In a free-particle approximation we can write for the CM kinetic energy

$$E_{ke} = \hbar^2 K^2 / 2M. \qquad (6.70)$$

The relative motion is hydrogen atom like with quantum numbers $n = 1, 2, 3, \ldots$ and $\ell = 0, 1, 2, \ldots, n-1$. The continuum states describe free electron and hole under Coulomb attraction.

Fig. 6.20:

6.3.1. Exciton Effect at M_0 Critical Points

Let us assume spherical free-electron like conduction band for electrons

$$E_e(\mathbf{k}_e) = E_g + \hbar^2 k_e^2 / 2m_e \qquad (6.71)$$

and

$$E_h(\mathbf{k}_h) = E_g + \hbar^2 k_h^2 / 2m_h\,. \qquad (6.72)$$

The two-particle exciton wavefunction can be written in terms of *Bloch functions* of electron and holes, $\psi_{\mathbf{k}_e}(\mathbf{r}_e)$ and $\psi_{\mathbf{k}_h}(\mathbf{r}_h)$, as

$$\Psi(\mathbf{r}_e, \mathbf{r}_h) = \Sigma_{\mathbf{k}_e,\mathbf{k}_h} C(\mathbf{k}_e, \mathbf{k}_h)\, \psi_{\mathbf{k}_e}(\mathbf{r}_e)\, \psi_{\mathbf{k}_h}(\mathbf{r}_h) \qquad (6.73)$$

but "better" with *localized Wannier functions* $a_{\mathbf{R}_e}(\mathbf{r}_e)$ and $a_{\mathbf{R}_h}(\mathbf{r}_h)$, as

$$\Psi(\mathbf{r}_e, \mathbf{r}_h) = \Sigma_{\mathbf{k}_e,\mathbf{k}_h} \Phi(\mathbf{R}_e, \mathbf{R}_h)\, a_{\mathbf{R}_e}(\mathbf{r}_e)\, a_{\mathbf{R}_h}(\mathbf{r}_h), \qquad (6.74)$$

where $\Phi(\mathbf{R}_e, \mathbf{R}_h)$ is the *exciton envelope wavefunction.* This can be separated as

$$\Phi(\mathbf{R}_e, \mathbf{R}_h) = \psi(\mathbf{R})\, \phi(\mathbf{r}),$$

where $\psi(\mathbf{R})$ is the CM part and $\phi(\mathbf{r})$ is the relative motion part, where

$$\mathbf{R} = (m_e \mathbf{R}_e + m_h \mathbf{R}_h) / M \quad \text{and} \quad \mathbf{r} = \mathbf{R}_e - \mathbf{R}_h\,. \qquad (6.76)$$

The corresponding Schrödinger equations are

Total energy is a sum of the two above eigenenergies,

$$E = E_R + E_r .$$

The first one of these is the "free-particle" kinetic energy (6.70)

$$E_R(\mathbf{K}) = \hbar^2 K^2 / 2M \qquad (6.78a)$$

of the "free-particle" wavefunction

$$\psi_{\mathbf{K}}(\mathbf{R}) = N^{-1/2} \exp(i\mathbf{K}\cdot\mathbf{R}). \qquad (6.78b)$$

Following the model of hydrogen atom we can write for the relative motion

$$E_r(n) = E_r(\infty) - R^* / n^2, \qquad (6.80)$$

where $E_r(\infty)$ is minimum energy of the continuum states, the "zero energy" for $E_R(\mathbf{K})$. As this is the lowest electron excitation energy from valence to conduction band without forming a bound exciton, $E_r(\infty) = E_g$. R^* is the *excitonic Rydberg constant,* defined as

$$R^* = -\frac{1}{2}\left(\frac{e^2}{4\pi\varepsilon_o\varepsilon}\right)^2 \frac{\mu}{\hbar^2} = \frac{\mu}{m\varepsilon^2} R_H, \qquad (6.81)$$

where $R_H = 1/2$ Ha $= 1$ Ry ≈ 13.6 eV is the *hydrogen atom Rydberg constant* and m is the free electron mass. Note, that $\mu^{-1} = m_e^{-1} + m_h^{-1}$.

The relative motion wavefunctions are, of course, the hydrogenic ones

$$\phi_{n\ell m}(\mathbf{r}) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\varphi), \qquad (6.79)$$

where $\mathbf{r} = (r,\theta,\varphi)$, $R_{n\ell}(r)$ are the associate Laguerre polynomials and $Y_{\ell m}(\theta,\varphi)$ are the spherical harmonics.

By combining all of the above we obtain

$$\Phi_{\mathbf{K}n\ell m}(\mathbf{R},\mathbf{r}) = N^{-1/2} \exp(i\mathbf{K}\cdot\mathbf{R})\, R_{n\ell}(r)\, Y_{\ell m}(\theta,\varphi) \qquad (6.82)$$

and

$$E_{\mathbf{K}n} = E_g + \hbar^2 K^2 / 2M - R^* / n^2. \qquad (6.83)$$

In real semiconductors:

6.4. Phonon contribution to ε

Consider next the phonon polarization contribution to the complex dielectric function ε. Let us model "optically active" phonons by oscillation of a collection of identical charged *simple harmonic oscillators* (SHO). Assume isotropically and uniformly distributed SHOs of density N, with mass and charge M and Q, respectively.

By denoting the displacement vector of SHO by $\mathbf{u}$ the equation of free motion becomes

$$M\,\ddot{\mathbf{u}} = -K\,\mathbf{u} \qquad \text{or} \qquad \ddot{\mathbf{u}} + \omega_0^2\,\mathbf{u} = 0,$$

where $\omega_0^2 = K/M$ is the (square root of) resonance or natural frequency.

<u>Transverse Phonons, TO</u>

Now, consider the phonon response to the (transverse) electric field of plane wave form

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0 \exp[i(\mathbf{k}\cdot\mathbf{r} - \omega t)]. \tag{6.97}$$

The equation of motion becomes then

$$M\,\ddot{\mathbf{u}} = -K\,\mathbf{u} + Q\,\mathbf{E}. \tag{6.98}$$

The steady-state solution to this is

$$\mathbf{u}(\mathbf{r},t) = \mathbf{u}_0 \exp[i(\mathbf{k}\cdot\mathbf{r} - \omega t)],$$

whose substitution to (6.98) $\ddot{\mathbf{u}} + \omega_T^2\,\mathbf{u} = Q/M\,\mathbf{E}$ leads to

The macroscopic polarization

$$\mathbf{P} = NQ\,\mathbf{u} \tag{6.101}$$

gives the electric displacement

$$\mathbf{D} = \varepsilon_0\,\mathbf{E} + \mathbf{P} = \varepsilon_0\varepsilon\,\mathbf{E} \tag{6.102}$$

or in scalar form

If we include the low frequency contribution of electrons, $\varepsilon_\infty = \varepsilon_{electr}(0)$, the Eq. (6.103) takes form

$$\varepsilon(\omega) = \varepsilon_\infty + NQ^2 / [\varepsilon_0 M (\omega_T^2 - \omega^2)], \qquad (6.105)$$

provided that $\omega << E_g/\hbar$.

Longitudinal Phonons, LO

To allow longitudinal polarization without corresponding external field requires that $\varepsilon(\omega_L) = 0$. From (6.105) we obtain