G Effective-Mass Theory

The effective-mass theory or approximation (EMA), also termed the envelope function approximation, is widely used for calculating the electronic properties of carriers in potentials in an otherwise periodic crystal. The strength of the method is that the complexities of the periodic potential are hidden in the effective-mass tensor m^*_{ij}. The effective-mass theory is a useful approximation for the treatment of shallow impurities (Sect. 7.5) or quantum wells (Sect. 11.3.2) with a potential that is slowly varying with respect to the scale of the lattice constant.

For the lattice-periodic potential, the Schrödinger equation

$$H_0 \Psi_{n\mathbf{k}} = E_n(\mathbf{k}) \Psi_{\mathrm{n}\mathbf{k}} \tag{G.1}$$

is solved by the Bloch wave $\Psi_{n\mathbf{k}}$. With a perturbing potential V, the Schrödinger equation reads

$$(H_0 + V)\, \Psi_{n\mathbf{k}} = E_n(\mathbf{k}) \Psi_{\mathrm{n}\mathbf{k}} \; . \tag{G.2}$$

According to Wannier's theorem [1484], the solution is approximated by the solution of the equation

$$[E_n(-\mathrm{i}\nabla) + V]\, \Phi_n = E\, \Phi_n \; . \tag{G.3}$$

The dispersion relation is expanded to second order as described in Appendix F. The function Φ_n is termed the *envelope function* since it varies slowly compared to the lattice constant and the exact wavefunction is approximated (in lowest order) by

$$\Psi(\mathbf{r}) = \Phi_n(\mathbf{r}) \, \exp(\mathrm{i}\mathbf{k}\mathbf{r}) \, u_{n0}(\mathbf{r}) \; . \tag{G.4}$$

M. Grundmann, *The Physics of Semiconductors*, 2nd ed., Graduate Texts in Physics, DOI 10.1007/978-3-642-13884-3_30,