the first 13 reciprocal-lattice vectors for fcc and 14 for bcc. The resulting energy levels are remarkably insensitive to the choice of splitting parameter.[16] Only the few levels near the bottom of the d band for which approximation (6) becomes important are noticeably β sensitive. However, these levels have converged to within about 0.002 Ry for the value of $\beta = 0.9$ used in the present calculations. Table I lists the resulting values of the TB overlap parameters and their energy derivatives. It is seen that we need only retain out to second nearest neighbors for fcc and third for bcc.

The model Hamiltonian reproduces the energy levels[12] below X_4, to within a rms accuracy of 0.005 Ry for fcc (81 levels) and 0.006 Ry for bcc (74 levels). This success of the simple resonance parameter scheme should make it extremely useful in providing accurate transition-metal band structures and wave functions, under change of volume or structure,[10] once the good physical parameters E_d and W have been found.

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*Work supported by the United Kingdom Ministry of Technology. Present address: Department of Physics, Imperial College, Prince Consort Road, London S.W.7.

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PHYSICAL REVIEW B VOLUME 2, NUMBER 8 15 OCTOBER 1970

Influence of Surface Force-Constant Changes on Surface-Mode Frequencies

S. W. Musser and K. H. Rieder
Österreichische Studiengesellschaft für Atomenergie Institut Metallurgie, Reaktorzentrum Seibersdorf, Austria

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Investigations of the dynamical properties of metallic crystals with free surfaces have been performed on the basis of a Born–von Karman model with atomic interactions up to second nearest neighbors including noncentral forces. The effect of a variation of the force constants near the surface on the surface-mode dispersion relations is analyzed. The calculations were based on a nonstandard Green's-function technique. Results are presented for the (100) surface of nickel. Surface modes are shown to exist below and above the cyclic frequency band as well as in a gap within the bulk region. The consequences of the fulfillment of the conditions of rotational invariance for the surface-mode dispersion relations are demonstrated.

I. INTRODUCTION

Within the last year several theoretical studies of surface vibrational modes of crystal lattices have been published. For example, Tong and Maradudin[1] have investigated a NaCl crystal slab using the rigid-ion model introduced by Kellermann. Allen *et al.*[2,3] have performed extended calculations for monatomic crystal slabs with atoms interacting through a Lennard-Jones (12, 6) potential, thus gaining a realistic description of noble gas crystals.

In investigating localized surface modes another topic has also been of great interest, namely, the effect of isotopic surfaces, i.e., of surface layers consisting of atoms with masses different from the mass of the bulk atoms, but with no changes in the forces between atoms near the surface.[2–5] It is evident that an analysis of the influence of changed atomic force constants near the surface on surface-mode dispersion relations is of similar importance in connection with adsorbed or chemically bound surface layers. LEED experiments[6] have shown that a change of force constants has also to be taken into account near clean crystal surfaces.[7] However, to the author's knowledge, no systematic study in this direction has been carried out. Therefore we want to present in this paper results of our investigations concerning surface-mode frequencies of crystals with changed forces between atoms near the surface, but without considering surface atoms with changed masses.

Besides, we show that the fulfillment of the conditions of rotational invariance imposed on the atomic force constants near the surface is of importance for the exact description of surface-mode dispersion relations not only in the long-wavelength limit but also through nearly the whole Brillouin zone.

II. LATTICE MODEL

In the papers cited above[1–3] the calculations have been based on models restricted to central forces and therefore the validity of the Cauchy relations is assumed implicitly. These relations are well satisfied for the alkali halides and the noble gas crystals. For metals, however, there are strong deviations from the Cauchy relations and a model with central forces only cannot yield correct results. But since the great difficulties in the theory of lattice dynamics of metals prohibit first-principle calculations of dynamical surface effects, we think that a method for computing surface-mode frequencies on the basis of a realistic Born–von Karman model is of interest. The importance of such calculations is particularly emphasized by the fact that the progress in LEED experiments may soon provide data about the properties of surface modes of metal crystals.

In our calculations of the vibrational modes of fcc metallic crystals with free (100) surfaces we have used a force constant model with central forces between first and second nearest neighbors (coupling constants C_1 and C_2) and with angular forces of the DeLaunay type[8] between first nearest neighbors (coupling constant A). The introduction of these three coupling constants makes it possible to match exactly the elastic properties of the bulk.[7] Furthermore, it is known from neutron scattering data, that the phonon dispersion relations of the bulk modes of various fcc metals are reproduced by our model with rather good accuracy (Ni,[9] Cu, Ag,[10] Pt, and Au[11]).

At the surface the angular forces are modified in order to ensure the fulfillment of the conditions of rotational invariance. A detailed description of this modification is given in Ref. 7 (surface model SURF 1). As has been proved by Ludwig and Lengeler,[12] the fulfillment of the conditions of rotational invariance for the atomic force constants for atoms near the surface[13] is necessary for consistency between the long-wavelength limit of the acoustic surface modes and the Rayleigh modes of the continuum theory.

To study the influence of the rotational invariance conditions on all parts of the surface-mode dispersion relations, we have performed additional calculations using a model with unchanged coupling constants near the surface. This model SURF 0 is not rotationally invariant. We have based our calculations upon a model with angular forces of the DeLaunay type, because a model with angle bending forces as described by Clark *et al.*[14] leads automatically to a rotationally invariant surface model and therefore prohibits the study of the influence of rotational invariance on surface-mode frequencies.

A comparison between the mean square displacements of surface atoms measured by LEED experiments[6] and those computed from force constant models shows that the interactions between atoms near the surface are different from those in the bulk of the crystal.[7] In our computations this fact has been taken into consideration by a variation of the central force coupling constant between an atom in the surface layer and its nearest neighbors in the second layer (surface coupling constant C_1^{12}). Since the values of the coupling constants C_1 are much larger than the values of the coupling parameters C_2 and A, our assumption seems to be a good approach to reality.

For bcc metals a calculation of surface-mode frequencies from a rotationally invariant Born–von Karman model including angle bending forces according to Ref. 14 has been performed already by Gazis and Wallis.[15] However, these authors did not allow for modified coupling constants between atoms near the surface.

III. THEORETICAL PROCEDURE

In order to make the problem of calculating surface-mode frequencies amenable to computation, we consider a slab-shaped crystal of finite thickness. We assume the customary cyclic boundary conditions with respect to translations parallel to the surfaces. Thus all vibrations of the slab may be classified by a two-dimensional wave vector $k_\parallel$ with components parallel to the surfaces. Using two-dimensional Fourier transformation we can reduce the dynamical matrix of the crystal slab to matrices of lower dimension. These matrices display the same structure as the dynamical matrix of a crystal with a point defect. Consequently, a Green's-function method analogous to that used in the theory of defect modes is applicable for the computation of surface-mode frequencies. For the problem under consideration, we used a modification of the standard Green's-function method.

As is well known, phonon frequencies are determined by the classical time-independent equations of motion (given, for instance, in Refs. 16 and 7). We start from a short-hand matrix formulation of these equations:

$$\underline{\underline{L}}(\omega^2)\,\underline{u}=\underline{0}\ . \tag{1}$$

$\underline{\underline{L}}(\omega^2)$ is the coefficient matrix, $\underline{u}$ the vector formed by the atomic displacements of all atoms of the crystal. In the case of a crystal with a point defect, $\underline{\underline{L}}(\omega^2)$ can be replaced by a sum of two matrices

$$\underline{\underline{L}}(\omega^2)=\underline{\underline{L}}^{(0)}(\omega^2)+\delta\underline{\underline{L}}(\omega^2)\ , \tag{2}$$

where $\delta\underline{\underline{L}}(\omega^2)$ can be written in the following partitioned form:

$$\delta\underline{\underline{L}}(\omega^2)=\begin{pmatrix}\underline{\underline{0}} & \underline{\underline{0}}\\ \underline{\underline{0}} & \delta\underline{\underline{L}}_{dd}(\omega^2)\end{pmatrix}\ . \tag{3}$$

Under these assumptions the phonon frequencies of Eq. (1) are more easily obtained from another matrix equation formed by submatrices belonging to the defect space [lower right-hand corner of the right-hand side of Eq. (3)]:

$$[\underline{\underline{1}}+\underline{\underline{G}}^{(0)}_{dd}(\omega^2)\,\delta\underline{\underline{L}}_{dd}(\omega^2)]\,\underline{u}_d=\underline{0}\,. \tag{4}$$

$\underline{\underline{G}}^{(0)}_{dd}(\omega^2)$ denotes a submatrix of the Green's function

$$\underline{\underline{G}}^{(0)}(\omega^2)=\underline{\underline{L}}^{(0)}(\omega^2)^{-1}\ . \tag{5}$$

The necessary and sufficient condition for nontrivial solutions of Eq. (4),

$$\det[\underline{\underline{1}}+\underline{\underline{G}}^{(0)}_{dd}(\omega^2)\,\delta\underline{\underline{L}}_{dd}(\omega^2)]=0\,, \tag{6}$$

is for our purposes replaced by the equation

$$\text{eigenvalue}\,[\underline{\underline{G}}^{(0)}_{dd}(\omega^2)\,\delta\underline{\underline{L}}_{dd}(\omega^2)]=-1\,. \tag{7}$$

For the use of Eq. (7) the summands of the left-hand side of Eq. (2) are defined in the following way: $\underline{\underline{L}}^{(0)}(\omega^2)$ represents the coefficient matrix of the crystal slab with free surfaces, but with no central force constant changes at the surface ($C_1^{12}=C_1$). $\delta\underline{\underline{L}}(\omega^2)$ is the perturbation matrix resulting from the replacement of the coupling constant C_1 by the surface coupling constant C_1^{12}. Since all elements of $\delta\underline{\underline{L}}(\omega^2)$ are proportional to the difference

$$\Delta C_1=C_1^{12}-C_1\ , \tag{8}$$

we define[17]

$$\delta\underline{\underline{L}}(\omega^2)=\Delta C_1\,\delta\underline{\underline{L}}^{R}(\omega^2)\ . \tag{9}$$

By inserting $\delta\underline{\underline{L}}^{R}_{dd}(\omega^2)$ into Eq. (7) we get

$$\text{eigenvalue}\ [\underline{\underline{G}}^{(0)}_{dd}(\omega^2)\,\delta\underline{\underline{L}}^{R}_{dd}(\omega^2)]=-1/\Delta C_1\ . \tag{10}$$

This relation renders immediately the desired functional dependence $\omega^2=\omega^2(C_1^{12})$ between the surface-mode frequencies and the surface coupling constant C_1^{12}.

For evaluating $\underline{\underline{G}}^{(0)}_{dd}(\omega^2)$ an inversion of the coefficient matrix $\underline{\underline{L}}^{(0)}(\omega^2)$ is necessary. This is performed by applying the matrix partitioning technique described in Ref. 7 to the following decomposition of $\underline{\underline{L}}^{(0)}(\omega^2)$:

$$\underline{\underline{L}}^{(0)}(\omega^2)=\underline{\underline{L}}^{\text{cycl}}(\omega^2)+\delta\underline{\underline{L}}^{\text{surf}}(\omega^2)\ . \tag{11}$$

The crystal slab with two free surfaces (and $C_1^{12}=C_1$) is thus considered as a defect of the slab with an additional cyclic boundary condition perpendicular to the surface [coefficient matrix $\underline{\underline{L}}^{\text{cycl}}(\omega^2)$]. The nonvanishing elements of the defect matrix $\delta\underline{\underline{L}}^{\text{surf}}(\omega^2)$ are confined to the defect region given in Eq. (3).

Our problem may also be solved from Eq. (6) by using the standard Green's-function technique

$$\text{Det}\ [\underline{\underline{1}}+\underline{\underline{G}}^{\text{cycl}}_{dd}(\omega^2)\,\delta\underline{\underline{L}}^{\text{total}}_{dd}(\omega^2)]=0\ . \tag{12}$$

$\underline{\underline{G}}^{\text{cycl}}(\omega^2)$ is the Green's function of the slab with an additional cyclic boundary condition perpendicular to the surfaces. $\delta\underline{\underline{L}}^{\text{total}}$ is the sum of the defect matrices defined in Eqs. (9) and (11),

$$\delta\underline{\underline{L}}^{\text{total}}(\omega^2)=\delta\underline{\underline{L}}^{\text{surf}}(\omega^2)+\delta\underline{\underline{L}}(\omega^2)\ . \tag{13}$$

If we would have used Eq. (12) for evaluating the dependence of the surface-mode frequencies on the surface coupling constant C_1^{12}, we would have been forced to select values for C_1^{12} and to solve Eq. (12) for each choice independently.

Owing to the localized character of surface modes (perpendicular to the surface), their frequencies approach asymptotic values when the thickness of the crystal slab increases. Since both surfaces of the slab are equivalent, each branch of the corresponding semi-infinite crystal is split into two branches with frequencies nearly equal, if the thickness of the slab is sufficiently great. In evaluating the asymptotic frequencies of the surface modes we could restrict ourselves to a 20-layer crystal for most of the wave vectors $k_{\parallel}$. Therefore a Green's-function method is more convenient for numerical use than the difference equation method due to Feuchtwang[18] used also by Gazis and Wallis.[15]

IV. RESULTS

We have calculated surface-mode dispersion relations for the (100) surface of a nickel crystal for modes propagating in the [01] direction. For wave vectors in this direction there exist two kinds of vibrations which have opposite parity with respect to a reflection at the mirror plane (001). In this paper we deal only with surface modes of odd parity and restrict our discussion to force constant ratios C_1^{12}/C_1 between 0.5 and 1.5.

Due to their localized character, surface modes exist in regions of $(k_{\parallel}, \omega)$ space free from modes of the cyclic crystal. Each cyclic mode is labeled by a three-dimensional vector $\vec{k}$. As we use for the classification of the modes only the components $k_{\parallel}$ parallel to the surface, the component $k_{\perp}$ perpendicular to the surface can vary independently. This yields a continuum of cyclic frequencies for each vector $k_{\parallel}$. In Fig. 1 the resulting cyclic frequency band for the [01] direction direction is shown for nickel. There are three regions where no bulk modes exist: below and above the cyclic band as well as in a gap near the Brillouin-zone boundary $\bar{M}$.

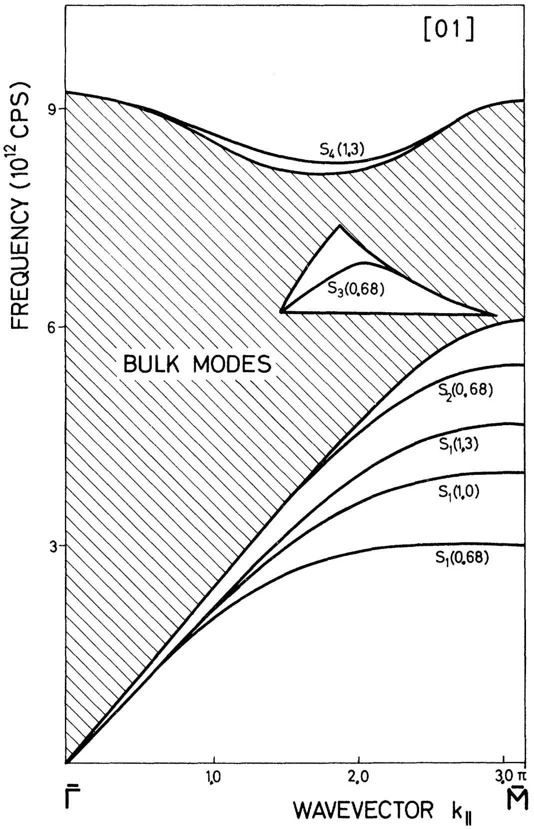

FIG. 1. Frequency–versus–wave-vector diagram along the [01] direction for the (100) surface of a Ni crystal. Surface-mode dispersion relations derived from the rotationally invariant model SURF 1 are given for the coupling constant ratios $C_1^{12}/C_1 = 0.68$, 1.0, and 1.3.

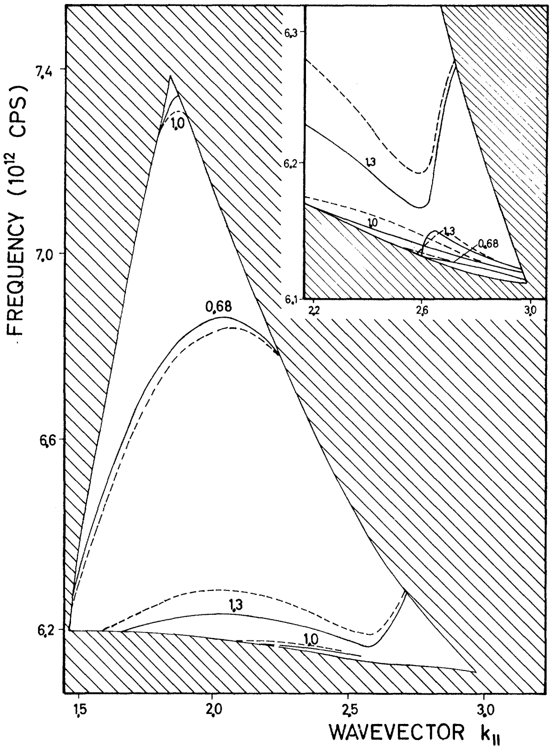

FIG. 2. Surface modes of vibration within the gap. Lower right-hand corner of the gap is enlarged in the upper right-hand corner of the figure. The solid lines correspond to the model SURF 1, the broken lines to SURF Ø.

We have found surface vibrational modes to exist in all three outband regions, the form of the dispersion relations being drastically influenced by the surface coupling constants C_1^{12}. In the figures we show the dispersion relations of the surface modes for the coupling constant ratios $C_1^{12}/C_1 = 1.3$, 1.0, and 0.68; each branch of the surface modes is labeled by the corresponding coupling constant ratio. The ratio $C_1^{12}/C_1 = 0.68$ has been derived[7] from the experimental value of the mean square displacement of nickel surface atoms.[6] Therefore, the results obtained with this value will exhibit the situation at a clean nickel surface.

In the following we refer mainly to the physically reasonable model SURF 1, reference to SURF Ø is always explicitly stated. Figure 1 exhibits the general features of our results. In Figs. 2 and 3

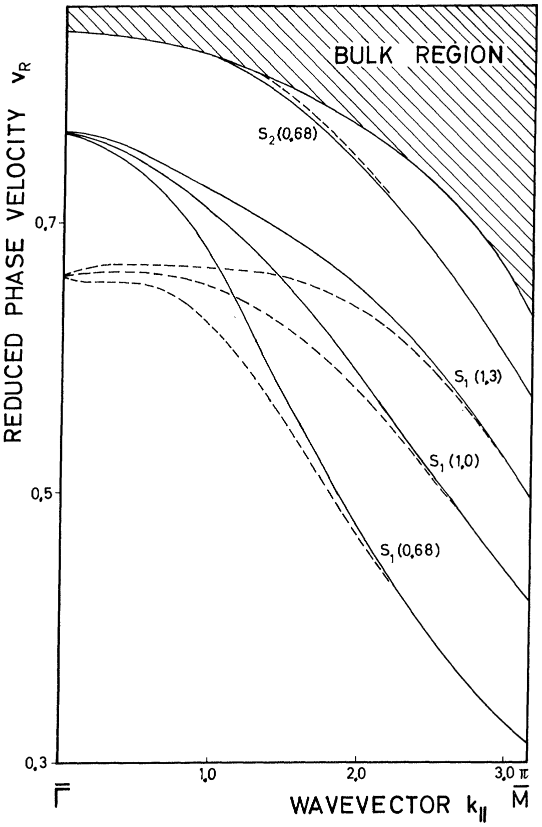

FIG. 3. Reduced phase velocity of surface modes below the cyclic region and lower boundary of the cyclic region versus wave vector $k_{\parallel}$. Solid lines correspond to the model SURF 1, the dashed lines to SURF 0.

the full lines correspond to the model SURF 1, the broken lines refer to SURF 0.

Above the cyclic region surface modes (S_4) can only appear for coupling constant ratios $C_1^{12}/C_1 > 1$. For $C_1^{12}/C_1 = 1.3$ surface modes exist only for a limited range of wave vectors (see Fig. 1). Their frequencies lie very close above the upper boundary of the cyclic region. With increasing ratio C_1^{12}/C_1 the range of wave vectors increases and the frequencies of the modes are shifted towards higher values. The model SURF ϕ shows similar results, the frequencies of the surface modes lie close below those derived from SURF 1.

The dispersion relations of surface modes *in the gap* (S_3) are shown in detail in Fig. 2. For each of the three coupling constant ratios plotted there exist two branches. The dispersion relations obtained with the model SURF 0 display the same structure, though with somewhat different frequency values.

Below the cyclic region one surface-mode branch (S_1) exists for all wave vectors, yielding the Rayleigh modes in the long-wavelength limit. A second branch (S_2) appears only for ratios $C_1^{12}/C_1 < 1$ and is limited to wave vectors near the Brillouin-zone boundary. With decreasing ratio C_1^{12}/C_1 the range of wave vectors for this branch spreads from the zone boundary $\bar{M}$ towards the center of the zone while the frequencies of the modes decrease. For $C_1^{12}/C_1 = 1$ the branch S_2 degenerates into a single bulk mode at the zone boundary with the frequency of lowest inband mode.

The importance of the fulfillment of the conditions of rotational invariance for the correct determination of the dispersion relations of the surface modes below the cyclic region is demonstrated in Fig. 3. Contrary to Fig. 1, as ordinate scale a reduced phase velocity v_R is chosen, which is defined by the ratio between the phase velocity v_{ph} of the surface modes given by[19]

$$v_{\text{ph}} = \tfrac{1}{2} a\omega(k_{\parallel})/k_{\parallel} \tag{14}$$

and the sound velocity

$$v_s = (c_{44}/\rho)^{1/2} \; . \tag{15}$$

It can be seen from Fig. 3 that the rotationally invariant model SURF 1 yields a much larger value for v_R at the zone center $\bar{\Gamma}$ than the model SURF 0. The discrepancy between the two models gradually disappears when $k_{\parallel}$ approaches the zone boundary $\bar{M}$.

The results of our lattice dynamical calculations of the value of v_R at the zone center $\bar{\Gamma}$ should be compared with the values derived from calculations based on the theory of elasticity as well as with experimental values. However, as we found in the literature experimental data only for copper, we have also calculated with both of our models the long-wavelength limit of v_R for copper. Again the model SURF 0 yields an essential lower value of 0.53 than the model SURF 1, from which we derived the value 0.73. The latter value is in very good agreement both with the value of 0.69 calculated by Gazis *et al.*[20] from elastic data and with the value of 0.68 measured by Lim and Farnell.[21]

At the point $\bar{M}$, for modes with odd parity, lattice symmetry has two consequences, which are independent from a special force constant model: (a) Disregarding accidental degeneracy, modes vibrate either parallel or perpendicular to the surface. (b) For modes perpendicular to the surface two groups of layers parallel to the surface vibrate independently – those with the layer numbers $n = 1, 3, 5, \ldots$ and those with $n = 2, 4, 6, \ldots$. At this special point the surface modes S_1 and S_2 vibrate perpendicular to the surface, S_2 is the surface mode of the even layers, S_1 that of the odd layers.

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Echo Expansion in the Theory of Alloys*

Richard M. More and Klaus Hacker†
Department of Physics, University of Pittsburgh, Pittsburgh, Pennsylvania 15213

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We have obtained a systematic expansion for the trace of the Green's function of electrons moving in a disordered alloy. In our expansion, the terms are classified by a path length which, for some models, takes on discrete values. The expansion is strongly convergent for large complex energies, but seems to be surprisingly useful even for nearly real energies. We present numerical calculations of the density of states for a one-dimensional system.

I. INTRODUCTION

Imagine emitting a pulse of sound from a point into some inhomogeneous environment and then waiting a short time t for the echoes. The result may be calculated *exactly*, knowing the properties of the environment within an influence sphere of radius $\frac{1}{2}ct$ about the initial point, where c is an appropriate sound velocity. We contrast this soluble problem with the very difficult one of reliably calculating the exact sonic dispersion relation in an inhomogeneous medium.

A qualitatively similar situation occurs for electrons in a disordered (or partially disordered) alloy. Of course, there is no strict limit on the velocity of motion of an electron (in a nonrelativistic theory). Nevertheless, over short time intervals, the motion is still essentially confined within an influence sphere, and this suggest the possibility of making a *local* calculation of some aspect of the electron dynamics. In this paper, we explore this possibility. The results are quite simple and interesting.

First, we have obtained a perfectly systematic and convergent "echo" expansion of the trace of the electron Green's function for complex energy z:

$$\operatorname{Tr}G(z)=\sum_L f_L(z)\, e^{ikL}, \quad k\equiv\sqrt{z}\ . \tag{1.1}$$

We consider noninteracting electrons moving in the presence of many "atomic" potentials V_n, with kinetic energy $H_0=p^2/2m$. In the present paper, we limit ourselves to one-dimensional problems with δ-function potentials on the sites of a fixed lattice. None of these limitations are essential in the present method. We define the Green's func-