Supplementary Material for

"Tunable RKKY interaction in 30° twisted bilayer graphene"

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I. LANCZOS METHOD

In this work we employ the Lanczos method in real space by which we can obtain numerically the lattice Green's function.The key procedure of the Lanczos method is to find out a basis set in which the tight-binding Hamiltonian of the system becomes a tridiagonal matrix. In so doing, we firstly choose a normalized seed state $|f_0\rangle$, then construct a new state orthogonal with $|f_0\rangle$ using the following formulas:

$$|F_1\rangle = \hat{H}|f_0\rangle - |f_0\rangle\langle f_0|\hat{H}|f_0\rangle = \hat{H}|f_0\rangle - a_0|f_0\rangle, \tag{S1}$$

$$|f_1\rangle = \frac{1}{b_1}|F_1\rangle, \tag{S2}$$

where $a_0 = \langle f_0|\hat{H}|f_0\rangle$, and $b_1 = \langle f_0|\hat{H}|f_1\rangle$ is the normalization coefficient of the state $|f_1\rangle$. Apparently, $|f_1\rangle$ is orthogonal to $|f_0\rangle$. It is easy to get the recursive relation when $n \geqslant 2$

$$|F_n\rangle = \hat{H}|f_{n-1}\rangle - a_{n-1}|f_{n-1}\rangle - b_{n-1}|f_{n-2}\rangle, \tag{S3}$$

$$|f_n\rangle = \frac{1}{b_n}|F_n\rangle, \tag{S4}$$

with the recursive coefficients:

$$a_n = \langle f_n|\hat{H}|f_n\rangle \tag{S5}$$

$$b_n = \langle f_{n-1}|\hat{H}|f_n\rangle. \tag{S6}$$

We can prove that every new state obtained by Eqs. (S3) and (S4) is normalized and orthogonal to the preceding ones.

On the basis of $\{|f_0\rangle, |f_1\rangle, |f_2\rangle, \cdots\}$ the tight-binding Hamiltonian of the system becomes a tridiagonal matrix which takes a form as

$$H = \begin{bmatrix} a_0 & b_1 & 0 & \cdots \\ b_1 & a_1 & b_2 & \cdots \\ 0 & b_2 & a_2 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{bmatrix}. \tag{S7}$$

The retarded Green's function matrix is then defined as $G^r(\varepsilon) = (\varepsilon - H + i\eta)^{-1}$. In the numerical calculations we set the infinitesimal $\eta = 0.001|t|$ which is small enough to guarantee the convergence of the calculated Green's functions. The first diagonal element of such a Green's function can be written as

$$G^r_{00}(\varepsilon) = \langle f_0|\hat{G}^r(\varepsilon)|f_0\rangle = \frac{D_1}{D}, \tag{S8}$$

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where D is the determinant of the matrix $[\varepsilon - H + i\eta]$. And D_i for $i \geq 1$ is the determinant of the matrix by taking out both the first i rows and first i columns of $[\varepsilon - H + i\eta]$. We can expand D by using Laplace theorem, i.e.

$$D = (\varepsilon + i\eta - a_0)D_1 - b_1^2 D_2. \tag{S9}$$

So we can express $G_{00}^r(\varepsilon)$ as

$$G_{00}^r(\varepsilon) = \frac{1}{\varepsilon + i\eta - a_0 - b_1^2 \frac{D_2}{D_1}}. \tag{S10}$$

Analogously, D_i can be expanded in terms of D_{i+1} and D_{i+2} as

$$D_i = (\varepsilon + i\eta - a_i)D_{i+1} - b_{i+1}^2 D_{i+2}. \tag{S11}$$

Then we can get $G_{00}^r(\varepsilon)$ by using the continued fraction expansion method. In actual calculations, we have to take a cutoff of the tridiagonal Hamiltonian matrix as long as the retarded Green's function is converged. Namely, a_∞ and b_∞ are terminated at a_N and b_N respectively, with a sufficiently large N. Then we have

$$G_{00}^r(\varepsilon) = \cfrac{1}{\varepsilon + i\eta - a_0 - \cfrac{b_1^2}{\varepsilon + i\eta - a_1 - \cfrac{b_2^2}{\varepsilon + i\eta - a_2 - \cdots - b_{N-1}^2 \Sigma(\varepsilon)}}}, \tag{S12}$$

where

$$\Sigma(\varepsilon) = \frac{\varepsilon - i\sqrt{4b_N^2 - (\eta - a_N)^2} - a_N}{2b_N^2}. \tag{S13}$$

If we construct the seed state in the manner $|f_0\rangle = c_1|\alpha \boldsymbol{R}\rangle + c_2|\alpha' \boldsymbol{R'}\rangle$ with c_1 and c_2 being the arbitrary normalized coefficients, the obtained Green's function $G_{00}^r(\varepsilon)$ is associated with the ones used in Eq.(**??**), i.e.

$$G_{00}^r(\varepsilon) = |c_1|^2 G^r_{\alpha\boldsymbol{R},\alpha\boldsymbol{R}}(\varepsilon) + |c_2|^2 G^r_{\alpha'\boldsymbol{R'},\alpha'\boldsymbol{R'}}(\varepsilon) + c_1^* c_2 G^r_{\alpha\boldsymbol{R},\alpha'\boldsymbol{R'}}(\varepsilon) + c_1 c_2^* G^r_{\alpha'\boldsymbol{R'},\alpha\boldsymbol{R}}(\varepsilon), \tag{S14}$$

Then, by altering the normalized coefficients and repeating the above Lanczos procedure, we can finally obtain the Green's functions $G^r_{\alpha\boldsymbol{R},\alpha'\boldsymbol{R'}}(\varepsilon)$ and $G^r_{\alpha'\boldsymbol{R'},\alpha\boldsymbol{R}}(\varepsilon)$.

Finally, it is necessary to check the convergence of the numerical results of RKKY interaction with respect to N, the recursion cutoff in Lanczos method. If the numerical results always depend on N sensitively, it means that a result with any given N still suffer from the finite cluster effect. Hence the Lanczos method fails to study numerically the RKKY interaction of the system under our consideration. We have already checked the convergence. Fortunately, we find that in any case the cutoff $N = 1500$ is large enough to result in a convergent result of RKKY interaction which is almost independent of the further increase of N. Such a convergence is exemplified by the numerical results in Fig.S1 where the dependence of the calculated RKKY interaction on N is shown for two typical cases.

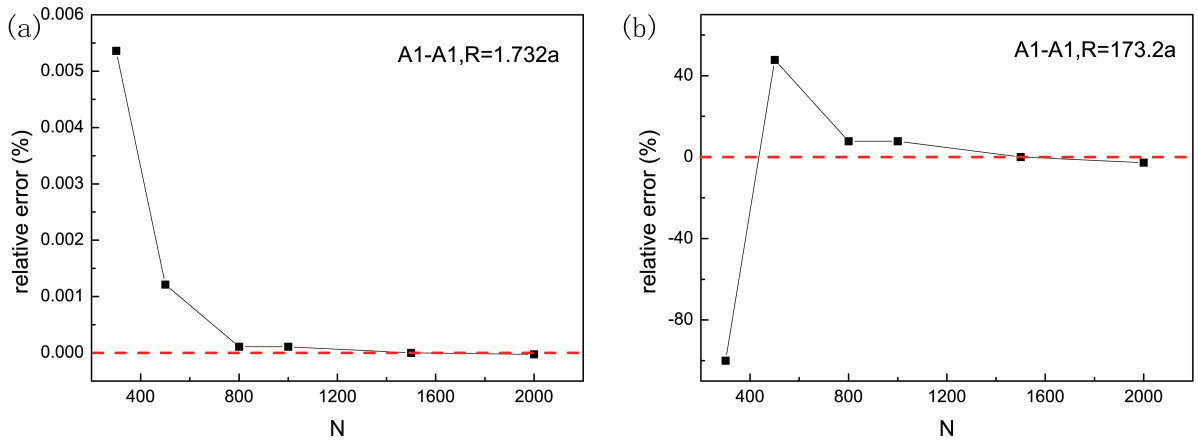

FIG. S1: (Color online) Illustration of the convergence of the calculated RKKY interaction in 30° TBG with respect to the recursion cutoff N. (a) $J_{A1\text{-}A1}(R)$ with the relevant parameter fixed at $R = 1.732a$ and (b) $J_{A1\text{-}A1}(R)$ with $R = 173.2a$. In both cases convergence is well achieved at $N = 1500$.