12-1 Path-integral Theory for Photoemission Spectra of Electron-phonon Coupled Systems

The electron-phonon (e-ph) interaction is a basic problem in the solid state physics. It has been simulated by a large amount of researches, but still a lot of questions are unanswered. One of the most fascinating ones is how the e-ph interaction influences the electronic energy band structures, and finally determines a material to be an insulator, metal or superconductor. Since the photoemission spectra (PES) and angle resolved photoemission spectra (ARPES) can directly probe the structure of electronic energy band with high resolution, they have become one of the most important measurements for the experimental studies [1].

In the theoretical aspect, it is now well known, these spectra are nothing, but the Lehmann's representation of the one-body Green's function. However, the spectra calculated by the conventional theories, like the mean-field and perturbative approximation methods, are significantly different from the experimental ones. Recent experiments of ARPES on Be(0001) surface [2] (Fig. 1) and $Bi_2Sr_2CaCu_2O_8$ [3] show that, the spectra take sharp two-headed asymmetric Lorentzians at the Fermi level (E_F), and become broad Gaussians at the band bottom. This spectral change from two-headed asymmetric Lorentzian to broad Gaussian is quite unexpected and difficult to be explained by the conventional theories mentioned above, because the high-order e-ph scattering processes are not properly considered in these theories.

To clarify the mechanism of this spectral evolution, we develop a new path-integral theory [4] to calculate the ARPES. This is the first work in the world that the ARPES from E_F to band bottom are completely and exactly calculated, since in our theory, we take into account all kinds of e-ph scattering processes, and no other approximation is applied.

We start from the two-dimensional Holstein model, whose Hamiltonian is given as

$$H = -T \sum_{<l,l'>} \sum_{\sigma} (a_{l\sigma}^+ a_{l'\sigma} + a_{l'\sigma}^+ a_{l\sigma}) - \mu \sum_{l\cdot\sigma} n_{l\sigma}$$
$$+ \sum_{l} \left(\frac{P_l^2}{2m} + \frac{1}{2} m\omega_0^2 Q_l^2 \right) - S \sum_{l,\sigma} Q_l \left(n_{l\sigma} - \frac{\bar{n}}{2} \right).$$

From this Hamiltonian, we first calculate the one-body Green's function of electron by the path-integral theory, then derive the spectral function by the analytic continuation. The electronic transfer energy T and phonon energy ω_0 are taken as 0.25 eV and 0.025 eV, respectively. In Fig. 2, we show the calculated ARPES at the band bot-

tom (a) and E_F (b). The blue curves are obtained by our path-integral, and shaded ones are by the perturbation theory. In the perturbation theory, since the high order e-ph scattering processes are omitted, it gives almost same spectral shape in both panels. In contrast, our path-integral has taken into account all kinds of e-ph scattering processes, so our results well reproduce the spectral evolution from broad Gaussian at band bottom to two-headed asymmetric Lorentzian at E_F.

From a general point of view, a hole close to E_F is the most stable one in the band, it can stay there for a long lifetime, being almost free from the scatterings with phonons. Therefore, the photoemission spectrum near E_F gives a Lorentzian form characterized by the coherent plane-wave-like peak. While, for a hole at the band bottom, multiple e-ph scatterings are more likely to be aroused. Consequently, the hole is dressed by thick phonon cloud, and the spectral shape becomes a broad Gaussian distribution with an incoherent nature. A statistical average over these processes then gives us the spectral evolution of the ARPES.
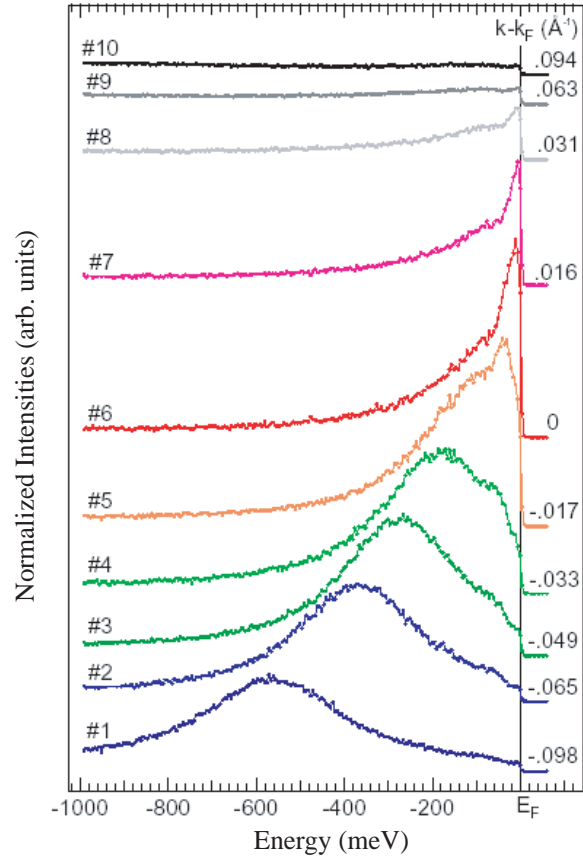

Figure 1
Experimental ARPES measured on the Be(0001) surface along the $\bar{\Gamma}\bar{M}$ symmetry line of the surface Brillouin zone (after Hengsberger *et al.* [2]). It is clearly represented that the spectra evolves from broad Gaussian at band bottom to two headed asymmetric Lorentzian at Fermi level.
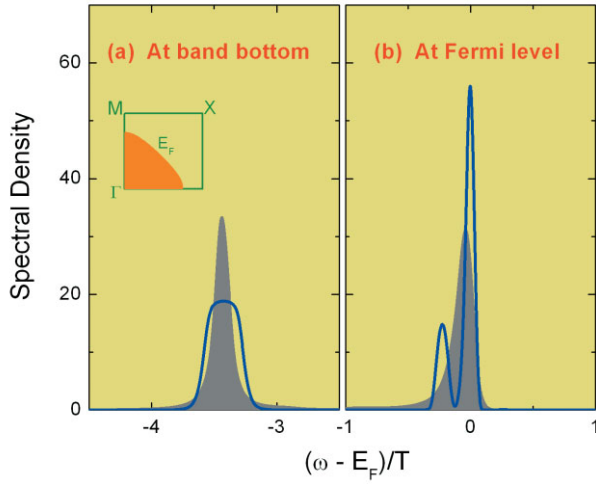
Figure 2
Calculated ARPES at the band bottom (a) and Fermi level (b). Our path-integral theory (blue curves) well reproduces the characteristic spectral change, while the perturbation theory (shaded curves) gives almost same spectra. The inset shows the Brillouin zone and Fermi surface.

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12-2 New Many-body Theory by the Superposition of Non-orthogonal Slater Determinants

Developing new many-body theories has been one of the central problems in both physics and chemistry. At present, we have the real-space density-matrix renormalization group method, dynamical mean-field theory, and quantum Monte Carlo simulation to explore the many-body effects. However, these methods have strong restrictions on their applications, such as dimensionality and particle filling. Therefore, we still need more tractable and applicable theories.

Here, I introduce a new variational approach to the accurate description of the electron correlations, called the resonating Hartree-Fock (Res-HF) method [1-3]. This method approximates a many-body wave-function by the superposition of non-orthogonal Slater determinants (S-dets). The non-orthogonality enables us to describe the large quantum fluctuations efficiently, since each S-det naturally includes the full-electron-excitation effects from other S-dets.

In the Res-HF method, the broken-symmetry S-dets are used to generate the Res-HF wave-function. As the resonance of different kinds of broken-symmetry S-dets should stabilize the many-body states, the Res-HF wave-function $|\psi>$ is preliminarily expressed by

$$| \psi> = \sum_{n=1}^{N_s} C_n |\varnothing_n >,$$

where the number of S-dets is given by N_s and $|\varnothing_n >$ represents a constituting broken-symmetry S-det. The orbitals of every S-det, as well as the superposition coefficients, are variationally determined. However, this is not sufficient, since each $|\varnothing_n >$ breaks symmetry of the system. We should make projections for each $|\varnothing_n >$, so that the Res-HF wave-function belongs to an irreducible representation of the system. Such projections depend on the symmetry of the system.

As a demonstration, I apply the Res-HF method to the 1-D single-band Hubbard model, where we have the exact Lieb-Wu solutions for both the half-filled and doped cases [4,5]. Its Hamiltonian is given by

$$H = -t\sum_{l=1}^{N}(a_{l\sigma}^{+} a_{l+1\sigma} + a_{l+1\sigma}^{+} a_{l\sigma}) + U\sum_{l=1}^{N} n_{l\uparrow} n_{l\downarrow}$$

where N represents the system size. In the following,

Table 1 The ground state energies of the 1-D half-filled and doped Hubbard systems. The correlation energy explained by each method is denoted by κ (%)

		$N=N_e=30$	κ	$N=30, N_e=26$	κ	$N=30, N_e=22$	κ
U=2	RHF	-23.2671		-26.1642		-26.8921	
	Res-HF	-25.3436	98.1	-27.9979	98.5	-28.4268	98.9
	Exact	-25.3835		-28.0253		-28. 4441	
U=4	RHF	-8.2671		-14.8975		-18.8254	
	Res-HF	-17.0542	97.5	-21.5720	94.1	-24.1582	95.5
	Exact	-17.2335		-21.9868		-24.4057	
U=8	RHF	21.7329		7.6358		-2.6921	
	Res-HF	-9.5378	99.0	-15.4059	97.2	-19.5552	95.5
	Exact	-9.8387		-16.0761		-20.3462	

symmetry group. P^s represents the spin projection of the constituting S-dets onto the exact singlet eigen-states.

In Table 1, I show the ground state energies of the half-filled and doped Hubbard systems. Here, RHF denotes the restricted HF state, which satisfies the full symmetries of the system. N_e represents the number of electrons. It is remarkable that for both the half-filled and doped systems, the Res-HF wave-functions can describe more than 94% of the correlation energies in all the correlation regimes.

Next, I show in Fig. 3 the spin correlation functions obtained by the Res-HF wave-functions for $U = 4$. The long-range behaviors are enlarged in the inset, where the crosses show the exact behaviors. We can see that the Res-HF wave-functions describe the exact spin correlation structures very nicely for both the half-filled and doped systems.

Thus, I have shown that both the correlation energies and correlation structures are well described by the Res-HF wave-functions. Since the Res-HF method does not suffer any problems from the dimensionality and filling, it can be a powerful tool for the studies of the interacting Fermion systems.

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Figure 3
Spin correlation functions for $N = N_e = 30$ (a), $N = 30$ and $N_e = 26$ (b), and $N = 30$ and $N_e = 22$ (c). The close-up of the long-range behavior is shown in the inset of each figure, where the crosses show the exact long-range behavior

all the energies are normalized by the transfer energy t. In this study, a periodic boundary condition is imposed. Therefore, the system has the D_N symmetry. Here, I focus on the ground state with $N=30$ sites which satisfies the $^1A_1$ symmetry. In this case the Res-HF wave-function is explicitly represented by

$$|\psi> = \sum_{n=1}^{N_S} C_f \sum_{m=0}^{N-1} P^s T^m (1+R) |\emptyset_n>,$$

where the operator T makes the translation of the S-det by one site, while R represents the C_2 rotation in the D_N