2-nd Workshop on Nanoscience: Carbon-Related Systems and Nanomaterials

July 4-7, 2012, NCTS, NCKU

Band-structure of graphene above the vacuum level

Vladimir U. Nazarov

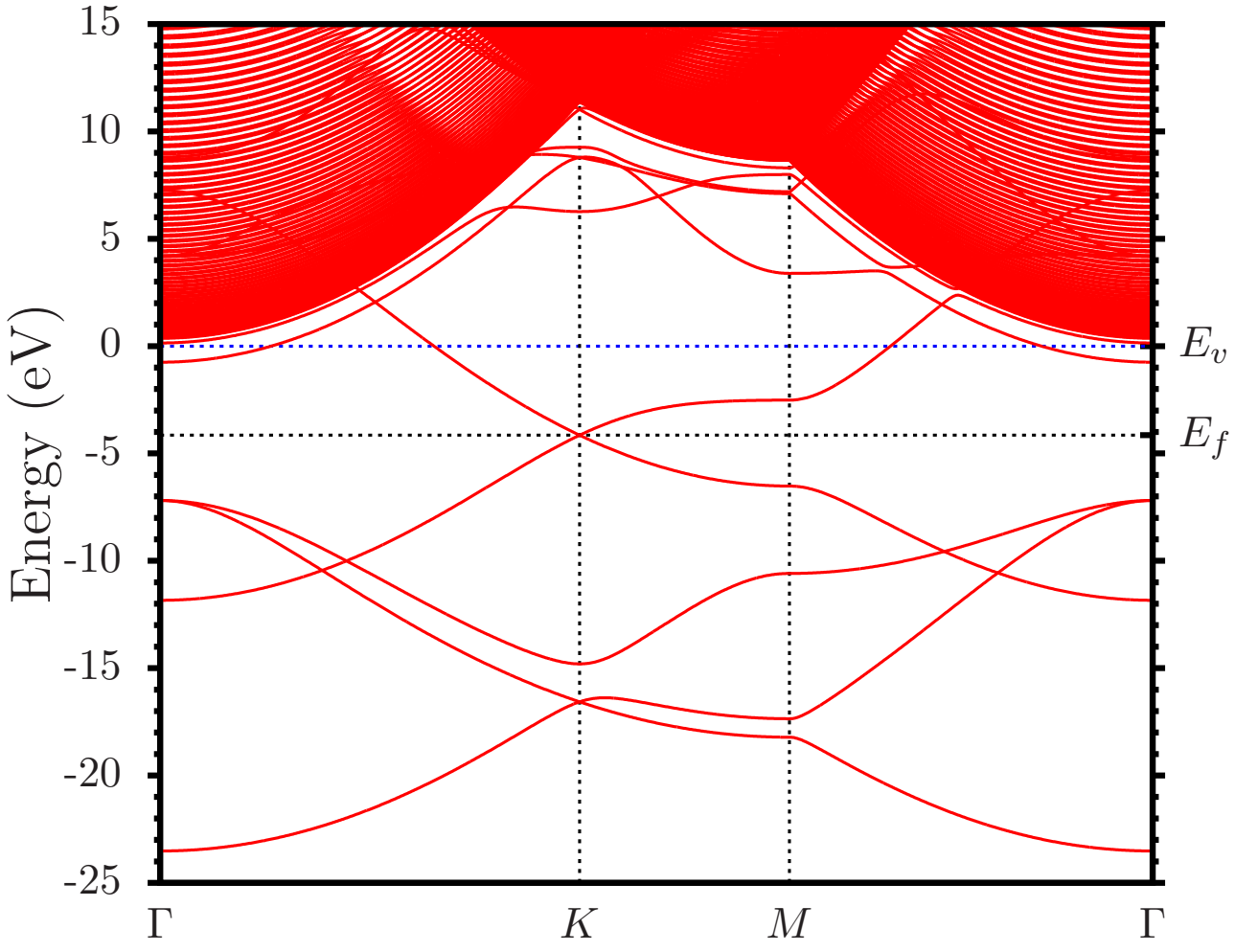
Research Center for Applied Sciences, Academia Sinica
Taiwan

In collaboration with:

Eugene Kogan, Bar-Ilan University, Ramat-Gan, Israel;

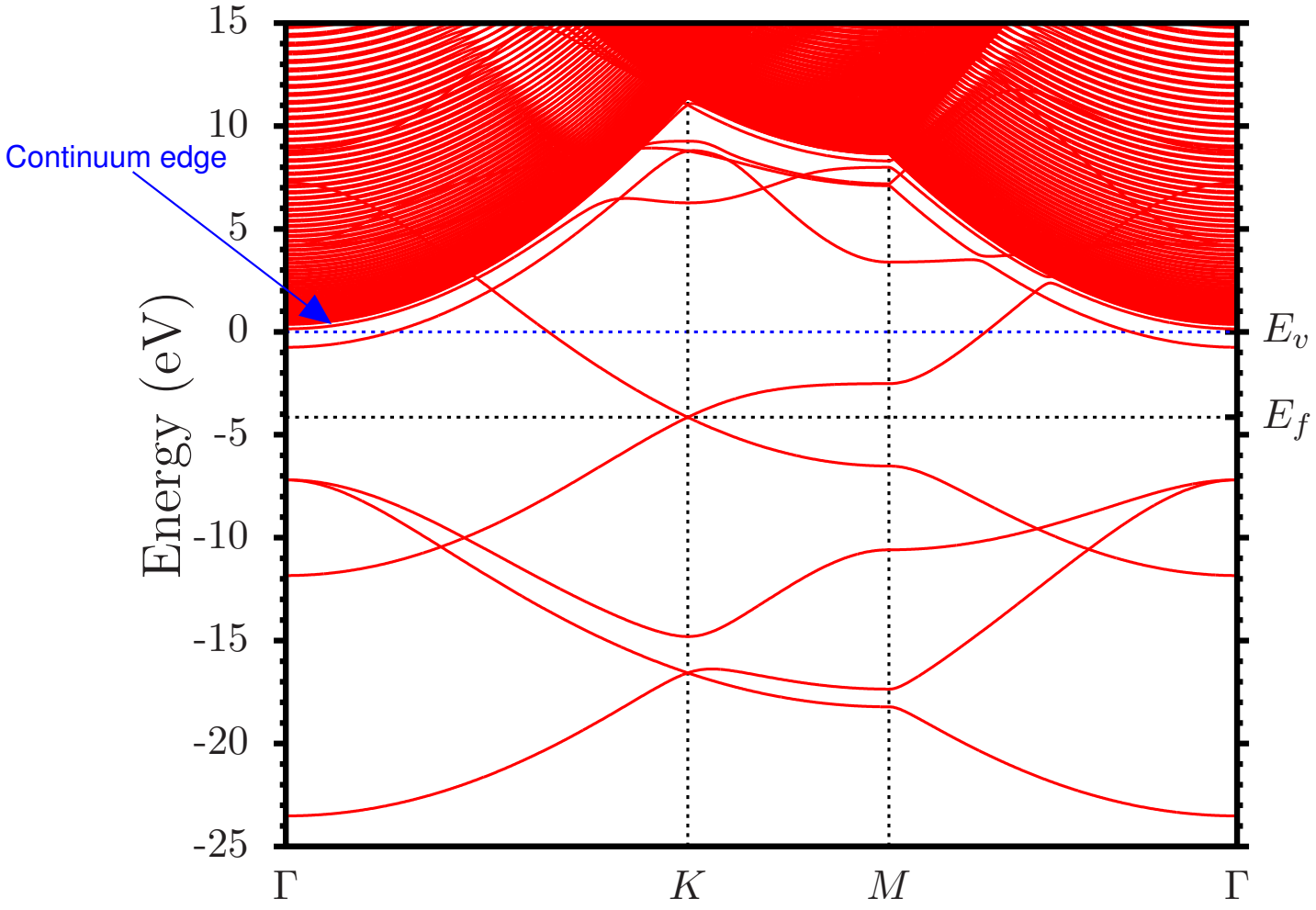
Vyacheslav Silkin, Eugene Krasovskii, Donostia International Physics Center, San Sebastian, Spain.

Motivation



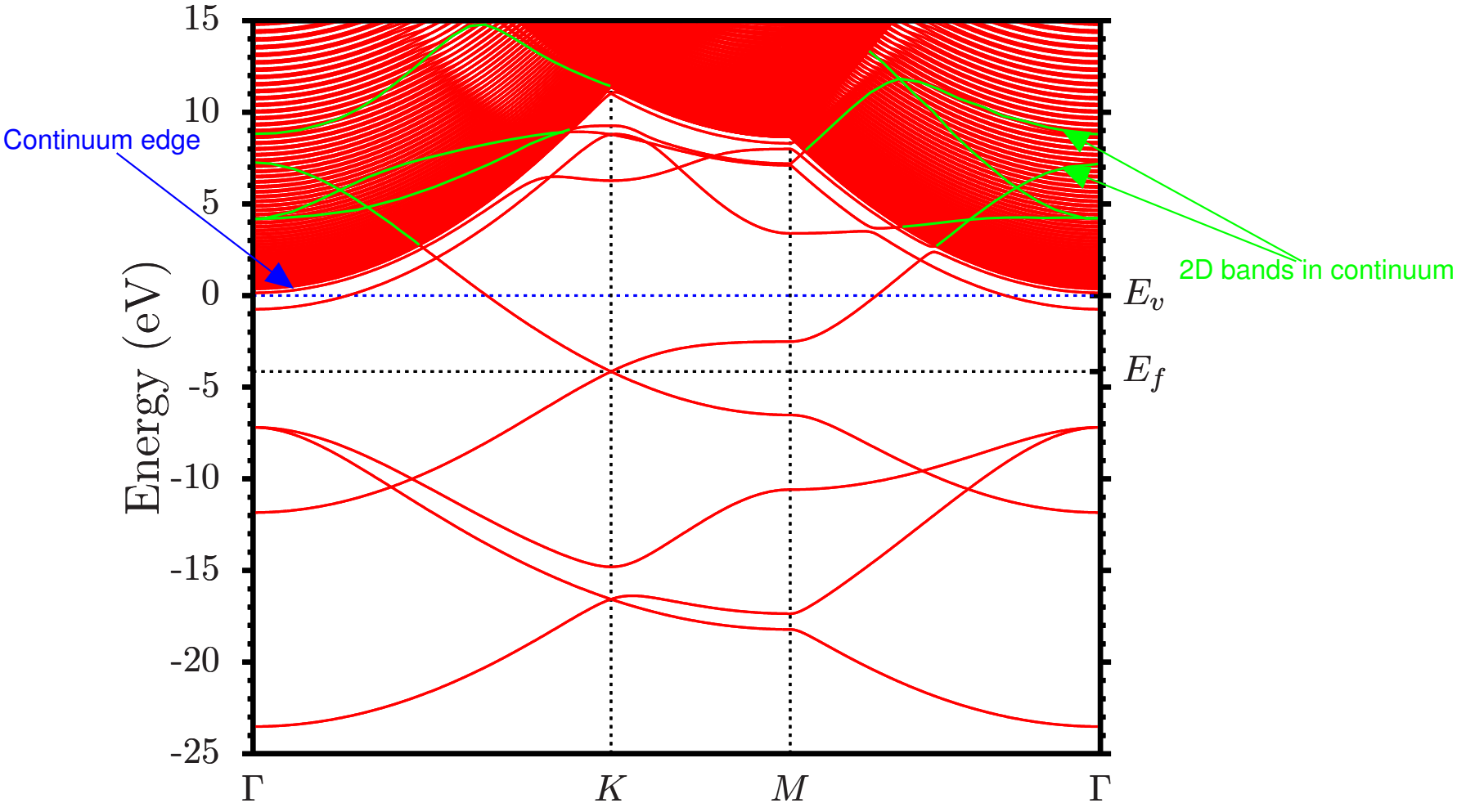
Ab initio band-structure of graphene.

Motivation



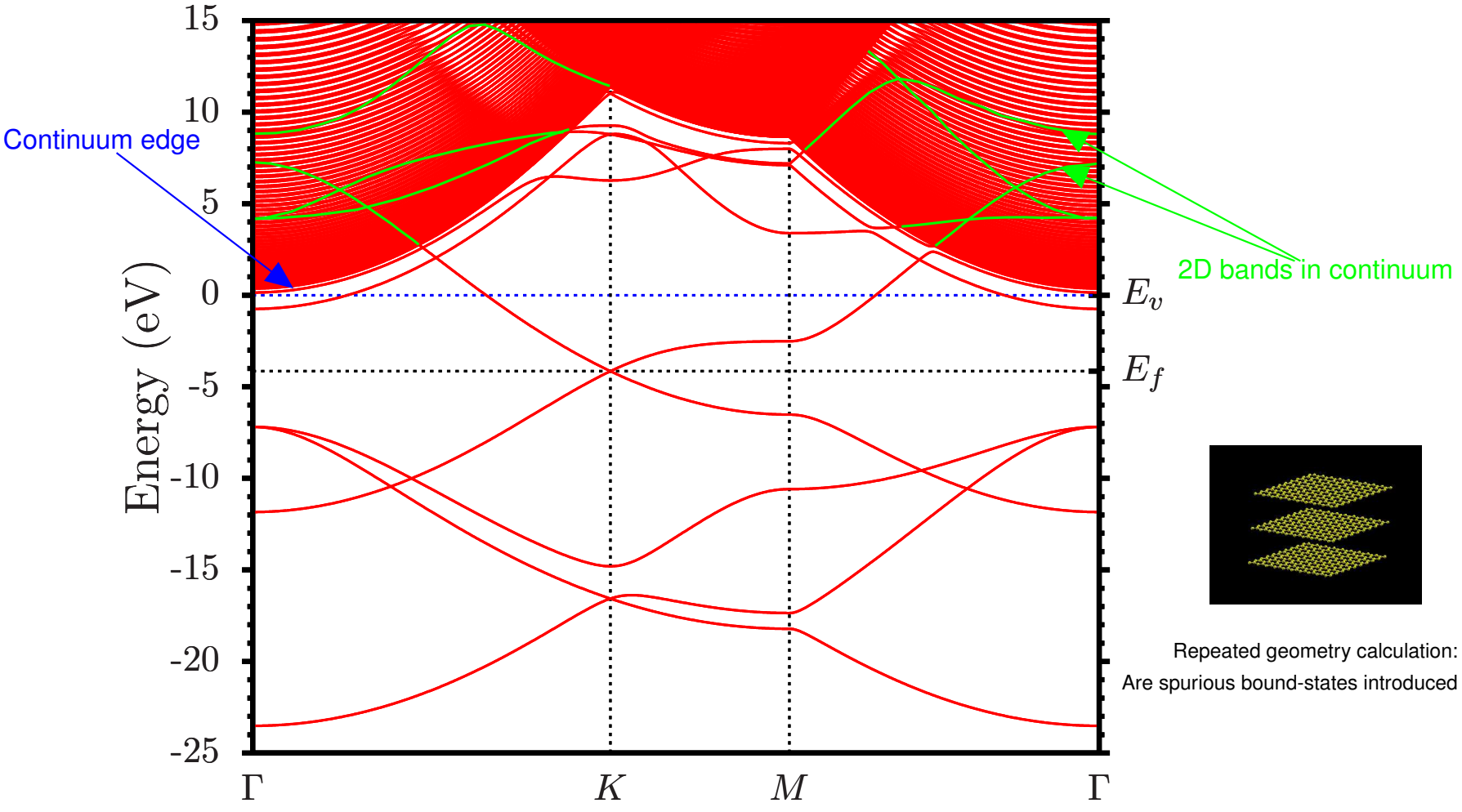
Ab initio band-structure of graphene.

Motivation



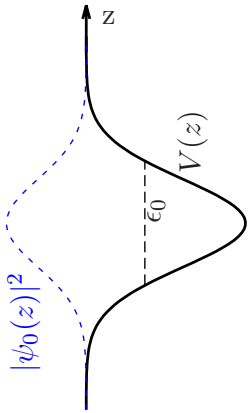
Ab initio band-structure of graphene.

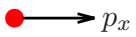
Motivation



Repeated geometry calculation:
Are spurious bound-states introduced ?

Ab initio band-structure of graphene.

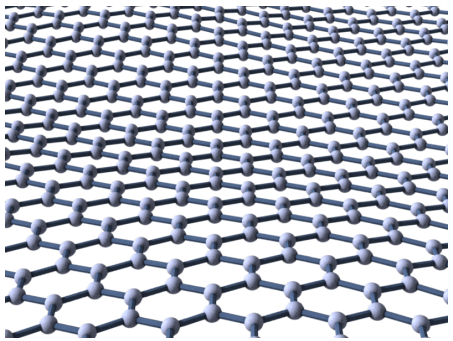




$$\psi(x,z) = \psi_0(z) \times e^{ip_x x}$$
$$E = \epsilon_0 + \frac{p_x^2}{2m}$$

In the case of a potential well in z direction and a uniform potential in xy plane, two perpendicular motions decouple.

Therefore, states bound in z direction, may have arbitrarily large energy due to the lateral motion of an electron.



Does this change and how if a laterally periodic potential is applied ?

Obviously, the in-plane and the perpendicular motions do couple in the presence of a periodic lateral potential.

We consider a model system with the potential

$$V(\mathbf{r}) = V(\mathbf{r}_\parallel) \times \delta(z), \tag{1}$$

where $V(\mathbf{r}_\parallel)$ is a 2D periodic function. By Fourier transform

$$V(\mathbf{r}_\parallel) = \sum_{\mathbf{G}} V_{\mathbf{G}}\, e^{i\mathbf{G}\cdot\mathbf{r}_\parallel}. \tag{2}$$

$V_{\mathbf{0}}$ is chosen negative to ensure the existence of a bound-state in z direction.

We are solving the single-particle Schrödinger equation

$$\left[-\frac{1}{2}\Delta + V(\mathbf{r}_\parallel)\delta(z)\right]\psi(z,\mathbf{r}_\parallel) = E\psi(z,\mathbf{r}_\parallel). \tag{3}$$

Solutions localized near and continuous across the $z = 0$ plane are

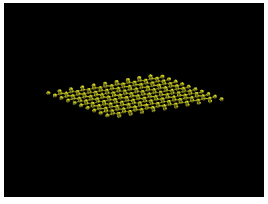
$$\psi(z,\mathbf{r}_\parallel) = \sum_{\mathbf{G}} a_{\mathbf{G}} e^{-\sqrt{(\mathbf{G}+\mathbf{k})^2 - 2E}\,|z|} e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}_\parallel} \tag{4}$$

where $a_{\mathbf{G}}$ satisfy the system of linear equations

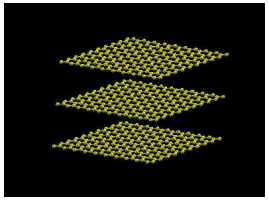
$$\sum_{\mathbf{G}'} V(\mathbf{G}-\mathbf{G}')a_{\mathbf{G}'} = -\sqrt{(\mathbf{G}+\mathbf{k})^2 - 2E}\, a_{\mathbf{G}}. \tag{5}$$

Eqs. (5) constitute a non-linear eigenvalue problem with respect to the eigenvalue E.

Stand-alone vs. repeated geometry



Stand-alone 2D-periodic layer.



Repeated geometry representation.

Bound-states above the vacuum level are resolved inside the continuous spectrum. Price: Non-linear eigenvalue problem.

Continuous spectrum and bound-states are intermixed above the vacuum level. Conventional (linear) eigenvalue problem.

$$\sum_{\mathbf{G}'} V(\mathbf{G}-\mathbf{G}')a_{\mathbf{G}'} = -\sqrt{(\mathbf{G}+\mathbf{k})^2 - 2E}\, a_{\mathbf{G}}. \qquad (6)$$

First, if $E > (\mathbf{G}+\mathbf{k})^2/2$ with an arbitrary $\mathbf{G}$ then the eigenvalue problem involves complex matrix elements. We, however, prove the following

Lemma

The problem (6) admits no resonance solutions, i.e., all the eigenvalues E are real.

Proof.

$$\sum_{\mathbf{G}\mathbf{G}'} a^*_{\mathbf{G}'} V(\mathbf{G}-\mathbf{G}')a_{\mathbf{G}'} = -\sum_{\mathbf{G}} \sqrt{(\mathbf{G}+\mathbf{k})^2 - 2E}\, |a_{\mathbf{G}}|^2. \qquad (7)$$

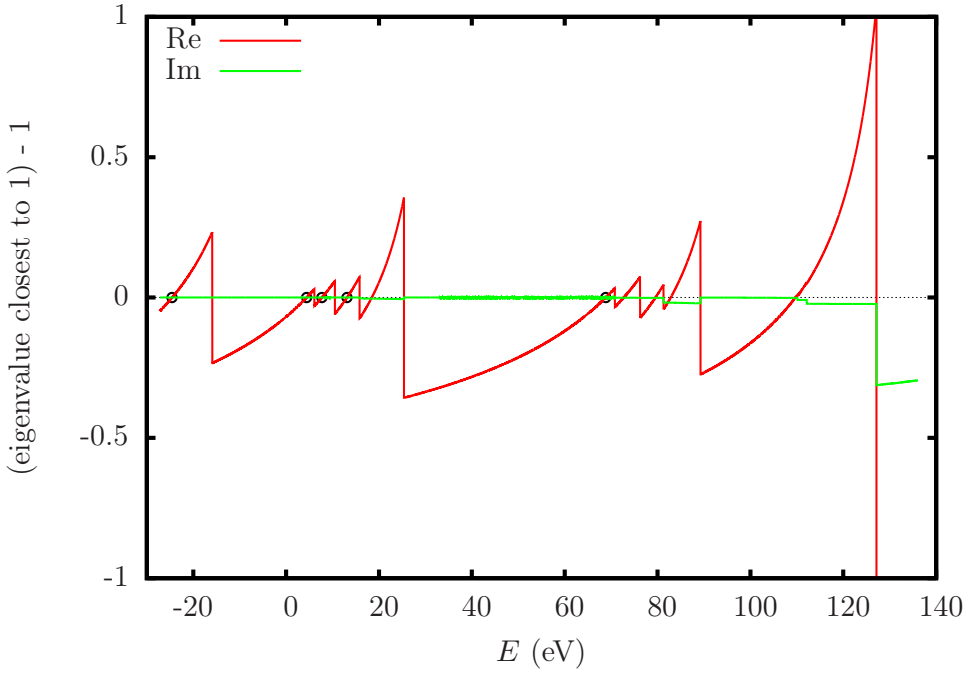
□

We are numerically solving the non-linear eigenvalue problem

$$\sum_{\mathbf{G}'} B_{\mathbf{G}\mathbf{G}'}(E) a_{\mathbf{G}'} = a_{\mathbf{G}}, \tag{8}$$

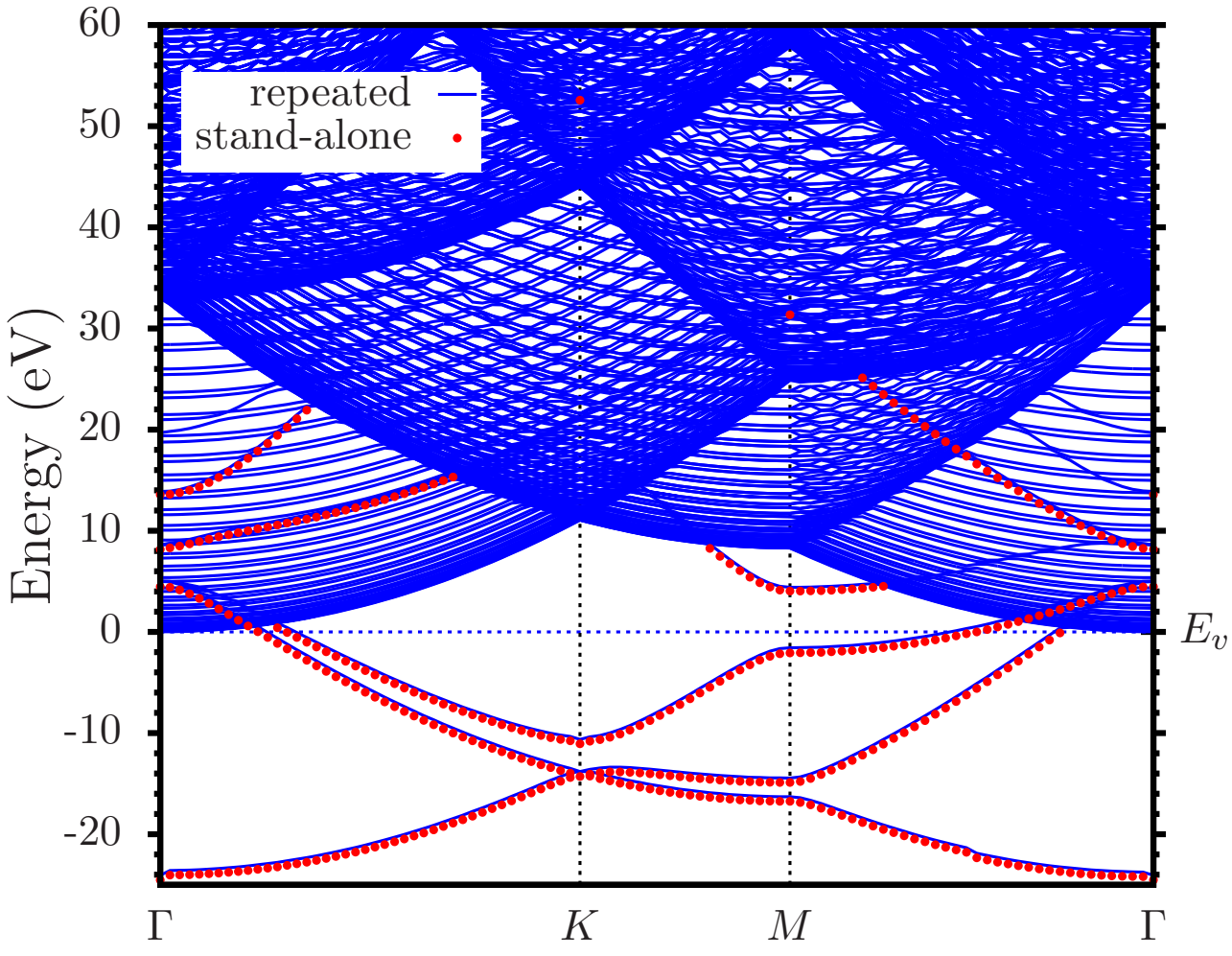
where

$$B_{\mathbf{G}\mathbf{G}'}(E) = -\frac{V(\mathbf{G}-\mathbf{G}')}{\sqrt{(\mathbf{G}+\mathbf{k})^2 - 2E}}. \tag{9}$$



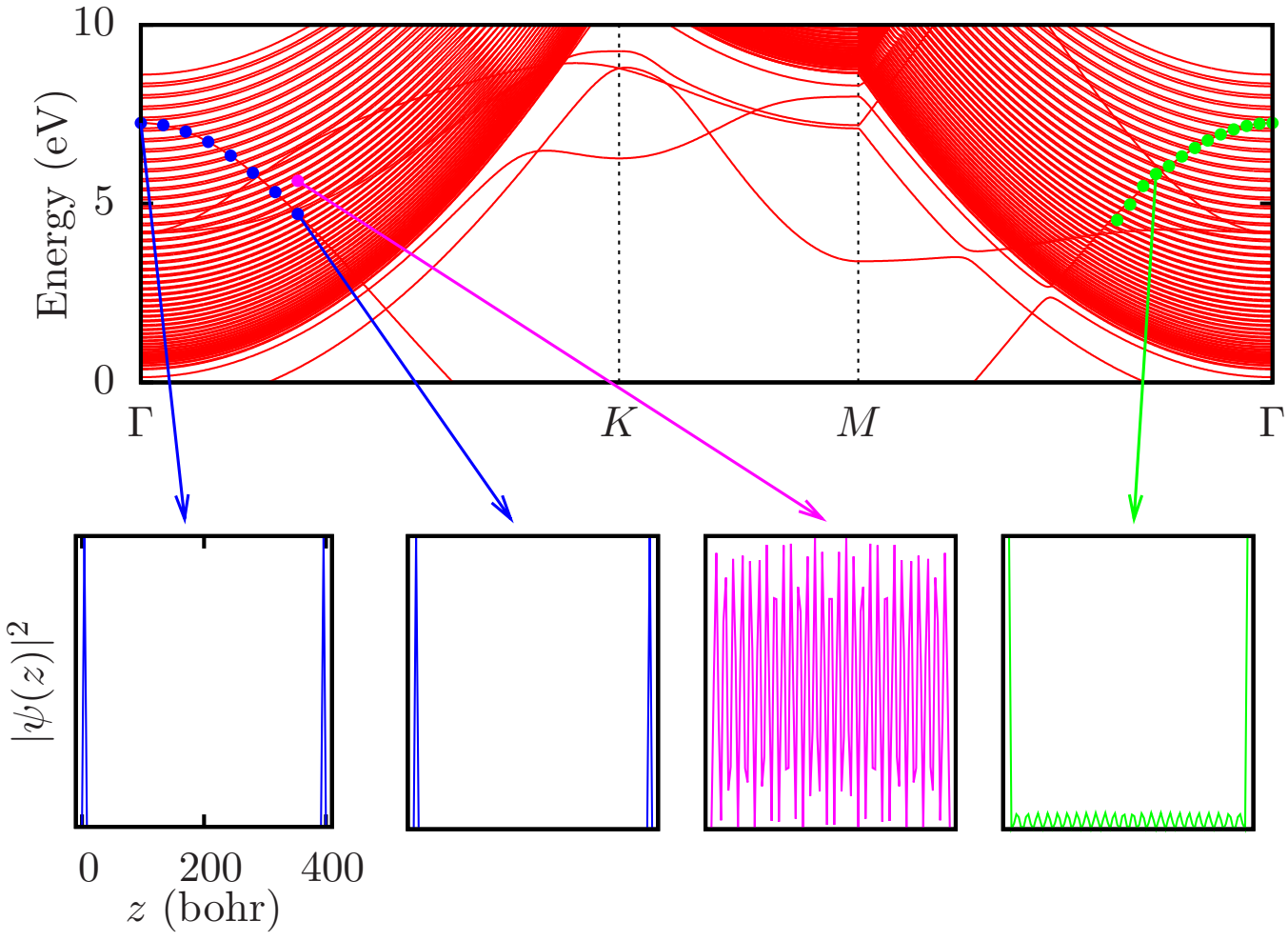
The eigenvalue of matrix B as a function of E.

Model band-structure



Model band-structure of a single periodic layer (red points) and layers in repeated-geometry (blue lines).

Projection on the *ab initio* graphene problem



z-dependence of the wave-functions of the states above the vacuum level obtained in the repeated geometry calculation.

Conclusions

- Our analysis shows that the graphene band-structure is affected drastically by the possibility for an electron above the vacuum level to escape from the layer;
- Whether or not at a particular $\mathbf{k}$ point a state above the vacuum level is bounded to the graphene layer is determined by the symmetry of that point.