# Theoretical study on angle-resolved photoemission spectroscopy of graphite

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## Introduction

Graphite is an important mother system for carbon-based nano-materials such as carbon nanotube and fullerene. Insight into this material has been attracting considerable research interests. Recently, the high resolution angle-resolved photoemission spectroscopy (ARPES) is performed on graphite [1-3], and a sharp peak is observed just on the Fermi surface ($E_F$) at K point of Brillouin zone. While away from $E_F$, its intensity declines dramatically. Below this peak, another small peak also appears, but its intensity is almost constant. One of the possible origins for this asymmetric two peak structure in ARPES is the many-body effect in graphite, which results in a side peak nearby $E_F$, as has been observed in several other materials [4]. However, it is also known that there is a weak interplay between the carbon planes, which introduces a splitting of the conduction band of graphite [5], and might be another origin for the two peak structure. In this work, we theoretically study these two effects on graphite, aiming to clarifiy the nature of this spectral structure.

## Model and Methods

To address the many-body effect on graphite, in this work, we consider a many electron system coupled with the lattice vibrations (phonons). We calculate the ARPES on the single graphene sheet and the bi-layer graphite system based on a half-filled Holstein type model,

$$H = -t\sum_{<n,n>}\sum_{\sigma}(a^{+}_{n\sigma}a_{n'\sigma}+a^{+}_{n'\sigma}a_{n\sigma})+\omega_0\sum_n b^{+}_n b_n \,, \qquad (1)$$
$$-\mu\sum_{n,\sigma}a^{+}_{n\sigma}a_{n\sigma}+g\sum_{n,\sigma}a^{+}_{n\sigma}a_{n\sigma}(b^{+}_n+b_n)$$

where $a^{+}_{n\sigma}$ ($a_{n\sigma}$) is the creation (annihilation) operator of an electron with a spin $\sigma$ at the carbon site $n$, and $t$ is the electronic transfer energy. In this system, the electrons hop between two nearest neighboring sites, denoted by $\langle n,n'\rangle$, and couple to the Einstein phonons localized at each site $n$, with a frequency $\omega_0$. $b^{+}_n$ ($b_n$) is the phonon operators, and $g$ is the electron-phonon (e-ph) coupling constant.

From the theoretical point of view, the spectral function can be derived from the single-particle Green's function,

$$G_{n,n',\sigma}(\tau) = -\left\langle T_\tau a_{n\sigma}(\tau)a^{+}_{n'\sigma}\right\rangle \,, \qquad (2)$$

where $\tau$ means imaginary time, $a_{n\sigma}(\tau)$ is the Heisenberg representation of $a_{n\sigma}$, and $T_\tau$ is the time ordering operator. In our theory, the Green's function of Eq. (2) is calculated by the quantum Monte Carlo (QMC) simulation method with a hybrid algorithm [6]. After the Fourier transformation of Green's function,

$$G_\sigma(\mathbf{p},\tau) = \frac{1}{N}\sum_{n,n'} e^{i\mathbf{p}\cdot(\mathbf{R}_n-\mathbf{R}_{n'})}G_{n,n',\sigma}(\tau) \,, \qquad (3)$$

we obtain the electronic spectral function [$\equiv A_\sigma(\mathbf{p},\omega)$] for a given momentum $\mathbf{p}$ through the analytic continuation as,

$$G_\sigma(\mathbf{p},\tau) = \int_{-\infty}^{\infty}\frac{e^{-\omega\tau}}{1+e^{-\omega\beta}}A_\sigma(\mathbf{p},\omega)\,d\omega \,. \qquad (4)$$

## Results and Discussion

Our calculation shows that in the case of graphene sheet, the ARPES is characterized by a sharp peak at the K point as shown in Fig. 1(a). In the bi-layer graphite case, when the inter-layer electronic transfer ($\equiv t_\perp$) is introduced, intensity of this sharp peak decreases as shown in Fig. 1(b) with $t_{//}$ being the intra-layer transfer, as a result of the band splitting. Thus, it can be inferred that the central sharp peak is primarily due to the two-dimensional electronic behavior, while the other structure nearby it is due to the bulk effect, or inter-layer correlation.

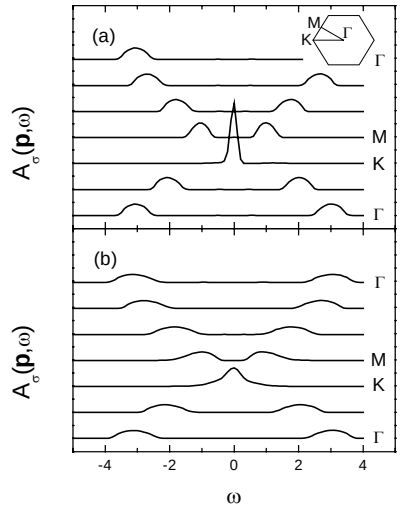


*Fig. 1.*

Fig. 1: Calculated ARPES of (a) graphene sheet, and (b) bi-layer graphite ($t_\perp = 0.5t_{//}$).

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