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# Electron energy-loss spectroscopy of quasi-2D crystals: Beyond the energy-loss functions formalism

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Inelastic scattering of the medium-energy (~10-100 eV) electrons underlies the method of the high-resolution electron energy-loss spectroscopy (HREELS), which has been successfully used for decades to characterize pure and adsorbate-covered surfaces of solids. With the emergence of graphene and other quasi-two-dimensional (Q2D) crystals, HREELS could be expected to become a major experimental tool to study this class of materials. We, however, identify a critical flaw in the theoretical picture of the HREELS of Q2D crystals in the context of the inelastic scattering only (``energy-loss functions" formalism), in contrast to its justifiable use for bulk solids and surfaces. The shortcoming is the neglect of the elastic scattering, which we show is inseparable from the inelastic one, and which, affecting the spectra dramatically, must be taken into account for the meaningful interpretation of the experiment. With this motivation, we build a theory of the simultaneous inelastic and elastic electron scattering at Q2D crystals. We apply this theory to HREELS of graphene, revealing an important effect of the strongly coupled excitation of the  $\pi + \sigma$  plasmon and elastic scattering resonances [1]. Our results open a path to the consistent and interpretable study of the elementary excitations in crystalline mesoscopic materials by means of HREELS, with its supreme resolution on the meV energy-scale, which is far beyond the capacity of the now overwhelmingly used EELS in transmission electron microscope [2].

#### References

- 1. V. U. Nazarov, E. E. Krasovskii, and V. M. Silkin (2013), Scattering resonances in two-dimensional crystals with application to graphene. *Phys. Rev.* B 87:041405(R).
- 2. V. U. Nazarov, V. M. Silkin, E. E. Krasovskii (2017) Probing mesoscopic crystals with electrons: One-step simultaneous inelastic and elastic scattering theory, *Phys. Rev.* B 96: 235414.

## **Recent Publications**

- 1. V. U. Nazarov (2017) Quasi-low-dimensional electron gas with one populated band as a testing ground for time-dependent density-functional theory of mesoscopic systems, Physical Review Letters 118:236802.
- 2. V. U. Nazarov (2016) Exact exact exchange potential of two- and one-dimensional electron gases beyond the asymptotic limit, *Physical Review* B 93:195432.

## **Biography**

Vladimir U. Nazarov, (Ph.D.-physics), now is an Associate Research Fellow at the Research Center for Applied Sciences, Academia Sinica, Taiwan. He got his B. Sc in physics, M. Sc physics from the Far-Eastern National University, Vladivostok, Russia, and his Ph.D. degree from the Institute for Automation and Control Processes, Far-Eastern Branch of Russian Academy of Sciences, Vladivostok, Russia. Currently Dr. Vladimir Nazarov's researches focus on the fundamentals of Time-Dependent Density-Functional Theory (TDDFT) and its applications to optics and transport in bulk materials and low-dimensional structures. Dr. Vladimir Nazarov has his Habilitation (in Russia, Doctor of Physical and Mathematical Sciences) from the Far-Eastern National University, Russia. The past positions of Dr. Vladimir Nazarov include the Leading Researcher at the Institute for Automation, Far-Eastern Branch of Russian Academy of Sciences, the Associate Professor at Kyushu Institute of Technology, Japan, Visiting Professor at the Institute for Solid State Physics, Japan, and Visiting Professor at Chonnam National University, South Korea

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