Electron scattering by confined LO polar phonons in a quantum well

B. K. Ridley
Department of Physics, University of Essex, Colchester CO4 3SQ, United Kingdom
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A simple model is used to highlight the main features of electron scattering in a quantum well via the Fröhlich interaction with confined LO polar optical phonon modes. It is shown that the scalar potential field associated with strongly confined modes is different from that assumed by other authors, and consequently quite different results are obtained. One of the possible interface modes is shown to be mainly responsible for intrasubband scattering in thin wells, and as a result the scattering rate is proportional to the density of states and this increases with diminishing well width.

I. INTRODUCTION

Light-scattering data indicate that optical phonons in GaAs quantum wells in the GaAs-$Al_xGa_{1-x}As$ system are confined (see review by Klein[1]), and this is supported by theory.[2] Several authors have pointed out that such confinement, leading to the presence of guided modes and interface modes, can reduce the strength of the Fröhlich interaction with electrons,[4-6] and also give rise to resonant effects in capture and intersubband processes.[7,8] The scattering of electrons by guided modes differs significantly from that by bulk modes. For example, while the bulk-mode interaction predicts intersubband scattering rates smaller than intrasubband scattering rates, the reverse is the case for the guided-mode interaction.[9] This is an important difference. Unfortunately, but inevitably, realistic theoretical models are heavily numerical, and the various factors which contribute to this difference are not always transparent. It is therefore one of the purposes of this paper to present a simple model of the electron-phonon interaction when the phonons are confined, in order to bring out the essential features of that interaction and to provide analytic formulas for estimating rates.

But perhaps more important is highlighting the disparity between different theoretical models. The difference between confined modes in a layer sandwiched between two layers of a different solid and those of an ionic slab as described by Fuchs and Kliewer[10] is clear. Fuchs-Kliewer modes have antinodes at the interfaces whereas confined modes in a layered material tend to have nodes at the interface. In such a situation the lowest-order mode ($m=1$) contributes significantly to intrasubband scattering and although the rate is reduced from that with bulk modes, the reduction is not large.[5] For well-confined guided modes in a layered material, on the other hand, the rate is reduced by an order of magnitude, as we will show. This is because only the $m=2$ mode is able to effect an intrasubband transition. All models agree that in a system such as GaAs/$Al_xGa_{1-x}As$ some modes can be extremely well confined in the GaAs layer.

Thus one can assume that the optical displacement of the ions in a guided mode is of the form

$$u_z \sim \sin(q_z z), \quad 0 \le z \le L$$

with $q_z = m\pi/L$. The difference arises in the choice of the scalar potential field associated with this displacement. Lassnig and Zawadski,[11] Sawaki,[6] and Wendler and Pechstedt[12] obtain a potential of the same form, and this leads to the $m=1$ mode being dominant in intrasubband scattering. In our simple model, which is based on the continuum model of Babiker,[2] the potential for guided modes is of the form

$$\phi \sim \cos(q_z z) ,$$

and this leads to profoundly different conclusions; for example, it is the $m=2$ mode, not the $m=1$ mode, which dominates intrasubband scattering as far as guided modes are concerned.

Another concern is the role of interface modes. All models agree that such modes may exist. Nevertheless, it is usually assumed that the guided modes are completely confined, implying zero amplitude at the interfaces. Strictly, then, such an assumption rules out the existence of interface modes, but they are nevertheless admitted to the models, and indeed play a significant role. This apparent inconsistency requires some justification and we will attempt to do this.

II. THE ELECTRON-PHONON INTERACTION

We will assume that the effective-mass model is adequate to describe electrons in a single quantum well, and that the continuum model serves to describe the optical vibrations. The simplifying features consist of assuming that both electrons and phonons are totally confined within the layer forming the quantum well. The quasi-two-dimensional (quasi-2D) electron wave function is then

$$\psi(\mathbf{r},z) = \left[\frac{2}{V}\right]^{1/2} U(\mathbf{r},z) e^{i\mathbf{k}\cdot\mathbf{r}} \sin(k_z z), \quad 0 \le z \le L \tag{1}$$

where $\mathbf{r}$ is a position vector lying in the plane of the layer,

z lies along the direction perpendicular to the plane, V is the cavity volume, and $U(\mathbf{r},z)$ is the cell-periodic part of the Bloch function. The wave vector $\mathbf{k}$ lying in the plane is unrestricted, but because of the assumption that the electron is totally confined,

$$k_z=\frac{n\pi}{L}\ , \tag{2}$$

where L is the width of the layer.

To begin with, let us ignore the existence of interface modes, and deal only with guided modes. Assuming that the optical vibration is totally confined means that the component of optical displacement transverse to the layer is of the form

$$u_z(\mathbf{Q})=\hat{\mathbf{z}}A(\mathbf{Q})e^{i\mathbf{q}\cdot\mathbf{r}}\sin(q_z z)\ , \tag{3}$$

where $\mathbf{Q}$ is the total wave vector such that

$$Q^2=q^2+q_z^2\ , \tag{4}$$

with

$$q_z=m\frac{\pi}{L},\quad m=1,2,\ldots, \tag{5}$$

and $\hat{\mathbf{z}}$ is a unit vector. We assume that the boundary conditions are such as to produce nodes at the interfaces. (By assuming this we rule out the existence of interface modes. We return to this later.) The displacement along the layer must be such that the mode is truly longitudinal with zero electric displacement. For such a mode the electric field is given by

$$\epsilon=-\frac{e^*}{V_0\epsilon_0}\mathbf{u}=-\nabla\phi\ , \tag{6}$$

where e^* is the Callen effective charge, V_0 is the volume of the unit cell, ϵ_0 is the permittivity of free space, and ϕ is the associated scalar potential. Since the displacement is a gradient of a scalar field its curl must vanish, and hence

$$\mathbf{u}_{\mathbf{r}}(\mathbf{Q})=\mathbf{B}(\mathbf{Q})e^{i\mathbf{q}\cdot\mathbf{r}}\cos(q_z z)\ , \tag{7}$$

with

$$\frac{A(\mathbf{Q})}{B(\mathbf{Q})}=\frac{iq_z}{q}\ . \tag{8}$$

The mode amplitude can now be found by relating the total energy in the cavity to that of an equivalent simple harmonic oscillator. Thus

$$E=\tfrac{1}{2}\omega^2\overline{M}\int\mathbf{u}^*(\mathbf{Q})\cdot\mathbf{u}(\mathbf{Q})d\mathbf{r}\,dz=\tfrac{1}{2}\omega^2\overline{M}\chi(\mathbf{Q})\ , \tag{9a}$$

whence

$$|A(\mathbf{Q})|^2+|B(\mathbf{Q})|^2=\frac{2}{N}\chi(\mathbf{Q})\ , \tag{9b}$$

where ω is the oscillator angular frequency, $\overline{M}$ is the reduced mass, $\chi(\mathbf{Q})$ is the coordinate for the simple harmonic oscillator, and N is the number of unit cells in the cavity. It follows from Eqs. (8), (9), and (6) that

$$\phi(\mathbf{Q})=-\frac{ie^*}{V_0\epsilon_0}\left[\frac{2}{N}\right]^{1/2}\frac{\chi(\mathbf{Q})}{Q}e^{i\mathbf{q}\cdot\mathbf{r}}\cos(q_z z) \tag{10}$$

and the total potential is

$$\phi=-\frac{e^*}{V_0\epsilon_0}\left[\frac{2}{N}\right]^{1/2}\sum_{\mathbf{Q}}\frac{1}{Q}[i\chi(\mathbf{Q})e^{i\mathbf{q}\cdot\mathbf{r}}\cos(q_z z)+\text{c.c.}]\ . \tag{11}$$

The Fröhlich interaction then gives the scattering rate:

$$W=\frac{2\pi}{\hbar}\int|\langle\mathbf{k}'|e\phi|\mathbf{K}\rangle|^2\delta(E'-E)dN_f\ . \tag{12}$$

Processing the matrix element is standard and leads to the usual conservation of crystal momentum in the plane; with that implied, we obtain

$$W=\frac{e^2\omega_L}{2\pi L}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_s}\right][n(\omega_L)+\tfrac{1}{2}\mp\tfrac{1}{2}]\times\sum_{q_z,k_z'}G^2(q_z)\int\int\frac{q}{q^2+q_z^2}\delta(E'-E)dq\,d\theta\ , \tag{13}$$

where ϵ_∞ and ϵ_s are the permittivities at high and low frequencies, respectively, $n(\omega_L)$ is the phonon occupation factor, the upper sign is for absorption and the lower for emission, and

$$G(q_z)=\int_0^L\psi'(\mathbf{r},z)\cos(q_z z)\psi(\mathbf{r},z)dz\ . \tag{14}$$

This integral determines momentum conservation in the z direction. With the electron wave functions given by Eqs. (1) and (2), $G=0$ unless

$$q_z=\begin{cases}|k_z'\pm k_z|, & k_z'\neq k_z & (15)\\ 2k_z, & k_z'=k_z\ , & (16)\end{cases}$$

when $G^2(q_z)=\frac{1}{4}$. Equations (15) and (16) describe intersubband and intrasubband scattering, respectively. They show that crystal momentum is conserved. In terms of quantum numbers they become

$$m=\begin{cases}|n'\pm n|, & n'\neq n & (17)\\ 2n, & n'=n\ , & (18)\end{cases}$$

where m is the phonon mode number, n is the number of the subband containing the initial electron state, and n' refers to the subband containing the final state.

The integration over q and θ is straightforward and we can write the result as follows:

$$W=\tfrac{1}{2}W_0\left[\frac{\hbar\omega_L}{E_1}\right]^{1/2}\frac{\pi^2}{L^2}[n(\omega_L)+\tfrac{1}{2}\mp\tfrac{1}{2}]\times\sum_{q_z}\left[q_z^4+2q_z^2k^2\left[2\pm\frac{\hbar\omega^*}{E_k}\right]+\left[\frac{\hbar\omega^*}{E_k}\right]^2k^4\right]^{-1/2}, \tag{19}$$

where

$$E_1=\frac{\hbar^2\pi^2}{2m^*L^2} \tag{20}$$

is the energy of the lower subband minimum, E_k $(=\hbar^2 k^2/2m^*)$ is the kinetic energy in the plane of the electron before scattering, and

$$\mp\hbar\omega^* = E_{n'} - E_n \mp \hbar\omega_L \ , \tag{21}$$

where E_n is the energy of the initial subband minimum, and $E_{n'}$ is that containing the final state. The basic rate W_0 is given by

$$W_0 = \frac{e^2}{4\pi\hbar}\left[\frac{2m^*\omega_L}{\hbar}\right]^{1/2}\left[\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right] , \tag{22}$$

and the sum in Eq. (19) is over all allowed values of q_z.

III. RATES FOR LOW QUANTUM NUMBERS

In many quasi-2D situations we are mainly interested in the scattering rates involving the two lowest subbands. Equation (19) yields simple analytic solutions for the intraband scattering rate in the lowest subband and the interband rate involving a transition from $n=2$ to $n=1$.

Consider first the intrasubband rate when the energy of the electron is just enough to emit a phonon, and let us suppose that emission is the only process allowed. Then with $\hbar\omega^* = \hbar\omega_L$, $E_k = \hbar\omega_L$, and $q_z = 2k_z$, we obtain

$$W = \tfrac{1}{2}W_0\left[\frac{\hbar\omega_L}{E_1}\right]^{1/2}\frac{1}{4+(\hbar\omega_L/E_1)} \ . \tag{23}$$

The only mode which can contribute to intrasubband transitions is the $m=2$ guided mode.

For the intersubband rate we assume the electron is at the bottom of band 2, and again only emission is allowed. (We assume $E_2 - E_1 \geq \hbar\omega_L$.) Then $\hbar\omega^* = E_1 - E_2 + \hbar\omega_L$, $E_k = 0$, and $q_z = (k_z \pm k_z)$, and we obtain

$$W = \tfrac{1}{2}W_0\left[\frac{\hbar\omega_L}{E_1}\right]^{1/2}\left[\frac{1}{4-(\hbar\omega_L/E_1)} + \frac{1}{12-(\hbar\omega_L/E_1)}\right] . \tag{24}$$

Contributions are obtained solely from $m=1$ modes. (Note that our assumption that $E_2 - E_1 \geq \hbar\omega_L$ implies that $\hbar\omega_L/E_1 \leq 3$.)

These rates are plotted for GaAs as a function of well width in Fig. 1. Unlike the situation for bulk modes, for guided modes the intraband rate is *less than* the interband rate. The magnitude of the intersubband rate is not much different from that obtained with bulk modes, but the intraband rate is less by an order of magnitude. The latter comes about not only because of the effect of confinement on the magnitude of q_z but also because symmetry rules out any interaction with the lowest-order mode. This result is markedly different from that obtained with ionic slab modes.[5] One reason for this is that slab modes have antinodes at the surface. Interchanging cosine for sine in Eq. (11) increases the rate by an order of magnitude. The other reason is that interface modes make a contribution in ionic slabs but they are at present ruled out in our simple model.

IV. RATE FOR HIGH QUANTUM NUMBERS

As the bulk situation is approached, the importance of intrasubband processes diminishes. In the limit we can neglect them altogether and replace the summation in Eq. (19) with an integral over final states. For simplicity we consider an electron scattering from the bottom of a subband so that $E_k = 0$, and once again, for brevity, deal with emission only. Then

$$W = \tfrac{1}{2}W_0\left[\frac{\hbar\omega_L}{E_1}\right]^{1/2}\frac{\pi^2}{L^2} \times \int_{k'_{z_{\min}}}^{k'_{z_{\max}}} [(k_z \pm k'_z)^2 - (k'^2_z - k_z^2 + k_0^2)]^{-1} dk' \frac{L}{\pi} \ , \tag{25}$$

where we have substituted $q_z^2 = (k_z \pm k'_z)^2$, replaced $E_{n'}$ and E_n in favor of k'_z and k_z, introduced $k_0^2 = \hbar\omega_L/(\hbar^2/2m^*)$, and replaced the summation step by $dk'L/\pi$. The lower limit refers to the wave vector of the lowest subband and as $L \to \infty$ this can safely be put to zero. The upper limit is the highest subband to which an emission is possible, i.e.,

$$k'_{z_{\max}} = k_z\left[1 - \frac{\hbar\omega_L}{E}\right]^{1/2} , \tag{26}$$

where E is the energy of the initial state (the subscript z becomes redundant here). The integration is straightforward and gives the correct bulk result:

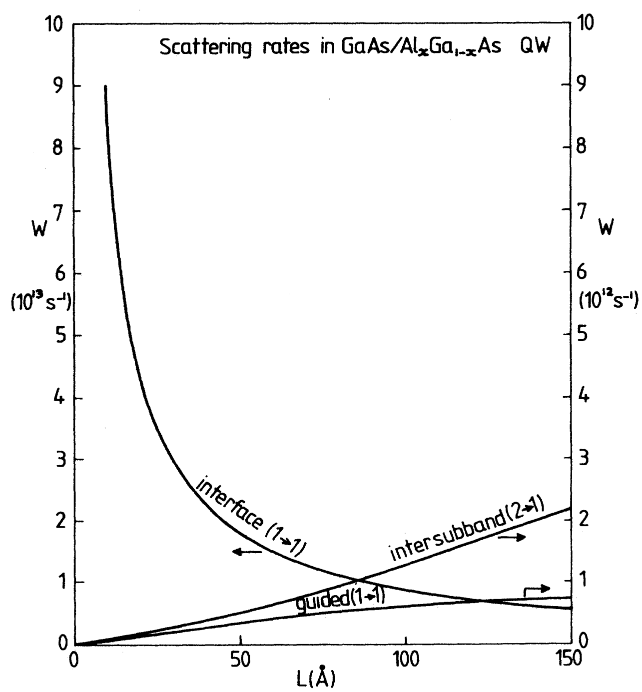

FIG. 1. Scattering rates in the GaAs/Al$_x$Ga$_{1-x}$As quantum well.

$$W=W_0\left[\frac{\hbar\omega_L}{E}\right]^{1/2}\sinh^{-1}\{[(E/\hbar\omega_L)-1]^{1/2}\} . \quad (27)$$

The calculation of absorption is equally straightforward and again gives the bulk result.

This successful extrapolation to the bulk solution is satisfactory, but it cannot be used as an argument for the detailed correctness of our model. The reason for this is that it depends on the conservation of crystal momentum, but this need not be rigorous. For a cosine potential conservation of momentum is exact, which is the case in our model. For a sine potential, such as one obtains for the Fuchs-Kliewer model and other models, conservation of momentum is not exact, but it approaches exactness with increasing well width. Thus whatever the detailed properties of a model may be in the quasi-2D regime, the bulk result will always be recoverable.

V. INTERFACE MODES

It is evident that our simple model, which assumes that the ionic displacement at the interface is zero, cannot describe interface modes and their interaction with electrons. In general such modes will exist and their importance in determining the strength of the electron-phonon interaction will be enhanced as the well width decreases, in view of the weakening of the interaction with guided modes. It is therefore important to relax our assumption of strict confinement in order to allow interface modes to appear. If the amplitude of interface modes remains small it may then be reasonable to keep the assumption of strict confinement to describe the guided modes while admitting interface modes.

We can show that this approximation is valid for $GaAs/Al_xGa_{1-x}As$ by considering the hydrodynamic boundary conditions at the interfaces for an interface mode. Using the approach in Sec. II we can show that only two LO interface modes exist and they have optical displacements and scalar potentials when u_z is small at the interfaces given by an even and an odd solution, respectively.

Even solution:

$$u_z(\mathbf{Q})=i\left[\frac{2}{N}\right]^{1/2}\frac{\alpha e^{i\mathbf{q}\cdot\mathbf{r}}\chi(\mathbf{Q})\cosh\{\alpha[z-(L/z)]\}}{[(q^2+\alpha^2)\gamma-(q^2-\alpha^2)]^{1/2}} , \quad (28)$$

$$\mathbf{u}_r(\mathbf{Q})=\left[\frac{2}{N}\right]^{1/2}\frac{\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}}\chi(\mathbf{Q})\sinh\{\alpha[z-(L/z)]\}}{[(q^2+\alpha^2)\gamma-(q^2-\alpha^2)]^{1/2}} , \quad (29)$$

$$\phi(\mathbf{Q})=\frac{-ie^*}{V_0\epsilon_0}\left[\frac{2}{N}\right]^{1/2}\frac{e^{i\mathbf{q}\cdot\mathbf{r}}\chi(\mathbf{Q})\sinh\{\alpha[z-(L/z)]\}}{[(q^2+\alpha^2)\gamma-(q^2-\alpha^2)]^{1/2}} . \quad (30)$$

Odd solution:

$$u_z(\mathbf{Q})=i\left[\frac{2}{N}\right]^{1/2}\frac{\alpha e^{i\mathbf{q}\cdot\mathbf{r}}\chi(\mathbf{Q})\sinh\{\alpha[z-(L/z)]\}}{[(q^2+\alpha^2)\gamma+(q^2-\alpha^2)]^{1/2}} , \quad (31)$$

$$\mathbf{u}_r(\mathbf{Q})=\left[\frac{2}{N}\right]^{1/2}\frac{\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}}\chi(\mathbf{Q})\cosh\{\alpha[z-(L/z)]\}}{[(q^2+\alpha^2)\gamma+(q^2-\alpha^2)]^{1/2}} , \quad (32)$$

$$\phi(\mathbf{Q})=-i\frac{e^*}{V_0\epsilon_0}\left[\frac{2}{N}\right]^{1/2}\times\frac{e^{i\mathbf{q}\cdot\mathbf{r}}\chi(\mathbf{Q})\cosh\{\alpha[z-(L/z)]\}}{[(q^2+\alpha^2)\gamma+(q^2-\alpha^2)]^{1/2}} , \quad (33)$$

where $\gamma=\sinh(\alpha L)/\alpha L$. The parameter α is obtained from[2]

$$\frac{(\beta_2/\beta_1)(\rho_2/\rho_1)(q_\Delta^2+\alpha^2-q^2)\alpha}{(q^2-\alpha^2)\{q_\Delta^2+\alpha^2+q^2[(\beta_2/\beta_1-1)]\}^{1/2}}=\begin{cases}\coth(\alpha L/2) & \text{(odd)}\\ \tanh(\alpha L/2) & \text{(even)} ,\end{cases} \quad (34)$$

where ρ_1,ρ_2 are the densities of the well and barrier materials, respectively, and β_1,β_2 are the acoustic velocities. The wave vector q_Δ is defined as follows:

$$q_\Delta^2=\frac{\omega_1^2-\omega_2^2}{\beta_1^2} , \quad (35)$$

where ω_1,ω_2 are the LO frequencies at the zone center.

For the transverse displacements to be small at the interfaces it is clear from Eqs. (28) and (31) that α must be small. Thus if we wish to maintain the approximation that the guided modes are totally confined we must for consistency ensure that any solution describing an interface mode has $\alpha\rightarrow0$, and is compatible with our assumption for guided modes. For the latter it is necessary that the frequency disparity be large, i.e., $q_\Delta^2\gg q^2+q_L^2$. With this condition, only the odd solution is allowed, and a consistent solution can be obtained with

$$\alpha\approx\frac{q}{(q_\Delta L/2)^{1/2}} \quad (36)$$

provided $(q_\Delta L/2)\gg1$. For GaAs $q_\Delta=3.66\times10^7$ cm^{-1}, and so the condition holds for $L\gg5.5$ Å. Since this is virtually the condition for the continuum approximation to hold we may conclude that, within that approximation, an interface mode exists under conditions which are compatible with heavily confined guided modes. (Note, however, that the latter cannot exist when $q_z\rightarrow q_\Delta$, i.e., confinement becomes weaker with increase of mode number $m=q_zL/\pi$.)

The scattering rate associated with the odd mode with $\alpha\rightarrow0$ is readily obtained, viz.,

$$W=W_0\frac{(\hbar\omega_LE_1)^{1/2}}{\hbar\omega^*}G^2(\alpha) , \quad (37)$$

$$G(\alpha)=\alpha^2\left[\frac{\cos^2[(k_z'-k_z)L/2]}{\alpha^2+(k_z'-k_z)^2}-\frac{\cos^2[(k_z'+k_z)L/2]}{\alpha^2+(k_z'+k_z)^2}\right] . \quad (38)$$

$G(\alpha)$ is negligible except for an intrasubband transition and then, with $\alpha^{-2} \gg 4k_z^{-2}$, $G(\alpha)=1$, whence

$$W = W_0 \left[\frac{E_1}{\hbar\omega_L} \right]^{1/2} . \tag{39}$$

This rate is independent of kinetic energy in the plane and is much larger than that associated with guided modes in narrow wells (Fig. 1). Indeed, it is simply proportional to the density of states in the lowest band. (Note that this rate vanishes as $L \to \infty$. There is no interface component in the bulk situation.) The interface mode, as in the case of Fuchs-Kliewer modes, is acting here essentially like an $m=0$ guided mode (apart from a numerical factor).

VI. DISCUSSION

It is clear that interface modes can justifiably be included in a model containing totally confined guided modes. It is also clear that modes of the latter type are associated with a Fröhlich potential field which must have antinodes at the interfaces, and as a result such modes cannot scatter totally confined electrons within a subband with anything like the strength of bulk modes. As a consequence, scattering within a subband is effected principally by the interface mode with odd displacement symmetry (and hence even potential symmetry), with a rate which increases with diminishing well width. Scattering between subbands is entirely determined in our model by guided modes and hence this rate drops with diminishing well width.

These conclusions are at variance with the models of Lassnig and Zawadski,[11] Sawaki,[6] and Wendler and Pechstedt,[12] which appear to contain non-Fröhlich potentials. These models also ignore the variation of frequency with wave vector and rely on the dielectric discontinuity to describe interface modes. For longitudinally polarized optical modes the permittivity function $\epsilon(\omega)$ is zero, which is true on both sides of the interface. There is thus no dielectric discontinuity. Without taking into account dispersion it would not be possible to describe the quantized LO modes of the system, defined by $\epsilon(\omega)=0$, correctly.

Our simple model cannot claim to represent reality very closely. Neither electrons nor phonons will be totally confined. Processes forbidden by strict selection rules will become allowed, but at the expense of oscillator strength elsewhere. Nevertheless, the broad outline should remain. The odd interface mode will tend to dominate intrasubband processes, guided modes intersubband processes; with the intrasubband rate, as for bulk modes, greater than the intersubband rate. As a consequence of the role of the interface mode in the intrasubband process, the rate increases with diminishing well width, following the increase in density of states.

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