5.10 Theory

Our theory group of the Photon Factory in IMSS of KEK, has been established about 15 years ago, and at present, it is composed of one professor, two research associates, a few post-doctoral researchers, and several PHD course students of the School of Materials Structure Science in the Graduate University for Advanced Study (So-ken-dai). Its research activity is widely concerned with various theoretical problems of solid state physics, especially with the theoretical solid state optics, which expands from the hard and the soft x-ray regions to the visible region, and often extends even to the infrared region. Practical studies in these recent 5 years are concentrated to two main themata, the path integral theory for the photo-electron emission spectrum, and the theory for photo-induced structural phase transitions.

5-10-1 Coexistence of both coherent and incoherent peaks in photoemission spectra of intermediately correlated many-electron systems

We have theoretically studied various one-, two- and three-dimensional half-filled Hubbard models from the weak correlation cases to the strong ones, and calculated the Lehmann's spectra of the momentum-specified one-electron Green's functions, as well as the total density of states (DOS), using the quantum Monte Carlo method. In the region of intermediate correlation strength, we have found the DOS has new characteristic peaks near the Fermi level, in addition to the well-known upper and lower Hubbard-band peaks. We have shown that these new peaks near the Fermi level comes from quasi-coherent states, while the upper and lower Hubbard-band peaks comes from strongly incoherent ones. This multi-peaked structure, appearing only in the intermediate region, is shown to be quite insensitive to the dimensionality. Finally, we have compared our results with the static single impurity model, and have given a rough and intuitive explanation for the origin of this newly obtained multi-peaked structure. Our results also qualitatively agree with the recent photoemission experiments on $CaVO_3$ and $SrVO_3$ crystals.

References

[1] M. Yamazaki, N. Tomita and K. Nasu, *J. Phys. Soc. Jpn.,* **72** (2003) 611.
[2] K. Ji, H. Zheng and K. Nasu, *Phys. Rev. B,* **68**(2003) 035117.
[3] K. Nasu, M. Yamazaki,N. Tomita, H. Zhao and C. Wu, *J. Ele. Spe. Rel. Pheno.*, **136** (2004) 49.

5-10-2 New path-integral theory for evolution of momentum specified photoemission spectra from broad Gaussian to two-headed Lorentzian due to electron-phonon coupling

Using a new path-integral theory, we have studied the momentum specified photoemission spectra (MSPES) of one- and two-dimensional metallic many-electron systems, coupled with the Einstein phonons. The multiple scatterings of electrons due to phonons are shown to completely dominate the MSPES, even if the electron-phonon coupling strength is intermediate. These multiple scatterings result in spectral evolution from a broad Gaussian to a two-headed asymmetric Lorentzian as the momentum changes from the band bottom to the Fermi one ($\equiv P_F$). We have also found that this two-headed structure near P_F becomes most distinct in the two dimensional non-half-filled cases with no charge density wave gap. These results qualitatively agree with recent experiments of MSPES of the Be(0001) surface and $Bi_2Sr_2CaCu_2O_8$.

References

[3] K. Ji, H. Zheng and K. Nasu, *Phys. Rev. B*, **70** (2004) 85110.
[4] K. Ji and K. Nasu, *J. Ele. Spe. Rel. Pheno.*, **144 –147** (2005) 1233.

5-10-3 Theory for difference between photoinduced phase and thermally excited phase

A possible difference between the photo-induced phase and the thermally excited one is studied by using a two-dimensional extended Peierls-Hubbard model, which includes a strong electron-phonon coupling and a on-site inter-electron repulsion, as well as an anharmonic lattice potential. Because of this anharmonicity, the system undergoes a first order phase transition from an insulating CDW state to a metallic one at a high temperature. Although some sign of an SDW order is expected to appear due to this repulsion, it is always hidden in any equilibrium phases of the present system. In fact, it is hidden, not only in the CDW ground state, but also in this metallic one, since the high temperature itself destroys the SDW order, far before the CDW-metal transition occurs. While, a photo-excitation at low enough temperature is shown to generate a local metastable SDW domain. Therefore, to observe the presence of such the Coulomb interaction and the resultant broken symmetry, a non-equilibrium photo-induced phase is shown to be most straightforward. Thus, the photo-induced phase transition can make an interaction appear as a broken symmetry only in this phase, even though this interaction is almost completely hidden in all the equilibrium phases from low temperature to high ones.

References

[5] P. Huai and K. Nasu, *J. Phys. Soc. Jpn.*, **71**(2002) 1182.

5-10-4 Theory for pattern formation dynamics in photoinduced structural phase transitions

We have theoretically studied the formation dynamics of exciton domain patterns organized in optically excited 2-dimensional many-exciton system, which is strongly coupled with an Einstein-phonon, and also im-

mersed in a reservoir. It is shown that the exciton may proliferate quite rapidly by several successive photon-pulse excitation, and the resultant pattern becomes something like a fjord structure. Moreover, the further proliferation can occurr by filling up this structure even when the excitation is already turned off. We also have investigated the effect of anisotropy of inter-exciton interaction on the efficiency of the proliferation. Consequently, we have concluded that the strong anisotropy leads to the very efficient proliferation and makes the resultant photo-induced structural phase transition vast and successful, as compared with isotropic cases.

References

[6] K. Nasu, *Physics Letters A,* **320** (2004) 286.

5-10-5 Photogeneration of super-para-electric large polarons in dielectrics with soft-anharmonic T_{1U} phonons

In connection with the recent experiments on photo-enhancements of the electronic conductivity and the quasi-static electric susceptibility of $SrTiO_3$, we have theoretically studied global versus local parity violation of a photogenerated electron in this dielectric. The photogenerated electron, being quite itinerant in the 3d band of Ti, is assumed to couple weakly but quadratically with soft-anharmonic T_{1U} phonons in this dielectric. The electron is also assumed to couple strongly but linearly to the breathing (A_{1g}) type high energy phonons. We will show that these two types of electron-phonon (e-p) couplings result in two types of polarons, a "super-para-electric large polaron" with a quasi-global parity violation, and an "off-center type self-trapped polaron" with only a local parity violation. These two states are shown to be separated by an adiabatic potential barrier, if these e-p couplings are short in their force ranges. Without the T_{1U} phonon, these two states reduce to the well-known large polaron and the self-trapped one, both of which have even parities. We have also shown that this super-para-electric large polaron enhances both the electronic conductivity and the quasi-static electric susceptibility, in qualitative agreements with the experiments.

References

[7] K. Nasu, Y. Qiu, C.Q. Wu and K. Nasu, *Phys. Rev. B*, **67** (2003) 174111; **72**(2005) 224105.

5-10-6 Photo-induced structural phase transition from a layered semi-metal to an insulator through inter-layer charge-transfer excitations in the visible region

In connection with the recent discovery of a new photo-induced phase with a novel inter-layer bond in a graphite crystal, we theoretically clarify the mechanism of this non-equilibrium phase transition, in terms of the lattice relaxation and the proliferation of photo-generated inter-layer charge-transfer excitations. This excitation is in the visible region, and at the Franck-Condon state, the resultant electron-hole pair, spanning neighboring two layers, is quite unstable, being easily dissipated into the 2d-semimetallic continuum electronic states, as plus and minus free carriers. However, by a small but finite probability, the electron and the hole are shown to become stable, as the lattice relaxation proceeds, being bound with each other, just like an exciton, through the inter-layer Coulomb attraction, and self-localize at a certain point of layer by contracting the inter-layer distance only around them. Thus, a local inter-layer bond is formed and a pseudo-energy-gap opens at the Fermi level, or a tiny insulating domain appears. Through further pulse excitations by several visible photons, this tiny domain is shown to proliferate stepwise up to a new insulating phase, wherein more than 1000 carbon atoms are included, and the inter-layer distance is greatly contracted in it. The relation between this new phase and the conventional graphite-diamond conversion is also clarified.

References

[8] Phys.Rev.B 2006 in press