

# 15

## *Probing Vibrational Energy Relaxation in Proteins Using Normal Modes*

Hiroshi Fujisaki, Lintao Bu, and John E. Straub

### CONTENTS

15.1 Introduction .....	301
15.2 Cytochrome c .....	302
15.3 QCF Approach .....	303
15.3.1 Fermi's Golden Rule .....	304
15.3.2 Quantum Correction Factor .....	305
15.3.3 NM Calculations for Cyt c .....	306
15.3.4 Application to VER of the CD Bond in Cyt c .....	307
15.3.5 Fluctuation of the CD Bond Frequency .....	308
15.4 Reduced Model Approach .....	309
15.4.1 Reduced Model for a Protein .....	310
15.4.2 Maradudin–Fein Formula .....	311
15.4.3 Third-Order Coupling Elements .....	312
15.4.4 Width Parameter .....	313
15.4.5 Temperature Dependence .....	315
15.5 Discussion .....	315
15.5.1 Comparison with Experiment .....	315
15.5.2 Validity of Fermi's Golden Rule .....	316
15.5.3 Higher-Order Coupling Terms .....	317
15.6 Summary .....	318
Acknowledgments .....	320
References .....	320

### 15.1 Introduction

The harmonic (or normal mode (NM)) approximation has been a powerful tool for the analysis of few and many-body systems where the essential

301













































