

Contents

Chapter 0 Introduction	1
Chapter 1 Linear Density Response	3
1.1 Non-Relativistic Hamiltonian	3
1.1.1 The Lagrangian for many-body systems	3
1.1.2 Canonical momentum	3
1.1.3 Non-relativistic Hamiltonian	4
1.1.4 Quantization of the electromagnetic field	4
1.1.5 Intrinsic spin in the magnetic field	5
1.1.6 Born-Oppenheimer approximation	5
1.1.7 Model Hamiltonian for electrons	6
1.2 Non-Resonant Inelastic Photon Scattering	7
1.2.1 Time dependent perturbation theory (TDPT)	7
1.2.2 Inelastic photon scattering	8
1.3 Linear Density Response	12
1.3.1 Density-density response function	12
1.3.2 Excitation energy of N-particle system	14
1.3.3 Connection with dynamic structure factor	16
1.4 Time-Dependent Density-Functional Theory	18
1.4.1 Density-functional theory (DFT)	18
1.4.2 Kohn-Sham response function	21
1.4.3 Meaning of Kohn-Sham response function	23
1.4.4 Application to phonon calculation	25
Chapter 2 Excitons in NiO and CoO	28
2.1 Introduction	28
2.2 Geometric structure	30
2.3 Electronic structure	31
2.3.1 LDA+U method	31
2.3.2 Band structure	33

- with
lent
68
- Fig. 2.72 $\chi(q \sim 7\text{\AA}^{-1}, q \sim 7\text{\AA}^{-1}; \omega)$, the results of the Hartree-Fock case weighting by the Fourier transforms of Wannier functions at $q \sim 7\text{\AA}^{-1}$ for CoO. 81
- Fig. 2.73 q -dependence of the imaginary parts of χ for the Hartree-Fock case in CoO with the energies at (a) 1.37eV, (b) 2.32eV, (c) 2.81eV, and (d) 3.17eV. Averaging over cubic equivalent anti-ferromagnetic domain is imposed. 82
- Fig. 3.1 Cubic structure of PbTiO_3 . 86
- Fig. 3.2 Tetragonal structure of PbTiO_3 . 86
- Fig. 3.3 Tetragonal structure of $\text{Pb}_{0.75}\text{Ca}_{0.25}\text{TiO}_3$. 87
- Fig. 3.4 Primitive unit cell of cubic $\text{Pb}_{0.5}\text{Ca}_{0.5}\text{TiO}_3$. 87
- Fig. 3.5 Phonon dispersion curves of tetragonal PTO corresponding to Type I and Type II calculations (see in the text) are shown as solid and dotted curves, respectively. Open symbols (circles, triangles)[85] and solid symbols (circles[71], diamonds[83], squares[84]) denote various experimental data. 91
- Fig. 3.6 Sound velocities of longitudinal (L) and two shear waves (S1 and S2) of tetragonal PTO in (a) a-b and (b) a-c planes. Shear wave polarizes nearly perpendicular (parallel) to the plane is represented as S1 (S2). Brillouin scattering experiment data[72] and calculations based on experimental and theoretical relaxed geometries are plotted as dashed, solid and dotted lines, respectively. 93
- Fig. 3.7 TO1 mode of cubic PbTiO_3 with frequency $215i \text{ cm}^{-1}$. The direction of wave vector q is pointed out on the right-hand side of the plot. 97

