

Theory of valence-band Auger spectra: GaAs(110)[†]

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In order to establish the utility of Auger line-shape analysis as a probe of local electronic structure at surfaces, we propose the study of GaAs(110) 1×1 . This surface is of interest because extensive theoretical studies of GaAs band structure, both bulk and surface, are available, because the 1×1 nature of this surface's "reconstruction" permits a relatively unambiguous determination of its atomic geometry, and because the local densities of states (LDOS's) on the Ga and As atoms are very different. We calculate the Ga and As $M_1M_{4,5}V$ and $M_{2,3}M_{4,5}V$ Auger line shapes for GaAs(110) and show that they differ considerably from one another, reflecting the differing angular-momentum compositions of the Ga and As LDOS's and the facts that valence s -electron emission is favored in the $M_1M_{4,5}V$ case while s - and p -electron emission are roughly equally weighted in the $M_{2,3}M_{4,5}V$ lines.

I. INTRODUCTION

Until now the main tool used in the study of surface electronic structure has been ultraviolet-photoemission spectroscopy (UPS). However, UPS has the disadvantage that it is not a "local" probe, that is, it involves the excitation of electrons in extended states with a spatial coherence large compared to a surface unit cell. [The fact that this is true is evident from the apparent importance of the momentum conservation law in determining peak positions in photoemission energy distributions (PED's) at low photon energies.¹] The reason that the "nonlocality" of UPS is disadvantageous is that chemical bonding is typically a local phenomenon and, thus, in trying to understand surface chemistry one wants to be able to measure the "local density of states" (LDOS) at potential bonding sites.

We are, therefore, led to consider the possibility of using Auger-electron spectroscopy (AES) as a probe of the valence-electron structure at a surface. AES is unique among the electron spectroscopies of solids in that it is simultaneously: (i) surface sensitive, at least if one looks at the lower-energy Auger lines; (ii) a core-level spectroscopy and, therefore, a local probe; and (iii) a probe of the *occupied* part of the valence bands. On the other hand, there are two features of AES which have, in the past at least, made it seem rather unattractive as anything other than a tool for the analysis of surface atomic composition. In particular, Auger spectra are typically accompanied by substantial "background," and they are smeared because of inelastic scattering of Auger electrons before they emerge from a solid. Recently, however, strides have been taken in AES

data reduction which, reasonably unambiguously, enable one to obtain AES spectra in integral form with background removed and inelastic loss features deconvoluted away.²

For the few materials whose Auger spectra have been treated in this manner [including Si,³ Al,² and Li (Ref. 4)] it has been found that the reduced ("intrinsic") experimental Auger spectra do not generally agree in shape with the predictions of the usual DOS models. For the case of the $L_{2,3}VV$ Auger lines of Si(111) and Si(001), this phenomenon can be explained in terms of the strong dependence of Auger matrix elements on the *angular* momentum character of the electrons involved.^{5,6} Specifically, the fact that the valence bands of Si are strongly s like at lower energies and p like at higher energies, coupled with the fact that the matrix elements involving only p electrons are dominant, is believed to explain the fact that the Si $L_{2,3}VV$ lines look quite similar to the self-fold of the p -like part of the Si DOS and not to the self-fold of the full DOS.^{5,6} Moreover, one has reason to believe that a similar matrix-element effect explains the nature of the observed Al (Ref. 7) and Li (Ref. 4) spectra.

With the possibility established of obtaining agreement between calculated and measured Auger spectra for broad-band materials,⁸ we extend our investigation in this paper to the question of how the locality of the Auger phenomenon might be useful by turning our attention to a binary compound, GaAs, so that we can compare the spectra originating on each of the atomic constituents. GaAs(110) is a particularly interesting surface to study in this regard in that:

(i) although the GaAs(110) surface forms a 1×1 structure in equilibrium whose atomic geometry

should, therefore, be relatively easy to determine, the arrangement of the Ga and As atoms for this surface has not been convincingly determined until recently.⁹⁻¹² Comparison of low-energy-electron diffraction (LEED) and ultraviolet-photoemission theory and experiment by Tong *et al.*¹¹ and by Pandey *et al.*,¹² respectively, have now shown that a partial relaxation of the surface in which the Ga-As bonds are rotated by 20°, with the As's moving out of the ideal surface, is probably the correct geometry. One would hope that additional electron spectroscopic information would confirm this picture, and would also eventually help to answer related questions such as the nature of the oxidation process on GaAs(110).¹³

(ii) The electronic structure of GaAs is well known for the bulk material.¹⁴ It has been intensively investigated for various surfaces,^{15,16} and is of a character ideally suited to the question of how a *local* probe of electronic structure might be useful. Specifically, even though the LDOS's for both Ga and As (in whatever atomic layer) show essentially the same three major structures, the

angular-momentum decomposition of these LDOS's (see Fig. 1) reveals a striking contrast for the two species. For Ga, we find that the lowest-energy (≈ -10 eV) feature in the LDOS is roughly equally divided between *s* and *p* character. On the other hand, for As this peak is considerably larger and is of virtually pure *s* character. The middle (~ -5 eV) peak in the Ga LDOS is essentially an *s*-like peak, while in the As LDOS the corresponding structure is of *p* character. Finally, the uppermost broad structure in both species's LDOS's are predominantly associated with *p* electrons. These conclusions are true not only for the first layer LDOS's, shown in Fig. 1, but for the Ga and As LDOS's of all the layers of the GaAs crystal. We show below how these contrasting angular-momentum decomposed LDOS's should manifest themselves in contrasting Auger lineshapes from Ga and As, as a consequence of the dependence of Auger matrix elements on angular momentum.

The remainder of this paper is organized as follows: In Sec. II we review briefly the method which we have used to calculate Auger line shapes and discuss the question of which lines in the Ga and As Auger spectra are likely to be most useful. In Sec. III we present the various calculated Ga and As Auger line shapes and compare them to the Ga and As LDOS's for the outer layers of a GaAs (110) surface.

II. DESCRIPTION OF THE CALCULATION

The method used to calculate GaAs Auger line shapes is identical to that which was applied in our previous calculations for clean Si surfaces^{5,6} and has been described in detail in Ref. 5 and 6. The assumptions which underlie the model are: (i) that the most important contributions to the Auger matrix elements come from the immediate vicinity of the decaying core hole, and that, therefore, it is sufficient to calculate these matrix elements using *atomic* wave functions; (ii) that the independent-electron model provides a sufficiently accurate description of the final, two-hole states which result from an Auger decay, i.e., that hole-hole repulsion effects can be dropped; and finally (iii) that final-state multiple scattering may be ignored insofar as one considers only angle-integrated Auger spectra.

The statement in assumption (i) that the most important contributions to the Auger matrix elements come from the immediate vicinity of the decaying core state can be verified by direct numerical calculation (cf. also Ref. 6). However, to date the supposed corollary that one may therefore use atomic wave functions rather than Wannier functions to calculate these matrix elements has not proven, in practice, to be true.⁶ Thus, it is

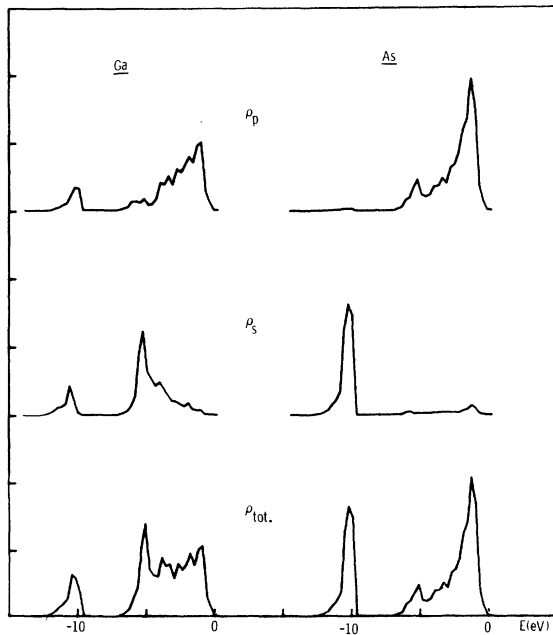


FIG. 1. Angular-momentum decomposition of the local densities of states at the outermost Ga and As layers of a GaAs(110) surface. The As curves are drawn to half the scale of Ga curves. Energies are measured from the valence-band maximum. The GaAs(110) surface is assumed to be relaxed, as described in the main text, with the As atoms having moved outward into the vacuum and the Ga atoms inward relative to the ideal position of the outermost crystal plane. A full description of the LCAO calculation which produces these curves may be found in Ref. 12.

TABLE II. Energies E (Ref. 14) and widths (Ref. 15), of the M -shell core levels of Ga and As.

	E_{3s}	$\hbar\Gamma_{3s}$	$E_{3p\ 1/2}$	$\hbar\Gamma_{3p\ 1/2}$	$E_{3p\ 3/2}$	$\hbar\Gamma_{3p\ 3/2}$	E_{3d}	$\hbar\Gamma_{3d}$
Ga	158	2.5	107	2.9	103	2.4	18	1.2
As	204	2.7	147	2.4	141	2.5	41	1.4

mation may be obtainable from them, and finally, that core level spin-orbit splitting may require further data reduction before one can obtain an experimental valence-band LDOS.

The lowest energy, and thus the most surface sensitive Auger lines of GaAs, correspond to the MMV and MVV transitions. Consulting Table II which lists the energies¹⁹ and widths²⁰ of the Ga and As M levels, we deduce the following facts:

(a) The Ga $M_{4,5}VV$ transition lies so low in energy that only electrons from the uppermost part of the valence bands will be able to escape from the solid because of it. The As $M_{4,5}VV$ transition will produce electrons from the full valence band, but they will emerge at sufficiently low energies that they may well lie on a rapidly varying background which would be difficult to remove from the data.

(b) The M_1VV and $M_{2,3}VV$ transitions for both Ga and As are likely to be too weak to be seen because the probability of the Coster-Kronig $M_1M_{2,3}V$, $M_1M_{4,5}V$, and $M_{2,3}M_{4,5}V$ decays can be expected to be high²¹ causing M_1 and $M_{2,3}$ holes to be filled long before an M_1VV or $M_{2,3}VV$ transition can occur.

(c) The $M_1M_{2,3}V$ lines of Ga and As will overlap one another and since the ratio of 3s-level binding energies of As and Ga is only 1.3, it would be difficult to separate the As and Ga data by performing experiments at various incident-beam energies for which the probabilities of M_1 -hole creation on Ga and As were different. Additionally, of the MMV lines, the $M_1M_{2,3}V$'s are the broadest, because they involve two core levels which are broadened by Coster-Kronig transitions, and at the same time, the $M_1M_{2,3}V$ lines are spin-orbit split.

(d) On the other hand, $M_1M_{4,5}V$ Auger electrons from Ga and As should not overlap each other at all in energy. Lifetime broadening effects on the $M_1M_{4,5}V$ lines should be somewhat less severe than for the $M_1M_{2,3}V$ transitions because only one Coster-Kronig decaying level is involved, and there are no spin-orbit splitting effects in the $M_1M_{4,5}V$ case.

(e) Finally, for the $M_{2,3}M_{4,5}V$ lines, matters are somewhat worse. Here, depending on how much broadening there is, there will be some overlap in energy of the Ga and As lines, and spin-

orbit splitting will be significant.

We conclude from this analysis that of the various possible MMV and MVV decays of GaAs, the ones most likely to provide useful information are the $M_1M_{4,5}V$ and $M_{2,3}M_{4,5}V$ lines. Accordingly, it is these transitions for which we present numerical results in Sec. III.

III. NUMERICAL RESULTS: THE $M_1M_{4,5}V$ AND $M_{2,3}M_{4,5}V$ AUGER LINES OF GaAs(110)

Calculated Ga and As $M_1M_{4,5}V$ and $M_{2,3}M_{4,5}V$ Auger line shapes for our relaxed GaAs(110) 1×1 surface are presented in Figs. 2 and 3. Focusing attention on the curves on the left-hand sides of these figures, which do not include the effects of lifetime broadening or (in Fig. 3) spin-orbit splitting of the Ga and As 3p levels, one notes that there are marked differences, in both cases, between the expected Ga and As lineshapes.

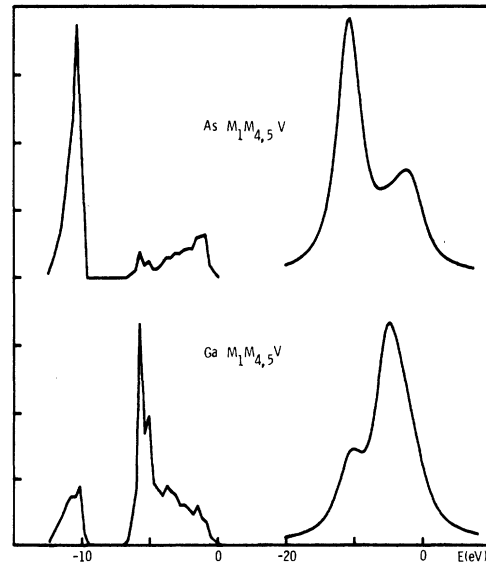


FIG. 2. Calculated Ga and As $M_1M_{4,5}V$ Auger spectra for GaAs(110) 1×1 . The curves on the right-hand side were obtained by folding those on the left with Lorentzians of widths ~ 4 eV (cf. Table II). Note that the scale on the abscissa for the broadened curves is twice that for the unbroadered ones. For all the curves shown, incidentally, we used a mean free path of 7 Å.

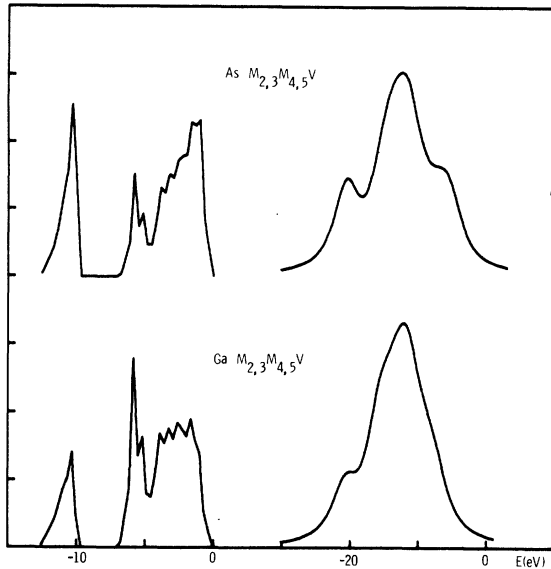


FIG. 3. Calculated Ga and As $M_{2,3}M_{4,5}V$ Auger spectra for GaAs(110) 1×1 . The curves on the right-hand side were obtained from those on the left by folding with Lorentzians of 4eV width and by including the effects of the 4- and 6-eV splittings of the $3p$ levels in Ga and As, respectively. (In each case the contributions of the $3p_{3/2}$ and $3p_{1/2}$ levels were assumed to be in their statistical proportion, 2:1.) Note that the scale of the abscissa for the curves on the right-hand side is twice that for the curves on the left. Also, note that these curves were calculated for a 7-Å mean free path.

These differences reflect the different angular momentum character of the LDOS's for the two atomic species.

In Fig. 2 it is evident that for both Ga and As the matrix elements for $M_1M_{4,5}N_1$ transitions dominate those for $M_1M_{4,5}N_{2,3}$ decays; i.e., the s -like parts of the valence bands are enhanced relative to the p -like parts in the Auger lineshapes as compared to what one sees in the LDOS's (cf. Fig. 1). Thus, the As $M_1M_{4,5}V$ line is predominantly a single narrow peak coming from about 10 eV below the valence-band maximum, while the Ga $M_1M_{4,5}V$ line has its largest peak at ~ -5 eV and smaller structures on either side of it.

In Fig. 3 we see that the situation for the $M_{2,3}M_{4,5}V$ lines is somewhat different. Here, the contributions to the line shapes for both Ga and As from the p -like components of the valence bands are considerably stronger. Thus, the As $M_{2,3}M_{4,5}V$ line is more of a two-peaked structure than in the $M_1M_{4,5}V$ case and similarly for Ga.

Unfortunately, when the effects of lifetime broadening and spin-orbit splitting are taken into account, the differences between the various MMV lines are made less distinct. However, as shown

in the curves on the right-hand sides of Figs. 2 and 3, they should still be quite readily visible in experimental data.

In order to understand why the curves of Figs. 2 and 3 look as they do, we begin by consulting Table I, which presents values of atomically calculated radial matrix elements $\mathcal{R}_\kappa(l_f l_i l_1 l_2)$ (where l_f and l_i are the orbital angular momenta of the final Auger electron and initial core hole, respectively, where l_1 and l_2 are the angular momenta of the final holes, one in a $3d$ core level and the other in the valence band, and where the integer κ represents the angular-momentum transfer) for the Ga and As $M_1M_{4,5}V$ and $M_{2,3}M_{4,5}V$ Auger decays. In order to decide if any of these matrix elements might be dominant, one must recall²² that each \mathcal{R} is always accompanied, when one calculates a transition rate, by the factor $(2\kappa + 1)^{-1}$. Thus, the \mathcal{R} 's with the smallest value of κ tend to be the most important. Looking at Table I(a), one notes that for the $M_1M_{4,5}V$ transitions (because of angular momentum and parity conservation) there is only one $\mathcal{R}_\kappa(l_f l_i l_1 l_2)$ for which $\kappa = 0$, namely, $\mathcal{R}_0(2002)$, and that this matrix element is for decays involving a valence-band s electron. None of the other \mathcal{R} 's is as large as $\mathcal{R}_0(2002)$ after being multiplied by $(2\kappa + 1)^{-1}$. Thus, we anticipate that s -like valence electrons will be most prominent in the $M_1M_{4,5}V$ lines, which indeed they are.

A similar analysis may be made of the \mathcal{R} 's in Table I(b) for the $M_{2,3}M_{4,5}V$ lines. Here there are two large matrix elements involving p -like valence electrons, $\mathcal{R}_0(2112)$ and $\mathcal{R}_1(2121)$, but also two comparably significant elements involving valence electrons of s character, $\mathcal{R}_1(1102)$ and $\mathcal{R}_1(1120)$. Thus, for the $M_{2,3}M_{4,5}V$ lines one can understand why the s - and p -like parts of the valence band are roughly comparable in importance.

These arguments can be given in more detail using the simplified version of the independent-electron theory of Auger line shapes of Ref. 6. There it is shown that if the off-diagonal LDOS matrix²³ component $F_{(0,0),(1,0)}$ [where the subscripts (l, m) refer to orbital angular momentum components and thus $F_{(0,0),(10)}$ means F_{s,p_z} and, e.g., $F_{(0,0),(0,0)} = \rho_s$, the s -like part of the ordinary LDOS] is small, then any core-core-valence Auger line shape for an s - p -band solid can be given as a linear combination of LDOS components for the decaying ion. Accordingly, making use of the fact that $F_{(0,0),(1,0)}$ is generally small for our model of GaAs(110) 1×1 , and of our analysis of which matrix elements are most important for the $M_1M_{4,5}V$ and $M_{2,3}M_{4,5}V$ lines, we can write rather simple expressions for these line shapes, which agree quite well with the line shapes calculated using the exact theory of Ref. 6. Specifically, we

have for the partial width for producing $M_1M_{4,5}V$ Auger electrons at energy E from ions at depth Z , the approximate formula,

$$\hbar\Gamma_{M_1M_{4,5}V}(E, Z) \approx 16\pi R \left[\rho_s \left(\sum_{m_f} \tilde{B}_{22m_f} \right) [\mathcal{R}_0^2(2002) - \frac{1}{5}\mathcal{R}_0(2002)\mathcal{R}_2(2020)] + C_p \right]. \quad (1)$$

In Eq. (1), R is the rydberg, C_p is a rather complicated expression for the small contributions of the p electrons to the line shape,²⁴ and \tilde{B}_{11^12m} is a factor describing the escape probability of the Auger electron, given by²⁵

$$\tilde{B}_{11^12m} \equiv \frac{1}{2} \left(\frac{(2l_1+1)(2l_2+1)(l_1-m)!(l_2-m)!}{l_1+m)!(l_2+m)!} \right)^{1/2} \times \int_0^1 dx P_{l_1}^m(y(x)) P_{l_2}^m(y(x)) e^{-z/\lambda y(x)} \quad (2)$$

In Eq. (2), λ is the inelastic mean free path, the quantity $y(x)$ is given by

$$y(x) \equiv [(Ex^2 + V_0)/(E + V_0)]^{1/2}, \quad (3)$$

where V_0 is the inner potential, and the $P_l^m(z)$ are associated Legendre polynomials.

For the $M_{2,3}M_{4,5}V$ transitions we obtain a similarly simple formula, viz.,

$$\begin{aligned} \hbar\Gamma_{M_{2,3}M_{4,5}V}(E, Z) = & (16\pi R/3) \left\{ \frac{2}{3}\rho_s \tilde{B}_{000} [\mathcal{R}_1^2(1102) + \mathcal{R}_1^2(1120) - \mathcal{R}_1(1102)\mathcal{R}_1(1120)] + 5\rho_p \tilde{B}_{000} \mathcal{R}_0^2(2112) \right. \\ & + [\rho_{(1,0)} (\frac{1}{5}\tilde{B}_{221} + \frac{2}{15}\tilde{B}_{220}) + (\rho_{(1,1)} + \rho_{(1,-1)}) (\frac{1}{5}\tilde{B}_{222} + \frac{1}{10}\tilde{B}_{221} + \frac{1}{30}\tilde{B}_{220})] \\ & \left. \times [\frac{4}{3}\mathcal{R}_1^2(2121) - 2\mathcal{R}_1(2121)\mathcal{R}_0(2112)] \right\}, \quad (4) \end{aligned}$$

in which the $\rho_{(l,m)}$ are the components of the p -like LDOS, i.e.,

$$\rho_p \equiv \rho_p(E - E_{3d} + E_{3p}, Z) \equiv \sum_{m=-1}^1 \rho_{(1,m)}(E - E_{3d} + E_{3p}, Z). \quad (5)$$

Note that in deriving Eq. (4), one must use the identity, cf. Eq. (2),

$$\sum_{m=-l}^l \tilde{B}_{11^1m} \equiv (2l+1)\tilde{B}_{000}.$$

Equations (1) and (4) will provide a useful format for parametrizing experimental data. That is, if one has confidence in calculated LDOS's of Ga and As for a GaAs(110) surface, then by fitting theory and experiment via Eqs. (1) and (4), one may determine the experimental values of the important radial Auger matrix elements. This sort of information will be very helpful in trying to understand the differences between Auger matrix elements for an isolated atom and those for the same atom when it resides in a solid.⁶

IV. DISCUSSION

We have shown that the differences in the LDOS's on Ga and As atoms in GaAs(110) 1×1 should result in rather large differences in the Ga and As

$M_1M_{4,5}V$ and $M_{2,3}M_{4,5}V$ Auger line shapes from this surface. An experimental confirmation of this prediction would be an important step toward the development of valence-band Auger spectroscopy as a tool for obtaining *local* DOS information from surfaces. At the same time an experimental determination of the Auger line shapes of GaAs(110) would be useful insofar as it might confirm or cast doubt on models of GaAs(110) surface relaxation,⁹⁻¹² and also in that it would permit a determination of the Auger matrix elements of Ga and As to compare with theory.

On the other hand, GaAs is perhaps not the most attractive material for an Auger study. The Auger lines in GaAs, particularly the $M_1M_{2,3}V$ lines, tend to overlap somewhat, and are quite broad due to the rapidity of all the possible *MMV* Coster-Kronig transitions. We have investigated GaAs(110) theoretically because it is the only binary compound surface for which an empirical LCAO band-structure calculation has been performed using an atomic geometry that is reasonably well established.^{11,12} Experimentally, however, at least at the outset, compounds of lighter elements, whose Auger lines are more widely separated and are also less broadened might make more attractive objects of investigation.

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- ²¹This is evidenced by their widths in Table II.
- ²²Reference 6, Eqs. (3.4) and (3.5).
- ²³The LDOS matrix is defined by
- $$F_{(l,m), (l',m')} (E, Z) = \sum \delta(E - E_s) c_{(l,m)}(s, Z) \times c_{(l',m')}^*(s, Z),$$
- where the sum on *s* covers occupied states and where *c* is the amplitude for an electron of orbital angular momentum (*l*, *m*) on an atom at depth *Z* in state *s*. Note that $F_{(l,m), (l,m)}$ is thus just the (*l*, *m*) component of the ordinary LDOS.
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- ²⁵We have assumed here collection of Auger electrons from all 2π of azimuth and over 0 to $\frac{1}{2}\pi$ of polar angle. Relaxation of the latter assumption is a trivial matter theoretically; but relaxation of the former assumption would make the numerics considerably more complicated.