Modeling the space-charge-layer boundary of a forward-biased junction

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In a p-n junction under forward bias, however large or small, the space-charge-layer boundaries are well defined in the sense that surfaces exist on both sides of the junction at which electric field reverses. Each zero-field surface lies within a layer of space charge attributable exclusively to imbalance of the excess-carrier densities. With the assumption of negligible recombination, an analytical solution for the boundary regions can be written. The solution defines surfaces lying on either side of each zero-field surface, separated from it by distances that are bias independent. The analytical solution for the boundary region has been joined to a numerical solution for the balance of the sample. The analytical solution defines clearly the position at which quasineutrality gives way to gross space charge.

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I. INTRODUCTION

The carrier field, and potential profiles of p-n junctions have been the subjects of extensive numerical calculations because of difficulties inherent in the general analytical problem. Middlebrook has presented analytical approximations for the reverse-biased junction—specifically for the case of the collector junction of a bipolar transistor in forward-active operation. The forward-biased junction, however, presents a simpler problem. This is true because electric field undergoes reversal at both space-charge-layer boundaries; the fact that transport of both carrier types is purely diffusive at these surfaces provides a point of entry for an analysis. Guckel et al. have explored the existence of these zero-field surfaces to treat the abrupt junction under forward bias. We shall do so also. Their treatment, however, differs from ours in two major respects: (1) they focused primarily on the region of significant depletion and "inversion," in the case of an asymmetric junction that lies near the metallurgical junction. We focused on the region at the boundary of the space-charge layer and on the adjacent quasineutral region that extends all the way to the corresponding ohmic contact. (2) They produced approximate analytical solutions for a wide range of doping relationships in the abrupt junction. We made simplifying assumptions and provided an exact analytical solution for the boundary and quasineutral regions. We then combined our exact solution with a more recent numerical solution for the region of heavy depletion to achieve an overall result. While this result does not have general applicability because of our restrictive assumptions, it nonetheless does provide a kind of modeling insight into the behavior of carrier populations that is very difficult to extract from purely numerical studies, and even from approximate analytical studies.

The zero-field surfaces whose presence we exploit exist for any forward bias, high or low. But as the first (and major) simplification, we shall assume low-level conditions. For further simplification of the problem, let us consider a one-dimensional symmetric step-junction in a semiconductor material of very high carrier lifetime. Now, the reason for the existence of the zero-field surfaces can be appreciated by considering these factors: inside the zero-field surfaces (i.e., in a direction toward the metallurgical junction), field direction is set by the junction's double layer of ionic charge; in the end regions, the field arises to counter majority-carrier diffusion, and this requires a field sense opposite to that associated with the double layer that embraces the junction.

II. THE MODEL

Figure 1 shows the situation we wish to examine. Here, for illustration, we have arbitrarily selected a sample and a bias level so that the distance from a zero-field surface to the corresponding ohmic contact is ten extrinsic Debye lengths.

In addition to symmetric doping, we assume end regions of equal length and ideal ohmic contacts to each. Let us consider these contacts to provide surfaces at which equilibrium carrier densities are preserved, and the semiconductor material between them to have infinite lifetime. For steady-state bias, then, we must have continuity of and throughout the sample; there are no sources or sinks for carriers of either type within the semiconductor. In Fig. 1(b), portions of the hole and electron profiles are shown with linear axes. Since low-level conditions are assumed, it is of course necessary to create a huge gap in the ordinate in order to depict both populations. Let us focus on the right-hand side. Linear profiles for minority carriers in both end regions are dictated by the assumptions above. Further, the hole (minority-carrier) profile remains linear well into the space-charge region: this is because \( E(x) \) must rise to a value that is several orders of magnitude larger than the nearly constant field in the end region before hole drift becomes significant. Refer to Fig. 1(b) once more. The hole density in the region two or so Debye lengths thick lying to the left of \( x = 0 \) differs by a small factor (less than 2) from the hole density an equal distance to the right of \( x = 0 \). Electric field assumes a nearly constant value in the end region [Fig. 1(a)]. But there the product \( p(x)E(x) \) is by assumption so small that drift current is negligible; thus the assertion above is a plausible one. Below we shall offer quantitative verification that \( J_{p,n} \) remains essentially diffusive well into the space-charge region.
In the end region to a small degree and in the boundary region (i.e., in the vicinity of the boundary of the space-charge layer) to a much larger degree, the densities of excess-carrier populations are unequal. This is represented by the difference between the excess-electron (majority-carrier) profile and the excess-hole profile as shown in Fig. 1(c). The \( n(x) \) profile must necessarily pass through a maximum and then head down steeply to meet its orders-of-magnitude lower boundary value at the other side of the space-charge layer. Note that we have chosen to place the origin of the \( x \) coordinate at one of the surfaces where electric field changes sign.

Figure 1(d) shows in qualitative fashion the two components of electron current density throughout the sample. Proceeding from right to left we observe that the rightward (particle) diffusion of electrons constitutes a negative conventional current-density component. The electric field mentioned in Sec. I moves electrons leftward, to yield a positive and larger drift component of electron density. Note that where the maximum in \( n(x) \) is located [Fig. 1(c)], \( J_{\text{drift}} \) is purely field induced [Fig. 1(d)], and where \( E(x) \) vanishes [Fig. 1(e)] the electron current is purely diffusive. Extrema in both components occur somewhere to the right of the metallurgical junction; then \( J_{\text{drift}} \) fades away while \( J_{\text{os}} \) settles down to become \( J_{\text{os}} \), this occurring (as noted above) well before the other space-charge boundary is reached. The two current-component curves are symmetric about \( 1/2(L_o) \).

A similar pair of curves could be sketched for holes, but have been omitted from Fig. 1(d) in the interest of clarity. They would, of course, be symmetric about \( 1/2(L_o) \).

It is worthwhile to consider the variation of the current profiles in Fig. 1(d) as a function of bias voltage \( V \). In the low-level regime, the end-region currents grow exponentially with \( V \) via the factor \( \exp [qV/(kT)] \). In the transition region, the values also grow with \( V \) but by a smaller factor. For example, at the metallurgical junction the electron density grows as \( \exp [qV/(kT)] \) and the field declines slowly, approximately according to the power-law prescription \( \psi \sim V^{1/2} \), where \( \psi \) is the contact potential. Thus, electron drift current at the junction is proportional to the product of these factors and is slower growing than end-region currents (in a relative rather than absolute sense) on account of both factors. The electron diffusion component at the junction is
always larger by the amount \( J_{n,\text{int}} \), which of course grows purely exponentially. As bias increases, the extrema in the current components move closer to the metallurgical junction.

We should point out that it is not essential to assume infinite lifetime between the ohmic contacts to carry out a useful analysis. We can, for example, substitute a sample with long end regions and large but finite lifetime. Then we merely substitute the carrier diffusion lengths (assumed equal) for \( X_e \) and achieve an analysis of the junction’s boundary region having approximately equal validity. We still, however, neglect recombination in the space-charge region. But let us return to the infinite-lifetime case. The minority-carrier profiles in the end regions are linear and symmetric about the metallurgical junction. Symmetry requires, then, that the respective minority-carrier currents in these regions are related by letting \( b = \mu_n/\mu_p \), by

\[
J_{n,\text{int}} = b J_{p,\text{int}}. \tag{1}
\]

It follows from the above current-continuity argument that this relationship holds throughout the sample, regardless of the minority or majority status of a given carrier, a point made for the case of electrons in Fig. 1(d).

Now let us apply Eq. (1) at \( x = 0 \):

\[
J_{n,\text{int}}(0) = b J_{p,\text{int}}(0), \tag{2}
\]

both of these currents are purely diffusive because electric field is zero at this surface. It follows from this fact that

\[
\frac{dn'}{dx} \bigg|_{x=0} = -\frac{dp'}{dx} \bigg|_{x=0}, \tag{3}
\]

fact that we shall presently employ. (The prime indicates excess-carrier density.) Through the interval \( 0 < x < X_e \), however, \( J_{n,\text{int}} \) contains both diffusion and drift components, while \( J_{p,\text{int}} \) remains purely diffusive because of the low-level assumption. Hence for the entire interval we may write

\[
qD_n \frac{dn'(x)}{dx} + q\mu_n n_0 E(x) = qD_p \frac{p'(0)}{X_e}, \tag{4}
\]

where the symbols have their usual meanings.

But we may also write

\[
E(x) = \frac{q}{e} \int_0^x [p'(x_t) - n'(x_t)] \, dx_t, \tag{5}
\]

cause the disparity between the excess-carrier densities constitutes the “source charge” responsible for the field in \( 0 < x < X_e \) interval. Hence, from Eqs. (4) and (5), and Einstein’s relation

\[
\frac{[x]}{x} + \frac{q}{kT} n_0 \int_0^x [p'(x_t) - n'(x_t)] \, dx_t = \frac{q D_p}{X_e}, \tag{6}
\]

\[
\frac{[x]}{x} + \frac{1}{L_D^2} \int_0^x [p'(x_t) - n'(x_t)] \, dx_t = \frac{q D_p}{X_e} = 0, \tag{7}
\]

where \( L_D \) is the extrinsic Debye length. Differentiating,

\[
\frac{d^2 [x]}{dx^2} + \frac{1}{L_D^2} [p'(x) - n'(x)] = 0. \tag{8}
\]

It is evident from the foregoing assumptions and Fig. 1(c) that the excess-hole density may be written throughout the interval of interest as

\[
p'(x) = p(x) - p'(0) = \frac{x - X_e}{X_e}. \tag{9}
\]

Substituting this expression into Eq. (8) produces an equation having a solution of the form

\[
n'(x) = A e^{-x/X_p} + B e^{x/X_p} = \frac{p'(0)}{X_e} \frac{x - X_e}{X_e}. \tag{10}
\]

As one boundary condition we impose Eq. (3). To provide a second boundary condition we define the position \( x = X_e \) by means of the expression

\[
p'(X_e) = n'(0). \tag{11}
\]

The geometrical meaning of this definition is clearly indicated in Fig. 1(c). Applying these boundary conditions then gives us

\[
n'(x) = p'(0) \left\{ \frac{L_D}{2X_e} \left[ 2 \frac{X_e}{L_D} \right] e^{x/L_D} \right. - \left. \frac{L_D}{2X_e} \left[ 2 \frac{X_e}{L_D} \right] e^{-x/L_D} \right\} \frac{x - X_e}{X_e}. \tag{12}
\]

The dependence of \( X \) upon \( X_e \), can be evaluated by evaluating Eq. (12) at \( x = X_e \), where \( n' = 0 \):

\[
\frac{L_D}{2X_e} \left( 2 \frac{X_e}{L_D} \right) e^{X_e/L_D} - \frac{L_D}{2X_e} \left( 2 \frac{X_e}{L_D} \right) e^{-X_e/L_D} = 0.
\]

Whence,

\[
\frac{X_e}{L_D} = \frac{1}{2} \ln \left( \frac{2 \left( X_e/L_D \right)}{2 - \left( X_e/L_D \right)} \right). \tag{13}
\]

The quantity \( (X_e / L_D) \) approaches the value of 2.0 very quickly. For example, for the absurdly low value \( (X_e / L_D) = 3 \), we find that \( (X_e / L_D) = 1.99 \). And for \( (X_e / L_D) = 10 \), that \( (X_e / L_D) = 1.9999999999 \). Consequently we can, for most practical purposes, substitute \( (X_e / L_D) = 2 \) into Eq. (12), to yield

\[
n'(x) = p'(0) \left( \frac{x - X_e}{X_e} \right) - \frac{L_D}{X_e} e^{-x/X_p}. \tag{15}
\]

Next, let us define the position \( x = -X_e \), by writing \( n'(-X_e) = 0 \). Once more the geometrical significance of this boundary definition can be seen in Fig. 1(c). The subscript “i” stands for “inner”. This is a logical boundary because ionic space charge is felt to its left. To its right there are sufficient majority electrons present to neutralize the charge of the \( p_i \) equilibrium holes plus the net donor atoms, assumed fully ionized. In the region \(-X_e < x < 0\), electrons are once more transported by both drift and diffusion. Let us assume that throughout this range the minority holes still have low enough density so that their transport remains purely diffusive. We shall examine this assumption below. Under these conditions then, all of the steps leading to the solution for \( n'(x) \), Eq. (15), remain equally valid, so this expression may be considered to apply throughout the entire interval \(-X_e < x < X_e\). Once more, excess-carrier mismatch provides the “source charge” for the [now leftward-directed] electric field.

Evaluating Eq. (15) at \( x = -X_e \) yields

\[
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\[ n'( -X_c) = 0 = \rho'(0) \left( \frac{X_c + X_i}{X_c} - 2 \frac{L_D}{X_c} e^{X_i/L_D} \right) \]  

(16)

From this expression we learn that

\[ \frac{X_i}{L_D} = \ln \left( \frac{X_c + X_i}{2L_D} \right) \]  

(17)

Because \( X_c > X_i \), typically, and because of the logarithmic insensitivity of the right-hand side to \( X_c \), this is readily solved by iteration to give the result plotted in Fig. 2. To an excellent approximation, the thickness of the inner layer of excess-carrier charge grows logarithmically with \( X_c \), which is, in turn, approximately sample half-length for a long sample at bias levels in excess of \(-0.1 \, \text{V}\).

Next let us examine the validity of our assumption that the minority profile may be assumed linear to and beyond (i.e., even inside) the position \( -X_c \). From Eqs. (9) and (15) we have

\[ \rho'(x) = \rho'(0) 2 \frac{L_D}{X_c} e^{-x/L_D} \]  

(18)

Integrating this expression from \( -X_c \) to 0, and then from 0 to \( X_c \), and then dividing the first result by the second, gives the ratio of the charge in the inner layer to that in the entire region from the zero-field surface to the ohmic contact. Via Gauss's law, then, it gives the ratio

\[ \frac{E(-X_c)}{E(X_c)} \approx \frac{X_c}{2L_D} - 1 \]  

(19)

where the approximation assumes \( X_c \geq 10 \, L_D \). Evidently from Eq. (19) our assumption of a linear majority hole profile is valid if \( X_c \) is not too large. That is, it holds for some intermediate range, such as \( 10 < (X_c/L_D) < 10^9 \), failing ultimately when \( E(-X_c) \) becomes large enough to produce a nonnegligible drift current.

**III. DISCUSSION AND EXTENSION OF THE MODEL**

Further questions deserve to be addressed. First, just where in the boundary region of the space-charge layer does one apply the well-known boundary conditions, such as those of Shockley,\(^{11}\) Fletcher,\(^{12}\) or Misawa.\(^{13}\) Here we should note parenthetically that the Fletcher and Misawa conditions are fully equivalent,\(^{14}\) and at low level, both asymptotically approach the Shockley conditions.

Since we have assumed low-level conditions in the present analysis, it can be said that only the Shockley boundary conditions are relevant. However, the qualitative character of the carrier profiles is unaltered as we make the transition into high-level conditions. That is (continuing to focus on the right-hand side in Fig. 1), \( \rho(x) \) will remain monotonic in the region of interest; \( E(x) \) will vanish at a surface where we choose to place the x origin; the slopes of the carrier profiles at \( x = 0 \) will continue to have magnitudes that are equal; \( n(x) \) will exhibit a maximum near \( x = 0 \), etc. In view of these facts, it is worthwhile to inquire about the most appropriate choice of boundary location for purposes of applying the high-level boundary conditions as well as low-level conditions.

The Fletcher conditions invoke a voltage \( V_f \) that is the difference between the junction's diffusion potential and the actual boundary-to-boundary potential difference when the junction is under bias. From the field profile in Fig. 1(e) it is evident that a potential extremum exists at \( x = 0 \) when the junction is under bias. Thus the choice of \( x = 0 \) as the boundary leads to an unambiguous value for \( V_f \).

The Misawa conditions, on the other hand, invoke the Fermi-level "splitting", or the separation of the two quasi-Fermi levels in the transition region. This, too, is a very clearly defined quantity in high-lifetime samples. A given quasi-Fermi level is flat not only through the transition region but well into the quasineutral region on the side where the carrier in question has minority status. Basically this is true because, for all but extremely low-level biases, the minority densities in the boundary portion of the quasineutral region are orders of magnitude larger than in the ohmic contact portion; thus orders-of-magnitude lower gradients of the quasi-Fermi level will be required in the former region.
as compared to the latter. Thus it is that the zero-field surface is a logical choice as the boundary when one considers the potential difference specified in either the Misawa or Fletcher boundary conditions.

The second consideration is somewhat less concise. Both Fletcher and Misawa address four unknowns, namely, both carrier densities at both boundaries. Two of the necessary equations are Boltzmann-type equations. The other two are neutrality equations applied at the two boundaries. But it is evident in Fig. 1(c) that strict neutrality does not exist at \( x = 0 \). From Eq. (18),

\[
p'(0) - n'(0) = \frac{2L_D}{X_c}.
\]

(20)

Thus by increasing \( \{X_c/L_D\} \) or \( \{L_D/L_D\} \), the neutrality assumption can be made valid to any arbitrary degree. But for a short sample, the neutrality assumption is poor. We point out, however, that space-charge density falls rapidly as we depart farther from the junction. At \( x = X_c \), merely two Debye lengths farther from the junction, we have

\[
p'(X) - n'(X) = \frac{2L_D}{X_c} e^{-X/X_c} = (0.135)p'(0) \frac{2L_D}{X_c},
\]

(21)

so that the space-charge density has declined nearly an order of magnitude. These findings suggest that the zero-field surface constitutes a good choice as a meaningful space-charge-layer boundary for a wide range of practical cases.

Next, let us pose a second key question. Just where in the boundary region is the surface that separates a region of quasineutrality from a region of gross space charge. Let us adopt as the criterion for quasineutrality the condition that the space-charge density resulting from excess-carrier mismatch be less than the charge associated with the excess-hole density at \( x = 0 \) by the factor \( K \). That is,

\[
p'(x) - n'(x) = [p'(0)]/K.
\]

(22)

Using Eq. (18) we find that

\[
\frac{x}{L_D} = -\ln \left[ \frac{X_c}{(12L_DK)} \right].
\]

(23)

This relationship is plotted in Fig. 3 for various values of \( K \).

A problem in the present analysis is that the zero-field surface advances toward the metallurgical junction as forward bias is increased. In other words, the position of the origin is bias dependent. As a consequence \( X_c \), the distance from the origin to the ohmic contact is also bias dependent. A reasonable way to deal with this complication is to specify a particular sample and then to observe the dependence of \( X_c \) upon bias.

First, let us arbitrarily select a symmetric junction sample wherein \( N = 10^{15} \) cm\(^{-3} \). Also, choose a sample half-length, \( X_e = (100)L_D \). Next, let us define the position \( x = -X_e \) as the position where \( n \) has dropped to the value 0.9 \( n_o \). In other words, we shall press our analytical solution to serve inward even beyond the point \( x = -X_e \). The subscript in \( X_e \) stands for "numerical", since it is at this point that we shall splice a numerical solution computed from the metallurgical junction toward \( X_e \) with the analytical solution computed from \( x = 0 \) toward \( X_e \). The numerical solutions for forward-biased junctions developed by Lee and Warner\(^6\) are convenient for present purposes. They showed that equilibrium solutions can be employed for low-level for-

![FIG. 3. Position of a critical surface as a function of \( X_c/L_D \) with \( K \) as a parameter. \( K \) is defined as the ratio of the charge associated with the excess-hole density at \( x = 0 \) to the space-charge density at the critical plane resulting from excess-carrier mismatch.](image-url)
ward-bias cases with negligible error. Figure 4(a) compares the equilibrium solution so employed with the analytical solution, which, from Eq. (15), can be written

\[ n(x) = n_0 + \frac{p'(0)}{X_s/L_D} \left( \frac{X_s - x}{L_D} - 2e^{-x/L_D} \right). \] (24)

By the definition of \( X_s \) we may write

\[ n(-X_s) = 0.9n_0 = n_0 + \frac{p'(0)}{X_s/L_D} \left( \frac{X_s}{L_D} - \frac{X_s}{L_D} - 2e^{-x'/L_D} \right). \] (25)

The quantity \( p'(0) \) may be computed for a voltage between 0.1 and 0.4 V using the usual low-level prescription; then the corresponding value of \( X_s/L_D \) and \( X_s'/L_D \) are readily found by iteration. For 0.4 V, the respective values are 87.3 and -8.5, as can be seen in Fig. 4(a). Note that when the two curves have been joined at \( n = 0.9 \ n_0 \), they match very closely. The slope of the analytical solution is

\[ \frac{dn}{dx} \bigg|_{-x_s} = \frac{p'(0)}{L_D} \left( \frac{2}{X_s/L_D} \right)^{x'/L_D} - \frac{1}{X_s/L_D} \]

\[ = 1.00 \times 10^{14}/\text{cm}^3 \ L_D, \] (26)

and that of the numerical solution is \( 0.91 \times 10^{14}/\text{cm}^3 \ L_D \), both computed at \(-X_s\), so the match is satisfactory.

In Fig. 4(b) the same data are presented, but with the ordinate scale expanded by a factor of 100 to show details of the analytical solution analogous to those in Figs. 1(b) and 1(c). Figure 4(c), then, shows the data of Fig. 1(a) once more, but with the ordinate scale compressed by a factor of 10 to show the carrier profile throughout the transition region. Finally, Fig. 4(d) shows how the positions of the several critical points in the analytical solution move spatially as forward bias is varied. Curiously, the origin's location depends linearly on applied bias. As 0.5 V is approached, high-level conditions commence in this particular sample. Also, for bias values below 0.1 V, the assumption of a flat minority-carrier quasi-Fermi level (upon which our computation of

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FIG. 4. (a) Comparing analytical solution for carrier density in boundary region (solid line) with equilibrium numerical solution for sample with half-length \( X_s = 100 \ L_D \), with \( n_0 = 10^{14}/\text{cm}^3 \), and with forward voltage \( V = 0.4 \) V. Curves have been matched at \( n \) 0.9. (b) Data of part (a) with ordinate scale expanded by a factor of 100 to show details of analytical solution analogous to those in Figs. 1(b) and 1(c). (c) Data of part (a) with ordinate scale compressed by a factor of 10 to show electron-density profile throughout transition region. (d) Dependence of solution critical points upon forward-bias voltage. The meanings of these symbols are as follows: \( n(-X_s) = 0.9n_0 \); \( n(X_s) = n_0 \); at \( x = 0 \), \( E = 0 \); \( p'(X) = n(0) \). The spatial origin has been placed at the junction here for reference and comparison.
$\rho(0)$ is based] becomes poor. In addition, the plane of field reversal (i.e., the origin) retreats so far from the junction that further strain is placed on the assumption of a flat Fermi level. Hence the computations have been extended only from 0.1 to 0.4 V. If they were repeated for the range below 0.1 V, taking into account the effects just described, the plane of field reversal would approach $X^*$ as $V$ approaches zero.

IV. CONCLUSIONS

We have defined a simplified problem for which it is possible to obtain an exact analytical solution. The case selected is the symmetric step junction of high lifetime under low-level forward bias. The match of this analytical solution to an equilibrium numerical solution for the transition region is excellent, with the point where $n = 0.9 n_x$ taken as the point for joining the two solutions. It is shown that the plane of field reversal that always exists in the boundary region of a forward-biased junction is a logical and well defined location for applying boundary conditions. This zero-field surface lies within a "blanket" of space charge arising from excess-carrier mismatch. On the side toward the neutral region, this layer of space charge has a bias-independent thickness of $2L_D$. Also it is independent of the dimension $X_0$ (approximately the sample half-length), or of the carrier diffusion length in a sample of large but finite lifetime. On the side toward the junction, this layer of carrier charge increases logarithmically with $X_0$. If the sample is long enough so the $X_0$ may be regarded as bias independent, then the inner-layer thickness $Y$ is bias independent. For intermediate values of low-level bias, from 0.1 to 0.4 V, the surface of field reversal moves toward the metallurgical junction, linearly with increasing bias voltage.

It is shown that the transition from quasineutrality to gross space charge occurs at a position that is bias independent. The analysis permits determination of this position for any desired criterion for "quasineutrality". The principles employed in this analysis can also be employed to address the problem of the asymmetric step junction. For the problem of high-level bias, however, both the numerical and analytical approaches would have to be changed.

We believe that the kind of detailed modeling on a very small scale ("micromodeling") illustrated above will become increasingly relevant as device dimensions continue to shrink.

5A. deMarli, Solid-State Electron. 11, 33 (1968).
7M. S. Mock, Solid-State Electron. 15, 115 (1972).
15Plotted analytical examples illustrating this point are shown in Fig. 6 of Ref. 14.