THEORY OF THERMAL NEUTRON SCATTERING

The Use of Neutrons for the Investigation of Condensed Matter

W. Marshall and S. W. Lovesey

Atomic Energy Research Establishment
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PREFACE

In the last decade there has been a rapid expansion in the use of neutron-beam techniques to investigate the properties of solids, liquids, and gases. Nevertheless there is no easy access to the theory of neutron scattering from these materials, and workers in the subject are obliged to work through the original papers to get the necessary theoretical background. The intention of this book is therefore to give a comprehensive review of all the theory that is relevant to the interpretation of experiment.

Inevitably, the limitations of time and space have obliged us to omit many points of interest. We have given almost nothing on experimental techniques, on extinction, and on the refraction of long wavelength neutrons. Liquids are given a long chapter although they deserve a book to themselves. The discussion of critical phenomena is handicapped by the fact that many ideas and results are being published as the book goes to press; we have therefore been content to describe simple theories of critical phenomena and merely indicate some of the more recent work. Except in a few special cases we have not aimed to quote original references for the various ideas or observations which are described in the book. Parts of Chapter 6, on the theory of magnetic scattering from salts, and of Chapter 8, on the use of correlation functions in magnetic scattering, have not previously been published, as far as I know.

This is a book that has been started many times but finished only once. The first attempt was made in collaboration with my colleague Roger Elliott more than a decade ago. But we both found research too time-demanding for the more leisurely exercise of book-writing to be given any attention. A second attempt with Marty Blume as partner suffered the same fate. A third, solo, attempt was smothered by growing responsibilities and their demands for time.

The modest idea of these three early attempts was simply to revise, update, and extend the lecture notes that I had prepared for a course at Harvard in 1959. The fourth attempt started inauspiciously: Stephen Lovesey rejected the modest idea and argued for a fresh start altogether, not based on material written a decade earlier supplemented with miscellaneous lectures and notes I had prepared since then. His argument seemed logical but likely to set back the completion date for another decade. This pessimism was unfounded, because fifteen months later he produced a manuscript which, with little alteration, has now become this book.

W. M.

AERE, Harwell
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LIST OF IMPORTANT SYMBOLS

$A = \{(i+1)b^{(+)}+ib^{(-)}\}/(2i+1)$ (1.27 a)

$\quad = \bar{b}$ coherent scattering amplitude (1.28 a)

$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ basic vectors of unit cell (2.1)

$\hat{A}$ Hermitian operator (Appendix B)

$\hat{a}^+, \hat{a}$ Bose creation and annihilation operators (Chapters 3 and 4)

$A_{\alpha\beta}(l, l')$ second-order derivatives of crystal potential (4.3) and (4.26)

$\mathscr{A}_{\alpha\beta}(\mathbf{q})$ dynamical matrix (4.11 b) and (4.28)

$a_\lambda^\wedge(\mathbf{d}; \mathbf{k})$ tight binding transformation coefficients (5.72)

$B = 2\{b^{(+)}-b^{(-)}\}/(2i+1)$ (1.27 b)

$\hat{B}$ Hermitian operator (Appendix B)

$b^{(+)}$ scattering length for $i+\frac{1}{2}$ state } Chapter 1

$b^{(-)}$,, ,, $i-\frac{1}{2}$ state } Chapter 1

$\hat{b}$ scattering amplitude operator (1.26)

$\bar{b}$ coherent scattering length (1.24)

$\mathscr{b}_l = \bar{b}_l \exp[-\frac{1}{2}\langle\{\boldsymbol{\varkappa}.\hat{\mathbf{u}}(l, 0)\}^2\rangle]$ (15.7)

$B_s[x]$ Brillouin function (13.22)

$\hat{c}, \hat{c}^+$ Fermion operators for electrons (§ 5.5 and Chapter 9)

c velocity of light (Chapter 5), c concentration of impurities (Chapters 14 and 15)

C_P, C_V specific heats at constant pressure, C_P, and constant volume, C_V (Chapter 11)

c_ξ concentration of ξ isotope (1.21)

c_0 velocity of sound (11.138)

$$\operatorname{curl} \mathbf{A} \equiv \boldsymbol{\nabla}\times\mathbf{A} = \tilde{\mathbf{x}}\left(\frac{\partial A_z}{\partial y}-\frac{\partial A_y}{\partial z}\right)+\tilde{\mathbf{y}}\left(\frac{\partial A_x}{\partial z}-\frac{\partial A_z}{\partial x}\right)+\tilde{\mathbf{z}}\left(\frac{\partial A_y}{\partial x}-\frac{\partial A_x}{\partial y}\right)$$

$\mathbf{d}$ position vector of atom within unit cell (2.2)

$\mathbf{D}(\mathbf{m}-\mathbf{n})$ anisotropic exchange parameter (13.55)

$\mathscr{D}(\mathbf{q})$ Fourier transform of $\mathbf{D}(\mathbf{m}-\mathbf{n})$ (13.56)

D spin-wave stiffness (Chapter 9)

$D(T)$ temperature-dependent spin-wave stiffness (Chapter 9)

$\mathrm{d}\tilde{\mathbf{k}}' = \mathrm{d}\Omega$ (Chapters 1 and 2)

$\mathrm{d}\sigma/\mathrm{d}\Omega$ differential cross-section (§ 1.2 and Appendix A)

$\mathrm{d}^2\sigma/\mathrm{d}\Omega\mathrm{d}E'$ partial differential cross-section ((1.10) and Appendix A)

$\mathscr{D}^{(J)}_{MK}(\alpha\beta\gamma)$ rotation matrix (12.14)

$\operatorname{div}\mathbf{A} = \boldsymbol{\nabla}.\mathbf{A} = \dfrac{\partial A_x}{\partial x}+\dfrac{\partial A_y}{\partial y}+\dfrac{\partial A_z}{\partial z}$

E, E' initial and final energy of neutron, respectively (§ 1.2)
$\mathscr{E}_\lambda(\mathbf{k})$ band energy (5.46)
$\mathscr{E}$, $\mathscr{E}_\mathbf{q}$ reduced spin-wave energy (§ 9.6 (*b*) and § 15.2)
e charge of single electron
$\mathbf{E}$ electric field due to atomic electrons and nuclei in target ((5.1) and § 10.3)
E_λ, $E_{\lambda'}$ initial and final target energies (§ 1.2)

$f(\mathbf{k}, \mathbf{k}')$ scattering amplitude (1.8 b)
$F(\boldsymbol{\varkappa})$ atomic form factor ((5.15), § 5.3, (6.120), and (6.121))
$\mathscr{F}(\boldsymbol{\tau})$ magnetic unit-cell vector structure factor (7.16)
$\mathscr{F}_\mathrm{d}(\boldsymbol{\varkappa})$ vector form factor (7.21)
$F_\mathrm{N}(\boldsymbol{\tau})$ nuclear unit-cell structure factor (2.12)
$F_\mathrm{M}(\boldsymbol{\tau})$ magnetic unit-cell structure factor (7.27 a)
$F_\mathrm{E}(\boldsymbol{\tau})$ electrostatic unit-cell structure factor (10.56)
$F^{\alpha\beta}(\boldsymbol{\varkappa}, \omega)$ spin spectral weight function (Chapter 8 and (13.15))
$f(r)$ radial part of one-electron wave function (§ 5.2 and (6.19))

g gyromagnetic ratio, Landé splitting factor (5.24)
$g_{OP}(\omega)$ spectral weight function (§ B.5)
$g_{OP}(t) = \langle\hat{O}(t)\hat{P}(0)\pm\hat{P}(0)\hat{O}(t)\rangle$ Fourier transform of spectral weight function (Appendix B, (B.36))
$G^{<}_{OP}(\omega)$ spectral function of arbitrary operators $\hat{O}$ and $\hat{P}$ (Appendix B, (B.33 a))
$G^{>}_{OP}(\omega) = \exp(\hbar\omega\beta)G^{<}_{OP}(\omega)$ spectral function (Appendix B, (B.33 b) and (B.35))
$G^{(\pm)}_{OP}$ advanced $(-)$ and retarded $(+)$ thermal two-time Green functions (§§ 8.3 and B.8)
$G(\mathbf{r}, t)$ pair correlation function (3.9)
$G_\mathrm{s}(\mathbf{r}, t)$ self pair correlation function (3.19 a)
$G^\mathrm{cl}(\mathbf{r}, t)$ classical pair correlation function (3.21)
$G^\mathrm{cl}_\mathrm{s}(\mathbf{r}, t)$ classical self pair correlation function (3.20)
$\tilde{G}(\mathbf{r}, t) = G(\mathbf{r}, t+\frac{1}{2}\mathrm{i}\hbar\beta)$ (3.46)
$\bar{G}_\mathrm{s}(\mathbf{r}, t)$ ((3.59 a) and § 3.5)
$\bar{G}_\mathrm{d}(\mathbf{r}, t)$ ((3.59 b) and § 3.5)
$G'(\mathbf{r}, t)$ (3.26 a)
$G'_\mathrm{s}(\mathbf{r}, t)$ (3.27 a)

$g(\mathbf{r})$ static pair-distribution function (3.23)

$\text{grad}\,\phi = \nabla\phi = \tilde{\mathbf{x}}\dfrac{\partial\phi}{\partial x}+\tilde{\mathbf{y}}\dfrac{\partial\phi}{\partial y}+\tilde{\mathbf{z}}\dfrac{\partial\phi}{\partial z}$

$G'_l(\mathbf{r},t)$ (8.9)

$G_l(\mathbf{r},t)$ (8.9)

$\mathscr{H}$ quantum mechanical Hamiltonian

$\mathscr{H}$ classical Hamiltonian

H, $\mathbf{H}$ magnetic field (Chapters 8, 9, and 13, and Appendix B)

H_{A} single-ion anisotropy field (§ 9.6 (*a*))

h_{A} reduced single-ion anisotropy field (9.245)

$\hbar$ Planck's constant/2π

$\hat{\mathbf{i}}$ nuclear spin operator of magnitude i

I Coulomb matrix element (9.95)

$I(\boldsymbol{\varkappa},t)$ spatial Fourier transform of pair correlation function (3.15 b)

$I_{\text{s}}(\boldsymbol{\varkappa},t)$ spatial Fourier transform of self pair correlation function (11.2 b)

Im imaginary part

$\hat{\mathbf{J}} = \hat{\mathbf{L}}+\hat{\mathbf{S}}$ total angular momentum operator of magnitude J (§ 5.3 and Chapter 6)

$J(\mathbf{m}-\mathbf{n})$ exchange parameter in Heisenberg Hamiltonian between ions at lattice sites $\mathbf{m}$ and $\mathbf{n}$ (Chapter 9)

$\mathscr{J}(\mathbf{q})$ spatial Fourier transform of exchange parameter J (9.10 a)

$J^{(n)}$ moments of exchange parameter (9.240), see also $\overline{l^n}$

$j_K(x)$ spherical Bessel function of order K

$\bar{j}_K(\kappa)$ radial integral ((5.20) and (6.38))

$\mathbf{k}$ wave vector of incident neutron, electron momentum (Chapters 5 and 9)

$\mathbf{k}'$ wave vector of scattered neutron

k_{B} Boltzmann's constant

k_f electron wave vector at Fermi surface (§ 9.2)

$\bar{k}$, $\bar{k}'$ initial and final neutron wave vectors in centre of mass frame of reference (§ 12.2)

l cell indices } use also m, n, and k (2.1)
$\mathbf{l}$ lattice vector }

$\overline{l^n}$ moments of exchange parameter (9.22), see also $J^{(n}$

l orbital quantum number (Chapters 5 and 6)

$\hat{\mathbf{l}}$ electron orbital angular momentum operator (Chapter 6)

$\hat{\mathbf{L}}$ total orbital angular momentum operator of magnitude L (Chapter 5)

m mass of neutron
m_e mass of electron
M mass of nucleus
$M^\alpha = -g\mu_B\langle\hat{S}^\alpha\rangle$ magnetic moment
M_L, M_S total orbital and spin magnetic quantum numbers
$$-L \leqslant M_L \leqslant L, \quad -S \leqslant M_S \leqslant S$$
(Chapter 6)
m^*_λ effective mass (§ 5.5)

N number of unit cells in crystal (or nuclei of same type)
$n_j(\mathbf{q}) = [\exp\{\beta\hbar\omega_j(\mathbf{q})\}-1]^{-1}$ (4.18 a)
$n(\omega) = [\exp(\hbar\omega\beta)-1]^{-1}$ Bose factor
$\tilde{\mathbf{n}} = \mathbf{k}'\times\mathbf{k}/(k^2\sin\theta)$ (10.25)
n number of electrons in incomplete atomic shell (§ 6.3)
$\hat{n}_\nu$ particle number operator (5.50)
$N(k)$, $N(\lambda)$ incident flux of neutrons (§§ 1.1 and 2.4)

$\hat{O}$ arbitrary operator (Appendix B)
$\mathcal{O}$ = average over nuclear spin orientations (§ 10.4)

$\mathbf{P}$ polarization vector of incident neutrons (§ 10.1)
$\mathbf{P}'$ polarization vector of scattered neutrons (§ 10.2)
$\hat{\mathbf{p}} = -i\hbar\boldsymbol{\nabla}$ linear momentum operator (3.37)
$\hat{\mathscr{p}}$ linear momentum density operator (5.91), see also (6.3)
$\hat{\mathbf{p}}(l)$ nuclear momentum operator (4.16 b)
p_σ incident neutron spin probability (§§ 1.2 and 10.2)
p_λ probability distribution for initial target states (§ 1.2)
$\mathrm{P}\int$ principal part integral
$\mathbf{P}_\perp = \tilde{\boldsymbol{\varkappa}}\times(\mathbf{P}\times\tilde{\boldsymbol{\varkappa}})$ (10.79)
$P_{\alpha\beta}(l, l'; \omega)$ unperturbed phonon Green function (15.15)
$\mathscr{P}^j(\mathbf{q})$ (15.24)
$\mathscr{P}(\omega)$ reduced unperturbed phonon Green function (15.34)
$P(m, n; \mathscr{E})$ unperturbed ferromagnetic spin-wave Green function (15.87) and (15.89)
$\hat{P}$ arbitrary operator (Appendix B)

$\mathbf{q}$ reciprocal vector
$\hat{\mathbf{Q}}_\perp$ total magnetic interaction operator ((5.10) and § 6.4)
$\hat{\mathbf{Q}}$, where $\hat{\mathbf{Q}}_\perp = [\tilde{\boldsymbol{\varkappa}}\times(\hat{\mathbf{Q}}\times\tilde{\boldsymbol{\varkappa}})]$ ((5.12 a), (6.57), and § 6.4)
$\hat{\mathbf{Q}}^{(\mathrm{D})}$ dipole approximation to $\hat{\mathbf{Q}}$ ((5.19) and § 6.5)

$\mathbf{R}_{ld} = \mathbf{l}+\mathbf{d}$ position vector of nucleus (2.3)

$R_{AB}(t)$ relaxation function (Appendix B, § B.4)

$\mathscr{R}_{\mathbf{q}}(t)$ spin relaxation function ((8.31) and Chapter 13); see also (8.89)

$\mathscr{R}_{\mathbf{q}}(\omega)$ Fourier transform of spin relaxation function

r number of atoms in a unit cell (Chapter 2) and number of nearest-neighbour ions to given ion (Chapter 9)

Re real part

$\hat{S}$ spin operator of magnitude S for magnetic ion (Chapter 5)

$\hat{s}$ spin operator for a single electron (Chapter 5)

$\hat{\mathfrak{s}}(\mathbf{r})$ electron spin density operator (5.59)

$\hat{\mathfrak{s}}(\mathbf{q})$ Fourier transform of electron spin density operator (5.60)

$S(\boldsymbol{\varkappa}, \omega)$ scattering law (Chapter 3, nuclear, and Chapter 8, magnetic)

$\hat{S}^{\pm} = \hat{S}^{x} \pm i\hat{S}^{y}$ spin angular momentum raising and lowering operators

$\tilde{S}(\boldsymbol{\varkappa}, \omega) = \exp(-\frac{1}{2}\hbar\omega\beta)S(\boldsymbol{\varkappa}, \omega)$ (3.45)

$S_{\mathrm{i}}(\boldsymbol{\varkappa}, \omega)$ 'incoherent' nuclear scattering law (3.18)

$\hat{S}^{\alpha}_{\mathbf{q}} = \sum \exp(-i\mathbf{q}.\mathbf{l})\hat{S}^{\alpha}_{l}$ (Appendix B, (B.81 b), Chapters 5, 8, 9, and 13)

$\hat{S}^{\pm}_{\mathbf{q}} = \sum \exp(\mp i\mathbf{q}.\mathbf{l})\hat{S}^{\pm}_{l} = \hat{S}^{x}_{\pm\mathbf{q}} \pm i\hat{S}^{y}_{\pm\mathbf{q}}$ (Appendix B, (B.81), Chapters 9 and 13)

T absolute temperature $\beta = (k_{\mathrm{B}}T)^{-1}$

t time variable

t_1, t_2, t_3 reciprocal lattice indices (2.5)

Tr $\equiv$ trace

$T^{dd'}_{\Lambda\Lambda'}(\mathbf{l}-\mathbf{l}')$ (5.77)

$\hat{u}_{\alpha}(l, t)$ displacement operator (4.16 a) and (4.30)

$u_{\mathbf{k}\lambda}(\mathbf{r}) = \exp(-i\mathbf{k}.\mathbf{r})\psi_{\mathbf{k}\lambda}(\mathbf{r})$ periodic part of Bloch function (5.45 a)

$u_{\mathbf{q}}$, $\bar{u}_{\mathbf{q}}$ transformation coefficients (§§ 9.4, 9.6, and 9.7)

V volume of target

v_0 volume of unit cell (2.7)

$\hat{V}(\boldsymbol{\varkappa})$ Fourier transform of total neutron–target interaction potential (§ 1.2 and Appendix A)

$\hat{V}_{\mathrm{E}}(\boldsymbol{\varkappa})$ Fourier transform of total electrostatic interaction potential (10.24)

$\hat{V}_{\mathrm{N}}(\boldsymbol{\varkappa})$ Fourier transform of total nuclear interaction potential (§§ 1.3 and 1.4, and (10.20))

$\hat{V}_{\mathrm{M}}(\boldsymbol{\varkappa})$ Fourier transform of total magnetic interaction potential (§ 5.2 and (10.22))

$v_{\mathbf{q}}$, $\bar{v}_{\mathbf{q}}$ transformation coefficients (§§ 9.4, 9.6, and 9.7)

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v quantum numbers needed when the set $SM_{\mathrm{S}}\,LM_{\mathrm{L}}$ fail to define atomic state uniquely (6.49)
$\langle V(\mathbf{r})\rangle$ mean potential seen by neutron (2.14)
$\delta\hat{V}(\mathbf{r})$ deviation in potential from mean value (2.15)
$V(\boldsymbol{\tau}) = \int d\mathbf{r}\, \exp(i\boldsymbol{\tau}.\mathbf{r})\langle V(\mathbf{r})\rangle$ (2.20 b)
v_{ld} potential due to atom at site $\mathbf{R}_{ld}$ (2.26)

$W(\boldsymbol{\varkappa})$ Debye–Waller factor (4.35), (4.38) and (4.51)
$W_{k\to k'}$ Golden rule transition probability ((1.3) and Appendix B, § B.6)
$w(t), \bar{w}(t)$ width function (11.14)

$Y_Q^K(\theta, \phi)$ spherical harmonic of rank K and order Q: definition in accord with A. R. Edmonds, *Angular momentum in quantum mechanics*, Princeton University Press, 1960.

$Z = \mathrm{Tr}\exp(-\beta\mathscr{H})$ partition function
$Z(\omega)$ normalized vibrational density of states ((4.39) and Chapter 15)
Z number of electrons associated with ion (§ 10.3)
$z(\tau)$ number of reciprocal lattice vectors with magnitude $|\boldsymbol{\tau}| = \tau$ ((2.41) and Chapter 4, Table 4.3)

α (with β and γ) Euler angle (§ 12.1)
α (with β) Cartesian component index
α coefficient of thermal expansion (11.135)
$\hat{\boldsymbol{\alpha}}$ vector part of general interaction potential between neutron and target (10.26)

β (with α and γ) Euler angle (§ 12.1)
β (with α) Cartesian component index
$\beta = (k_{\mathrm{B}}T)^{-1}$
$\hat{\beta}$ scalar part of general interaction potential between neutron and target (10.26)

γ (with α and β) Euler angle (§ 12.1)
$\Gamma(\mathbf{q}, \omega)$ width in energy (§ 4.4, (9.79), (15.64), and Appendix C)
$r\gamma_{\mathbf{q}} = \sum \exp(i\mathbf{q}.\boldsymbol{\rho})$ (9.15)
$\gamma(\boldsymbol{\varkappa})$ Fourier transform of static pair distribution function (11.4 a)
$\gamma(t)$ (3.57) and (4.96)
$\hat{\Gamma}_{jj'}(t)$ (3.52)
$\Gamma_{\boldsymbol{\varkappa}}^{\alpha}$ width in energy (§ 13.3 (*d*), (*e*))
$\gamma = -1{\cdot}91$ gyromagnetic ratio of neutron (5.2)

Γ_n Bethe's notation for irreducible representations of cubic group (§§ 6.6 (*b*), 15.2)
$\Gamma_{\alpha\beta}(\mathbf{r}, t)$ (8.5)
$\gamma_{\alpha\beta}(l, t)$ (8.8)
$\gamma'_{\alpha\beta}(l, t)$ (8.8)

$\delta(x)$ Dirac delta function
$\delta_{l,m}$ Kronecker delta function
Δ band splitting (9.110 b)
$\Delta(\mathbf{q}, \omega)$ real part of self-energy (shift) (§ 4.4, (9.79), (15.64), and Appendix C)

$\epsilon^{\alpha\beta\gamma}$ antisymmetric unit tensor with three indices (10.35)
ϵ perturbation parameter (15.96)

$\zeta(n)$ Riemann's zeta function of order n (9.32)

$\tilde{\boldsymbol{\eta}}_{ld}(\boldsymbol{\varkappa})$ unit vector in direction of spin at site $\mathbf{R}_{ld}$ (7.23)
η, η' first, η, and second, η', viscosity coefficients (§ 11.4 (*b*))
η_B bulk viscosity coefficient (§ 11.4 (*b*))

$\theta(t)$ unit step function ((8.48) and Appendix B, (B.12))
θ scattering angle (§ 1.2)
θ, θ' shorthand for vSL and $v'S'L'$ defining terms of l^n (6.49)
$\bar{\theta}$ shorthand for $\bar{v}\bar{S}\bar{L}$ defining terms of l^{n-1} (6.49)

$\boldsymbol{\varkappa} = \mathbf{k}-\mathbf{k}'$ scattering vector (§ 1.3)
κ_S adiabatic compressibility (11.154)
κ_T isothermal compressibility (11.135)

λ perturbation parameter (15.3)
λ, Λ band indices (§ 5.5)
λ thermal conductivity (§ 11.4 (*b*))
λ, λ' quantum numbers specifying initial and final target states (§ 1.2 and Appendix A)

$\mu_B = e\hbar/2m_e c$ Bohr magneton (Chapter 5)
$\mu_N = e\hbar/2m_p c$ nuclear magneton (Chapter 5)
$\hat{\mu}$ magnetic moment operator (Chapter 5)
μ (together with ν) spherical coordinate index (Chapter 8 and Appendix B, § B.9)
μ reduced mass (§ 12.2)

ν (together with μ) spherical coordinate index (Chapter 8 and Appendix B, § B.9)

ξ isotope label (1.21)

$\Xi(\boldsymbol{\varkappa})$ Fourier transform of mean square moment fluctuation in random mixed system (14.6)

ρ perturbation parameter (15.96)

$\hat{\rho}$ density matrix (§ 10.2, Appendix B, § B.3)

ρ mean density (§§ 3.2, 11.1)

$\hat{\rho}(\mathbf{r},t) = \sum \delta\{\mathbf{r}-\hat{\mathbf{R}}_j(t)\}$ particle density operator (3.8)

$\hat{\rho}_{\mathbf{q}}(t) = \sum \exp\{-i\mathbf{q}\,.\,\hat{\mathbf{R}}_j(t)\}$ Fourier component of particle density operator (3.13)

$\boldsymbol{\rho}$ vector to nearest-neighbour ions (Chapter 9)

$\frac{1}{2}\hat{\boldsymbol{\sigma}}$ neutron spin operator (§ 1.4)

$\boldsymbol{\sigma}^j(\mathbf{q})$ phonon polarization vector for jth branch (4.11 a)

$\hat{\sigma}^\alpha$ Pauli matrices (§ 5.5)

σ, σ' initial and final neutron spin quantum numbers in cross-section; also, electron spin index (in §§ 5.5 and 9.3)

$\Sigma_{\mathbf{q}}(\omega)$ self-energy function (9.78) and Appendix C

$\sigma = \langle \hat{S}^z \rangle / S$ reduced moment (13.21)

$\sigma'_{\alpha\beta}$ stress tensor (11.130)

σ_c single (bound) nucleus coherent cross-section (§ 1.5)

$\sigma_i = \sigma - \sigma_c$ (Chapters 4 and 11)

σ_{ab} single (bound) nucleus absorption cross-section (§ 1.5 and Appendix A, § A.1)

σ total single (bound) nucleus cross-section

$\boldsymbol{\tau} = t_1\boldsymbol{\tau}_1 + t_2\boldsymbol{\tau}_2 + t_3\boldsymbol{\tau}_3$ reciprocal lattice vectors (2.5)

$\varphi_{\mathbf{k}\lambda\sigma}(\mathbf{r})$ Bloch function: λ band index, σ spin index (5.46)

$\phi_\Lambda(\mathbf{r}-\mathbf{R}_{ld})$ localized electron wave function (5.72 and § 9.3)

$\phi_{AB}(t)$ response function (Appendix B, § B.1 and (B.24 b))

$\phi_{\mathbf{q}}^{(\pm)}(t)$ wave vector dependent response function (Appendix B, § B.9 and Chapter 8)

$\phi_{\mathbf{q}}^{\alpha\beta}(t)$ wave vector dependent response function (8.29 b); see also (8.87)

χ_σ electron spin spinor (§ 5.5)

χ_0 susceptibility of an isolated ion (13.13)

$\chi_{AB}[\omega] = \chi'_{AB}[\omega] + i\chi''_{AB}[\omega]$ generalized susceptibility (Appendix B, § B.1)

$\chi_{\mathbf{q}}^{\alpha\beta}$ isothermal wave vector dependent susceptibility (Appendix B, (B.97))

$\chi_{\mathbf{q}}^{(\pm)}[\omega]$ generalized wave vector dependent susceptibility (Appendix B, (B.91) and (8.30 b)); see also (8.88)

$\chi^{\alpha\beta}[l, \omega]$ generalized susceptibility tensor (8.28 b)

$\Psi(\mathbf{q}, \omega)$ wave vector dependent susceptibility for liquid in hydrodynamic region (11.144)

$\hat{\psi}$, $\hat{\psi}^{+}$ particle field operators (5.56)

$\hbar\omega = \hbar^2(k^2 - k'^2)/2m$ energy lost by neutron (§ 1.2)

$\omega_j(\mathbf{q})$ frequency function of jth phonon branch (§ 4.1)

$\omega_{\mathbf{q}}$ frequency function for spin waves (Chapter 9)

$\Omega_{\mathbf{k}}$ frequency function for spin waves in itinerant electron system (§ 9.3 (*d*))

Ω solid angle

$\Omega(\mathbf{q})$ (§ 9.6 (*a*), (*b*))

$\overline{\omega^n}$ moments, of $F^{\alpha}(\boldsymbol{\varkappa}, \omega)$ (§ 13.3), of scattering law (§ 11.6)

CONTENTS

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