

14

Neutron Transfer Reactions

by

Ziad J. Azzam

Submitted to the Department of Electrical Engineering and Computer Science
in partial fulfillment of the requirements for the degree of

Master of Science in Electrical Engineering and Computer Science

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

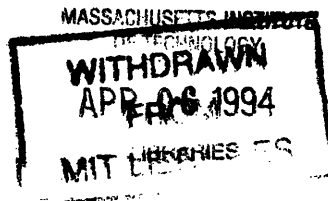
February 1994

© Massachusetts Institute of Technology 1994. All rights reserved.

Z. A.
Author
Z. A. Department of Electrical Engineering and Computer Science
January 31, 1994

P. L. H.
Certified by
Peter L. Hagelstein
Professor of Electrical Engineering and Computer Science
Thesis Supervisor

F. R. M.
Accepted by
Frederic R. Morgenthaler
Chairman, Departmental Committee on Graduate Students



Eng.

Neutron Transfer Reactions

by

Ziad J. Azzam

Submitted to the Department of Electrical Engineering and Computer Science
on January 31, 1994, in partial fulfillment of the
requirements for the degree of
Master of Science in Electrical Engineering and Computer Science

Abstract

A theory of second order reactions involving off-resonant intermediate states which contain virtual neutrons is studied. These reactions, so called *neutron transfer reactions*, have the potential to explain some of the anomalous effects observed in Pons-Fleischmann cells, namely excess heat and production of ^4He . A brief introduction to the various transfer operators and different reaction mechanisms is presented. The notion that a neutron can hop from one nucleus to another through second order coupling with continuum states raises the possibility of new reactions, as proposed by P. L. Hagelstein. This thesis studies issues related to the possible delocalization of virtual neutrons. We have focused on near-resonant exchange scattering of virtual neutrons and have made progress in the computation of the self-energy associated with this process.

Thesis Supervisor: Peter L. Hagelstein

Title: Professor of Electrical Engineering and Computer Science

Acknowledgments

I wish to thank my parents for their love and support.

I also wish to thank Professor Hagelstein for his patience and kindness.

Contents

1	Introduction	4
1.1	“Cold Fusion”, A Misnomer	6
1.2	Neutron Transfer Reactions	6
2	Neutron Transfer Reactions	9
3	Two-Step Reactions and Virtual Neutrons	16
3.1	Two-Step Second Order Reactions	16
3.2	Virtual Neutrons	18
4	Resonance Exchange Scattering	25
5	Hamiltonian for the Coupled System	30
6	Hartree-Fock and the Proper Self-Energy	35
7	Phonon Averaged Green’s Function Solution	45
7.1	Review of Phonon Averaging Techniques	46
7.2	Zero-Phonon Contribution to $\Sigma^*(\mathbf{k}, \mathbf{k}')$	49
7.3	Review of One-Phonon Exchange	51
7.4	One-Phonon Contribution to $\Sigma^*(\mathbf{k}, \mathbf{k}')$	53
7.5	Two-Phonon Contribution to $\Sigma^*(\mathbf{k}, \mathbf{k}')$	54
7.6	The Green’s Function Solution	56
7.7	Reaction Rates	57
8	Summary and Conclusion	60
8.1	Summary of Original Results	61

List of Figures

1-1	Two-step virtual neutron transfer reaction from a donor to an acceptor nucleus.	7
3-1	Two-step Raman process involving a virtual intermediate state. A laser which is mismatched to a transition frequency drives electrons from a ground state to a virtual intermediate state. The subsequent transition to a stable final state is driven by another laser.	17
3-2	Auxiliary functions f_1 and f_2	23
5-1	Feynman-like diagram for coherent coupled $d(\gamma, n)p$ and $^{105}Pd(n, \gamma)^{106}Pd$ reactions.	32
6-1	Lowest order proper self-energy $\Sigma_{(1)}^*(x, x')$	36
6-2	Full expansion for $\Sigma^*(x, x')$ in Hartree-Fock approximation.	36
6-3	Iterative definition of $\Sigma^*(x, x')$ in Hartree-Fock approximation.	37
6-4	Dyson's equation for G in Hartree-Fock approximation.	37

Chapter 1

Introduction

Pons and Fleischmann's claim of observation of heat generation of nuclear origin in electrolysis experiments in 1989 took the scientific community by surprise¹. From the outset, the claim was met with hostility and much skepticism. Critics have persistently maintained that the experimental reports were products of poorly designed experiments and that the observed effects were tarnished by poor signal to noise ratios. Criticisms, which in many cases have proven to be true, deepened in the early months following Pons and Fleischmann's claim because most laboratories failed to reproduce the effect.

The past several years however have seen a number of serious reports of observation of anomalies in metal deuteride systems². Rather than going into details of each experimental group's findings and techniques, we shall simply list some of the most significant observations claimed by these studies.

1. Excess heat production is the most significant claimed effect³. Many palladium elec-

¹M. Fleischmann and S. Pons, "Electronically Induced Nuclear Fusion of Deuterium", *J. Electroanal. Chem.*, **261**, 301 (1989).

S. Pons and M. Fleischmann, "Calorimetric Measurements of the Palladium/Deuterium System: Fact and Fiction", *Fusion Technol.*, **17**, 669 (1990).

S. Pons and M. Fleischmann, "Calorimetry of the Palladium-Deuterium System", *Proc. of the First Annual Conference on Cold Fusion*, p. 1, Salt Lake City, Utah, March 28-31, 1990.

S. Pons and M. Fleischmann, "Calorimetric Measurements on Palladium Based Cathodes Polarized in Heavy Water", presented at the *Second Conference on Cold Fusion*, Como, Italy, June 29-July 4, 1991.

²See reports in the *Third Annual Conference on Cold Fusion, ICCF3 Conference Proc.*, Nagoya, Japan, October 1992 and in the *Fourth Annual Conference on Cold Fusion, ICCF4 Conference Proc.*, Lahaina, Hawaii, December 1993.

³M. McKubre, R. Rocha-Filho, S. Smedley, F. Tanzella, S. Crouch-Baker, T. Passel and J. Santucci, "Isothermal Flow Calorimetric Investigations of the D/Pd System", *Proc. Second Annual Cold Fusion Conference*, Como, Italy, July 1991.

M. Fleischmann and S. Pons, *Proc. Third International Conference on Cold Fusion* Ed. H. Ikegami, Uni-

trollysis experiments carried out in a basic (LiOD) heavy water electrolyte report excess energy production, with some laboratories claiming energy generation in excess of 50 MJ/mole (or 500 eV/atom) of Pd⁴. No exothermic reaction of chemical nature is capable of producing heat of such magnitude. If these claims prove to be true, then it must be concluded that a reaction of nuclear origin is taking place.

2. Anomalous emissions of neutrons in electrolytic and gas-loaded metal deuterides have been reported⁵.
3. Additionally, there have been claims of excess tritium production⁶ (unaccompanied by neutron emission) as well as fast charged particles and anomalous gamma emissions⁷.
4. ⁴He production has been claimed⁸, though further confirmation of this phenomenon by independent experimental studies is warranted. ⁴He production is of particular significance because it is believed by some to be the leading candidate for a signal that dd-fusion in some form is indeed occurring.

These and other reports have attempted to address much of the criticism surrounding the “cold fusion” phenomenon, yet many questions are left unanswered. For instance, if the conjecture of deuteron fusion in the cells were correct, then the dominant reaction should follow one of these pathways :



versal Academy Press, Tokyo (1993).

M. Fleischmann and S. Pons, *Physics Letters A*, **176** 118 (1993).

⁴M. McKubre, S. Crouch-Baker, A. M. Riley, S. I. Smedley and F. L. Tanzella, *Proc. Third International Conference on Cold Fusion* Ed. H. Ikegami, Universal Academy Press, Tokyo (1993).

⁵H. O. Menlove, *Proc. First Annual Cold Fusion Conference*, Salt Lake City, March 1990; page 250.

⁶T. Claytor, “Tritium Generation in Pd-Si Systems”, presented at the Conference on Anomalous Nuclear Effects in Deuterium/Solid Systems, BYU, Oct. 1990.

⁷A. B. Karabut, Y. R. Kucherov, I. B. Savatimova, *Physics Letters A* **170** 265 (1992).

⁸M. Miles, B. Bush and D. Stilwell, “Calorimetric Principles and Problems in Measurements of Excess Power During Pd – D₂O Electrolysis”, to be published in the *Journal of Physical Chemistry E*, Feb. 17, (1994).

M. Miles and B. Bush, “Heat and Helium Measurements in Deuterated Palladium”, *Fourth Annual Conference on Cold Fusion, ICCF4 Conference Proc.*, Lahaina, Hawaii, December 1993.

D. Gozzi *et. al.* and S. Frullani *et. al.*, “Helium-4 Quantitative Measurements in the Gas Phase of Cold Fusion Electrochemical Cells”, *Fourth Annual Conference on Cold Fusion, ICCF4 Conference Proc.*, Lahaina, Hawaii, December 1993.

The levels of both neutron and tritium production observed in the experiments, however, are incommensurate with the excess heat production. Some have suggested that ^4He production may be the dominant pathway, yet how this could possibly be the case remains unknown. Ultimately, the major problem of “fusion” theories lies in their inability to account, either qualitatively or quantitatively, for the mechanism of the reactions responsible for the claimed anomalies. Consequently, an effort has been undertaken toward developing alternative theories which propose to explain many of the observed effects in Pons-Fleischmann cells and to provide details of the reaction mechanisms.

1.1 “Cold Fusion”, A Misnomer

In response to the deficiencies mentioned of theories pretending to explain the Pons-Fleischmann effect that are based on nuclear fusion, it is our conviction that the name “cold fusion”, which the field acquired from early speculations, is a misnomer. A new search for the mechanism responsible for the excess heat generation and other anomalous observations is thus warranted.

1.2 Neutron Transfer Reactions

In developing a new theory to seek to explain the Pons-Fleischmann effect, several issues must be addressed. The following is a list of some of the leading constraints or prerequisites which the present model faced.

1. As mentioned above, fusion theories have problems overcoming the Coulomb barrier. In order to circumvent this problem it has been proposed that the reactions within the cells involve the transfer of a neutral particle. The candidate in this case is the neutron. The charge neutrality of the neutron allows it, potentially, to be absorbed/emitted from acceptor/donor lattice sites without having to overcome an overwhelming Coulomb barrier. A typical proposed neutron transfer reaction (shown in Fig. 1-1) would involve transfer from a donor nucleus such as deuterium to an acceptor nucleus, such as ^2H , ^6Li , ^{10}B and Pd isotopes, as well as others.
2. The two-step reactions should proceed through a virtual intermediate state. The reaction pathway involving on-shell real neutrons would naturally suffer significant

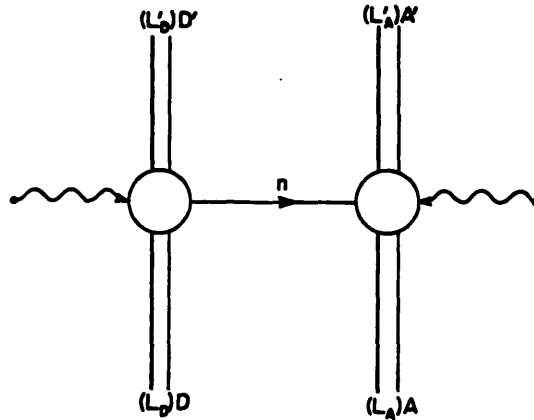


Figure 1-1: Two-step virtual neutron transfer reaction from a donor to an acceptor nucleus.

loss of neutrons, requiring some mechanism within the theory to continually supply these neutrons⁹. By demanding that the neutrons be virtual in nature this problem is avoided altogether. In addition, with transfer reactions involving real neutrons, one expects primary and secondary capture gammas to be present. So far, the reported levels of gammas in Pons-Fleischmann cells are incommensurate with the levels of energy generation. Finally, for real neutrons, there exists the physical handicap of having to overcome the binding energy of the donor nucleus (2.225 MeV for the deuteron). Once again, neutrons undergoing transfer reactions through virtual intermediate states escape this limitation, since it may be possible for the continuum neutron states to be driven off-resonance in the intermediate stage of a two-step reaction. This situation is analogous in some ways to Raman scattering where, instead of a neutron, the laser driven transition involves an electron passing through a virtual intermediate state¹⁰.

3. The transfer of nuclear energy to the lattice is proposed to occur through frequency shifting of the lattice normal phonon modes. This process is inherently highly nonlinear, which may require a non-perturbative approach to the problem.
4. The original proposal assumed that the transitions were driven by the long wavelength electric or magnetic field. It has been found, more recently, that the strong interaction between the neutrons and the nuclei occupying the lattice sites is responsible for the proposed neutron transfer reactions, (see chapters 4 and 7).

⁹P. L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two-Step Reactions and Virtual Neutrons", MIT, submitted to *Fusion Tech.*, November, (1992).

¹⁰See chapter 3.

The assumptions and preconditions listed above have guided the proposed neutron transfer theory, and at the same time have helped to overcome many of the barriers that stood in the way of a “contradiction-free” theory to explain the Pons-Fleischmann anomalies.

This work undertakes the dual task of, firstly, reviewing the fundamental concepts developed by P. L. Hagelstein in his effort to develop a theory of neutron transfer reactions¹¹, to which end chapters 2, 3 and 4 are dedicated; and, secondly, deriving a Green’s function solution to the problem of the virtual neutron in the presence of a lattice. In chapter 5, the Green’s function formulation of the virtual neutron problem is presented and the total system Hamiltonian developed, leading to the sixth and seventh chapters where the Hartree-Fock approximation scheme is adopted to derive approximations useful to study the virtual neutron Green’s function.

In striving toward presenting as complete a picture as possible of the new theory to explain the Pons-Fleishmann phenomenon, and since this effort was initiated by P. L. Hagelstein a few years before my joining the project, this work, naturally, contains much material that is a review. The original research which constitutes the *thesis* is presented in chapters 5, 6 and much of chapter 7. The essential new result is contained in the formal derivation of the one-phonon contribution to the proper self-energy of the neutron/lattice system (see Eq. (7.44)). This result was used to derive an expression for the many-body Green’s function. Additionally, the proper self-energy expression was used to estimate the neutron transfer reaction rate for the case of electromagnetic interaction as well as that of the strong interaction.

¹¹P.L. Hagelstein, “Coherent and Semi-Coherent Neutron Transfer Reactions I: The Interaction Hamiltonian”, *Fusion Tech.* **22**, 172-180, (1992).

P.L. Hagelstein, “Coherent and Semi-Coherent Neutron Transfer Reactions II: Transition Operators”, submitted to *Fusion Tech.*, (1992).

P.L. Hagelstein, “Coherent and Semi-Coherent Neutron Transfer Reactions III: Phonon Generation”, *Fusion Tech.*, May 1993.

P.L. Hagelstein, “Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two Step Reactions and Virtual Neutrons”, submitted to *Fusion Tech.* November (1992).

Chapter 2

Neutron Transfer Reactions

The original proposal by P.L. Hagelstein for neutron transfer reactions involved single-step first order reactions whereby coherent transfer of energy to and from the lattice occurred with each neutron capture or ionization reaction¹. The analysis is facilitated by the use of second quantized field operators for the neutrons and the donor and acceptor nuclei. In the case of neutrons, one may define the field operators $\hat{\Psi}_n(\mathbf{r})$ and $\hat{\Psi}_n^\dagger(\mathbf{r})$ in the following manner:

$$\hat{\Psi}_n(\mathbf{r}) = \sum_{\alpha_n} \sum_{\mathbf{k}} \hat{b}_{n,\alpha_n,\mathbf{k}} \Phi_{n,\alpha_n,\mathbf{k}}(\mathbf{r}) \quad , \quad (2.1)$$

$$\hat{\Psi}_n^\dagger(\mathbf{r}) = \sum_{\alpha_n} \sum_{\mathbf{k}} \hat{b}_{n,\alpha_n,\mathbf{k}}^\dagger \Phi_{n,\alpha_n,\mathbf{k}}^*(\mathbf{r}) \quad , \quad (2.2)$$

where $\hat{b}_{n,\alpha_n,\mathbf{k}}$ and $\hat{b}_{n,\alpha_n,\mathbf{k}}^\dagger$ are Schrodinger picture single neutron annihilation and creation operators, $\Phi_{n,\alpha_n,\mathbf{k}}(\mathbf{r})$ and $\Phi_{n,\alpha_n,\mathbf{k}}^*(\mathbf{r})$ are spatial wavefunctions, and α_n represents the neutron spin quantum number.

In the case of nuclei, the following field operators are defined:

$$\hat{\Psi}_X(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_i \sum_{\alpha_X} \hat{b}_{X,\alpha_X}(i) \Phi_{X,\alpha_X}(\mathbf{r}_1 - \hat{\mathbf{R}}_i, \dots, \mathbf{r}_N - \hat{\mathbf{R}}_i) \quad , \quad (2.3)$$

$$\hat{\Psi}_X^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_i \sum_{\alpha_X} \hat{b}_{X,\alpha_X}^\dagger(i) \Phi_{X,\alpha_X}^*(\mathbf{r}_1 - \hat{\mathbf{R}}_i, \dots, \mathbf{r}_N - \hat{\mathbf{R}}_i) \quad , \quad (2.4)$$

¹This chapter is a review of the following articles:

P.L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions I: The Interaction Hamiltonian", *Fusion Tech.* **22**, 172-180, (1992),

P.L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions II: Transition Operators", submitted to *Fusion Tech.*, (1992),

P.L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions III: Phonon Generation", *Fusion Tech.*, May 1993

where $\hat{\mathbf{R}}_i$ is the time-dependent center of mass position operator at site i . Operators $\hat{\Psi}_X(\mathbf{r}_1, \dots, \mathbf{r}_N)$ and $\hat{\Psi}_X^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_N)$ destroy and annihilate respectively nucleon X at lattice site i .

With the field operators defined, the evaluation of the interaction Hamiltonian for neutron capture and emission in a lattice may proceed. The process involves a free neutron being captured by nucleus Y (of nuclear mass $N - 1$) forming nucleus X (atomic mass N) and vice versa. In the case of a magnetic dipole transition, the interaction Hamiltonian is given by the following expression:

$$\begin{aligned} \hat{H}_{-\mu \cdot \mathbf{B}} = & \int d^3\mathbf{r}_1 \dots \int d^3\mathbf{r}_N \left[\hat{\Psi}_Y^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \wedge \hat{\Psi}_n^\dagger(\mathbf{r}_N) \right] \left[- \sum_j \mu_j \cdot \mathbf{B}(\mathbf{r}_j) \right] \hat{\Psi}_X(\mathbf{r}_1, \dots, \mathbf{r}_N) \\ & + \int d^3\mathbf{r}_1 \dots \int d^3\mathbf{r}_N \hat{\Psi}_X^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_N) \left[- \sum_j \mu_j \cdot \mathbf{B}(\mathbf{r}_j) \right] \\ & \times \left[\hat{\Psi}_Y^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \wedge \hat{\Psi}_n(\mathbf{r}_N) \right] . \end{aligned} \quad (2.5)$$

Substituting in the expressions for the field operators derived earlier yields the following expression for the interaction Hamiltonian:

$$\begin{aligned} \hat{H}_{-\mu \cdot \mathbf{B}} = & \sum_i \sum_{\alpha_n} \sum_{\alpha_X} \sum_{\alpha_Y} \sum_{\mathbf{k}} \hat{b}_{n,\alpha_n,\mathbf{k}}^\dagger \hat{b}_{Y,\alpha_Y}^\dagger(i) \hat{b}_{X,\alpha_X}(i) \hat{U}_{Y,n,X}^{\alpha_Y,\alpha_n,\alpha_X}(i) \\ & + \sum_i \sum_{\alpha_n} \sum_{\alpha_X} \sum_{\alpha_Y} \sum_{\mathbf{k}} \hat{b}_{X,\alpha_X}^\dagger(i) \hat{b}_{n,\alpha_n,\mathbf{k}} \hat{b}_{Y,\alpha_Y}(i) \hat{U}_{X,Y,n}^{\alpha_X,\alpha_Y,\alpha_n}(i) . \end{aligned} \quad (2.6)$$

The $\hat{U}(i)$'s are called magnetic dipole potential operators and are defined by the following relations:

$$\begin{aligned} \hat{U}_{Y,n,X}^{\alpha_Y,\alpha_n,\alpha_X}(i) = & \int \dots \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N \left[\Phi_{Y,\alpha_Y}^*(\mathbf{r}_1 - \hat{\mathbf{R}}_i^{Y_i}, \dots, \mathbf{r}_{N-1} - \hat{\mathbf{R}}_i^{Y_i}) \wedge \Phi_{n,\alpha_n,\mathbf{k}}^*(\mathbf{r}_N) \right] \\ & \left[- \sum_j \mu_j \cdot \mathbf{B}(\mathbf{r}_j) \right] \Phi_{X,\alpha_X}(\mathbf{r}_1 - \hat{\mathbf{R}}_i^{X_i}, \dots, \mathbf{r}_N - \hat{\mathbf{R}}_i^{X_i}) , \end{aligned} \quad (2.7)$$

$$\hat{U}_{X,Y,n}^{\alpha_X,\alpha_Y,\alpha_n}(i) = \left[\hat{U}_{Y,n,X}^{\alpha_Y,\alpha_n,\alpha_X}(i) \right]^\dagger . \quad (2.8)$$

At this point it is of interest to apply these results to a study of the effects on the lineshape of the lattice. After all, any macroscopic energy that may be exchanged between

the nucleons and the lattice should manifest itself in a shift in the lattice lineshape. Fortunately, in this regard, the work of Lamb may be used for reference². In his study of *resonant* neutron capture processes in a lattice, Lamb arrived at the following expression for the lineshape:

$$W(E) \sim \sum_{\alpha} \sum_{\beta} \frac{g(\{\alpha\}) |\langle \{\beta\} | e^{i\mathbf{k}_p \cdot \mathbf{R}_i} | \{\alpha\} \rangle|^2}{[E - E_0 - \Delta E(\alpha, \beta)]^2 + \frac{1}{4}(\hbar\Gamma)^2} \quad , \quad (2.9)$$

where α and β refer to lattice phonon states, $g(\{\alpha\})$ and $g(\{\beta\})$ are the probability functions that the lattice is in state α or β respectively, E is the energy of the emitted gamma, E_0 is the resonance energy and, finally, $\hbar\Gamma$ is the homogeneous linewidth. The $|\langle \{\beta\} | e^{i\mathbf{k}_p \cdot \mathbf{R}_i} | \{\alpha\} \rangle|^2$ term which appears in the numerator represents the gamma emission recoil matrix element. In order to adapt Lamb's results to the study of *non-resonant* neutron capture in a lattice, recoil term in Eq. (2.9) should be replaced by the magnetic dipole transition operators $\hat{U}(i)$ shown in Eq. (2.7). The emission lineshape for the case of non-resonant neutron capture is thus given by:

$$W(E) \sim \sum_{\alpha} \sum_{\beta} \frac{g(\{\alpha\}) |\langle \{\beta\} | \hat{U}(i) | \{\alpha\} \rangle|^2}{[E - E_0 - \Delta E(\alpha, \beta)]^2 + \frac{1}{4}(\hbar\Gamma)^2} \quad . \quad (2.10)$$

The expression for $\hat{U}(i)$ in Eq. (2.7) may be approximated by the product of a *primary recoil* term, $e^{i(\mathbf{k}_p - \mathbf{k}_n) \cdot \mathbf{R}_i}$, a *Duschinsky operator*, $e^{-i\hat{S}_D}$, and a free-space matrix element $\langle \alpha_Y \alpha_n | -\boldsymbol{\mu} \cdot \mathbf{B} | \alpha_X \rangle$,³

$$\hat{U}(i) \sim \langle \alpha_Y \alpha_n | -\boldsymbol{\mu} \cdot \mathbf{B} | \alpha_X \rangle e^{i(\mathbf{k}_p - \mathbf{k}_n) \cdot \mathbf{R}_i} e^{-i\hat{S}_D} \quad . \quad (2.11)$$

The Duschinsky operator (named after Duschinsky⁴ who studied electronic transitions in polyatomic molecules) accounts for differences in modes between initial and final phonon states. We thus end up with the following simplified form for the lineshape of non-resonant

²W. E. Lamb, "Capture of Neutrons by Atoms in a Crystal", *Phys. Rev.* **55**, 190 (1939).

³For a more detailed discussion of the Duschinsky effect and a more exact treatment of $\hat{U}(i)$ refer to the article by P.L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions II: Transition Operators", submitted to *Fusion Tech.*, (1992).

⁴F. Duschinsky, "Zur Deutung der Elektronenspektren mehratomiger Molekule I. Uber das Franck-Condon-Prinzip", *Acta Physicochimica U.R.S.S.* **7**, 551 (1937).

neutron capture processes:

$$W(E) \sim \sum_{\alpha} \sum_{\beta} \frac{g(\{\alpha\})|\langle\{\beta\}|e^{i(\mathbf{k}_p-\mathbf{k}_n)\cdot\hat{\mathbf{R}}_i}e^{-i\hat{S}_D}|\{\alpha\}\rangle|^2}{[E - E_0 - \Delta E(\alpha, \beta)]^2 + \frac{1}{4}(\hbar\Gamma)^2} . \quad (2.12)$$

Analysis has shown that the primary recoil term alone is incapable of mediating macroscopic energy transfer to or from the lattice. For example, in a thermal lattice phonon generation due to gamma recoil is well understood, yet the total energy transfer is on the atomic scale. Transferring a large number of phonons in succession is preempted by an exponentially decaying phonon mode occupation function ($f \sim \left[\frac{H_{\alpha\beta}}{\Delta E}\right]^{2n}$); and transferring the energy via a nonperturbative process requires that the acceptor nucleon in the lattice have a relative kinetic energy on the order of MeV, which is certainly highly improbable. We are thus forced to look at the Duschinsky term as the primary means for the mediation of large energy transfer.

In general, the Duschinsky operator translates and rotates phonon modes. It has the property:

$$e^{-i\hat{S}_D} \Psi(\mathbf{q}) \equiv \Psi(\mathbf{A} \cdot \mathbf{q} + \mathbf{b}) . \quad (2.13)$$

In the case of neutron capture reactions, the appropriate Duschinsky operator only rotates, and therefore is given by

$$e^{-i\hat{S}_D} \Psi(\mathbf{q}) \equiv \Psi(\mathbf{A} \cdot \mathbf{q}) . \quad (2.14)$$

Before evaluating the matrix elements of the Duschinsky operator, an expression for the rotation matrix \mathbf{A} must be determined. This is achieved by expressing the initial state lattice mode, $q_m^{(i)}$, in terms of the final state lattice mode $q_m^{(f)}$. The initial and final lattice center of mass positions are given by

$$\mathbf{R}_j = \mathbf{R}_j^{0,i} + \sum_m \mathbf{u}_m^{(i)}(j) q_m^{(i)} , \quad (2.15)$$

$$\mathbf{R}_j = \mathbf{R}_j^{0,f} + \sum_m \mathbf{u}_m^{(f)}(j) q_m^{(f)} , \quad (2.16)$$

where \mathbf{u}_m are displacement vectors, m is the phonon mode index and j is the phonon index.

$q_m^{(i)}$ can be expressed in terms of $q_m^{(f)}$ through the relation

$$q_m^{(i)} = \sum_j \sum_{m'} [\mathbf{v}_m^{(i)}(j)]^T \cdot \mathbf{u}_{m'}^{(f)}(j) q_{m'}^{(f)}(j) + \sum_j [\mathbf{v}_m^{(i)}(j)]^T \cdot (\mathbf{R}_j^{0,f} - \mathbf{R}_j^{0,i}) \quad , \quad (2.17)$$

where $\mathbf{R}_j^{0,i}$ and $\mathbf{R}_j^{0,f}$ are the initial and final equilibrium lattice position vectors respectively. $\mathbf{v}_m(j)$ is related to the displacement vector $\mathbf{u}_m(j)$ through the following identity:

$$\sum_j \mathbf{v}_m^T(j) \cdot \mathbf{u}_{m'}(j) = \delta_{m,m'} \quad . \quad (2.18)$$

Using the above equation, together with the orthonormality property of the displacement vectors

$$\sum_j M_j \mathbf{u}_m^T(j) \cdot \mathbf{u}_{m'}(j) = M \delta_{m,m'} \quad , \quad (2.19)$$

where M is the “mass” assigned to the phonon modes, one arrives at the following expression relating the adjoint vectors to the displacement vectors:

$$\mathbf{v}_m(j) = \frac{M_j}{M} \mathbf{u}_m(j) \quad . \quad (2.20)$$

The expression for the Duschinsky rotation matrix follows from Eqs. (2.17) and (2.20),

$$A_{m,m'} \simeq [A^{-1}]_{m,m'}^T = [\mathbf{v}_m^{(i)}(j)]^T \cdot \mathbf{u}_{m'}^{(f)}(j) + \left(\frac{M_j^{(f)}}{M_j^{(i)}} - 1 \right) [\mathbf{v}_m^{(i)}(0)]^T \cdot \mathbf{u}_{m'}^{(f)}(0) \quad , \quad (2.21)$$

where we have defined $j = 0$ to be the lattice site where neutron transfer occurred.

At this point the matrix elements of the Duschinsky operator, M_{fi} , may be determined. These are defined by the relation

$$M_{fi} \equiv \int \Psi_f^*(\mathbf{q}) e^{-i\hat{S}_D} \Psi_i(\mathbf{q}) d^3\mathbf{q} \quad , \quad (2.22)$$

where Ψ_i is given by

$$\Psi_i \equiv F(\mathbf{q}, \mathbf{p}) \Phi[0] \quad . \quad (2.23)$$

$F(\mathbf{q}, \mathbf{p})$ is a function of creation and annihilation operators, and $\Phi[0]$ is the phonon ground

state. Defining $f(\mathbf{q}, \mathbf{p})$ as

$$f(\mathbf{q}, \mathbf{p})e^{-i\hat{S}_D} \equiv e^{-i\hat{S}_D} F(\mathbf{q}, \mathbf{p}) \quad , \quad (2.24)$$

results in the following expression for M_{fi} :

$$M_{fi} = \sum_l \int \Psi_f^*(\mathbf{q}) f(\mathbf{q}, \mathbf{p}) \Psi_i(\mathbf{q}) d^3\mathbf{q} \int \Psi_l^*(\mathbf{q}) e^{-i\hat{S}_D} \Phi[0] d^3\mathbf{q} \quad . \quad (2.25)$$

The first integral in the above equation represents phonons being created. This effect is expected to be weak because of the limitations on the number of phonons one may “squeeze” in a given mode and for other factors discussed earlier in this chapter. It is in the second integral where most of the energy transfer mediation is expected to occur. The integral itself displays the Duschinsky operator’s ability to exchange initial phonons with final phonons of different energies.

In conclusion, it has been demonstrated that the Duschinsky transformation is indeed capable of mediating significant transfer of energy (of order MeV) between microscopic nuclei and a macroscopic lattice during neutron transfer reactions. The Duschinsky operator’s capacity to shift the energy of a highly excited phonon is key to the success of the model. Nevertheless, certain conditions still need to be satisfied before the Duschinsky transformation could take effect. Most important is the requirement that the lattice contain a significant amount of impurities. The presence of an impurity band near the frequency of the localized mode is paramount, since it allows a large number of modes to jump the gap between the D modes and the T continuum modes during a neutron transfer reaction⁵. The model fails however to account for reactions involving neutron ionization reactions. The original speculation by P.L. Hagelstein was that the lattice itself provided the energy needed to ionize the neutron. It was found that the sign of the energy transfer in this model prohibits lattice-induced neutron ionization. Consequently, further development of the neutron transfer theory focused on second order processes involving virtual intermediate neutrons.

It is worth mentioning that, very recently, new mechanisms have been found that can lead to lattice-induced neutron ionization. The advent of these mechanisms, however, does

⁵For a detailed look at the conditions on the lattice, and why ground state and thermal lattices are excluded in the model, refer to the article by P.L. Hagelstein, “Coherent and Semi-Coherent Neutron Transfer Reactions III: Phonon Generation”, *Fusion Tech.*, May 1993.

not alter the many advantages of working with second order theories involving virtual neutrons.

Chapter 3

Two-Step Reactions and Virtual Neutrons

3.1 Two-Step Second Order Reactions

Two types of second order reactions exist. The first type involves processes whereby a neutron is captured onto a lattice first, followed by an ionization reaction. Second order reactions of this nature involve intermediate states that are driven off-resonance, or in other words, the reaction channel involves the transfer of *virtual neutrons*. The alternative of course involves *real neutrons* with the ionization reaction taking place first followed by a neutron capture reaction. The former channel is more promising, mainly because it allows us the freedom of dictating high reaction rates without having to account for the supply of neutrons. Second order reactions involving virtual intermediate states are hardly a new field in physics; among their many applications is Raman spectroscopy shown schematically in Fig. 3-1.

We shall follow the standard approach to two-step mechanisms¹. Consider an *initial state*, before any reaction has taken place, consisting of a donor nucleus, an acceptor nucleus and a lattice in its ground state. Let this initial state be denoted by the Hamiltonian H_0

¹This chapter is a summary of the article by P.L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two-Step Reactions and Virtual Neutrons", submitted to *Fusion Tech.* November (1992).

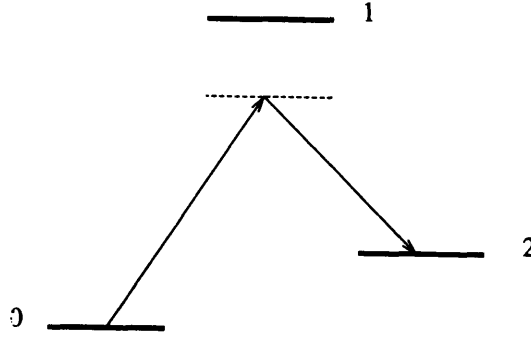


Figure 3-1: Two-step Raman process involving a virtual intermediate state. A laser which is mismatched to a transition frequency drives electrons from a ground state to a virtual intermediate state. The subsequent transition to a stable final state is driven by another laser.

and the wavefunction Ψ_0 . The *intermediate state* consists of a donor which has donated, a free neutron, an acceptor nucleus and a highly excited lattice. It is represented by the Hamiltonian H_1 and the wavefunction Ψ_1 . Finally, there is the *final state* which includes a donor nucleus which has donated, an acceptor nucleus which has accepted and a highly excited lattice; Hamiltonian H_2 and wavefunction Ψ_2 denote the final state. Transitions between the three states are governed by the following coupled Schrodinger equations:

$$i\hbar \frac{\partial}{\partial t} \Psi_0 = H_0 \Psi_0 + H_{01} \Psi_1 \quad , \quad (3.1)$$

$$i\hbar \frac{\partial}{\partial t} \Psi_1 = H_1 \Psi_1 + H_{10} \Psi_0 + H_{12} \Psi_2 \quad , \quad (3.2)$$

$$i\hbar \frac{\partial}{\partial t} \Psi_2 = H_2 \Psi_2 + H_{21} \Psi_1 \quad . \quad (3.3)$$

We wish to solve the above three equations with the ultimate goal being to derive an expression for the spatial dependence of the virtual neutron wavefunction, $\psi_n(\mathbf{r}_n)$. Once an expression for $\psi_n(\mathbf{r}_n)$ is found, we can determine the range of the virtual neutrons, which is key to the success of the model.

One method of solving the coupled Schrodinger equations is to first eliminate Ψ_1 . Before doing that however, a few assumptions must be made.

1. The difference between initial and final state energies is small, so we may set $E_0 \approx E_2$.

2. The energy of the intermediate state, E_1 , is higher than the initial state energy, E_0 , by an order of MeV's.
3. The transition Hamiltonians (H_{nm} $n, m = 0, 1, 2$) are time-independent.

Consequently, the intermediate state will be driven off-resonance with energy E_0 ; or in other words

$$\Psi_1 \sim e^{-\frac{iE_0 t}{\hbar}} . \quad (3.4)$$

Substituting this into Eq. (3.2) leads to the result

$$\begin{aligned} (E_0 - H_1)\Psi_1 &= H_{10}\Psi_0 + H_{12}\Psi_2 \\ \implies \Psi_1 &= (E_0 - H_1)^{-1}H_{10}\Psi_0 + (E_0 - H_1)^{-1}H_{12}\Psi_2 . \end{aligned} \quad (3.5)$$

The above expression for Ψ_1 , when substituted into Eqs. (3.1) and (3.3), yields the following identities:

$$i\hbar \frac{\partial}{\partial t} \Psi_0 = [H_0 + H_{01}(E_0 - H_1)^{-1}H_{10}]\Psi_0 + H_{01}(E_0 - H_1)^{-1}H_{12}\Psi_2 , \quad (3.6)$$

$$i\hbar \frac{\partial}{\partial t} \Psi_2 = [H_2 + H_{21}(E_0 - H_1)^{-1}H_{12}]\Psi_2 + H_{21}(E_0 - H_1)^{-1}H_{10}\Psi_0 . \quad (3.7)$$

3.2 Virtual Neutrons

Next we turn our attention toward deriving the spatial dependence of the virtual neutron wavefunction, $\psi_n(\mathbf{r}_n)$. To do that, we first look at a toy model. Consider the problem of a deuteron embedded in a lattice and surrounded by a static magnetic field. Let Ψ_0 be the probability amplitude of the state consisting of a deuteron in a lattice; and let Ψ_1 be the probability amplitude of the state consisting of a proton in a lattice plus a free neutron. We may approximate Ψ_0 as a product of the neutron wavefunction and the proton wavefunction. As a result we have the following relations:

$$\Psi_0|_{spatial} = \psi_D , \quad (3.8)$$

$$\Psi_1|_{spatial} = \psi_n \times \psi_p , \quad (3.9)$$

where

$$\psi_p(\mathbf{r}_p) = \left(\frac{\alpha_p}{\pi}\right)^{\frac{3}{4}} e^{-\frac{\alpha_p|\mathbf{r}_p|^2}{2}} , \quad (3.10)$$

$$\psi_D(\mathbf{r}_p, \mathbf{r}_n) = \left(\frac{\alpha_D}{\pi}\right)^{\frac{3}{4}} \left(\frac{\beta_D}{\pi}\right)^{\frac{3}{4}} e^{-\frac{\alpha_D|\mathbf{r}_p+\mathbf{r}_n|^2}{2}} e^{-\frac{\beta_D|\mathbf{r}_p-\mathbf{r}_n|^2}{2}} . \quad (3.11)$$

Substituting the above four equalities into the Schrodinger equation for the neutron wavefunction

$$(\Delta E - H_n)\psi_n = \langle \psi_p | -\mu \cdot \mathbf{B} | \psi_D \rangle , \quad (3.12)$$

results in the following equation, which is the generating formula for the neutron wavefunction:

$$(\Delta E - H_n)\psi_n(\mathbf{r}_n) = \langle {}^1S, 0 | -\mu \cdot \mathbf{B} | {}^3S, M_S \rangle \left[\frac{4\alpha_p\alpha_D}{\pi^2} \right]^{\frac{3}{4}} \sqrt{V_N} e^{-\frac{(\alpha_p+\alpha_D)|\mathbf{r}_n|^2}{2}} . \quad (3.13)$$

ΔE is the off-resonant neutron energy, which in this case is equal to the binding energy of the deuteron ($\Delta E = -2.225$ MeV), and V_N is a constant given by $V_N = \left(\frac{\pi}{\beta_D}\right)^{\frac{3}{2}}$.

The next task involves the examination of the formula in Eq. (3.13) in the context of various systems. The two systems to be studied are the free space model and the perfect crystal model.

In the free space case Eq. (3.13) simplifies to

$$\left[\frac{\hbar^2 \nabla^2}{2M_n} + \Delta E \right] \psi_n(\mathbf{r}_n) = \langle {}^1S, 0 | -\mu \cdot \mathbf{B} | {}^3S, M_S \rangle \left[\frac{4\alpha_p\alpha_D}{\pi^2} \right]^{\frac{3}{4}} \sqrt{V_N} e^{-\frac{(\alpha_p+\alpha_D)|\mathbf{r}_n|^2}{2}} . \quad (3.14)$$

Since $|\Delta E|$ is expected to be far greater than the kinetic energy of the neutron, the latter may be dropped out of equation. The approximate solution to the neutron wavefunction is thus given by

$$\psi_n(\mathbf{r}_n) \approx \frac{\langle {}^1S, 0 | -\mu \cdot \mathbf{B} | {}^3S, M_S \rangle}{\Delta E} \left[\frac{4\alpha_p\alpha_D}{\pi^2} \right]^{\frac{3}{4}} \sqrt{V_N} e^{-\frac{(\alpha_p+\alpha_D)|\mathbf{r}_n|^2}{2}} . \quad (3.15)$$

A more exact solution to the neutron wavefunction may be reached by solving the Green's function equation

$$\left[\frac{\hbar^2 \nabla^2}{2M_n} + \Delta E \right] G(\mathbf{r}_n, \mathbf{r}'_n) = \delta^3(\mathbf{r}_n - \mathbf{r}'_n) , \quad (3.16)$$

and using the result for $G(\mathbf{r}_n, \mathbf{r}'_n)$ in the total ψ_n solution given by

$$\psi_n(\mathbf{r}_n) = \langle {}^1S, 0 | -\boldsymbol{\mu} \cdot \mathbf{B} | {}^3S, M_S \rangle \left[\frac{4\alpha_p \alpha_D}{\pi^2} \right]^{\frac{3}{4}} \sqrt{V_N} \int d^3\mathbf{r}'_n G(\mathbf{r}_n, \mathbf{r}'_n) e^{-\frac{(\alpha_p + \alpha_D)|\mathbf{r}_n|^2}{2}}. \quad (3.17)$$

As it turns out, Eq. (3.16) has an exact solution²,

$$G(\mathbf{r}_n, \mathbf{r}') = -\frac{1}{4\pi} \frac{2M_n}{\hbar^2} \frac{e^{-\sqrt{\frac{2M_n|\Delta E|}{\hbar^2}}|\mathbf{r}_n|}}{|\mathbf{r}_n|}. \quad (3.18)$$

The decaying exponential in the above expression for $G(\mathbf{r}_n, \mathbf{r}')$ gives us a measure of the distance the neutron is able to travel. This distance is of the order $\left(\frac{\hbar^2}{2M_n|\Delta E|}\right)^{\frac{1}{2}}$, which for $|\Delta E| = 2.225 \text{ MeV}$ evaluates to roughly 3.05 fm. Clearly this is far too small a distance to be of any use to us and we must seek other models.

The perfect lattice model is an obvious alternative to the free space model just discussed³. The presence of the lattice adds a periodic potential, $V(\mathbf{r})$, to the system Hamiltonian. Eq. (3.16) thus mutates into the following form:

$$\left[\frac{\hbar^2 \nabla^2}{2M_n} + \Delta E - V(\mathbf{r}) \right] G(\mathbf{r}, \mathbf{r}') = \delta^3(\mathbf{r} - \mathbf{r}'). \quad (3.19)$$

One may construct the Green's function from a superposition of the eigenfunctions, $\phi(\mathbf{k}, \mathbf{r})$, of the Hamiltonian $H = \frac{\hbar^2 \nabla^2}{2M_n} - V(\mathbf{r})$ to obtain

$$G(\mathbf{r}, \mathbf{r}') = - \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\phi(\mathbf{k}, \mathbf{r}) \phi^*(\mathbf{k}, \mathbf{r}')}{|\Delta E| + E(\mathbf{k})}. \quad (3.20)$$

Using this result, one may define the *difference Green's function* as such:

$$\Delta G(\mathbf{r}, \mathbf{r}') = - \int \frac{d^3\mathbf{k}}{(2\pi)^3} \left[\frac{\phi(\mathbf{k}, \mathbf{r}) \phi^*(\mathbf{k}, \mathbf{r}')}{|\Delta E| + E(\mathbf{k})} - \frac{\phi_0(\mathbf{k}, \mathbf{r}) \phi_0^*(\mathbf{k}, \mathbf{r}')}{|\Delta E| - E_0(\mathbf{k})} \right], \quad (3.21)$$

where $\phi_0(\mathbf{k}, \mathbf{r})$ is the eigensolution of the unperturbed Hamiltonian ($V(\mathbf{r}) = 0$), and $E_0(\mathbf{k})$ is its associated eigenvalue. To obtain some idea on the long range part of the neutron wave-function, the difference Green's function should be evaluated in the context of Bragg scattering. Bragg scattering, afterall, is potentially the strongest interaction that may occur

²P.L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two-Step Reactions and Virtual Neutrons", submitted to *Fusion Tech.* November (1992).

³Note that henceforth the subscript n on the position coordinate for the neutron will be dropped.

between the neutron and the lattice⁴.

The first order contribution to the integrand in Eq. (3.21) is given by

$$\Delta G(\mathbf{r}, \mathbf{r}') = -\frac{1}{|\Delta E|} \int \frac{d^3\mathbf{k}}{(2\pi)^3} [\phi(\mathbf{k}, \mathbf{r})\phi^*(\mathbf{k}, \mathbf{r}') - \phi_0(\mathbf{k}, \mathbf{r})\phi_0^*(\mathbf{k}, \mathbf{r}')] \quad , \quad (3.22)$$

which evaluates to zero. The second order contribution is nonzero and is given by:

$$\Delta G(\mathbf{r}, \mathbf{r}') = -\frac{1}{|\Delta E|^2} \int \frac{d^3\mathbf{k}}{(2\pi)^3} [E(\mathbf{k})\phi(\mathbf{k}, \mathbf{r})\phi^*(\mathbf{k}, \mathbf{r}') - E_0(\mathbf{k})\phi_0(\mathbf{k}, \mathbf{r})\phi_0^*(\mathbf{k}, \mathbf{r}')] \quad . \quad (3.23)$$

Bragg theory tells that the integrand in Eq. (3.23) becomes significant in the region where

$$|\mathbf{k}|^2 \approx |\mathbf{K} - \mathbf{k}|^2 \quad , \quad (3.24)$$

where \mathbf{K} is the reciprocal lattice vector. Now, let \mathbf{K} point along the z -axis, and separate $d^3\mathbf{k}$ into one component that is parallel to \mathbf{K} (call that k_{\parallel}) and two components which are normal to \mathbf{K} (k_{\perp} 's). Along the two directions normal to \mathbf{K} the neutron is essentially confined, and thus any contribution to the integrand in Eq. (3.23) coming from the k_{\perp} 's may be ignored. Eq. (3.23) therefore simplifies to

$$\Delta G(\mathbf{r}, \mathbf{r}') = -\frac{1}{|\Delta E|^2} \sum_{\mathbf{K}} \delta^2(\mathbf{r}_{\perp} - (\mathbf{r}')_{\perp}) \int_{\Delta k_{\parallel}} \frac{dk_{\parallel}}{(2\pi)} [E(\mathbf{k})u(\mathbf{k}, \mathbf{r})u^*(\mathbf{k}, \mathbf{r}') - E_0(\mathbf{k})u_0(\mathbf{k}, \mathbf{r})u_0^*(\mathbf{k}, \mathbf{r}')] \quad , \quad (3.25)$$

where

$$\phi_0(\mathbf{k}, \mathbf{r}) \equiv e^{i(k_x x + k_y y)} u_0(\mathbf{k}, \mathbf{r}) \quad , \quad (3.26)$$

$$\phi(\mathbf{k}, \mathbf{r}) \equiv e^{i(k_x x + k_y y)} u(\mathbf{k}, \mathbf{r}) \quad . \quad (3.27)$$

Next $u(\mathbf{k}, \mathbf{r})$ is expressed as

$$u(\mathbf{k}, \mathbf{r}) = c_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + c_{\mathbf{k}-\mathbf{K}} e^{i(\mathbf{k}-\mathbf{K})\cdot\mathbf{r}} \quad (3.28)$$

and a solution for the expansion coefficients $c_{\mathbf{k}}$ and $c_{\mathbf{k}-\mathbf{K}}$ sought by solving the following

⁴For further details on Bragg neutron states and the perturbative evaluation of the integral in Eq. (3.21) refer to the article by P.L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two-Step Reactions and Virtual Neutrons", submitted to *Fusion Tech.* November (1992).

two eigenvalue equations and normalization condition:

$$\frac{\hbar^2|\mathbf{k}|^2}{2M_n}c_{\mathbf{k}} + V_{-\mathbf{K}}c_{\mathbf{k}-\mathbf{K}} = E(\mathbf{k})c_{\mathbf{k}} \quad , \quad (3.29)$$

$$V_{\mathbf{K}}c_{\mathbf{k}} + \frac{\hbar^2|\mathbf{k}-\mathbf{K}|^2}{2M_n}c_{\mathbf{k}} = E(\mathbf{k})c_{\mathbf{k}-\mathbf{K}} \quad . \quad (3.30)$$

$$|c_{\mathbf{k}}|^2 + |c_{\mathbf{k}-\mathbf{K}}|^2 = 1 \quad . \quad (3.31)$$

After some manipulations⁵ one ends up with the following expression for the *long range component* of ΔG :

$$\begin{aligned} \Delta G(\mathbf{r}, \mathbf{r}') = & -\frac{1}{|\Delta E|^2} \sum_{\mathbf{K}} \delta^2(\mathbf{r}_{\perp} - (\mathbf{r}')_{\perp}) \frac{|\mathbf{K}|\xi_{\mathbf{K}}}{\pi} \left\{ |V_{\mathbf{K}}| \sin\left[\frac{1}{2}\mathbf{K} \cdot (\mathbf{r} - \mathbf{r}')\right] f_1(\xi_{\mathbf{K}}\mathbf{K} \cdot (\mathbf{r} - \mathbf{r}')) \right. \\ & \left. + \frac{1}{2} \left[V_{\mathbf{K}}^* e^{\frac{i\mathbf{K} \cdot (\mathbf{r} + \mathbf{r}')}{2}} + V_{\mathbf{K}} e^{-\frac{i\mathbf{K} \cdot (\mathbf{r} + \mathbf{r}')}{2}} \right] f_2(\xi_{\mathbf{K}}\mathbf{K} \cdot (\mathbf{r} - \mathbf{r}')) \right\} . \quad (3.32) \end{aligned}$$

$\xi_{\mathbf{K}}$ is a dimensionless parameter defined as

$$\xi_{\mathbf{K}} \equiv \frac{2M_n|V_{\mathbf{K}}|}{\hbar^2|\mathbf{K}|^2} \quad , \quad (3.33)$$

and f_1 and f_2 are auxiliary functions defined by

$$f_1(t) \equiv \frac{\pi}{2t} [I_1(t) - L_1(t)] \quad (3.34)$$

$$f_2(t) \equiv 1 - \frac{\pi}{2} [I_1(t) - L_1(t)] \quad (3.35)$$

where $I_1(t)$ and $L_1(t)$ are modified first order Bessel and Struve functions respectively. Fig. 3-2 above illustrates the two functions⁶. The result in Eq. (3.32) demonstrates that the presence of the lattice does indeed alter the spatial component of the neutron wavefunction, ψ_n , inducing a *long range contribution* on the order of *microns*. To see that, consider the characteristic length which may be extracted from the formula in Eq. (3.32):

$$L \sim \frac{\hbar^2|\mathbf{K}|^2}{2M_n} \frac{1}{|V_{\mathbf{K}}||\mathbf{K}|} \quad . \quad (3.36)$$

⁵For details see article by P.L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two-Step Reactions and Virtual Neutrons", submitted to *Fusion Tech.* November (1992).

⁶M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, Dover Publications, Inc., New York (1972).

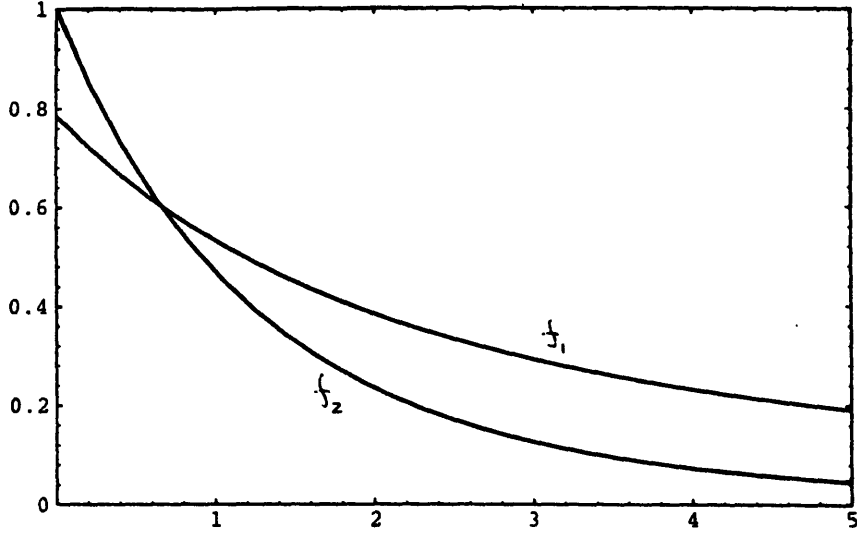


Figure 3-2: Auxiliary functions f_1 and f_2 .

$|\mathbf{K}|$ is given by

$$|\mathbf{K}| = \frac{2\pi}{a} \quad , \quad (3.37)$$

where a is the interstitial distance in the lattice, which in the case of palladium is roughly 4\AA . Following an order of magnitude argument we deduce that the term $\frac{\hbar^2|\mathbf{K}|^2}{2M_n} \frac{1}{|V_{\mathbf{K}}|} \sim 10^5$, resulting in a value for the neutron delocalization length, L , of $(10^5 \frac{a}{2\pi})$, or a few microns.

For the moment it seems as though the problem of the virtual neutron's localization has been resolved. With a potential to travel distances of a few microns, the neutrons can easily maneuver from site to site across the lattice, undergoing capture and ionization reactions. This picture, though convenient, is sadly misguided, namely because we have yet to address the issue of the probability that a virtual neutron attaining such a degree of delocalization. To do that, we turn our attention to second order gamma emissions. Since they are a product of the capture of neutrons onto lattice sites, second order gamma production rates are an ideal indicator of the neutron transfer reaction rates.

The total probability that the neutron is delocalized is given by

$$P = \sum_{\mathbf{K}} \sum_{\mathbf{K}'} P_{\mathbf{K},\mathbf{K}'} \quad , \quad (3.38)$$

where

$$\begin{aligned}
p_{\mathbf{K},\mathbf{K}'} &= \int [\Delta\psi_n^{(\mathbf{K})}(\mathbf{r})]^* \Delta\psi_n^{(\mathbf{K}')}(r) d^3\mathbf{r} \\
&= \left(\frac{2}{\pi}\right)^3 \left[\frac{\langle {}^1S, 0 | \mu \cdot \mathbf{B} | {}^3S, M_S \rangle}{|\Delta E|} \right]^2 \left| \frac{V_{\mathbf{K}}}{\Delta E} \right|^2 \\
&\times \left[\frac{(\alpha_p \alpha_D)^{\frac{2}{3}} V_N |\mathbf{K}| \zeta_{\mathbf{K}}}{(\alpha_p + \alpha_D)^2} \right] \left(e^{-\frac{|\mathbf{K}|^2}{4(\alpha_p + \alpha_D)}} \right) \int_{-\infty}^{\infty} (f_1^2(x) + f_2^2(x)) dx \quad . \quad (3.39)
\end{aligned}$$

Once again, an order of magnitude argument leads to the following approximation:

$$\begin{aligned}
p_{\mathbf{K},\mathbf{K}'} &\sim \left[\frac{\mu \cdot \mathbf{B}}{|\Delta E|} \right]^2 \left| \frac{V_{\mathbf{K}}}{\Delta E} \right|^2 \left(\frac{V_N}{V_A} \right) \left\{ \frac{|V_{\mathbf{K}}|}{\frac{\hbar^2 |\mathbf{K}|^2}{2M_n}} \right\} \\
&\sim [10^{-12}]^2 |10^{-14}|^2 (10^{-9}) \{10^{-5}\} = 10^{-66} \quad . \quad (3.40)
\end{aligned}$$

Consequently, despite the presence of considerable delocalization in the virtual neutron wavefunction, it has been determined that the associated neutron transfer reaction rate is negligible, roughly of the order of 10^{-59} or 10^{-60}sec^{-1} per deuteron in the lattice. Avenues for the possible enhancement of the transfer reaction rate must therefore be sought. Resonance exchange scattering is proposed as the most suitable candidate for the task.

Chapter 4

Resonance Exchange Scattering

Thus far it has been determined that while it is possible to impart a significant degree of delocalization to the virtual neutron, the total probability of such a delocalization occurring remains prohibitively small. It seems unlikely that any fine tuning of the parameters which introduced into the calculations could solve the problem. Fundamental surgical alterations to the theory are in order, requiring the introduction of new physical phenomena. Clearly the obvious route is to look for some form of resonance effect. Specifically, the situation where a virtual neutron, which had originated from a certain nucleus, is subsequently absorbed by another nucleus identical to the original donor nucleus shall be studied. The proposed process, first introduced by P. L. Hagelstein¹, is given the title of *resonance exchange scattering*.

Consider the coupled equations

$$i\hbar \frac{\partial}{\partial t} \Psi_0 = H'_0 \Psi_0 + H_{01} \Psi_1 \quad (4.1)$$

$$i\hbar \frac{\partial}{\partial t} \Psi_1 = H'_1 \Psi_1 + H_{10} \Psi_0 \quad (4.2)$$

describing resonant capture and re-emission of a virtual neutron onto a nucleus. These equations bear resemblance to the coupled Schrodinger equations derived at the end of section 3.1 (see Eqs. (3.6) and (3.7)), with the exception that the interaction Hamiltonian, H_{10} , now includes the *resonant* case where a neutron emitted by a deuteron is subsequently captured onto a proton. The Hamiltonian H'_1 may be expressed as a sum of the self-energy

¹See sections 7, 8 and 9 of the article by P. L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two-Step Reactions and Virtual Neutrons", submitted to *Fusion Tech.* November (1992).

term, H_1 , and an exchange potential as such:

$$H'_1 = H_1 + H_{10}(E_0 - H_0)^{-1}H_{01} \quad . \quad (4.3)$$

If we are looking at a truly resonant capture, then the term $E_0 - H_0$ will vanish leaving an infinite term in the expansion of the Hamiltonian. To circumvent this problem a slightly off-resonance case will be studied, whereby $E_0 - H_0$ will be replaced by a small energy parameter δE . With this in mind, we turn our attention to the Green's function. The incorporation of the resonance phenomenon in the theory simply adds an exchange operator, $W(\mathbf{r})$, to the Green's function equation defined in Eq. (3.19). The new Green's function now satisfies the relation

$$\left[\frac{\hbar^2 \nabla^2}{2M_n} + \Delta E - V(\mathbf{r}) - W(\mathbf{r}) \right] G(\mathbf{r}, \mathbf{r}_0) = \delta^3(\mathbf{r} - \mathbf{r}_0) \quad , \quad (4.4)$$

where $W(\mathbf{r})$ is given by²

$$W(\mathbf{r}_n)\psi_n(\mathbf{r}_n) \approx \sum_i \langle \psi_p^{(i)}(\mathbf{r}_p) | -\mu \cdot \mathbf{B} | \Psi_D^{(i)}(\mathbf{r}_p, \mathbf{r}_n) \rangle \frac{1}{\delta E} \langle \Psi_D^{(i)}(\mathbf{r}'_p, \mathbf{r}'_n) | -\mu \cdot \mathbf{B} | \psi_p^{(i)}(\mathbf{r}'_p) \psi_n(\mathbf{r}'_n) \rangle \quad . \quad (4.5)$$

Our goal is to demonstrate that the addition of this exchange operator will lead to an acceleration of the virtual neutron transfer reaction rate. In order to achieve that, we must first choose an appropriate form for the proton and deuteron wavefunctions, $\psi_p(\mathbf{r}_p)$ and $\Psi_D(\mathbf{r}_p, \mathbf{r}_n)$.

The parameterization of $\psi_p(\mathbf{r}_p)$ and $\Psi_D(\mathbf{r}_p, \mathbf{r}_n)$ for the case of localized neutrons was addressed in section 3.2 (see Eqs. (3.10) and (3.11)). Substituting these relations into Eq. (4.5) above results in

$$W(\mathbf{r}_n)\psi_n(\mathbf{r}_n) = \sum_{M_S} \left| \langle {}^1S, 0 | -\mu \cdot \mathbf{B} | {}^3S, M_S \rangle \right|^2 \left[\frac{4\alpha_p\alpha_D}{\pi^2} \right]^{\frac{3}{2}} \frac{V_N}{\delta E} \\ \times \sum_i e^{-\frac{(\alpha_p+\alpha_D)|\mathbf{r}_n-\mathbf{R}_i|^2}{2}} \int d^3\mathbf{r}_0 e^{-\frac{(\alpha_p+\alpha_D)|\mathbf{r}_0-\mathbf{R}_i|^2}{2}} \psi_n(\mathbf{r}_0) \quad . \quad (4.6)$$

It is immediately obvious that in this form $W(\mathbf{r})$ leads to no enhancement of the reaction

²P.L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two-Step Reactions and Virtual Neutrons", submitted to *Fusion Tech.* November (1992).

rate. To appreciate that, operate with $W(\mathbf{r})$ on a plane wave to obtain

$$W(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{\mathbf{K}} W_{\mathbf{k}-\mathbf{K},\mathbf{k}} e^{i(\mathbf{k}-\mathbf{K})\cdot\mathbf{r}} \quad , \quad (4.7)$$

where $W_{\mathbf{k}-\mathbf{K},\mathbf{k}}$ is given by³

$$\begin{aligned} W_{\mathbf{k}-\mathbf{K},\mathbf{k}} &= \sum_{M_S} \left| \langle {}^1S, 0 | -\boldsymbol{\mu} \cdot \mathbf{B} | {}^3S, M_S \rangle \right|^2 \left[\frac{16\alpha_p\alpha_D}{(\alpha_p\alpha_D)^2} \right]^{\frac{3}{2}} \frac{V_N}{V_{cell} \delta E} \\ &\times e^{-\frac{|\mathbf{k}|^2}{2(\alpha_p+\alpha_D)}} e^{-\frac{|\mathbf{k}-\mathbf{K}|^2}{2(\alpha_p+\alpha_D)}} \sum_i e^{i\mathbf{K}\cdot\mathbf{R}_i} \quad , \end{aligned} \quad (4.8)$$

V_{cell} being the volume of the lattice unit cell. Consequently, the analysis presented in the case of Bragg scattering in section 3.2 applies here, with the only difference being that instead of a simple periodic potential $V_{\mathbf{K}}$, there exists an additional periodic term $W_{\mathbf{k}-\mathbf{K},\mathbf{k}}$. The reaction rate, therefore, looks something like

$$\begin{aligned} \Gamma_{tot} &\sim N_D \left[\frac{\boldsymbol{\mu} \cdot \mathbf{B}}{|\Delta E|} \right]^2 \left| \frac{W_{\mathbf{k}-\mathbf{K},\mathbf{k}}}{\Delta E} \right|^2 \left(\frac{V_N}{V_A} \right) \left\{ \frac{|W_{\mathbf{k}-\mathbf{K},\mathbf{k}}|}{\frac{\hbar^2 |\mathbf{K}|^2}{2M_n}} \right\} \Gamma_{Pd} \\ &\sim 10^{21} \times 10^{-71} = 10^{-50} \text{sec}^{-1} \quad . \end{aligned} \quad (4.9)$$

It seems, once again, that we are faced with very low reaction rates. However there is an avenue that could salvage the model. So far, we have proposed the electromagnetic interaction to be the predominant force in the coupling between the virtual neutrons and lattice nuclei. The matrix element of the electromagnetic force we have been studying (which appears as $\boldsymbol{\mu} \cdot \mathbf{B}$ in the above formula) is of order magnitude 10^{-6} eV or so. If we switch to a picture where the principle interaction between neutrons and the lattice is *strong* in nature, then situation becomes quite different. This would mean, of course, that protons and deuterons no longer play a role in the transfer mechanism. Larger nuclei, like tritium, Pd and Li isotopes and others will now couple strongly to the virtual neutrons.

The strength of the *strong* force (which is sometimes referred to as the *nuclear* force since it is responsible for the binding of the nucleus) is measured by looking at the strong coupling between nucleons and various mesons. More specifically, it is believed that the strong

³P. L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two-Step Reactions and Virtual Neutrons", submitted to *Fusion Tech.* November (1992).

interaction between two nucleons arises through the exchange of virtual mesons. Since these virtual particles have mass, there is a minimum amount by which energy conservation must be violated during the exchange process; $\Delta E > m_\pi c^2$ where m_π is the mass of the pion, which is the lightest known meson⁴:

$$m_{\pi^\pm} c^2 = 139.576 \pm 0.011 \text{ MeV} \quad (4.10)$$

$$m_{\pi^0} c^2 = 134.972 \pm 0.012 \text{ MeV} \quad (4.11)$$

An upper limit on the range of the strong interaction may be obtained from m_π :

$$\Delta r < \frac{\hbar}{m_\pi c} \approx 1.4 \times 10^{-13} \text{ cm} \quad (4.12)$$

Of importance to us here is the actual strength of the strong force. Theoretical models predict the *OPEP* (One Pion Exchange Potential) to be of the form⁵

$$V_s = \left(\frac{1}{3}\right) \frac{g^2}{\hbar c} m_\pi c^2 (\hat{\tau}_1 \cdot \hat{\tau}_2) \left[(\hat{\sigma}_1 \cdot \hat{\sigma}_2) + \left(1 + \frac{3}{\mu r} + \frac{3}{(\mu r)^2}\right) \hat{S}_{12} \right] \frac{e^{-\mu r}}{\mu r} \quad (4.13)$$

where $\hat{\tau}$ is the isospin operator and \hat{S}_{12} is the tensor force operator,

$$\hat{S}_{12} = \frac{1}{r^2} \left[3(\hat{\sigma}_1 \cdot \hat{r})(\hat{\sigma}_2 \cdot \hat{r}) - (\hat{\sigma}_1 \cdot \hat{\sigma}_2) r^2 \right] \quad (4.14)$$

Of course, r is the distance separating the interacting nucleons and $\frac{g^2}{\hbar c}$ is the strong coupling constant, which, for the pion exchange, is given by

$$\frac{g^2}{\hbar c} = 0.081 \quad (4.15)$$

Thus we conclude that the matrix element of the strong force V_s , which is proposed to replace the $\mu \cdot \mathbf{B}$ term in Eq. (4.9) and in the formula for $W_{\mathbf{k}-\mathbf{K}, \mathbf{k}}$ in Eq. (4.8), has magnitude on the order of a few keV or so. With this in mind, we recalculate the neutron transfer

⁴A. deShalit and H. Feshbach, "Theoretical Nuclear Physics I: Nuclear Structure", John Wiley and Sons, Inc., 1974; pages 11 - 18 .

⁵A. deShalit and H. Feshbach, "Theoretical Nuclear Physics I: Nuclear Structure", John Wiley and Sons, Inc., 1974; Eqs. (3.5)-(3.7).

reaction rate to obtain

$$\begin{aligned}\Gamma_{tot} &\sim N_D \left[\frac{V_s}{|\Delta E|} \right]^2 \left| \frac{W_{\mathbf{k}-\mathbf{K},\mathbf{k}}^{(s)}}{\Delta E} \right|^2 \left(\frac{V_N}{V_A} \right) \left\{ \frac{|W_{\mathbf{k}-\mathbf{K},\mathbf{k}}^{(s)}|}{\frac{\hbar^2 |\mathbf{K}|^2}{2M_n}} \right\} \Gamma_{Pd} \\ &\sim 10^{21} \times 10^{+1} = 10^{22} \text{sec}^{-1} \quad .\end{aligned}\tag{4.16}$$

This reaction rate is enormous, which leads us to believe that the transfer mechanism in and of itself does not hinder the progress of the heat producing reactions. The bottle-neck, as it were, lies somewhere else. We shall see in the coming sections that it is the limitation on the number of phonons that may participate in the neutron exchange reactions which slows down the process.

The remaining chapters are dedicated toward constructing a more formal approach to the neutron/lattice coupling problem in the presence of the $W(\mathbf{r}_n$ exchange term in the Hamiltonian. Our aim is to devise an appropriate approximation scheme that would allow us to derive an expression for the neutron Green's function associated with the near-resonance exchange term in the Hamiltonian. Once an estimate for the Green's function is found, the associated transfer reaction rate may be determined. The scheme which shall be adopted is based on infinite order Brillouin-Wigner perturbation theory. It will be used to derive an estimate for the self-energy, and subsequently the Green's function.

Chapter 5

Hamiltonian for the Coupled System

In this chapter we turn our attention toward constructing the Green's function and Hamiltonian representing the virtual neutron in a lattice system.

The analysis is facilitated by the use of second quantized field operators for the neutrons and the donor and acceptor nuclei introduced in chapter 2 (see Eqs. (2.1) - (2.4)). In the case of neutrons, we defined the field operators $\hat{\Psi}_n(\mathbf{r})$ and $\hat{\Psi}_n^\dagger(\mathbf{r})$ in the following manner:

$$\begin{aligned}\hat{\Psi}_n(\mathbf{r}) &= \sum_{\alpha_n} \sum_{\mathbf{k}} \hat{b}_{n,\alpha_n,\mathbf{k}} \Phi_{n,\alpha_n,\mathbf{k}}(\mathbf{r}) \quad , \\ \hat{\Psi}_n^\dagger(\mathbf{r}) &= \sum_{\alpha_n} \sum_{\mathbf{k}} \hat{b}_{n,\alpha_n,\mathbf{k}}^\dagger \Phi_{n,\alpha_n,\mathbf{k}}^*(\mathbf{r}) \quad ,\end{aligned}$$

where, as a reminder, $\hat{b}_{n,\alpha_n,\mathbf{k}}$ and $\hat{b}_{n,\alpha_n,\mathbf{k}}^\dagger$ are Schrodinger picture single neutron annihilation and creation operators, $\Phi_{n,\alpha_n,\mathbf{k}}(\mathbf{r})$ and $\Phi_{n,\alpha_n,\mathbf{k}}^*(\mathbf{r})$ are Fock space wavefunctions, and α_n represents the neutron spin quantum number.

In the case of nuclei, we defined the following field operators:

$$\begin{aligned}\hat{\Psi}_X(\mathbf{r}_1, \dots, \mathbf{r}_N) &= \sum_i \sum_{\alpha_X} \hat{b}_{X,\alpha_X}(i) \Phi_X^{\alpha_X}(\mathbf{r}_1 - \hat{\mathbf{R}}_i, \dots, \mathbf{r}_N - \hat{\mathbf{R}}_i) \quad , \\ \hat{\Psi}_X^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_N) &= \sum_i \sum_{\alpha_X} \hat{b}_{X,\alpha_X}^\dagger(i) \Phi_X^{*\alpha_X}(\mathbf{r}_1 - \hat{\mathbf{R}}_i, \dots, \mathbf{r}_N - \hat{\mathbf{R}}_i) \quad ,\end{aligned}$$

where $\hat{\mathbf{R}}_i$ is the time-dependent center of mass position operator at site i . Operators $\hat{\Psi}_X^i(\mathbf{r}_1, \dots, \mathbf{r}_N)$ and $[\hat{\Psi}_X^i(\mathbf{r}_1, \dots, \mathbf{r}_N)]^\dagger$ destroy and annihilate nucleon X at lattice site i re-

spectively.

A formal expression for the many-body Green's function in terms of the neutron and donor and acceptor nuclear field operators follows immediately;

$$G_n(\mathbf{r}, \mathbf{r}_1, \dots, \mathbf{r}_N; \mathbf{r}', \mathbf{r}'_1, \dots, \mathbf{r}'_N) = -i \langle \Phi_0 | \left[\hat{\Psi}_{A'}^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_N) \hat{\Psi}_n(\mathbf{r}) \hat{\Psi}_A(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \right] \times \left[\hat{\Psi}_{D'}^\dagger(\mathbf{r}'_1, \dots, \mathbf{r}'_{N-1}) \hat{\Psi}_n^\dagger(\mathbf{r}') \hat{\Psi}_D(\mathbf{r}'_1, \dots, \mathbf{r}'_N) \right] | \Phi_0 \rangle \quad (5.1)$$

In formulating the full system Hamiltonian, H , we shall adopt three classifications: H_{nuclei} , which includes the contributions of all the donor and acceptor nuclei in the lattice; $H_{neutrons}$, representing the contributions of the neutrons to the total energy and $H_{phonons}$ depicting the phonon contribution to the total energy. $H_{neutrons}$ includes a kinetic energy term $[H_n]_{K.E.}$, a potential energy term depicting the presence of the lattice, which we shall call $[H_n]_{Bragg}$ since Bragg scattering is the strongest conventional interaction between the neutron and the lattice, and finally a magnetic dipole transition term, $H_{-\mu \cdot \mathbf{B}}$, containing the Duschinsky operator responsible for mediating the energy transfer in the cells. It is this magnetic dipole term which interests us most. More specifically we shall pay special attention to the resonance exchange term which results from a second order expansion of the magnetic dipole term.

H_{nuclei} is simply the sum of the energy deficits for the neutron transitions over all participating donor and acceptor nuclei. Therefore, by inspection, H_{nuclei} is given by

$$\begin{aligned} H_{nuclei} &= \sum_D \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N (\hbar\omega_D) \hat{\Psi}_D^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_N) \hat{\Psi}_D(\mathbf{r}_1, \dots, \mathbf{r}_N) \\ &+ \sum_{D'} \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N (\hbar\omega_{D'}) \hat{\Psi}_{D'}^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_N) \hat{\Psi}_{D'}(\mathbf{r}_1, \dots, \mathbf{r}_N) \\ &+ \sum_A \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_{N-1} (\hbar\omega_A) \hat{\Psi}_A^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \hat{\Psi}_A(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \\ &+ \sum_{A'} \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_{N-1} (\hbar\omega_{A'}) \hat{\Psi}_{A'}^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \hat{\Psi}_{A'}(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \quad . \quad (5.2) \end{aligned}$$

To illustrate some of these transition energy gaps or deficits, consider as an example the palladium electrolysis experiments in which heat production is observed. The conjecture is that the excess energy is produced from $d(\gamma, n)p$ coupled with $^{104}\text{Pd}(n, \gamma)^{105}\text{Pd}$ and $^{105}\text{Pd}(n, \gamma)^{106}\text{Pd}$ reactions, as illustrated in Fig. 5-1. The associated energy transfers for these reactions are 2.225 MeV, -7.09 MeV and -9.56 MeV respectively.

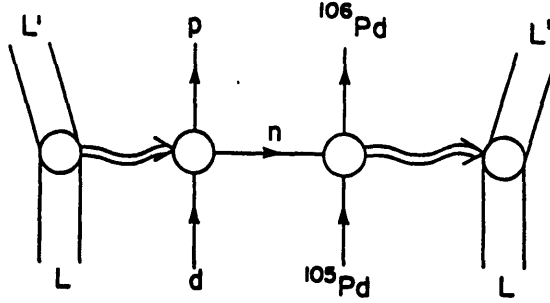


Figure 5-1: Feynman-like diagram for coherent coupled $d(\gamma, n)p$ and $^{105}\text{Pd}(n, \gamma)^{106}\text{Pd}$ reactions.

As far as the terms contributing to $H_{neutrons}$ are concerned, $[H_n]_{K.E.}$ and $[H_n]_{Bragg}$ may be readily expressed in terms of the neutron field operator. $[H_n]_{K.E.}$ represents the non-interacting part of the Hamiltonian, or in other words, it is the energy contribution by the neutrons in the free space model. In free space, the neutron eigenfunctions are plane waves ($\psi_n \sim e^{i\mathbf{k}\cdot\mathbf{r}}$) with eigenvalues $\frac{\hbar^2|\mathbf{k}|^2}{2M_n}$, M_n being the mass of the neutron. It follows that $[H_n]_{K.E.}$ is given by

$$[H_n]_{K.E.} = \sum_{\alpha_n} \int d^3\mathbf{r} \hat{\Psi}_n^\dagger(\mathbf{r}) \left(\frac{-\hbar^2 \nabla^2}{2M_n} \right) \hat{\Psi}_n(\mathbf{r}) \quad . \quad (5.3)$$

$[H_n]_{Bragg}$ may be defined as follows:

$$[H_n]_{Bragg} = \sum_{\alpha_n} \int d^3\mathbf{r} \hat{\Psi}_n^\dagger(\mathbf{r}) V(\mathbf{r}) \hat{\Psi}_n(\mathbf{r}) \quad , \quad (5.4)$$

where $V(\mathbf{r})$ is simply the periodic lattice potential.

The case of the magnetic dipole transition potential was visited in chapter 2. Our calculations led us to the following expression for the interaction Hamiltonian (see Eqs. (2.5)-(2.8)):

$$\begin{aligned} H_{-\mu\cdot\mathbf{B}} = & \sum_i \sum_{\alpha_n} \sum_{\alpha_D} \sum_{\alpha_{D'}} \sum_{\mathbf{k}} \hat{b}_{n,\alpha_n,\mathbf{k}}^\dagger \hat{b}_{D',\alpha_{D'}}^\dagger(i) \hat{b}_{D,\alpha_D}(i) \hat{U}_{D',n,D}^{\alpha_{D'},\alpha_n,\alpha_D}(i) \\ & + \sum_i \sum_{\alpha_n} \sum_{\alpha_A} \sum_{\alpha_{A'}} \sum_{\mathbf{k}} \hat{b}_{A',\alpha_{A'}}^\dagger(i) \hat{b}_{n,\alpha_n,\mathbf{k}} \hat{b}_{A,\alpha_A}(i) \hat{U}_{A',A,n}^{\alpha_{A'},\alpha_A,\alpha_n}(i) \quad . \end{aligned}$$

Finally, there is the phonon contribution to the total energy. In the strictest sense, if

we wanted to take into account changes in the lattice caused by the interactions with the neutrons, then we would have to define Hamiltonian of the form

$$H_{phonons} = \sum_i \frac{\hat{\mathbf{P}}_i^2}{2\hat{m}_i} + \sum_{i<j} \hat{V}_{ij} \quad , \quad (5.5)$$

where \hat{m}_i is the phonon “mass” operator and \hat{V}_{ij} is the exchange potential. In this case diagonalizing the Hamiltonian is not trivial, if at all possible. However, since lattice variations are not taken into account in our calculation of the proper self-energy (see chapter 6) and later on when we take phonon averages (see chapter 7), then the harmonic approximation is valid. Therefore we may assume $H_{phonons}$ to be of the form

$$H_{phonons} = \sum_{\mathbf{k},s} \hbar\omega_s(\mathbf{k}) \left(\hat{a}_{\mathbf{k},s}^\dagger \hat{a}_{\mathbf{k},s} + \frac{1}{2} \right) = \sum_{\mathbf{k},s} \hbar\omega_s(\mathbf{k}) \left(\hat{n}_s(\mathbf{k}) + \frac{1}{2} \right) \quad , \quad (5.6)$$

where $\hat{a}_{\mathbf{k},s}^\dagger$ and $\hat{a}_{\mathbf{k},s}$ are phonon creation and annihilation operators respectively¹. In addition, the magnetic dipole transition term itself includes phonon operators $\hat{\mathbf{r}}$ representing lattice phonon-neutron interaction.

Summing up all these terms yields the following expression for the aggregate virtual neutron/lattice system Hamiltonian:

$$\begin{aligned} H_{total} = & \sum_D \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N (\hbar\omega_D) \hat{\Psi}_D^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_N) \hat{\Psi}_D(\mathbf{r}_1, \dots, \mathbf{r}_N) \\ & + \sum_{D'} \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N (\hbar\omega_{D'}) \hat{\Psi}_{D'}^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_N) \hat{\Psi}_{D'}(\mathbf{r}_1, \dots, \mathbf{r}_N) \\ & + \sum_A \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_{N-1} (\hbar\omega_A) \hat{\Psi}_A^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \hat{\Psi}_A(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \\ & + \sum_{A'} \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_{N-1} (\hbar\omega_{A'}) \hat{\Psi}_{A'}^\dagger(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \hat{\Psi}_{A'}(\mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \\ & + \sum_{\alpha_n} \int d^3\mathbf{r} \hat{\Psi}_n^\dagger(\mathbf{r}) \left(\frac{-\hbar^2 \nabla^2}{2M_n} \right) \hat{\Psi}_n(\mathbf{r}) \\ & + \sum_{\alpha_n} \int d^3\mathbf{r} \hat{\Psi}_n^\dagger(\mathbf{r}) V(\mathbf{r}) \hat{\Psi}_n(\mathbf{r}) \\ & + \sum_{\mathbf{k},s} \hbar\omega_s(\mathbf{k}) \left(\hat{a}_{\mathbf{k},s}^\dagger \hat{a}_{\mathbf{k},s} + \frac{1}{2} \right) \end{aligned}$$

¹A detailed discussion on the theory of harmonic crystals, including the definitions of the phonon creation and annihilation operators in terms of the polarization vector $\epsilon_s(\mathbf{k})$ and frequency $\omega_s(\mathbf{k})$ (see Eqs. (7.30) and (7.31)), is provided in chapter 7.

$$\begin{aligned}
& + \sum_i \sum_{\alpha_n} \sum_{\alpha_D} \sum_{\alpha_{D'}} \sum_{\mathbf{k}} \hat{b}_{n,\alpha_n,\mathbf{k}}^\dagger \hat{b}_{D',\alpha_{D'}}^\dagger(i) \hat{b}_{D,\alpha_D}(i) \hat{U}_{D',n,D}^{\alpha_{D'},\alpha_n,\alpha_D}(i) \\
& + \sum_i \sum_{\alpha_n} \sum_{\alpha_A} \sum_{\alpha_{A'}} \sum_{\mathbf{k}} \hat{b}_{A',\alpha_{A'}}^\dagger(i) \hat{b}_{n,\alpha_n,\mathbf{k}} \hat{b}_{A,\alpha_A}(i) \hat{U}_{A',A,n}^{\alpha_{A'},\alpha_A,\alpha_n}(i) . \quad (5.7)
\end{aligned}$$

Chapter 6

Hartree-Fock and the Proper Self-Energy

In order to tackle the Green's function problem, we must choose an appropriate approximation scheme. A perturbative approach is always a viable option, however we have chosen to abandon the standard order by order perturbation calculation in favor of infinite order perturbation expansion. Hartree Fock theory is an example of such a scheme. The next few pages will be dedicated to the introduction and development of the principles of Hartree theory which concern us most in our calculations.

The Hartree-Fock approximation method is based on the assumption that one may simplify a given many-body problem by dividing it into a set of single-body particle equations. Alternatively, one may treat the individual particles as moving in single-particle potentials representing the mean interaction with all the other particles in the system¹.

The analysis of Hartree theory benefits from the use of Feynman diagrams and the concept of the self-energy. Consider then the proper self-energy term $\Sigma^*(x, x')$ for a single particle. To first-order, the contributions to $\Sigma^*(x, x')$ are precisely the terms which appear in the first order expansion of the many-body Green's function $G_{\alpha\beta}^{(1)}(x, x')$ and is displayed in diagrammatic form in Fig. 6-1².

Using this definition we may derive an expression for the full proper self-energy by

¹Alexander L. Fetter and John Dirk Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, Inc., New York, (1971).

²Fig. 6-1 is a reproduction of Fig. 10.1, Alexander L. Fetter and John Dirk Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, Inc., New York, (1971).

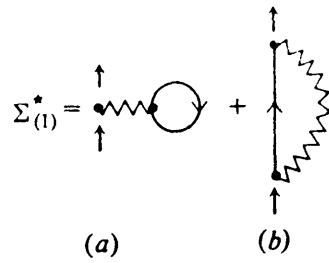


Figure 6-1: Lowest order proper self-energy $\Sigma_{(1)}^*(x, x')$.

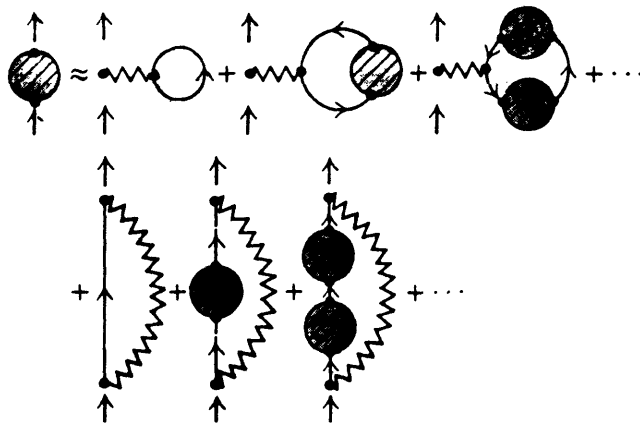


Figure 6-2: Full expansion for $\Sigma^*(x, x')$ in Hartree-Fock approximation.

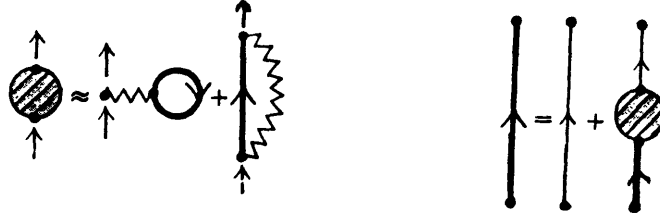


Figure 6-3: Iterative definition of $\Sigma^*(x, x')$ in Hartree-Fock approximation.

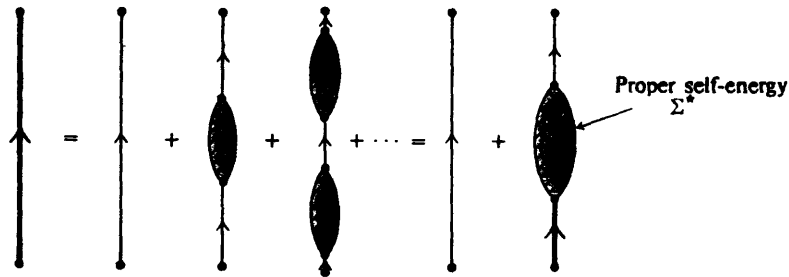


Figure 6-4: Dyson's equation for G in Hartree-Fock approximation.

inserting higher and higher orders of $\Sigma^*(x, x')$ into the lowest order diagram in the figure. The result is shown in Fig. 6-2³. The expansion may be recast in iterative form in the manner displayed in Figs. 6-3(a) and 6-3(b)⁴. Combining the two diagrams in Fig. 6-3 yields the general form for Dyson's equation in the Hartree-Fock scheme, shown in Fig. 6-4⁵.

Having defined Dyson's equation in the context of Hartree's theory, we are now in position to address the problem of the virtual neutron in a lattice. The total system Hamiltonian is given Eq. (5.7). The first seven terms in the expansion for H_{total} we choose to combine here to form what is called the *noninteracting potential*, H_0 . Therefore H_0 is

³Fig 7-2 is a reproduction of Fig. 10.2, Alexander L. Fetter and John Dirk Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, Inc., New York, (1971).

⁴Fig. 6-3 is a reproduction of Figs. 10.3 and 10.4, Alexander L. Fetter and John Dirk Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, Inc., New York, (1971).

⁵Fig 6-4 is a reproduction of Fig. 10.5, Alexander L. Fetter and John Dirk Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, Inc., New York, (1971).

given by

$$\begin{aligned}
H_0 &= \sum_D \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N (\hbar\omega_D) \hat{\Psi}_D^\dagger(\mathbf{r}_1 \dots \mathbf{r}_N) \hat{\Psi}_D(\mathbf{r}_1 \dots \mathbf{r}_N) \\
&+ \sum_{D'} \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N (\hbar\omega_{D'}) \hat{\Psi}_{D'}^\dagger(\mathbf{r}_1 \dots \mathbf{r}_N) \hat{\Psi}_{D'}(\mathbf{r}_1 \dots \mathbf{r}_N) \\
&+ \sum_A \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N (\hbar\omega_A) \hat{\Psi}_A^\dagger(\mathbf{r}_1 \dots \mathbf{r}_N) \hat{\Psi}_A(\mathbf{r}_1 \dots \mathbf{r}_N) \\
&+ \sum_{A'} \int d^3\mathbf{r}_1 \dots d^3\mathbf{r}_N (\hbar\omega_{A'}) \hat{\Psi}_{A'}^\dagger(\mathbf{r}_1 \dots \mathbf{r}_N) \hat{\Psi}_{A'}(\mathbf{r}_1 \dots \mathbf{r}_N) \\
&+ \sum_{\alpha_n} \int d^3\mathbf{r} \hat{\psi}_n^\dagger(\mathbf{r}) \left[-\frac{\hbar^2 \nabla^2}{2M_n} + V(\mathbf{r}) \right] \hat{\psi}_n(\mathbf{r}) + \sum_{\mathbf{k}, s} \hbar\omega_s(\mathbf{k}) \left(\hat{a}_{\mathbf{k}, s}^\dagger \hat{a}_{\mathbf{k}, s} + \frac{1}{2} \right) \quad . \quad (6.1)
\end{aligned}$$

Bear in mind that there is an implicit summation over the lattice index i in the definition of the phonon operators (see Eqs. (7.30) and (7.31)). The *interacting Hamiltonian*, H_1 , includes the last two terms in Eq. (5.7), which, using the approximation stated in Eq. (2.11), may be rewritten in the following form:

$$\begin{aligned}
H_1 &= \sum_i \sum_{\alpha_n} \sum_{\alpha_p} \sum_{\alpha_d} \sum_{\mathbf{k}} \langle \alpha_n, \alpha_p | -\mu \cdot \mathbf{B} | \alpha_d \rangle \hat{b}_{n, \alpha_n, \mathbf{k}}^\dagger \hat{b}_{p, \alpha_p}^\dagger(i) \hat{b}_{d, \alpha_d}(i) e^{i\mathbf{k} \cdot \hat{\mathbf{R}}_i} e^{-i\hat{S}_D} \\
&+ \sum_j \sum_{\alpha_{n'}} \sum_{\alpha_{p'}} \sum_{\alpha_{d'}} \sum_{\mathbf{k}'} \langle \alpha_{d'} | -\mu \cdot \mathbf{B} | \alpha_{n'}, \alpha_{p'} \rangle \hat{b}_{d, \alpha_{d'}}^\dagger(j) \hat{b}_{n, \alpha_{n'}, \mathbf{k}'} \hat{b}_{p, \alpha_{p'}}(j) e^{-i\mathbf{k}' \cdot \hat{\mathbf{R}}_j} e^{i\hat{S}_D} \quad (6.2)
\end{aligned}$$

I have introduced a slight change in indices in the above equation, by replacing the *generic* indices for donors and acceptors (D, D' and A, A') in Eq. (5.7) with *specific* indices for the deuterons and protons (d, d' and p, p').

Turning our attention to the Green's function for a moment, $G(\mathbf{x}, \mathbf{x}')$ is given by Dyson's equation⁶,

$$G(\mathbf{x}, \mathbf{x}') = G^0(\mathbf{x}, \mathbf{x}') + \int d^4x_1 d^4x_1' G^0(\mathbf{x}, x_1) \Sigma^*(x_1, x_1') G(x_1', \mathbf{x}') \quad . \quad (6.3)$$

We need develop a scheme that would allow us to deduce a form for the proper self-energy without having to solve for $G(\mathbf{x}, \mathbf{x}')$ first. In order to do that, define $\phi_j^0(\mathbf{r})$ to be the eigenfunction solution to the non-interacting Hamiltonian H_0 given in Eq. (6.1), with

⁶Alexander L. Fetter and John Dirk Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, Inc., New York, (1971); page 123 Eq. (10.3)

corresponding eigenenergies E_j^0 ;

$$H_0\phi_j^0(\mathbf{r}) = \left[-\frac{\hbar^2\nabla^2}{2M_n} + V(\mathbf{r}) \right] \phi_j^0(\mathbf{r}) = E_j^0\phi_j^0(\mathbf{r}) \quad . \quad (6.4)$$

Similarly, let $\phi_j(\mathbf{r})$ to be the eigenfunction solution to the full Hamiltonian. The equation for $\phi_j^0(\mathbf{r})$ which corresponds to Eq. (6.4) is⁷

$$E_j\phi_j(\mathbf{r}) = \left[-\frac{\hbar^2\nabla^2}{2M_n} + V(\mathbf{r}) \right] \phi_j(\mathbf{r}) + \int d^3\mathbf{r}' \hbar\Sigma^*(\mathbf{r}, \mathbf{r}')\phi_j(\mathbf{r}') \quad . \quad (6.5)$$

Eq. (6.5) may be redefined in the frequency domain by performing a Fourier transform. The result is that

$$E_j\phi_j(\mathbf{k}) = -\frac{\hbar^2\nabla_{\mathbf{k}}^2}{2M_n}\phi_j(\mathbf{k}) + V(\mathbf{k}) \otimes \phi_j(\mathbf{k}) + \hbar \sum_{\mathbf{k}'} \Sigma^*(\mathbf{k}, \mathbf{k}')\phi_j(\mathbf{k}') \quad , \quad (6.6)$$

where \otimes implies convolution. The above two equations will play a very important role in the ensuing calculations as they will be used in identifying the part which constitutes the proper self-energy operator of the neutron/lattice system in the Brillouin-Wigner approximation scheme.

This completes the formalism of Hartree-Fock's approach to the many-body problem. The challenge now is to be able to derive an expression for the proper self-energy term in Eq. (6.6) and thus obtain a solution for the Green's function. The Hamiltonian for the zero neutron and single neutron Fock space may be approximated as follows:

$$H = \begin{pmatrix} H_0 & 0 \\ 0 & H_0 \end{pmatrix} + \begin{pmatrix} 0 & H_1 \\ H_1 & 0 \end{pmatrix} \quad . \quad (6.7)$$

According to Brillouin-Wigner theory the Hamiltonian in Eq. (6.7) has eigenfunction solutions of the form

$$\Psi = \begin{pmatrix} \Psi_0 \\ \Psi_1 \end{pmatrix} = \begin{pmatrix} \Phi_0 \\ 0 \end{pmatrix} + \begin{pmatrix} \hat{Q} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \Psi_0 \\ \Psi_1 \end{pmatrix} \quad (6.8)$$

where Φ_0 is the eigenfunction of the non-interacting Hamiltonian H_0 , Ψ_0 contains no free

⁷Alexander L. Fetter and John Dirk Walecka, *Quantum Theory of Many-Particle Systems*, McGraw-Hill, Inc., New York, (1971); page 125 Eq. (10.17)

neutrons, $|\Psi_1\rangle$ contains a single free neutron and \hat{Q} is given by

$$\hat{Q} = 1 - |\Phi_0\rangle\langle\Phi_0| \quad . \quad (6.9)$$

Solving for $|\Psi_1\rangle$ yields

$$\left[E - H_0 - H_1[E - H_0]^{-1}(1 - |\Phi_0\rangle\langle\Phi_0|)H_1 \right] |\Psi_1\rangle = H_1|\Phi_0\rangle \quad . \quad (6.10)$$

Substituting the expansion for H_1 in Eq. (6.2) into Eq. (6.10) leads to the following result:

$$\begin{aligned} (E - H_0)|\Psi_1\rangle &= \sum_{i', i''} \sum_{\mathbf{k}', \mathbf{k}''} \sum_{\alpha_{n'}, \alpha_{n''}} \sum_{\alpha_{p'}, \alpha_{p''}} \sum_{\alpha_{d'}, \alpha_{d''}} \langle \alpha_{n'}, \alpha_{p'} | -\mu \cdot \mathbf{B} | \alpha_{d'} \rangle \\ &\times \left[\hat{b}_{p, \alpha_{p'}}^\dagger(i') \hat{b}_{d, \alpha_{d'}}(i') \hat{b}_{n, \alpha_{n'}, \mathbf{k}'}^\dagger e^{i\mathbf{k}' \cdot \hat{\mathbf{R}}_{i'}} e^{-i\hat{S}_D(i')} \right] \\ &\times [E - H_0]^{-1} (1 - |\Phi_0\rangle\langle\Phi_0|) \langle \alpha_{d''} | -\mu \cdot \mathbf{B} | \alpha_{n''}, \alpha_{p''} \rangle \\ &\times \left[\hat{b}_{p, \alpha_{p''}}(i'') \hat{b}_{d, \alpha_{d''}}^\dagger(i'') \hat{b}_{n, \alpha_{n''}, \mathbf{k}''} e^{-i\mathbf{k}'' \cdot \hat{\mathbf{R}}_{i''}} e^{i\hat{S}_D(i'')} \right] |\Psi_1\rangle \\ &= \sum_i \sum_{\mathbf{k}} \sum_{\alpha_n} \sum_{\alpha_p} \sum_{\alpha_d} \langle \alpha_n, \alpha_p | -\mu \cdot \mathbf{B} | \alpha_d \rangle \\ &\times \left[\hat{b}_{p, \alpha_p}^\dagger(i) \hat{b}_{d, \alpha_d}(i) \hat{b}_{n, \alpha_n, \mathbf{k}}^\dagger e^{i\mathbf{k} \cdot \hat{\mathbf{R}}_i} e^{-i\hat{S}_D(i)} \right] |\Phi_0\rangle \quad . \quad (6.11) \end{aligned}$$

In order to work with the above equation, we need a relation between state $|\Psi_1\rangle$ and state $|\Phi_0\rangle$. This may be achieved by assuming the following form for $|\Psi_1\rangle$:

$$|\Psi_1\rangle = \sum_i \sum_{\mathbf{k}} \sum_{\alpha_n} \sum_{\alpha_p} \sum_{\alpha_d} \left[\hat{b}_{p, \alpha_p}^\dagger(i) \hat{b}_{d, \alpha_d}(i) \phi_n(\mathbf{k}) \hat{b}_{n, \alpha_n, \mathbf{k}}^\dagger e^{i\mathbf{k} \cdot \hat{\mathbf{R}}_i} e^{-i\hat{S}_D(i)} \right] |\Phi_0\rangle \quad , \quad (6.12)$$

where I have used the shorthand

$$V_{\mu \cdot \mathbf{B}} = \langle \alpha_n, \alpha_p | -\mu \cdot \mathbf{B} | \alpha_d \rangle \quad .$$

$\phi_n(\mathbf{k})$ is the neutron wavefunction. The statement in Eq. (6.12) is obtained from an approximate first order perturbation expansion of $|\Psi_1\rangle$ in terms of $|\Phi_0\rangle$, according to

$$\Delta E |\Psi_1\rangle - H_1[E - H_0]^{-1} H_1 |\Psi_1\rangle = H_1 |\Phi_0\rangle$$

$$\begin{aligned}
\Rightarrow |\Psi_1\rangle &= [\Delta E - H_1[E - H_0]^{-1}H_1]^{-1} |\Phi_0\rangle \\
&= (\Delta E)^{-1}H_1|\Phi_0\rangle + (\Delta E)^{-2}H_1[E - H_0]^{-1}H_1H_1|\Phi_0\rangle + \dots
\end{aligned}$$

Eq. (6.12) is an approximation motivated by the observation that the lowest order expansion of $|\Psi_1\rangle$ is proportional to $H_1|\Phi_0\rangle$. The approximation itself is one that says that the system is weakly interacting, and that the free neutrons are given the freedom to scatter. Neutron "holes" are taken to be unperturbed, which is why no weighting function in index i appears in the approximation. The combination of Eqs. (6.12) and Eq. (6.11) produces the following equality:

$$\begin{aligned}
V_{\mu,\mathbf{B}}|\Phi_0\rangle &= \hat{b}_{p,\alpha_p}(i)\hat{b}_{d,\alpha_d}^\dagger(i)\hat{b}_{n,\alpha_n,\mathbf{k}}e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i}e^{i\hat{S}_D(i)}(E - H_0) \\
&\quad \times \left[\hat{b}_{p,\alpha_p}^\dagger(i)\hat{b}_{d,\alpha_d}(i)\phi_n(\mathbf{k})\hat{b}_{n,\alpha_n,\mathbf{k}}^\dagger e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_i}e^{-i\hat{S}_D(i)} \right] |\Phi_0\rangle \\
&- \sum_{i',i'',i'''} \sum_{\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \sum_{\alpha_{n'},\alpha_{n''},\alpha_{n'''}} \sum_{\alpha_{p'},\alpha_{p''},\alpha_{p'''}} \sum_{\alpha_{d'},\alpha_{d''},\alpha_{d'''}} |V_{\mu,\mathbf{B}}|^2 \\
&\quad \times \hat{b}_{p,\alpha_p}(i)\hat{b}_{d,\alpha_d}^\dagger(i)\hat{b}_{n,\alpha_n,\mathbf{k}}e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i}e^{i\hat{S}_D(i)}\hat{b}_{n,\alpha_{n'},\mathbf{k}'}^\dagger \\
&\quad \times \left[\hat{b}_{p,\alpha_{p'}}^\dagger(i')\hat{b}_{d,\alpha_{d'}}(i')\hat{b}_{n,\alpha_{n'},\mathbf{k}'}^\dagger e^{i\mathbf{k}'\cdot\hat{\mathbf{R}}_{i'}}e^{-i\hat{S}_D(i')} \right] \\
&\quad \times [E - H_0]^{-1}(1 - |\Phi_0\rangle\langle\Phi_0|) \\
&\quad \times \left[\hat{b}_{p,\alpha_{p''}}(i'')\hat{b}_{d,\alpha_{d''}}^\dagger(i'')\hat{b}_{n,\alpha_{n''},\mathbf{k}''}e^{-i\mathbf{k}''\cdot\hat{\mathbf{R}}_{i''}}e^{i\hat{S}_D(i'')} \right] \\
&\quad \times \hat{b}_{p,\alpha_{p'''}}^\dagger(i''')\hat{b}_{d,\alpha_{d'''}}(i''')\phi_n(\mathbf{k}''') \\
&\quad \times \hat{b}_{n,\alpha_{n'''},\mathbf{k}'''}^\dagger e^{i\mathbf{k}'''\cdot\hat{\mathbf{R}}_{i'''}}e^{-i\hat{S}_D(i''')}|\Phi_0\rangle \quad . \quad (6.13)
\end{aligned}$$

Consider now the first term on the right hand side of Eq. (6.13). It may be rewritten as

$$\hat{O}(E - H_0)|\Psi_1\rangle = [(E - H_0)\hat{O} + [\hat{O}, (E - H_0)]] |\Psi_1\rangle \quad , \quad (6.14)$$

where \hat{O} is an abbreviation for the operator $\hat{b}_{p,\alpha_p}(i)\hat{b}_{d,\alpha_d}^\dagger(i)e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i}e^{i\hat{S}_D(i)}$. But in the neutron problem, $(E - H_0)\hat{O}$ is expected to be dominant over the commutator term, since the energy scale of the former is of the order of MeV's ($\Delta E = -2.225$ MeV for the deuteron), whereas the latter is of atomic scale energy (of the order of a few eV's). Thus we may replace $\hat{b}_{p,\alpha_p}(i)\hat{b}_{d,\alpha_d}^\dagger(i)e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i}e^{i\hat{S}_D(i)}(E - H_0)$ in Eq. (6.13) with $(\Delta E - H_n)\hat{b}_{p,\alpha_p}(i)\hat{b}_{d,\alpha_d}^\dagger(i)e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i}e^{i\hat{S}_D(i)}$,

where H_n is the neutron energy. The result is given by

$$\begin{aligned}
V_{\mu\cdot\mathbf{B}}|\Phi_0\rangle &= (\Delta E - H_n)|\Phi_0\rangle\phi_n(\mathbf{k}) \\
&- \sum_{i',i'',i'''} \sum_{\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \sum_{\alpha_n',\alpha_n'',\alpha_n'''} \sum_{\alpha_{p'},\alpha_{p}'',\alpha_{p}'''} \sum_{\alpha_{d'},\alpha_{d}'',\alpha_{d}'''} |V_{\mu\cdot\mathbf{B}}|^2 \\
&\times \hat{b}_{p,\alpha_p}(i)\hat{b}_{d,\alpha_d}^\dagger(i)\hat{b}_{n,\alpha_n,\mathbf{k}}e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i}e^{i\hat{S}_D(i)} \\
&\times \left[\hat{b}_{p,\alpha_{p'}}^\dagger(i')\hat{b}_{d,\alpha_{d'}}(i')\hat{b}_{n,\alpha_n',\mathbf{k}'}e^{i\mathbf{k}'\cdot\hat{\mathbf{R}}_{i'}}e^{-i\hat{S}_D(i')} \right] \\
&\times [E - H_0]^{-1}(1 - |\Phi_0\rangle\langle\Phi_0|) \\
&\times \left[\hat{b}_{p,\alpha_{p''}}(i'')\hat{b}_{d,\alpha_{d''}}^\dagger(i'')\hat{b}_{n,\alpha_n'',\mathbf{k}''}e^{-i\mathbf{k}''\cdot\hat{\mathbf{R}}_{i''}}e^{i\hat{S}_D(i'')} \right] \\
&\times \hat{b}_{p,\alpha_{p'''}}^\dagger(i''')\hat{b}_{d,\alpha_{d'''}}(i''')\phi_n(\mathbf{k}''') \\
&\times \hat{b}_{n,\alpha_n''',\mathbf{k}'''}^\dagger e^{i\mathbf{k}'''\cdot\hat{\mathbf{R}}_{i'''}}e^{-i\hat{S}_D(i''')}|\Phi_0\rangle . \tag{6.15}
\end{aligned}$$

Multiply both sides of the above equation by $\langle\Phi_0|$ to obtain

$$\begin{aligned}
\langle\Phi_0|V_{\mu\cdot\mathbf{B}}|\Phi_0\rangle &= \langle\Phi_0|(\Delta E - H_n)|\Phi_0\rangle\phi_n(\mathbf{k}) \\
&- \langle\Phi_0| \sum_{i',i'',i'''} \sum_{\mathbf{k}',\mathbf{k}'',\mathbf{k}'''} \sum_{\alpha_n',\alpha_n'',\alpha_n'''} \sum_{\alpha_{p'},\alpha_{p}'',\alpha_{p}'''} \sum_{\alpha_{d'},\alpha_{d}'',\alpha_{d}'''} |V_{\mu\cdot\mathbf{B}}|^2 \\
&\times \hat{b}_{p,\alpha_p}(i)\hat{b}_{d,\alpha_d}^\dagger(i)\hat{b}_{n,\alpha_n,\mathbf{k}}e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i}e^{i\hat{S}_D(i)} \\
&\times \left[\hat{b}_{p,\alpha_{p'}}^\dagger(i')\hat{b}_{d,\alpha_{d'}}(i')\hat{b}_{n,\alpha_n',\mathbf{k}'}e^{i\mathbf{k}'\cdot\hat{\mathbf{R}}_{i'}}e^{-i\hat{S}_D(i')} \right] \\
&\times [E - H_0]^{-1}(1 - |\Phi_0\rangle\langle\Phi_0|) \\
&\times \left[\hat{b}_{p,\alpha_{p''}}(i'')\hat{b}_{d,\alpha_{d''}}^\dagger(i'')\hat{b}_{n,\alpha_n'',\mathbf{k}''}e^{-i\mathbf{k}''\cdot\hat{\mathbf{R}}_{i''}}e^{i\hat{S}_D(i'')} \right] \\
&\times \hat{b}_{p,\alpha_{p'''}}^\dagger(i''')\hat{b}_{d,\alpha_{d'''}}(i''')\phi_n(\mathbf{k}''') \\
&\times \hat{b}_{n,\alpha_n''',\mathbf{k}'''}^\dagger e^{i\mathbf{k}'''\cdot\hat{\mathbf{R}}_{i'''}}e^{-i\hat{S}_D(i''')}|\Phi_0\rangle . \tag{6.16}
\end{aligned}$$

Compare Eq. (6.16) above with Eq. (6.6). If we neglect the term on left hand side of Eq. (6.16), and remembering to sum over the i , α_p and α_d indices, the two equations become virtually identical. Consequently, we arrive an expression for the proper self-energy operator, $\Sigma^*(\mathbf{k}, \mathbf{k}''')$:

$$\begin{aligned}
\Sigma^*(\mathbf{k}''') &= \sum_{i,i',i'',i'''} \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''} \sum_{\alpha_n,\alpha_n'} \sum_{\alpha_p,\alpha_{p'},\alpha_{p}'',\alpha_{p}'''} \sum_{\alpha_d,\alpha_{d'},\alpha_{d}'',\alpha_{d}'''} \frac{1}{\hbar} |V_{\mu\cdot\mathbf{B}}|^2 \\
&\times \langle\Phi_0|\hat{b}_{p,\alpha_p}(i)\hat{b}_{d,\alpha_d}^\dagger(i)\hat{b}_{n,\alpha_n,\mathbf{k}}e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i}e^{i\hat{S}_D(i)}
\end{aligned}$$

$$\begin{aligned}
& \times \left[\hat{b}_{p,\alpha_p}^\dagger(i') \hat{b}_{d,\alpha_d}(i') \hat{b}_{n,\alpha_n,\mathbf{k}'}^\dagger e^{i\mathbf{k}' \cdot \hat{\mathbf{R}}_{i'}} e^{-i\hat{S}_D(i')} \right] \\
& \times [E - H_0]^{-1} (1 - |\Phi_0\rangle\langle\Phi_0|) \\
& \times \left[\hat{b}_{p,\alpha_p''}(i'') \hat{b}_{d,\alpha_d''}^\dagger(i'') \hat{b}_{n,\alpha_n,\mathbf{k}''} e^{-i\mathbf{k}'' \cdot \hat{\mathbf{R}}_{i''}} e^{i\hat{S}_D(i'')} \right] \\
& \times \hat{b}_{p,\alpha_p'''}^\dagger(i''') \hat{b}_{d,\alpha_d'''}(i''') \hat{b}_{n,\alpha_n,\mathbf{k}'''}^\dagger e^{i\mathbf{k}''' \cdot \hat{\mathbf{R}}_{i'''}} e^{-i\hat{S}_D(i''')} |\Phi_0\rangle \quad . \quad (6.17)
\end{aligned}$$

Consider the second and third lines of Eq. (6.17). A neutron of momentum \mathbf{k}' and spin $\alpha_{n'}$ is created out of the vacuum state $|\Phi_0\rangle$ in the third line, and another, of momentum \mathbf{k} and spin α_n annihilated in line two. This scenario may hold only if the two momenta and spins are equal, or, in other words, if the very same neutron which was created out of the vacuum is subsequently destroyed. The same argument applies to the neutron which is created and destroyed in the fifth and sixth lines of the equation. Consequently, Eq. (6.17) simplifies to

$$\begin{aligned}
\Sigma^*(\mathbf{k}, \mathbf{k}''') &= \sum_{i,i',i'',i'''} \sum_{\alpha_p,\alpha_{p'},\alpha_{p''},\alpha_{p'''} \alpha_d,\alpha_{d'},\alpha_{d''},\alpha_{d'''}} \sum_{\frac{1}{\hbar} |V_{\mu \cdot \mathbf{B}}|^2} \\
& \times \langle\Phi_0| \hat{b}_{p,\alpha_p}(i) \hat{b}_{d,\alpha_d}^\dagger(i) e^{-i\mathbf{k} \cdot \hat{\mathbf{R}}_i} e^{i\hat{S}_D(i)} \\
& \quad \times \left[\hat{b}_{p,\alpha_p'}^\dagger(i') \hat{b}_{d,\alpha_{d'}}(i') e^{i\mathbf{k} \cdot \hat{\mathbf{R}}_{i'}} e^{-i\hat{S}_D(i')} \right] \\
& \quad \times [E - H_0]^{-1} (1 - |\Phi_0\rangle\langle\Phi_0|) \\
& \quad \times \left[\hat{b}_{p,\alpha_{p''}}(i'') \hat{b}_{d,\alpha_{d''}}^\dagger(i'') e^{-i\mathbf{k}'' \cdot \hat{\mathbf{R}}_{i''}} e^{i\hat{S}_D(i'')} \right] \\
& \quad \times \hat{b}_{p,\alpha_{p'''}}^\dagger(i''') \hat{b}_{d,\alpha_{d'''}}(i''') e^{i\mathbf{k}''' \cdot \hat{\mathbf{R}}_{i'''}} e^{-i\hat{S}_D(i''')} |\Phi_0\rangle \quad . \quad (6.18)
\end{aligned}$$

We can expand the expression in Eq. (6.18) by splitting the \hat{Q} operator. Furthermore, for the sake of simplifying the notation I will use the symbol $\sum_{\{x\}}$ as a shorthand for $\sum_{x,x',x'',x'''}$. The final result is given by

$$\begin{aligned}
\Sigma^*(\mathbf{k}, \mathbf{k}''') &= \sum_{\{i\}} \sum_{\{\alpha_p\}} \sum_{\{\alpha_d\}} \frac{1}{\hbar} |V_{\mu \cdot \mathbf{B}}|^2 \\
& \times \langle\Phi_0| \left[\hat{b}_{p,\alpha_p}(i) \hat{b}_{d,\alpha_d}^\dagger(i) e^{-i\mathbf{k} \cdot \hat{\mathbf{R}}_i} e^{i\hat{S}_D(i)} \right] \\
& \quad \times \left[\hat{b}_{p,\alpha_{p'}}^\dagger(i') \hat{b}_{d,\alpha_{d'}}(i') e^{i\mathbf{k} \cdot \hat{\mathbf{R}}_{i'}} e^{-i\hat{S}_D(i')} \right] [E - H_0]^{-1} \\
& \quad \times \left[\hat{b}_{p,\alpha_{p''}}(i'') \hat{b}_{d,\alpha_{d''}}^\dagger(i'') e^{-i\mathbf{k}'' \cdot \hat{\mathbf{R}}_{i''}} e^{i\hat{S}_D(i'')} \right]
\end{aligned}$$

$$\begin{aligned}
& \times \left[\hat{b}_{p,\alpha_{p'''}}^\dagger(i''') \hat{b}_{d,\alpha_{d'''}}(i''') e^{i\mathbf{k}'''\cdot\hat{\mathbf{R}}_{i'''}} e^{-i\hat{S}_D(i''')} \right] |\Phi_0\rangle \\
- & \sum_{\{i\}} \sum_{\{\alpha_p\}} \sum_{\{\alpha_d\}} \frac{1}{\hbar} |V_{\mu\cdot\mathbf{B}}|^2 \\
& \times \langle \Phi_0 | \left[\hat{b}_{p,\alpha_p}(i) \hat{b}_{d,\alpha_d}^\dagger(i) e^{-i\mathbf{k}\cdot\hat{\mathbf{R}}_i} e^{i\hat{S}_D(i)} \right] \\
& \times \left[\hat{b}_{p,\alpha_{p'}}^\dagger(i') \hat{b}_{d,\alpha_{d'}}(i') e^{i\mathbf{k}\cdot\hat{\mathbf{R}}_{i'}} e^{-i\hat{S}_D(i')} \right] |\Phi_0\rangle \langle \Phi_0 | [E - H_0]^{-1} | \Phi_0\rangle \\
& \times \langle \Phi_0 | \left[\hat{b}_{p,\alpha_{p''}}(i'') \hat{b}_{d,\alpha_{d''}}^\dagger(i'') e^{-i\mathbf{k}''\cdot\hat{\mathbf{R}}_{i''}} e^{i\hat{S}_D(i'')} \right] \\
& \times \left[\hat{b}_{p,\alpha_{p'''}}^\dagger(i''') \hat{b}_{d,\alpha_{d'''}}(i''') e^{i\mathbf{k}'''\cdot\hat{\mathbf{R}}_{i'''}} e^{-i\hat{S}_D(i''')} \right] |\Phi_0\rangle \quad , \quad (6.19)
\end{aligned}$$

where we recall that $|V_{\mu\cdot\mathbf{B}}|^4$ is a shorthand for

$$|V_{\mu\cdot\mathbf{B}}|^2 = \langle \alpha_{n'} | \alpha_{p'} | - \mu \cdot \mathbf{B} | \alpha_{d'} \rangle \langle \alpha_{d''} | - \mu \cdot \mathbf{B} | \alpha_{n''}, \alpha_{p''} \rangle \quad . \quad (6.20)$$

Thus we have an explicit form for the proper self-energy for the neutron-lattice coupling. Note that the terms appearing in the expression for the proper self-energy in Eq. (6.19) are of the form $\langle \Phi_0 | \hat{\mathcal{O}}^2 | \Phi_0 \rangle - \langle \Phi_0 | \hat{\mathcal{O}} | \Phi_0 \rangle^2$.

Chapter 7

Phonon Averaged Green's Function Solution

So far we have put off the explicit evaluation of phonon averages. In this chapter we seek to understand the role which the phonons play in the theory; this will be done, primarily, by focusing on the techniques of phonon averaging. Our calculations will lead to expressions for the zero, one and two-phonon contributions to the the proper self-energy expression derived in Eq. (6.19). The results will show that the zero phonon piece vanishes while the single and higher order phonon averages do contribute to the proper self-energy of the system. The interpretation of these results fits well with the proposed neutron transfer theory.

Consider first the vanishing 0-phonon piece of the proper self-energy. The absence of phonon exchange means that there is no avenue for the virtual neutrons to scatter once they are created. This translates into a situation whereby the neutrons and the “holes” created in the lattice are always paired, since without phonon exchange, the neutron and “hole” will have matching momenta. This is equivalent to the free neutron being localized around the neutron “hole”. The presence of phonon exchange allows the neutrons to scatter off the lattice. Once phonon exchange occurs the momentum of the free neutrons acquires a component different than that of the holes and hence the pairing of free neutrons with the “holes” is broken. This, ultimately, is the basic mechanism proposed for delocalization of the virtual neutrons.

Another positive result which we obtained concerned the temperature dependence of the phonon averaged proper self-energy. We would expect the single and higher order phonon

piece of the self-energy to increase with temperature. An estimate for the temperature dependence of the 2-phonon contribution to the proper self-energy was found to be of the form

$$\Sigma_{(2)}^*(T) \sim \frac{e^{\hbar\omega_s(\mathbf{q})/k_B T}}{k_B T (e^{\hbar\omega_s(\mathbf{q})/k_B T} - 1)^2} ,$$

where $\omega_s(\mathbf{q})$ is the frequency of the normal mode of polarization s and wave-vector \mathbf{q} .

7.1 Review of Phonon Averaging Techniques

In this section we would like to review some of the standard results of phonon averaging theory¹. This material is intended to provide the reader with a brief review and will act as the background to the ensuing calculation of the zero and one phonon contributions to the proper self-energy.

Consider the problem of a neutron scattered by a crystal. We assume that the only degrees of freedom available to the crystal is motion of the ions about their equilibrium lattice positions. The composite neutron-ion system is described as follows:

$$\Psi_i = \psi_{\mathbf{p}}(\mathbf{r})\Phi_i = \frac{1}{\sqrt{V}} e^{i\frac{\mathbf{r}\cdot\mathbf{p}}{\hbar}} \Phi_i , \quad (7.1)$$

$$\Psi_f = \psi_{\mathbf{p}'}(\mathbf{r})\Phi_f = \frac{1}{\sqrt{V}} e^{i\frac{\mathbf{r}\cdot\mathbf{p}'}{\hbar}} \Phi_f , \quad (7.2)$$

$$\epsilon_i = E_i + \frac{p^2}{2M_n} , \quad (7.3)$$

$$\epsilon_f = E_f + \frac{(p')^2}{2M_n} , \quad (7.4)$$

where Ψ_i (Ψ_f) and ϵ_i (ϵ_f) are the initial (final) state and energy of the neutron-ion system, and \mathbf{p} and \mathbf{p}' are the incoming and outgoing momenta of the neutron.

The probability per unit time, P , for the neutron to scatter from \mathbf{p} to \mathbf{p}' is given by Fermi's Golden Rule which, to lowest order in perturbation expansion, leads to the

¹Neil W. Ashcroft and N. David Mermin, *Solid State Physics*, W.B. Saunders Co., 1976.

expression

$$P = \sum_f \frac{2\pi}{\hbar} \delta(\epsilon_f - \epsilon_i) |\langle \Psi_i | \mathcal{V} | \Psi_f \rangle|^2 . \quad (7.5)$$

\mathcal{V} is the neutron-ion interaction potential given by

$$\mathcal{V} = \sum_j v(\hat{\mathbf{R}}_j - \mathbf{R}_j^0) = \frac{1}{V} \sum_{\mathbf{k}, j} v_{\mathbf{k}} e^{i\mathbf{k} \cdot [\hat{\mathbf{R}}_j - \mathbf{R}_j^0]} . \quad (7.6)$$

$v_{\mathbf{k}}$ may be assumed constant (that is independent of \mathbf{k}) because of its limited range (typically nuclear dimensions), thus simplifying the expression for \mathcal{V} to

$$\mathcal{V} = \frac{2\pi \hbar^2 a}{M_n V} \sum_{\mathbf{k}, j} e^{i\mathbf{k} \cdot [\hat{\mathbf{R}}_j - \mathbf{R}_j^0]} . \quad (7.7)$$

Substituting this result into the equation for P gives

$$P_j = \frac{(2\pi \hbar)^3}{(M_n V)^2} \sum_f \delta(E_f - E_i + \hbar\omega) \left| \langle \Phi_i | e^{i\mathbf{k} \cdot \mathbf{R}_j^0} | \Phi_f \rangle \right|^2 , \quad (7.8)$$

where

$$\hbar\omega \equiv \frac{(p')^2}{2M_n} - \frac{p^2}{2M_n} \quad (7.9)$$

and

$$\hbar\mathbf{k} \equiv \mathbf{p}' - \mathbf{p} . \quad (7.10)$$

From the relationship between P and the scattering cross-section, $\frac{d\sigma}{d\Omega dE}$, we obtain the following relation for a given initial state i :

$$\frac{d\sigma}{d\Omega dE} = \frac{p'}{p} \frac{Na^2}{\hbar} S_i(\mathbf{k}, \omega) , \quad (7.11)$$

$S_i(\mathbf{q}, \omega)$ being the dynamical crystal structure which is given by²

$$S_i(\mathbf{k}, \omega) = \frac{1}{N} \sum_f \delta\left(\frac{E_f - E_i}{\hbar} + \omega\right) \left| \langle \Phi_i | e^{i\mathbf{k} \cdot \mathbf{R}_i^0} | \Phi_f \rangle \right|^2 . \quad (7.12)$$

At this point we assume the lattice to be in thermal equilibrium to begin with. We thus average the cross-section for a given state i over a Maxwell-Boltzmann distribution of

²Neil W. Ashcroft and N. David Mermin, *Solid State Physics*, W.B. Saunders Co., 1976.

equilibrium states. This means that $S_i(\mathbf{q}, \omega)$ will be replaced by its thermal average³

$$S(\mathbf{k}, \omega) = \frac{1}{N} \sum_{j,j'} e^{-i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_{j'})} \int \frac{dt}{2\pi} e^{i\omega t} \langle \langle e^{i\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_{j'})} e^{-i\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j)} \rangle \rangle, \quad (7.13)$$

where

$$\langle \langle \hat{O} \rangle \rangle = \frac{\sum e^{-\frac{B_i}{k_B T}} \langle \Phi_i | \hat{O} | \Phi_i \rangle}{\sum e^{-\frac{B_i}{k_B T}}}. \quad (7.14)$$

We now impose yet another condition that the crystal be *harmonic*, or in other words, that the position of any ion in the lattice at time t be a linear function of the positions and momenta of the other ions at time $t = 0$. This assumption allows us to use the identity

$$\langle \langle e^{\hat{A}} e^{\hat{B}} \rangle \rangle = e^{\frac{1}{2} \langle \langle \hat{A}^2 + \hat{B}^2 + 2\hat{A}\hat{B} \rangle \rangle} \quad (7.15)$$

for \hat{A} and \hat{B} linear in creation and annihilation operators. Applying this identity to the integrand in Eq. (7.13) yields the relation

$$\langle \langle e^{i\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_{j'})} e^{-i\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j)} \rangle \rangle = e^{\{-\frac{1}{2} \langle \langle [\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_{j'})]^2 \rangle \rangle - \frac{1}{2} \langle \langle [\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j)]^2 \rangle \rangle + \langle \langle [\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_{j'})][\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j)] \rangle \rangle\}}. \quad (7.16)$$

But with the harmonic condition we have

$$\langle \langle [\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_{j'})]^2 \rangle \rangle = \langle \langle [\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j)]^2 \rangle \rangle = \langle \langle [\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j^0)]^2 \rangle \rangle. \quad (7.17)$$

The quantity $\langle \langle [\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j^0)]^2 \rangle \rangle$ is defined to be the *Debye-Waller parameter*, W_D . Thus the expression for $S(\mathbf{k}, \omega)$ becomes⁴

$$S(\mathbf{k}, \omega) = e^{-W_D} \int \frac{dt}{2\pi} e^{i\omega t} \sum_j e^{-i\mathbf{k}\cdot\mathbf{R}_j^0} e^{\langle \langle [\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j^0)][\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j)] \rangle \rangle}, \quad (7.18)$$

where e^{-W_D} is known as the *Debye-Waller factor*. Expanding the exponential in the integrand of the above equation in a Taylor series we obtain

$$S_{(m)}(\mathbf{k}, \omega) = e^{-W_D} \int \frac{dt}{2\pi} e^{i\omega t} \sum_j e^{-i\mathbf{k}\cdot\mathbf{R}_j^0} \sum_{m=0}^{\infty} \frac{1}{m!} \left(\langle \langle [\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j^0)][\mathbf{k}\cdot\mathbf{u}(\mathbf{R}_j)] \rangle \rangle \right)^m. \quad (7.19)$$

³Neil W. Ashcroft and N. David Mermin, *Solid State Physics*, W.B. Saunders Co., 1976.

⁴Neil W. Ashcroft and N. David Mermin, *Solid State Physics*, W.B. Saunders Co., 1976.

The m 'th term in the above expansion corresponds to the contribution of the m -phonon process to the total cross-section.

7.2 Zero-Phonon Contribution to $\Sigma^*(\mathbf{k}, \mathbf{k}')$

We now examine the 0-phonon piece of the self-energy. In Eq. (6.19), we found an approximation to the proper self-energy, $\Sigma^*(\mathbf{k}, \mathbf{k}')$, for the neutron/lattice system. For the purposes of the present discussion the quantity $E - H_0$ may be replaced by δE , a small parameter representing the energy difference between the unperturbed and full Hamiltonian. This assumption, of course, is only valid for 0-phonon exchange. Moreover, we would like to make use of the expansion

$$e^{i\mathbf{k}\cdot\hat{\mathbf{R}}} = e^{i\mathbf{k}\cdot\mathbf{R}_i^0} e^{i\mathbf{k}\cdot(\hat{\mathbf{R}}_i^0 - \mathbf{R}_i^0)} \quad , \quad (7.20)$$

where I have defined \mathbf{R}_i^0 to be the equilibrium position of the ion at site i .

In order to calculate $\Sigma_{(0)}^*(\mathbf{k}, \mathbf{k}''')$ we must first determine the 0-phonon contribution to $S(\mathbf{k}, \omega)$. This is achieved by setting $m = 0$ in Eq. (7.19) and evaluating the integral. The result is

$$\begin{aligned} S_{(0)}(\mathbf{k}, \omega) &= e^{-W_D} \delta(\omega) N \sum_{\mathbf{K}} \delta_{\mathbf{k}, \mathbf{K}} \\ \Rightarrow \frac{d\sigma}{d\Omega} &= \int dE \frac{d\sigma}{d\Omega dE} = e^{-W_D} (Na)^2 \sum_{\mathbf{K}} \delta_{\mathbf{k}, \mathbf{K}} \quad , \end{aligned} \quad (7.21)$$

where \mathbf{K} is the reciprocal lattice vector. Knowing this, we may now evaluate $\Sigma_{(0)}^*(\mathbf{k}, \mathbf{k}''')$ which is given by

$$\begin{aligned} \Sigma_{(0)}^*(\mathbf{k}, \mathbf{k}''') &= \sum_{\{i\}} \sum_{\{\alpha_p\}} \sum_{\{\alpha_d\}} \frac{1}{\hbar \delta E} |V_{\mu\cdot\mathbf{B}}|^2 \\ &\times \langle \Phi_0 | \left[\hat{b}_{p, \alpha_p}(i) \hat{b}_{d, \alpha_d}^\dagger(i) e^{-i\mathbf{k}\cdot\mathbf{R}_i^0} e^{-W_D(\mathbf{k})} \right] \\ &\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i') \hat{b}_{d, \alpha_d}(i') e^{i\mathbf{k}\cdot\mathbf{R}_{i'}^0} e^{W_D(\mathbf{k})} \right] \\ &\quad \times \left[\hat{b}_{p, \alpha_p}(i'') \hat{b}_{d, \alpha_d}^\dagger(i'') e^{-i\mathbf{k}''\cdot\mathbf{R}_{i''}^0} e^{-W_D(\mathbf{k}'')} \right] \\ &\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i''') \hat{b}_{d, \alpha_d}(i''') e^{-i\mathbf{k}'''\cdot\mathbf{R}_{i'''}^0} e^{-W_D(\mathbf{k}''')} \right] | \Phi_0 \rangle \\ &- \sum_{\{i\}} \sum_{\{\alpha_p\}} \sum_{\{\alpha_d\}} \frac{1}{\hbar \delta E} |V_{\mu\cdot\mathbf{B}}|^2 \end{aligned}$$

$$\begin{aligned}
& \times \langle \Phi_0 | \left[\hat{b}_{p,\alpha_p}(i) \hat{b}_{d,\alpha_d}^\dagger(i) e^{-i\mathbf{k}\cdot\mathbf{R}_i^0} e^{-W_D(\mathbf{k})} \right] \\
& \quad \times \left[\hat{b}_{p,\alpha_p}^\dagger(i') \hat{b}_{d,\alpha_d}(i') e^{i\mathbf{k}\cdot\mathbf{R}_{i'}^0} e^{W_D(\mathbf{k})} \right] | \Phi_0 \rangle \\
& \times \langle \Phi_0 | \left[\hat{b}_{p,\alpha_p}(i'') \hat{b}_{d,\alpha_d}^\dagger(i'') e^{-i\mathbf{k}'''\cdot\mathbf{R}_{i''}^0} e^{-W_D(\mathbf{k}''')} \right] \\
& \quad \times \left[\hat{b}_{p,\alpha_p}^\dagger(i''') \hat{b}_{d,\alpha_d}(i''') e^{i\mathbf{k}'''\cdot\mathbf{R}_{i'''}^0} e^{W_D(\mathbf{k}''')} \right] | \Phi_0 \rangle , \quad (7.22)
\end{aligned}$$

where we defined $\delta E = E - H_0$ above.

Consider the first term on the right hand side of Eq. (7.22). Define the fermionic “hole” operator $\hat{c}_{\mathbf{k}}$ as

$$\hat{c}_{\mathbf{k}}^\dagger = \sum_i \hat{b}_{p,\alpha_p}^\dagger(i) \hat{b}_{d,\alpha_d}(i) e^{i\mathbf{k}\cdot\mathbf{R}_i^0} e^{W_D(\mathbf{k})} , \quad (7.23)$$

where, for the sake of simplicity, I have suppressed the α_p and α_d indices in $\hat{c}_{\mathbf{k}}$. Eq. (7.22) may now be expressed in the following simplified form:

$$\begin{aligned}
\Sigma_{(0)}^*(\mathbf{k}, \mathbf{k}''') &= \frac{1}{\hbar\delta E} \sum_{\{\alpha_p\}} \sum_{\{\alpha_d\}} |V_{\mu\cdot\mathbf{B}}|^2 \\
&\times \left[\langle \Phi_0 | \hat{c}_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}'''} \hat{c}_{\mathbf{k}'''}^\dagger | \Phi_0 \rangle - \langle \Phi_0 | \hat{c}_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger | \Phi_0 \rangle \langle \Phi_0 | \hat{c}_{\mathbf{k}'''} \hat{c}_{\mathbf{k}'''}^\dagger | \Phi_0 \rangle \right] , \quad (7.24)
\end{aligned}$$

But for fermionic hole operators

$$\langle \Phi_0 | \hat{c}_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}'''} \hat{c}_{\mathbf{k}'''}^\dagger | \Phi_0 \rangle \approx \langle \Phi_0 | \hat{c}_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger | \Phi_0 \rangle \langle \Phi_0 | \hat{c}_{\mathbf{k}'''} \hat{c}_{\mathbf{k}'''}^\dagger | \Phi_0 \rangle .$$

This corresponds to the physical statement that the neutron “hole” of momentum \mathbf{k} , which is created and destroyed by the $\hat{c}_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger$ pair of operators, is independent of the neutron “hole” of momentum \mathbf{k}''' . In this approximation the two terms on the right hand side of the Eq. (7.24) are approximately equal, which means that $\Sigma_{(0)}^*(\mathbf{k}, \mathbf{k}''') \approx 0$. We have thus argued that the 0-phonon contribution to the proper self-energy is projected out due to the presence of the \hat{Q} factor in the theory of Brillouin-Wigner. This result agrees with our expectations, since where no phonons are exchanged neutrons do not scatter and hence are completely localized about the lattice sites where they were created. In order to find the non-local part of the picture we must seek higher-order phonon contributions to the proper self-energy.

7.3 Review of One-Phonon Exchange

Before computing $\Sigma_{(1)}^*(\mathbf{k}, \mathbf{k}')$ we choose to review some standard results on one-phonon averaging techniques⁵. The 1-phonon contribution to the dynamical crystal structure, $S(\mathbf{k}, \omega)$, is given by the following expression:

$$S_{(1)}(\mathbf{k}, \omega) = e^{-W_D} \int \frac{dt}{2\pi} e^{i\omega t} \sum_j e^{-i\mathbf{k} \cdot \mathbf{R}_j^0} \langle \langle [\mathbf{k} \cdot \mathbf{u}(\mathbf{R}_j^0)] [\mathbf{k} \cdot \mathbf{u}(\mathbf{R}_j)] \rangle \rangle . \quad (7.25)$$

We need to evaluate the quantity $\langle \langle [\mathbf{k} \cdot \mathbf{u}(\mathbf{R}_j^0)] [\mathbf{k} \cdot \mathbf{u}(\mathbf{R}_j)] \rangle \rangle$. To do that we must refer to the quantum theory of harmonic crystals. The Hamiltonian for harmonic crystals is given by

$$H_{Harm} = \sum_j \frac{1}{2M} P^2(\mathbf{R}_j) + \frac{1}{2} \sum_{jj'} u_\mu(\mathbf{R}_j) V_{\mu\nu}(\mathbf{R}_j - \mathbf{R}_{j'}) u_\nu(\mathbf{R}_{j'}) . \quad (7.26)$$

Recall that in the case of a single or one-dimensional harmonic oscillator, the Hamiltonian, H , is given by

$$H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2 , \quad (7.27)$$

which is often redefined in terms of raising and lowering operators, \hat{a}^\dagger and \hat{a} , as such:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \hat{q} + i \sqrt{\frac{1}{2m\hbar\omega}} \hat{p} , \quad (7.28)$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \hat{q} - i \sqrt{\frac{1}{2m\hbar\omega}} \hat{p} , \quad (7.29)$$

$$\Rightarrow H = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) = \hbar\omega \left(\hat{n} + \frac{1}{2} \right) . \quad (7.30)$$

The procedure for harmonic crystals is very similar. Let $\omega_s(\mathbf{q})$ and $\epsilon_s(\mathbf{q})$ be the frequency and polarization vector respectively for the normal modes of polarization s and wave-vector \mathbf{q} . In analogy to the one-dimensional oscillator, we define

$$\hat{a}_{\mathbf{q},s} = \frac{1}{\sqrt{N}} \sum_j e^{-i\mathbf{q} \cdot \hat{\mathbf{R}}_j} \epsilon_s(\mathbf{q}) \left[\sqrt{\frac{M\omega_s(\mathbf{q})}{2\hbar}} \mathbf{u}(\hat{\mathbf{R}}_j) + i \sqrt{\frac{1}{2\hbar M\omega_s(\mathbf{q})}} \mathbf{P}(\hat{\mathbf{R}}_j) \right] , \quad (7.31)$$

⁵Neil W. Ashcroft and N. David Mermin, *Solid State Physics*, W.B. Saunders Co., 1976.

which is the phonon annihilation operator, and

$$\hat{a}_{\mathbf{q},s}^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{i\mathbf{q}\cdot\hat{\mathbf{R}}_j} \epsilon_s(\mathbf{q}) \left[\sqrt{\frac{M\omega_s(\mathbf{q})}{2\hbar}} \mathbf{u}(\hat{\mathbf{R}}_j) - i\sqrt{\frac{1}{2\hbar M\omega_s(\mathbf{q})}} \mathbf{P}(\hat{\mathbf{R}}_j) \right] , \quad (7.32)$$

which is the phonon creation operator. $\hat{a}_{\mathbf{q},s}$ and $\hat{a}_{\mathbf{q},s}^\dagger$ satisfy the commutation relations

$$[\hat{a}_{\mathbf{q},s}, \hat{a}_{\mathbf{q}',s'}^\dagger] = \delta_{\mathbf{q},\mathbf{q}'} \delta_{ss'} , \quad (7.33)$$

$$[\hat{a}_{\mathbf{q},s}, \hat{a}_{\mathbf{q}',s'}] = [\hat{a}_{\mathbf{q},s}^\dagger, \hat{a}_{\mathbf{q}',s'}^\dagger] = 0 . \quad (7.34)$$

Provided that the assumption of a lattice of “infinite” extent is valid, eqs. (7.31) and (7.32) may be inverted to yield

$$\mathbf{u}(\hat{\mathbf{R}}_j) = \frac{1}{\sqrt{N}} \sum_{\mathbf{q},s} \sqrt{\frac{\hbar}{2M\omega_s(\mathbf{q})}} (\hat{a}_{\mathbf{q}',s'} + \hat{a}_{-\mathbf{q},s}^\dagger) \epsilon_s(\mathbf{q}) e^{i\mathbf{q}\cdot\hat{\mathbf{R}}_j} , \quad (7.35)$$

$$\mathbf{P}(\hat{\mathbf{R}}_j) = -\frac{1}{\sqrt{N}} \sum_{\mathbf{q},s} \sqrt{\frac{\hbar M\omega_s(\mathbf{q})}{2}} (\hat{a}_{\mathbf{q}',s'} - \hat{a}_{-\mathbf{q},s}^\dagger) \epsilon_s(\mathbf{q}) e^{i\mathbf{q}\cdot\hat{\mathbf{R}}_j} . \quad (7.36)$$

H_{Harm} may now be expressed in terms of $\hat{a}_{\mathbf{q},s}$ and $\hat{a}_{\mathbf{q},s}^\dagger$ simply as

$$H_{Harm} = \sum_{\mathbf{q},s} \hbar\omega_s(\mathbf{q}) \left(\hat{a}_{\mathbf{q},s}^\dagger \hat{a}_{\mathbf{q},s} + \frac{1}{2} \right) = \sum_{\mathbf{q},s} \hbar\omega_s(\mathbf{q}) \left(\hat{n}_s(\mathbf{q}) + \frac{1}{2} \right) . \quad (7.37)$$

Using Eqs. (7.34) and (7.35) above and the identities,

$$\begin{aligned} \hat{a}_{\mathbf{q},s}(t) &= e^{-i\omega_s(\mathbf{q})t} \hat{a}_{\mathbf{q},s} , \\ \hat{a}_{\mathbf{q},s}^\dagger(t) &= e^{i\omega_s(\mathbf{q})t} \hat{a}_{\mathbf{q},s}^\dagger , \\ \langle\langle \hat{a}_{\mathbf{q}',s'}^\dagger \hat{a}_{\mathbf{q},s} \rangle\rangle &= n_s(\mathbf{q}) \delta_{\mathbf{q}\mathbf{q}'} \delta_{ss'} , \\ \langle\langle \hat{a}_{\mathbf{q},s} \hat{a}_{\mathbf{q}',s'}^\dagger \rangle\rangle &= [1 + n_s(\mathbf{q})] \delta_{\mathbf{q}\mathbf{q}'} \delta_{ss'} , \\ \langle\langle \hat{a}_{\mathbf{q},s}^\dagger \hat{a}_{\mathbf{q}',s'}^\dagger \rangle\rangle &= \langle\langle \hat{a}_{\mathbf{q},s} \hat{a}_{\mathbf{q}',s'} \rangle\rangle = 0 , \end{aligned}$$

we thus find that

$$S_{(1)}(\mathbf{k}, \omega) = e^{-W_D} \sum_s \frac{\hbar}{2M\omega_s(\mathbf{q})} [\mathbf{k} \cdot \epsilon_s(\mathbf{q})]^2 \{ [1 + n_s(\mathbf{q})] \delta(\omega + \omega_s(\mathbf{q})) + n_s(\mathbf{q}) \delta(\omega - \omega_s(\mathbf{q})) \} . \quad (7.38)$$

As a result the 1-phonon contribution to the cross-section is given by⁶:

$$\frac{d\sigma}{d\Omega dE} = N e^{-W_D} \frac{p}{p'} a^2 \sum_s \frac{1}{2M\omega_s(\mathbf{q})} [\mathbf{k} \cdot \boldsymbol{\epsilon}_s(\mathbf{q})]^2 \{ [1 + n_s(\mathbf{q})] \delta(\omega + \omega_s(\mathbf{q})) + n_s(\mathbf{q}) \delta(\omega - \omega_s(\mathbf{q})) \} , \quad (7.39)$$

which is a series of sharp delta-functions at the allowed final neutron energies, modulated by the Debye-Waller factor and scaled by the quantity $[\mathbf{k} \cdot \boldsymbol{\epsilon}_s(\mathbf{q})]^2$. This quantity contains information on the polarization vectors of the phonons involved in the reactions.

7.4 One-Phonon Contribution to $\Sigma^*(\mathbf{k}, \mathbf{k}')$

We now examine the 1-phonon piece of the proper self-energy, which is made up of four terms representing the four combinations in which a single phonon may be created and subsequently destroyed. $\Sigma_{(1)}^*(\mathbf{k}, \mathbf{k}''')$, in the case of a perfect crystal, is given by

$$\begin{aligned} \Sigma_{(1)}^*(\mathbf{k}, \mathbf{k}''') &= \sum_{\{i\}} \sum_{\{\alpha_p\}} \sum_{\{\alpha_d\}} \sum_{\mathbf{q}, s} \frac{|V_{\mu \cdot \mathbf{B}}|^2}{\hbar N} \\ &\times \langle \Phi_0 | \left[\hat{b}_{p, \alpha_p}(i) \hat{b}_{d, \alpha_d}^\dagger(i) e^{-i\mathbf{k} \cdot \mathbf{R}_i^0} e^{-W_D(\mathbf{k})} \right] \\ &\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i') \hat{b}_{d, \alpha_d}(i') e^{i\mathbf{k} \cdot \mathbf{R}_{i'}^0} e^{W_D(\mathbf{k})} \right] \\ &\quad \times \left(\frac{\hbar [\mathbf{k} \cdot \boldsymbol{\epsilon}_s(\mathbf{q})]^2}{2M\omega_s(\mathbf{q})} \right) \left(\frac{n_s(\mathbf{q})}{\hbar\omega_s(\mathbf{q})} \right) \\ &\quad \times \left[e^{i\mathbf{q} \cdot (\mathbf{R}_{i'''}^0 - \mathbf{R}_i^0)} + e^{i\mathbf{q} \cdot (\mathbf{R}_{i'''}^0 + \mathbf{R}_{i'}^0)} + e^{-i\mathbf{q} \cdot (\mathbf{R}_{i''}^0 + \mathbf{R}_i^0)} + e^{-i\mathbf{q} \cdot (\mathbf{R}_{i''}^0 - \mathbf{R}_{i'}^0)} \right] \\ &\quad \times \left[\hat{b}_{p, \alpha_p}(i'') \hat{b}_{d, \alpha_d}^\dagger(i'') e^{-i\mathbf{k}'' \cdot \mathbf{R}_{i''}^0} e^{-W_D(\mathbf{k}'')} \right] \\ &\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i''') \hat{b}_{d, \alpha_d}(i''') e^{i\mathbf{k}''' \cdot \mathbf{R}_{i'''}^0} e^{-W_D(\mathbf{k}''')} \right] | \Phi_0 \rangle , \quad (7.40) \end{aligned}$$

where $n_s(\mathbf{q})$ is the phonon expectation of operator $\hat{n}_s(\mathbf{q})$. Note that the \hat{Q} factor vanishes from the formula. The reason for this is that the creation of phonons alters the vacuum state $|\Phi_0\rangle$. Note that the phonon momentum shows up explicitly in the above equation, in conjunction with the free neutron momentum.

We can deduce a rough estimate for the temperature dependence of $\Sigma_{(1)}^*(\mathbf{k}, \mathbf{k}''')$ in the

⁶Neil W. Ashcroft and N. David Mermin, *Solid State Physics*, W.B. Saunders Co., 1976.

case of a thermal lattice by using

$$n_s(\mathbf{q}) = \frac{1}{e^{\hbar\omega_s(\mathbf{q})/k_B T} - 1} \quad , \quad (7.41)$$

where I have assumed a Bose-Einstein distribution. Substituting the above approximation into Eq. (7.40) yields

$$\begin{aligned} \Sigma_{(1)}^*(\mathbf{k}, \mathbf{k}''') &= \sum_{\{i\}} \sum_{\{\alpha_p\}} \sum_{\{\alpha_d\}} \sum_{\mathbf{q}, s} \frac{|V_{\mu \cdot \mathbf{B}}|^2}{\hbar N} \\ &\times \langle \Phi_0 | \left[\hat{b}_{p, \alpha_p}(i) \hat{b}_{d, \alpha_d}^\dagger(i) e^{-i\mathbf{k} \cdot \mathbf{R}_i^0} e^{-W_D(\mathbf{k})} \right] \\ &\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i') \hat{b}_{d, \alpha_d}(i') e^{i\mathbf{k} \cdot \mathbf{R}_{i'}^0} e^{W_D(\mathbf{k})} \right] \\ &\quad \times \left(\frac{\hbar[\mathbf{k} \cdot \boldsymbol{\epsilon}_s(\mathbf{q})]^2}{2M\omega_s(\mathbf{q})} \right) \left[\frac{1}{e^{\hbar\omega_s(\mathbf{q})/k_B T} - 1} \right] \\ &\quad \times \left[e^{i\mathbf{q} \cdot (\mathbf{R}_{i'''}^0 - \mathbf{R}_i^0)} + e^{i\mathbf{q} \cdot (\mathbf{R}_{i'''}^0 + \mathbf{R}_{i'}^0)} + e^{-i\mathbf{q} \cdot (\mathbf{R}_{i''}^0 + \mathbf{R}_i^0)} + e^{-i\mathbf{q} \cdot (\mathbf{R}_{i''}^0 - \mathbf{R}_{i'}^0)} \right] \\ &\quad \times \left[\hat{b}_{p, \alpha_p}(i'') \hat{b}_{d, \alpha_d}^\dagger(i'') e^{-i\mathbf{k}'' \cdot \mathbf{R}_{i''}^0} e^{-W_D(\mathbf{k}'')} \right] \\ &\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i''') \hat{b}_{d, \alpha_d}(i''') e^{i\mathbf{k}'' \cdot \mathbf{R}_{i'''}^0} e^{W_D(\mathbf{k}'')} \right] | \Phi_0 \rangle \quad . \quad (7.42) \end{aligned}$$

We may obtain an estimate on the magnitude of $\Sigma_{(1)}^*(\mathbf{k}, \mathbf{k}''')$ by substituting in typical values for the quantities appearing in the above formula. The result is

$$\begin{aligned} |\Sigma_{(1)}^*(\mathbf{k}, \mathbf{k}''')| &\approx \left| \frac{V_{\mu \cdot \mathbf{B}}}{\Delta E} \right|^2 \left(\frac{1}{k_B T} \right) \left(\frac{\bar{V}_n}{V_A} \right)^2 N_D N_{D'} \\ &\approx \left[\frac{10^{-6}}{10^6} \right]^2 (40) (10^{-9})^2 10^{15} 10^{21} = 4 \times 10^{-5} eV \quad . \end{aligned}$$

7.5 Two-Phonon Contribution to $\Sigma^*(\mathbf{k}, \mathbf{k}')$

As the name suggests, 2-phonon exchange involves the creation and subsequent annihilation of two phonons. There are two possible ways this could happen: the two phonons could both be produced at a single site and subsequently absorbed at another; or the two phonons may be born at different sites and then absorbed elsewhere. In all, there should be twelve terms in the expansion for 2-phonon piece of the proper self-energy. For the purpose of the present calculation, we choose to consider the one term where phonon \mathbf{q}' is produced at site i''' and subsequently absorbed at site i , while phonon \mathbf{q} is created at site i'' , later to

be absorbed at site i' . $\Sigma_{(2)}^*(\mathbf{k}, \mathbf{k}''')$ for that term is given by

$$\begin{aligned}
\Sigma_{(2)}^*(\mathbf{k}, \mathbf{k}''') &= \left(\frac{\hbar}{2M}\right)^2 \sum_{\{i\}} \sum_{\{\alpha_p\}} \sum_{\{\alpha_d\}} \sum_{\mathbf{q}, \mathbf{q}', s, s'} \frac{|V_{\mu \cdot \mathbf{B}}|^2}{\hbar N} \\
&\times \langle \Phi_0 | \left[\hat{b}_{p, \alpha_p}(i) \hat{b}_{d, \alpha_d}^\dagger(i) e^{-i\mathbf{k} \cdot \mathbf{R}_i^0} e^{-W_D(\mathbf{k})} \right] \\
&\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i') \hat{b}_{d, \alpha_d}(i') e^{i\mathbf{k} \cdot \mathbf{R}_{i'}^0} e^{W_D(\mathbf{k})} \right] \\
&\quad \times \left(\frac{[(\mathbf{k} + \mathbf{k}''') \cdot \boldsymbol{\epsilon}_s(\mathbf{q})][(\mathbf{k} + \mathbf{k}''') \cdot \boldsymbol{\epsilon}_{s'}(\mathbf{q}')] }{\omega_s(\mathbf{q})\omega_{s'}(\mathbf{q}')} \right) \left(\frac{n_{s'}(\mathbf{q}') - n_s(\mathbf{q})}{\hbar[\omega_{s'}(\mathbf{q}') - \omega_s(\mathbf{q})]} \right) \\
&\quad \times \left[e^{i\mathbf{q}' \cdot (\mathbf{R}_{i'''}^0 - \mathbf{R}_i^0)} e^{-i\mathbf{q} \cdot (\mathbf{R}_{i''}^0 - \mathbf{R}_{i'}^0)} \right] \\
&\quad \times \left[\hat{b}_{p, \alpha_p}(i'') \hat{b}_{d, \alpha_d}^\dagger(i'') e^{-i\mathbf{k}'' \cdot \mathbf{R}_{i''}^0} e^{-W_D(\mathbf{k}'')} \right] \\
&\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i''') \hat{b}_{d, \alpha_d}(i''') e^{i\mathbf{k}'' \cdot \mathbf{R}_{i'''}^0} e^{-W_D(\mathbf{k}''')} \right] | \Phi_0 \rangle . \quad (7.43)
\end{aligned}$$

For a thermal lattice, the quantity $\frac{n_{s'}(\mathbf{q}') - n_s(\mathbf{q})}{\hbar[\omega_{s'}(\mathbf{q}') - \omega_s(\mathbf{q})]}$ may be approximated as follows:

$$\frac{n_{s'}(\mathbf{q}') - n_s(\mathbf{q})}{\hbar[\omega_{s'}(\mathbf{q}') - \omega_s(\mathbf{q})]} \approx \frac{\partial n}{\partial E} = \frac{e^{\hbar\omega_s(\mathbf{q})/k_B T}}{k_B T (e^{\hbar\omega_s(\mathbf{q})/k_B T} - 1)^2} , \quad (7.44)$$

where, once again, I have assumed a Bose-Einstein distribution. Substituting the above approximation into Eq. (7.43) yields

$$\begin{aligned}
\Sigma_{(2)}^*(\mathbf{k}, \mathbf{k}''') &= \left(\frac{\hbar}{2M}\right)^2 \sum_{\{i\}} \sum_{\{\alpha_p\}} \sum_{\{\alpha_d\}} \sum_{\mathbf{q}, \mathbf{q}', s, s'} \frac{|V_{\mu \cdot \mathbf{B}}|^2}{\hbar N} \\
&\times \langle \Phi_0 | \left[\hat{b}_{p, \alpha_p}(i) \hat{b}_{d, \alpha_d}^\dagger(i) e^{-i\mathbf{k} \cdot \mathbf{R}_i^0} e^{-W_D(\mathbf{k})} \right] \\
&\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i') \hat{b}_{d, \alpha_d}(i') e^{i\mathbf{k} \cdot \mathbf{R}_{i'}^0} e^{W_D(\mathbf{k})} \right] \\
&\quad \times \left(\frac{[\mathbf{k} \cdot \boldsymbol{\epsilon}_s(\mathbf{q})]^2 [\mathbf{k}'' \cdot \boldsymbol{\epsilon}_{s'}(\mathbf{q}')]^2}{\omega_s(\mathbf{q})\omega_{s'}(\mathbf{q}')} \right) \left(\frac{e^{\hbar\omega_s(\mathbf{q})/k_B T}}{k_B T (e^{\hbar\omega_s(\mathbf{q})/k_B T} - 1)^2} \right) \\
&\quad \times \left[e^{i\mathbf{q}' \cdot (\mathbf{R}_{i'''}^0 - \mathbf{R}_i^0)} + e^{-i\mathbf{q} \cdot (\mathbf{R}_{i''}^0 - \mathbf{R}_{i'}^0)} \right] \\
&\quad \times \left[\hat{b}_{p, \alpha_p}(i'') \hat{b}_{d, \alpha_d}^\dagger(i'') e^{-i\mathbf{k}'' \cdot \mathbf{R}_{i''}^0} e^{-W_D(\mathbf{k}'')} \right] \\
&\quad \times \left[\hat{b}_{p, \alpha_p}^\dagger(i''') \hat{b}_{d, \alpha_d}(i''') e^{i\mathbf{k}'' \cdot \mathbf{R}_{i'''}^0} e^{-W_D(\mathbf{k}''')} \right] | \Phi_0 \rangle . \quad (7.45)
\end{aligned}$$

Of course, even though the above expression was derived and is expressed in terms of proton and deuteron creation and annihilation operators, it applies to any donor-acceptor

pair. $\Sigma_{(2)}^*(\mathbf{k}, \mathbf{k}''')$ in its more general form is thus given by

$$\begin{aligned}
\Sigma_{(2)}^*(\mathbf{k}, \mathbf{k}''') &= \left(\frac{\hbar}{2M}\right)^2 \sum_{\{i\}} \sum_{\{\alpha_A\}} \sum_{\{\alpha_D\}} \sum_{\mathbf{q}, \mathbf{q}', \mathbf{s}, \mathbf{s}'} \frac{|V_{\mu \cdot \mathbf{B}}|^2}{\hbar N} \\
&\times \langle \Phi_0 | \left[\hat{b}_{A, \alpha_A}(i) \hat{b}_{D, \alpha_D}^\dagger(i) e^{-i\mathbf{k} \cdot \mathbf{R}_i^0} e^{-W_D(\mathbf{k})} \right] \\
&\times \left[\hat{b}_{A, \alpha_{A'}}^\dagger(i') \hat{b}_{D, \alpha_{D'}}(i') e^{i\mathbf{k} \cdot \mathbf{R}_{i'}^0} e^{W_D(\mathbf{k})} \right] \\
&\times \left(\frac{[\mathbf{k} \cdot \boldsymbol{\epsilon}_s(\mathbf{q})]^2 [\mathbf{k}''' \cdot \boldsymbol{\epsilon}_{s'}(\mathbf{q}')]^2}{\omega_s(\mathbf{q}) \omega_{s'}(\mathbf{q}')} \right) \left(\frac{e^{\hbar\omega_s(\mathbf{q})/k_B T}}{k_B T (e^{\hbar\omega_s(\mathbf{q})/k_B T} - 1)^2} \right) \\
&\times \left[e^{i\mathbf{q}' \cdot (\mathbf{R}_{i'''}^0 - \mathbf{R}_i^0)} + e^{-i\mathbf{q} \cdot (\mathbf{R}_{i''}^0 - \mathbf{R}_{i'}^0)} \right] \\
&\times \left[\hat{b}_{A, \alpha_{A''}}(i'') \hat{b}_{D, \alpha_{D''}}^\dagger(i'') e^{-i\mathbf{k}''' \cdot \mathbf{R}_{i''}^0} e^{-W_D(\mathbf{k}''')} \right] \\
&\times \left[\hat{b}_{A, \alpha_{A'''}}^\dagger(i''') \hat{b}_{D, \alpha_{D'''}}(i''') e^{i\mathbf{k}''' \cdot \mathbf{R}_{i'''}^0} e^{-W_D(\mathbf{k}''')} \right] | \Phi_0 \rangle . \quad (7.46)
\end{aligned}$$

A similar order of magnitude argument to the one presented at the end of the last section may be used to obtain a rough estimate of the size of the 2-phonon piece. The result is

$$\begin{aligned}
|\Sigma_{(2)}^*(\mathbf{k}, \mathbf{k}''')| &\approx \left| \frac{V_{\mu \cdot \mathbf{B}}}{\Delta E} \right|^2 \left(\frac{1}{(k_B T)^2} \right) \left(\frac{V_n}{V_A} \right)^2 N_D N_{D'} \\
&\approx \left[\frac{10^{-6}}{10^6} \right]^2 (40)^2 (10^{-9})^2 10^{15} 10^{21} = 1.6 \times 10^{-3} eV .
\end{aligned}$$

7.6 The Green's Function Solution

The fact that we were able to reach an estimate for the proper self-energy for 0, 1 and 2-phonon exchange without having to undertake lengthy calculations is due largely to the universality of the method we have adopted for phonon averaging. Deriving an expression for the Green's function is now reduced to a simple substitution into Dyson's equation;

$$G(\mathbf{k}, \mathbf{k}''') = \frac{1}{[G^0(\mathbf{k}, \mathbf{k}''')]^{-1} - \Sigma^*(\mathbf{k}, \mathbf{k}''')} . \quad (7.47)$$

Thus we have accomplished what we had set out to do originally, namely to derive an expression for the Green's function which approximates the virtual neutron's interaction with the lattice. Notice the inherent splitting in the above equation of the *local* part of G , represented in the unperturbed Green's function G^0 , from the *nonlocal* part, generated by the exchange scattering term represented by the proper self-energy Σ^* . This splitting of

local and nonlocal part in the Green's function would naturally appear in the solution to the free neutron wavefunction.

7.7 Reaction Rates

In this we shall briefly examine the reaction rate for the neutron transfers which the 2-phonon self-energy average generates. The result will show that, in the case where the interaction between the neutron and the nucleus occupying the lattice site is predominantly due to the *strong* force, the reaction rate is enormous. This means that the proposed neutron transfer does not inhibit or slow down the processes within the Pons-Fleischmann cells in any way. As it turns out, it is the limitation on the number of phonons occupying a given mode and mediating the reaction which acts as the principle bottle-neck to the process.

We may obtain an estimate for the neutron transfer reaction rate simply by applying Fermi's Golden Rule just as we did on previous occasions in chapters 3 and 4 (see Eqs. (3.40) and (4.16)). The only difference now is that Σ^* , which represents the near-resonance exchange scattering in the problem, replaces the Bragg scattering term, $V_{\mathbf{K}}$ and the exchange term, $W_{\mathbf{k}-\mathbf{K},\mathbf{k}}$, in the formulas for Γ_{tot} in Eqs. (3.40) and (4.16) respectively.

We shall be examining the reaction rates generated by the 2-phonon averaged proper self-energy, since 2-phonon exchange interests us most in the theory. Using the expression for $\Sigma_{(2)}^*(\mathbf{k}, \mathbf{k}''')$ in Eq. (7.46) we arrive at the following estimate for the total reaction rate:

$$\begin{aligned} \Gamma &\approx N_D \left[\frac{V_{\mu \cdot \mathbf{B}}}{|\Delta E|} \right]^2 \left| \frac{\Sigma^*(\mathbf{k}, \mathbf{k}''')}{\Delta E} \right|^2 \left(\frac{V_N}{V_A} \right) \left\{ \frac{|\Sigma^*(\mathbf{k}, \mathbf{k}''')|}{\frac{\hbar^2 |\mathbf{k}''|^2}{2M_n}} \right\} \Gamma_{Pd} \\ &\approx \frac{1}{\hbar} N_D (N_A)^3 \frac{(V_{\mu \cdot \mathbf{B}})^8}{(\Delta E)^4} \left[\frac{V_N}{V_A} \right]^4 \left\{ \frac{e^{3\hbar\omega_A/k_B T}}{(k_B T)^3 (e^{3\hbar\omega_A/k_B T} - 1)^6} \right\} . \end{aligned} \quad (7.48)$$

Once again, as in Eq. (3.40), we plug in typical values for the quantities which appear in the above formula only to find that

$$\Gamma \approx (10^{16}) 10^{21} (10^{15})^3 \left(\frac{10^{-48}}{10^{24}} \right) [10^{-9}]^4 \left\{ \frac{1}{(40)^{-3}(25)^3} \right\} = 2 \times 10^{-27} \text{sec}^{-1} . \quad (7.49)$$

Clearly this rate is far too small. It amounts to, essentially, 2×10^{-48} transfer reactions per second per donor in the lattice!

There is a way out of this predicament, however, and that is if we consider the dominant

interaction between the neutron and the nuclei in the lattice to be *strong* in nature, just as we did in the latter part of chapter 4⁷. This requires that the participating donor and acceptor nuclei to be larger than the simple deuteron and proton, since these are incapable of interacting strongly with the free neutrons. Tritium, Pd and Li isotopes etc. are all possible candidates for the transfer reactions. As discussed in chapter 4, $V_{\mu \cdot \mathbf{B}}$ is now replaced by V_S (which is of order 10^7 or 10^8 larger) in the above formula. The reaction rate now becomes

$$\begin{aligned} \Gamma &\approx \frac{1}{\hbar} N_D (N_A)^3 \frac{(V_S)^8}{(\Delta E)^4} \left[\frac{V_N}{V_A} \right]^4 \left\{ \frac{e^{3\hbar\omega_A/k_B T}}{(k_B T)^3 (e^{3\hbar\omega_A/k_B T} - 1)^6} \right\} \\ &\approx (10^{16}) 10^{21} (10^{15})^3 \left(\frac{10^{24}}{10^{24}} \right) [10^{-9}]^4 \left\{ \frac{1}{(40)^{-3} (25)^3} \right\} = 2 \times 10^{45} \text{sec}^{-1}, \quad (7.50) \end{aligned}$$

which is enormous.

The free neutron transfer reaction rates may also be calculated using perturbation theory (see discussion following Eq. (6.12)). This calculation was carried out by P. L. Hagelstein, who arrived at the following expression for Γ :

$$\Gamma = \left(\frac{2\pi}{\hbar} \right) \left| \langle \Phi_2 | \hat{V} \hat{V} [E - H_0]^{-1} \hat{V} \hat{V} | \Phi_0 \rangle \right|^2 \rho(E_f), \quad (7.51)$$

where $\rho(E_f)$ is the density of states, and \hat{V} corresponds to H_1 in my notation. Estimates for the reaction rates derived from the above formula were

$$\begin{aligned} \Gamma &= \left(\frac{2\pi}{\hbar} \right) \frac{|\boldsymbol{\mu} \cdot \mathbf{B}|^2 |\mathbf{d} \cdot \mathbf{E}|^6}{\Delta E^4 \delta \epsilon^3} \left[\frac{V_n}{V_A} \right]^4 \frac{N_A N_A^2 N_D}{\sqrt{N_{ph}}} g(T) \\ &\approx 10^{16} \frac{[10^{-6}]^8}{[5 \times 10^6]^4 [3 \times 10^{-2}]^3} [10^{-9}]^4 \frac{[10^{15}]^3 10^{21}}{[1.5 \times 10^8]^{\frac{1}{2}}} \\ &= 5 \times 10^{-29} \text{sec}^{-1}, \quad (7.52) \end{aligned}$$

which compares favorably with the figure obtained in Eq. (7.49). A similar estimate for the rate in the case of the strong interaction from perturbation theory gave

$$\begin{aligned} \Gamma &= \left(\frac{2\pi}{\hbar} \right) \frac{|V_S(Pd)|^2 |V_S(Li)|^6}{\Delta E^4 \delta \epsilon^3} \left[\frac{V_n}{V_A} \right]^4 \frac{N_A N_A^2 N_D}{\sqrt{N_{ph}}} g(T) \\ &\approx 10^{16} \frac{[10^3]^8}{[7 \times 10^6]^4 [3 \times 10^{-2}]^3} [10^{-9}]^4 \frac{[10^{15}]^3 10^{21}}{[5 \times 10^6]^{\frac{1}{2}}} \end{aligned}$$

⁷See discussion on the *strong* interaction in chapter 4

$$= 7 \times 10^{43} \text{sec}^{-1} , \quad (7.53)$$

which, once again, agrees with the result we obtained in Eq. (7.50). The agreement between the two sets of results lends more credibility to the theory.

Thus we have argued that the underlying neutron transfer mechanism may hold up numerically. We had determined early on (see chapter 3) that the *Duschinsky matrix* introduced into the formalism was capable of mediating macroscopic energy transfer. With the reaction rate just estimated, we have demonstrated that the mechanism in and of itself does not inhibit the processes observed in the Pons-Fleischmann cells. The bottleneck is in the generation of phonon modes with high occupation.

Chapter 8

Summary and Conclusion

Pons and Fleischmann first claimed the observation of heat generation of nuclear origin in an electrolysis experiment in 1989. Early speculations focused on the possibility of low-temperature deuteron-deuteron fusion to explain the various reported anomalies. These theories however fail to account for the mechanism that would allow for the overwhelming Coulomb barrier to be overcome. An alternative theory based on second order reactions involving off-resonant intermediate states which contain virtual neutrons was proposed. The theory was pioneered by P. L. Hagelstein¹.

The present work began with a brief survey of the framework upon which Hagelstein's initial effort was built. The main features of the theory were:

1. The reactions involved the transfer of a neutral particle, namely the neutron, thus circumventing the problem of the Coulomb barrier.
2. Frequency shifting of a large number of phonons proved capable of mediating significant transfer of energy (of order MeV) between microscopic nuclei and a macroscopic lattice through use of the *Duschinsky* operator.
3. Because the theory required that the neutrons involved in the reactions be virtual in nature, a method had to be conceived in order to show that a significant amount of delocalization may be induced to these particles.

The original research presented in this work was aimed at verifying that neutron delocalization was in fact present. It was found that, by introducing a resonance exchange

¹See references for articles by P. L. Hagelstein at the end of chapter 1.

scheme into the theory, the neutrons could potentially achieve a range of a few microns. In order to insure that a sufficient number of these neutrons reach this degree of delocalization, we undertook the task of solving approximately for the Green's function of the full system Hamiltonian. Ultimately, an expression for the Green's function was obtained in terms of the self-energy which we had solved for explicitly in the one-phonon approximation scheme. Using the expression for the 1-phonon averaged proper self-energy, a reaction rate for the neutron transfer reactions was calculated for the case of electromagnetic interaction potential and the strong interaction potential. It was found that, in the instance where the interaction between the neutrons and the nuclei in the lattice was *strong*, the transfer reaction rate was enormous (of order 10^{25} reactions per second per donor in the lattice). For the magnetic dipole transition potential, on the other hand, the reaction rate was extremely low (of order 10^{-47} per second per deuteron in the lattice). Clearly, the focus of the theory must revolve around the strong interaction.

8.1 Summary of Original Results

1. The full system Hamiltonian, H_{total} , was expressed in terms of second quantized field operators for the neutrons and the donor and acceptor nuclei occupying the lattice sites (see Eq. (5.6)).
2. A formal expression for the many-body Green's function of the neutron/lattice system was obtained (see Eq. (5.1)).
3. We succeeded in extracting an approximation for the proper self-energy operator, $\Sigma^*(\mathbf{k}, \mathbf{k}')$, using infinite order Brillouin-Wigner perturbation theory, originally proposed by P.L. Hagelstein, (see Eq. (6.19)).
4. We looked at 0, 1 and 2-phonon averages for the proper self-energy of the system (see Eqs. (7.24), (7.42) and (7.46)) and saw that the 0-phonon piece vanished.
5. Using the result obtained for $\Sigma^*(\mathbf{k}', \mathbf{k}'')$ and Dyson's formula (see Eq. (7.47)), we arrived at a final expression for the exact many-body Green's function.
6. Finally, we succeeded in obtaining a rough estimate for the total neutron transfer reaction rate using the result obtained for $\Sigma_{(2)}^*(\mathbf{k}', \mathbf{k}''')$. This, in effect, is the key

result of the *thesis*, especially as a comparison of the reaction rates derived from the proper self-energy with those obtained from a perturbation expansion show remarkable agreement (see Eqs. (7.49) and (7.51), and Eqs. (7.50) and (7.52)). These results show that, while the reaction rate is negligible for electromagnetic interactions between the neutron and nuclei in the lattice (of order 10^{-48} per second per deuteron in the lattice), in the case of strong interactions, the reaction rate is enormous ($\sim 10^{24}$ per second per donor). We should not be alarmed that the rate is so large because all that it means is that the resonance exchange mechanism does not hinder the progress of the neutron transfers. The bottle-neck lies in the limited number of phonons mediating the reactions.

References

1. M. Fleischmann and S. Pons, "Electronically Induced Nuclear Fusion of Deuterium", *J. Electroanal. Chem.*, **261**, 301 (1989).
2. S. Pons and M. Fleischmann, "Calorimetric Measurements of the Palladium/Deuterium System: Fact and Fiction", *Fusion Tech.* **17**, 669 (1990).
3. S. Pons and M. Fleischmann, "Calorimetry of the Palladium-Deuterium System", *Proc. of the First Annual Conference on Cold Fusion*, p. 1, Salt Lake City, Utah, March 29-31, 1990.
4. S. Pons and M. Fleischmann, "Calorimetric Measurements on Palladium Based Cathodes Polarized in Heavy Water", presented at the *Second Annual Conference on Cold Fusion*, Como, Italy, June 29 - July 4, 1991.
5. M. Fleischmann and S. Pons, *Proc. Third International Conference on Cold Fusion*, Ed. Ikehami, Universal Academy Press, Tokyo (1993).
6. M. Fleischmann and S. Pons, *Physics Letters A*, **176** 118 (1993).
7. P. L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions I: The Interaction Hamiltonian", *Fusion Tech.* **22**, 172-180, (1992).
8. P. L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions II: Transition Operators", submitted to *Fusion Tech.*, (1992).
9. P. L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions III: Phonon Generation", to appear in *Fusion Tech.*, (1992).
10. P. L. Hagelstein, "Coherent and Semi-Coherent Neutron Transfer Reactions IV: Two Step Reactions and Virtual Neutrons", submitted to *Fusion Tech.* November, (1992).

11. M. McKubre, R. Rocha-Filho, S. Smedley, F. Tanzella, S. Crouch-Baker, T. Passel and J. Santucci, "Isothermal Flow Calorimetric Investigations of the D/Pd System", *Proc. Second Annual Cold Fusion Conference*, Como, Italy, July 1991.
12. M. McKubre, S. Crouch-Baker, A. M. Riley, S.I. Smedley and F. L. Tanzella, *Proc. Third International Conference on Cold Fusion*, Ed. H. Ikegami, Universal Academy Press, Tokyo (1993).
13. H. O. Menlove, *Proc. First Annual Cold Fusion Conference*, Salt Lake City, March 1990; page 250.
14. T. Claytor, "Tritium Generation in Pd-Si Systems", presented at the Conference on Anomalous Nuclear Effects in Deuterium/Solid Systems, BYU, Oct. 1990.
15. A. B. Karabut, Y. R. Kucherov, I. B. Savatimova, *Physics Letters A* **170** 265 (1992).
16. M. Miles, B. Bush and D. Stiwell, "Calorimetric Principles and Problems in Measurements of Excess Power During Pd-D₂O Electrolysis", to be published in the *Journal of Physical Chemistry E*, Feb. 17, (1994).
17. M. Miles and B. Bush, "Heat and Helium Measurements in Deuterated Palladium", *Fourth Annual Conference on Cold Fusion, ICCF4 Conference Proc.*, Lahaina, Hawaii, December 1993.
18. W. E. Lamb, "Capture of Neutrons by Atoms in a Crystal", *Phys. Rev.* **55**, 190 (1939).
19. F. Duschinsky, "Zur Deutung der Elektronenspektren mehratomiger Molekule I. Uber des Franck-Condon-Prinzip", *Acta Physiochimica U.R.S.S.* **7**, 551 (1937).
20. K. A. Brueckner and C. A. Levinson, "Approximate Reduction of the Many-Body Problem for Strongly Interacting Particles to a Problem of Self-Consistent Fields", *Phys. Rev.* **97**, 5 (1955).
21. K. A. Brueckner, "Many-Body Problem for Strongly Interacting Particles. II. Linked Cluster Expansion", *Phys. Rev.* **100**, 1 (1955).
22. K. A. Brueckner, R. J. Eden and N. C. Francis, "Theory of Neutron Reactions with Nuclei at Low Energy", *Phys. Rev.* **100**, 3 (1955).

23. K. A. Brueckner, "Properties of Nuclear Matter", *Phys. Rev* **109**, 4 (1958).
24. H. A. Bethe, "Nuclear Many-Body Problem", *Phys. Rev.* **103**, 5 (1956).
25. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, Dover Publications, Inc., New York (1972).
26. A. Deshalit and H. Feshbach, "Theoretical Nuclear Physics Volume I: Nuclear Structure", John Wiley and Sons, New York (1974).
27. Alexander L. Fetter and John Dirk Walecka, "Quantum Theory of Many-Particle Systems", McGraw Hill Inc., 1971.
28. Neil W. Ashcroft and N. David Mermin, *Solid State Physics*, W. B. Saunders Co., 1976.
29. D. A. Kirzhnits, "Field Theoretical Methods in Many-Body Systems", Pergamon Press Ltd., 1967.
30. T. D. Schultz, "Quantum Field Theory and the Many-Body Problem", Gordon and Breach Science Publishers, Inc.
31. John C. Inkson, "Many-Body Theory of Solids, An Introduction", Plenum Publ. Corp., 1984.
32. John W. Negele and Henry Orland, "Quantum Many-Particle Systems", Addison-Wesley Publ. Corp., 1988.
33. J. M. Jauch and F. Rohrlich, "Theory of Photons and Electrons", Addison-Wesley Publishing Company, Inc., Cambridge 42, Massachusetts 1955.
34. Suraj N. Gupta, "Quantum Electrodynamics", Gordon and Breach Science Publishers, Inc., New York 1977.
35. G. Kallen, "Quantum Electrodynamics", Springer-Verlag, Inc., New York 1972.
36. Lewis H. Ryder, "Quantum Field Theory", Cambridge Univ. Press, 1955.
37. V. L. Bonch-Bruевич and S. V. Tyablikov, "The Green Function Method in Statistical Mechanics", North-Holland Publishing Company, Amsterdam.

38. Richard D. Mattuck, "A Guide to Feynman Diagrams in the Many-Body Problem", McGraw-Hill Publishing Company Limited, McGraw-Hill House, Maidenhead, Berkshire, England 1967.