New Many-Body Theories On

Soft X-Ray
Spectroscopy

Of
Insulating Solids

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OF INSULATING SOLIDS**

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Preface

The x-ray spectroscopy has been quite an important tool to clarify peculiar electronic states of rushingly-synthesized new materials, such as high-temperature superconductors. As this experimental technique has been sophisticated enough to clarify the precise electronic structures, however, we have faced a serious problem that our conventional theories work only poorly on such new materials.

According to the linear response theorem, it has been believed that an externally-applied small perturbation, such as the x-ray absorbance, induces only small changes in the system, and we can clarify the electronic structures of the ground and excited states of these objective materials, by observing this response function. Even now, we can know the electronic structure only through this response function, but in these new materials, the real relationship between the external perturbation and its response becomes quite complicated.

For example, the energy resolution of the photoemission spectroscopy has now been reduced to less than 1 meV. Nevertheless, as will be mentioned in the following chapters in detail, the photoemission spectrum of the copper-oxide compound only has quite a broad and structure-less peak with a width of about 1 eV. Such an experimental result can never be explained by the conventional theories.

One of the most standard theories that deal with many-body

systems, is a mean-field approximation, in which the electron-electron interaction is reduced to the static self-consistent field. Thus, in this theory, we regard the interacting electrons as independent particles under this static self-consistent field.

Another conventional theory is a perturbation approach, in which the electron-electron interaction is renormalized into the electron mass. In this theory, we can regard the interacting electrons as independent particles with this renormalized mass.

When the electron-electron interaction is weak, these conventional theories can explain experiments well. However, through the recent x-ray spectroscopy, we have been confronting a serious problem that these conventional theories work quite poorly when the interaction is significantly strong. This difference, which makes the conventional concept of the independent electrons invalid, is called the strong many-body effect or electron correlation. In such a case, we have to change the concept of the independent electrons, and have to create a new theory, which can deal with the electron-electron interaction more appropriately.

In this book, we will introduce a new path-integral theory and clarify how the many-body effects change the conventional concept on the x-ray spectroscopy. We will also show that simple models, such as the Hubbard or extended Hubbard model, can consistently describe the light absorption and photoemission experiments on the real correlated materials quite nicely. We believe that such a consistent explanation for plural mutually-independent experiments is particularly important, since different experiments provide us complementary information on the electron correlation effects. To

establish the new theory, it is very important to explain different experiments consistently. We will see that the cooperative studies of experiments and theories on the x-ray spectroscopy can clarify the unconventional electronic states and the natures of the quantum fluctuations.

This book is organized as follows. General features and problems on the recent x-ray spectroscopy of the interacting electron systems are reviewed in Chap.1. The new path-integral theory is precisely derived in Chap.2. If the readers are interested only in phenomenological aspects on the spectroscopy, they can skip this chapter. In Chap.3, the photoemission spectroscopy on the strongly correlated electron systems is theoretically studied. We will show that the photoemission peak no longer corresponds to the band-like state in the strongly correlated electron systems. In Chap.4, we study the gap structures of the strongly correlated electron system by comparing the photoemission and light absorption spectra. In Chap.5, the light absorption spectra of Sr_2CuO_3 and Ni-Br complex are precisely studied to clarify the quantum fluctuations in the one-dimensional interacting electron systems. In Chap.6, we show that the simple model, such as the one-dimensional Hubbard or extended Hubbard model, can nicely describe the light absorption and photoemission spectra of the real correlated material comprehensively. Then, in Chap.7, the inelastic Raman and neutron scattering spectra of the strongly correlated electron system are studied. We show that the fluctuations, due to the nonlinear coupling between the spin and charge excitations, significantly affect these spectra. Chapter 8 is devoted to the electron correlation effects on the

characteristic x-ray radiation spectrum, while Chap.9 is devoted to phonon effects on the soft x-ray radiation spectrum. In these last two chapters, we show that the electron-electron scattering or electron-phonon scattering causes the dissipation in the photo-excited state. It is shown that the x-ray radiation spectrum is separated into the non-dissipated Raman and dissipated luminescence components.

We hope that this book helps the readers understand the x-ray spectroscopy for the strongly correlated electron systems and the natures of the correlated electrons.

Finally, we are grateful to Mr. Hugh Patton and Mr. Chad Patterson for their careful reading of the manuscript. We also wish to thank Mr. Yeow-Hwa Quek for his encouragement and advice in preparing the manuscript.

Norikazu Tomita and Keiichiro Nasu
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