orientation of the relative coordinate in both magnitude and direction. It also is real and vanishes when $\operatorname{Im}\epsilon=0$, as may be seen by using (3.24).

Finally we turn to the Q-space contribution of the collective modes. The single-particle excitations form a complete set for the solid. Addition of the collective modes makes the set of states of the solid over complete. However, it is useful to work with this over complete set since collective modes are not readily described by single-particle excitations. The Q-space excitations represent states of the solid which have carried off sufficient energy momentum from the c.p. to ionize it. We anticipate that the c.p. will have a bound state of atomic dimensions with energy and momentum components on the atomic scale. In that case the Q space will have single-particle or collective excitations with a spectrum which is greater than something set by the bound state of the c.p. (See the discussion at the beginning of Sec. II.) There is a redundancy in description in single-particle and collective modes, and excitations with sufficiently high energy momentum to be in Q space are better described by single-particle states. That is, collective excitations this high in the spectrum will decay rapidly to single-particle excitations, or, said another way, the coupling of the fast electron to higher excitations is through single-particle rather than collective modes. Then, the contribution to Q space from collective modes will be small and neglected.

At this point we may ask just how high the energy or velocity of the c.p. must be in order to satisfy the above requirements and the condition that the width be much smaller than the energy of the state. This last one is the most stringent requirement. It may be written

$$E_B>\Gamma=n_e\sigma_I v, \tag{3.27}$$

where E_B is the binding energy of the c.p. and is obtained in Sec. IV. The use of (3.9) in the high-velocity limit results in

$$\frac{\Gamma}{E_B}=2\pi(n_e a_0^3)\left(\frac{2\mathrm{Ry}}{E_B}\right)^2\frac{1}{\bar{v}}\ll 1\,, \tag{3.28}$$

where $\bar{v}=(\hbar/e^2)v$ and n_e is the electron density *in the channels* so that $n_e a_0^3<1$. Approximate values of E_B are obtained in Sec. IV, where it is shown to be less than 1 Ry. The result from (3.28) is then that $\bar{v}$ must be much greater than unity. This justifies our neglect of the plasma effects given in (3.25).

IV. NUMERICAL WORK

We now turn to the numerical problem of obtaining the eigenfunction of

$$[E-h(A)]\psi=0\,, \tag{4.1}$$

whose eigenvalue lies closest to the real axis. We then interpret this as the longest-lived state of the c.p. The procedure, outlined above, will be to deal with the Hermitian part of $h(A)$ first and then treat the absorptive part by first-order perturbation theory. Therefore the zero-order problem will yield only real eigenvalues. If we consider the Hermitian part of $h(A)$ we see that it contains the attractive potential of the proton and the screened strongly attractive potentials of the various strings. The latter are purely attractive since the Pauli principle is negligible for the combination of the fast electron and the electrons of the solid. From this we see that the zero-order solution will be either hydrogenlike states centered on the proton, or other kinds of states centered on the attractive strings. The latter may under some circumstances be more tightly bound than those centered on the proton. However, these will not be the states of interest since their maximum density will occur at the strings, so the absorptive part of the potential, $\mathcal{V}_I$, will have a large effect on them. That is, the approximation that the effect of $\mathcal{V}_I$ is small is expected to break down for states of this kind so that their true eigenvalues will be highly absorptive. Therefore, in treating the problem in zero order one cannot simply pick out the ground state of the problem as the one of interest. Instead, we must pick out the one which is most tightly bound to the proton. We do this by evaluating

$$\mathcal{E}_S^B=\langle\psi_S|\,H(A)\,|\psi_S\rangle \tag{4.2}$$

for each of the solutions (denoted by s) of (4.1) and choosing the one with the smallest $\mathcal{E}_S^B$. Here $H(A)$ is the hydrogenic Hamiltonian given by (3.2). Since this state will be the one most centered on the proton (away from the strings), it will also have the smallest decay rate, Γ.

The problem that remains is one of getting the solution to the eigenfunction and eigenvalues of the Hermitian part of $h(A)$, (3.1). We shall represent the "static potential" (3.4) plus the real part of $\mathcal{V}$ by the phenomenological form

$$\bar{V}=V_S+\mathrm{Re}\,\mathcal{V}=\sum_{\text{strings}}\int\frac{d\zeta}{a}\sum_i\frac{-z_i e^2}{|\vec{\mathrm{r}}-\vec{\mathrm{R}}|}e^{-\lambda_i|\vec{\mathrm{r}}-\vec{\mathrm{R}}|} \tag{4.3}$$

where a is the lattice parameter,

$$\vec{\mathrm{R}}=\vec{\mathrm{b}}+\hat{a}_z\zeta\,, \tag{4.4}$$

and $\vec{\mathrm{b}}$ is the coordinate of a string relative to the proton in a plane perpendicular to the direction of motion of the proton. The coordinate ζ is along the string and the integral $\int d\zeta/a$ is an average along that direction. The sum over i can be used to give a different term for each shell of the atom in the solid. That is, the sum of the attractive potential of the nucleus and the repulsive potential of the ith shell would produce a screened attractive part of strength z_i and screening length λ_i. The inclusion of many terms (strings and shells) makes our computation more complicated than seems warranted at this stage, so we have used a single-shell representation and kept many strings. We feel that this preserves the essential features of the computation. The phenomenological form for $\bar{V}$ is then

$$\bar{V}=-Z_2e^2\sum_{\text{strings}}\int\frac{d\zeta}{a}\;\frac{e^{-\lambda|\vec{\mathrm{r}}-\vec{\mathrm{R}}|}}{|\vec{\mathrm{r}}-\vec{\mathrm{R}}|}\,, \tag{4.5}$$

where λ is defined below.

We now specialize to a simple cubic lattice and illustrate with sodium. Sodium is actually a body-centered crystal, but when the string average is performed it effectively becomes a simple cubic crystal with channel width reduced by a factor $\sqrt{2}$ (see Fig. 1). We also note (Fig. 2) that the sum over strings can be broken into a sum over groups of four. That is, there are four nearest neighbors, $2\times 4=8$ next nearest, etc. Moreover, each group of four is arranged in a square centered on the proton. This is enough to show that the potential $\bar{V}$ (4.3) has the form

$$\begin{aligned}\bar{V}(r)&=\sum_M e^{4iM\phi}V_{4M}(r,\theta)\\&=\sum_{LM}Y_{L,4M}(\hat{r})V_{L,4M}(r)\,,\end{aligned} \tag{4.6}$$

where ϕ is the azimuthal angle around the z axis

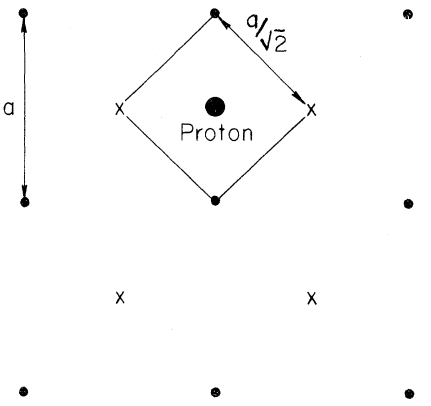

FIG. 1. Proper channel in a body-centered cubic crystal.

(the direction of motion).

We now proceed to an approximate solution of (4.1) by diagonalization in a finite basis set. The natural one to chose is the hydrogenic basis with nuclear charge Z

$$\psi = \sum_{\mu} a_\mu \phi_\mu(\vec{r}), \tag{4.7}$$

where

$$[H(A,Z) - W_\mu(Z)]\,\phi_\mu(\vec{r}) = 0 \tag{4.8}$$

and in spherical coordinates μ represents the usual three quantum numbers

$$\mu = (n, l, m).$$

This is a convenient and useful basis set in that it readily represents a state whose density is piled up at the atom. The other kind, those centered on strings, are also describable in this basis but need many terms. We are not interested in them here. In the limit of large Z our basis goes into the 1s state on Z, which is the correct result.

The matrix equation determining a_μ is

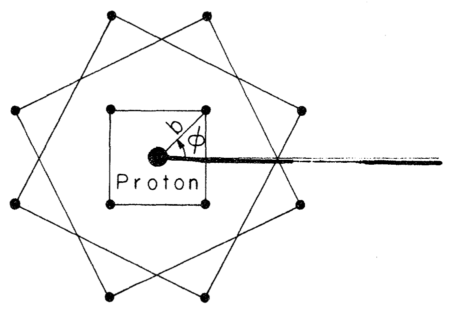

FIG. 2. Strings, showing nearest and next-nearest groups.

$$\sum_{\mu'} \{[E - W_\mu(Z)]\,\delta_{\mu\mu'} - V_{\mu\mu'}\} a_{\mu'} = 0\,, \tag{4.9}$$

with

$$V_{\mu\mu'} = (\phi_\mu, \bar{V}\phi_{\mu'}) = \sum_{LM} (\phi_\mu, V_{L,4M} Y_{L,4M} \phi_{\mu'})\,. \tag{4.10}$$

Using (4.3) in (4.9) and the invariance of the potential under the transformation

$$\vec{R} \rightarrow -\vec{R}$$

we find that (4.10) vanishes unless

$$l + l' = \text{an even integer}\,, \tag{4.11}$$

and we can similarly show that we must also have

$$L = \text{an even integer} \tag{4.12}$$

for nonvanishing matrix elements. We then expand the potential in spherical harmonics[10]

$$\frac{e^{-\lambda|\vec{r}-\vec{R}|}}{|\vec{r}-\vec{R}|} = 8\lambda \sum_{LM} i_L(\lambda s_<) k_L(\lambda s_>) Y^*_{LM}(\hat{R}) Y_{LM}(\hat{r})\,, \tag{4.13}$$

where $s_<(s_>)$ is the lesser (greater) of r and R. The functions i_L and k_L are related to the usual modified Bessel functions[10] by

$$\begin{Bmatrix} i_L \\ k_L \end{Bmatrix} = \frac{\pi}{2x} \begin{Bmatrix} I_{L+1/2} \\ K_{L+1/2} \end{Bmatrix}\,. \tag{4.14}$$

If we substitute (4.13) into (4.10) we obtain

$$V_{\mu\mu'} = -\left(\frac{2}{\pi}\right)^{1/2} \frac{64\lambda Z_2}{a} \sum_{LM} C(L; l'm'lm) \sum_{g} b_g^4 e^{-i4M\phi_g} [J_1(g) + J_2(g)], \tag{4.15}$$

where each g denotes a set of strings forming a square as in Fig. 2 and b_g is the distance from the proton to any one of the set of strings. The coefficient C, defined by[11]

$$C(L; l'm'lm) = (-1)^{m'} \left(\frac{(2l+1)(2l'+1)(2L+1)}{4\pi}\right)^{1/2} \times \begin{pmatrix} l & l' & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & l' & L \\ m & -m & M \end{pmatrix}, \tag{4.16}$$

is the Gaunt factor of atomic spectroscopy.[12] The radial integrals J are defined by

$$J_1 = \int_0^\infty dz\, P_{LM}\left(\frac{z}{\sqrt{1+z^2}}\right) k_L(\lambda b_g\sqrt{1+z^2}) \int_0^{\sqrt{1+z}\,^2} dr\, r^2$$

$$\times R_{n'l'}(b_g r) R_{nl}(b_g r) i_L(\lambda b_g r)\,,$$

$$J_2 = \int_1^\infty dr\, r^2 R_{n'l'}(b_g r) R_{nl}(b_g r) k_L(\lambda b_g r) \int_0^{\sqrt{r2-1}} dz\, P_{LM}$$

$$\times \left(\frac{z}{\sqrt{1+z^2}}\right) i_L(\lambda b_g\sqrt{1+z^2})\,. \qquad (4.17)$$

Standard techniques were used to evaluate the integrals and other factors of (4.15). The results are accurate to three significant figures or better. The diagonalization of (4.9) was performed and the eigenvalues obtained by the Jacobi method.[13]

A conventional value for the screening constant λ in (4.13) is the Bohr screening parameter[14] λ_B, whose derivation is based on Thomas-Fermi considerations for both the target and projectile atoms (in units of reciprocal Bohr radii),

$$\lambda_B = (Z^{2/3} + Z_2^{2/3})^{1/2}\,. \qquad (4.18)$$

This value is probably too large.[15] That is, it yields a string potential whose extension is too small, so we shall set

$$\lambda = \alpha\lambda_B \qquad (4.19)$$

and investigate λ as a function of α.

For sodium ($Z_2 = 11$) we use[16] $a = 4.28$ and note that $Z = 2$ yields results which are uninteresting for all reasonable values of α. That is, for $Z = 2$ the wave function of the c.p. is too small to significantly overlap the strings. Even for $\alpha = 0.33$ the wave function is essentially all $1s$.

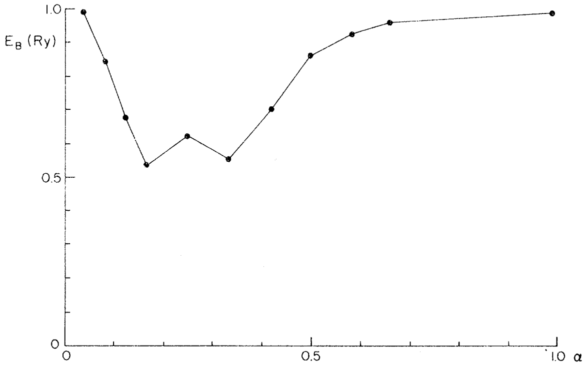

FIG. 3. Binding energy vs screening parameter α.

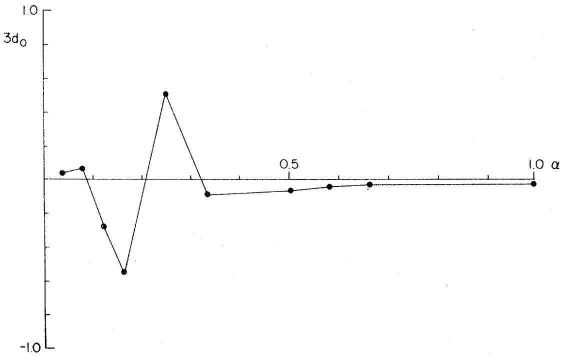

FIG. 4. Amplitude of the $3d_0$ state vs screening parameter α.

For $Z = 1$ we have calculated the eigenvalues of (4.9) with varying basis sizes ranging from 14 (including all the $n = 1, 2, 3$ states) to 30 (including the above and the $n = 4$ states) and varying values of α, and find that the difference in lowest eigenvalues is never more than a few percent. This accuracy is sufficient for our purposes. In Fig. 3 we show the binding energy, (4.2), versus α. As the screening length gets larger (smaller α) higher atomic states are introduced into the wave function and the binding energy drops. However, when λ becomes smaller, $\alpha < 0.3$, the binding energy rises again and the wave function becomes essentially $1s$ again. The reason for this may be seen as follows: If the potential $\overline{V}$ is a constant then there is no coupling in (4.9) and the ground state is purely $1s$. We may write $\overline{V}$ as

$$\overline{V} = \sum_s K_0(\lambda|r_\perp - R_\perp|)$$

$$= 2\sum_{m=0} K_m(\lambda R_\perp) I_m(\lambda r_\perp) e^{im\phi} \quad \text{for } r_\perp < R_\perp\,. \qquad (4.20)$$

The coupling to the $1s$ part of ψ can then be shown to vanish as λ^2 for small λ.

We feel that the important feature of Fig. 3 is the minimum in the binding energy versus α. The oscillation near $\alpha \sim 0.25$ is explained by Fig. 4, where it is seen that the amplitude for the $3d_0$ state becomes large there. That is, the wave function which is primarily $1s$ for larger α has a significant $3d$ component near $d \sim 0.25$. This phenomenenon is due to the overlap of the potential with the $1s$ state. The details are critically dependent upon the form of the potential $\overline{V}$, so that the results obtained with the crude form (4.20) should only be judged qualitatively.

The preceding considerations apply only to the bulk effect of the crystal on the c.p. The surfaces will also strongly affect the state of the c.p. in a way which is very difficult to determine since even for a completely clean surface the channel is distorted by the edge effects.

For this reason we have had difficulty in finding experiments which explore the distortion of the internal state of the c.p. by the channeling process only.

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