

Can photon Green's functions be integrated into a quantum kinetic theory?

We presented a method for the computation of photon Green's functions suitable for integration in a comprehensive quantum-kinetic theory of absorption and emission processes in layer-based nanostructures with applications in novel ultra-thin solar cell devices.

Can quantum computers simulate Green's function?

Although the development of quantum computers in the near future may enable us to compute energy spectra of classically intractable systems, methods to simulate the Green's function with near-term quantum algorithms have not been proposed yet.

How to calculate Green's function of a Hamiltonian on near-term quantum computers?

Here, we propose two methods to calculate the Green's function of a given Hamiltonian on near-term quantum computers. The first one makes use of a variational dynamics simulation of quantum systems and computes the dynamics of the Green's function in real time directly.

How is Green's function computed?

The first one makes use of a variational dynamics simulation of quantum systems and computes the dynamics of the Green's function in real time directly. The second one utilizes the Lehmann representation of the Green's function and a method which calculates excited states of the Hamiltonian.

Why is the Green's function important?

The Green's function plays a crucial role when studying the nature of quantum many-body systems, especially strongly correlated systems.

What is NEGF (non-equilibrium Green's function formalism)?

In both situations, the density and occupation of the entire spectrum of photonic modes needs to be determined for an optically open system. An elegant method ideally suited for this task is the non-equilibrium Green's function formalism (NEGF).

Simulation and the group of organic and hybrid solar cells at the Research Centre Jülich (Institute for Energy and Climate Research). Previously, he was a Junior Research Fellow at Imperial College London. His research interests include all aspects regarding the fundamental understanding of photovoltaic devices including their character-

The combinatorial growth of the Hilbert space makes the many-electron problem one of the grand challenges of theoretical physics. Progress relies on the development of non-perturbative methods, based on either wavefunctions or self energies. This made, in recent years, calculations for strongly correlated materials a

reality. These simulations draw their power ...

Photovoltaics (IEK-5), Forschungszentrum Jülich, 52425 Jülich, Germany e-mail: u.aeberhard@fz-juelich. Fig. 1. Model system used in the simulations. The gold reflector is only used for the optical simulation. Ohmic contacts are assumed for majority carriers. block minority carriers at the contacts by corresponding barrier

Forschungszentrum Jülich, D-52425 Jülich, Germany and; Zernike Institute for Advanced Materials, University of Groningen, NL-9747 AG Groningen, The Netherlands Kristel Michielsen Institute for Advanced Simulation, Jülich Supercomputing Centre, Forschungszentrum Jülich, D-52425 Jülich, Germany and; RWTH Aachen University, D-52062 ...

This thesis is concerned with the quantum mechanical investigation of a novel class of magnetic phenomena in atomic and nanoscale-sized systems deposited on surfaces or embedded in bulk materials that result from a competition between the exchange and the relativistic spin-orbit interactions. The thesis is motivated by the observation of novel spin-textures of one and two ...

solar cells in Prof. Michael Saliba's group. aInstitute for Photovoltaics (ipv), University of Stuttgart, 70569 Stuttgart, ... the external quantum efficiencies and (ii) the stabilities of these PeLEDs. The role of perovskite in lasing ... gator at the Forschungszentrum Jülich, Germany. He is renowned for his pioneering discoveries in

We can now show that an L^2 space is a Hilbert space. Theorem 2.3. For $p \geq 1$, an L^p space is a Hilbert Space only when $p = 2$. Proof : We see that the inner product, $\langle x, y \rangle = \sum_{n=1}^{\infty} x_n \overline{y_n}$ has a metric; $d(x, y) = \|x - y\|_2 = \sqrt{\sum_{n=1}^{\infty} |x_n - y_n|^2}$. This agrees with the definition of an L^p space when $p = 2$. An L^2 space is closed and therefore complete, so it follows that an L^2 space is a Hilbert

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This article reviews the application of the nonequilibrium Green's function formalism to the simulation of novel photovoltaic devices utilizing quantum confinement effects in low dimensional absorber structures. It covers well-known aspects of the ... **ABSTRACT** Quantum well solar cells have been introduced as high efficiency photovoltaic ...

Loosely speaking, if such a function G can be found for the operator L , then, if we multiply the equation 1 for the Green's function by $f(s)$, and then integrate with respect to s , we obtain, $(,) = () = ()$. Because the operator $=$ is linear and acts only on the variable x (and not on the variable of integration s), one may take the operator

outside of the integration, yielding $(\langle \cdot \rangle) = \langle \cdot \rangle$.

states only, the spin index in the electronic Green function can be suppressed; (ii) the perturbation H_{e-ph} does not mix different electronic bands or phononic modes, such that the interacting Green functions can still be represented by a single band/mode index. The bare Green functions of the unperturbed Hamiltonian $H_0 = H_e + H_{ph}$ are $G_0(k, \dots)$...

Hybrid Quantum Classical Simulations Dennis Willsch¹, Manpreet Jattana;², Madita Willsch³, Sebastian Schulz^{1,2}, Fengping Jin¹, Hans De Raedt;⁴, and Kristel Michiels^{2,3} ¹ Institute for Advanced Simulation, Jülich Supercomputing Centre, Forschungszentrum Jülich, 52425 Jülich, Germany

The light-matter interaction in planar nanostructures with applications in photovoltaic devices is investigated by means of a microscopic quantum-kinetic theory based on the non-equilibrium Green's function formalism. The Dyson and Keldysh equations for the Green's functions of photons are solved numerically. The result is used to couple the optical and ...

The first comprehensive overview over the NEGF modelling framework for solar cells is given in: [2] U. Aeberhard, Theory and simulation of quantum photovoltaic devices based on the non-equilibrium Green's function formalism, J. Comput. Electron. 10, 394 (2011). For a recent overview of applications to nanostructure photovoltaics:

⁴ Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Jülich, Germany ... elements as a function of the energy of the deuteron beam. We found that ¹¹B exhibits the highest neutron yield but more work has to be done regarding mechanical engineering and heat load aspects. According to the current state of

the photon collection in photovoltaic fluorescent collectors L. Pröbcke^{1,a}, G.C. Glaser¹, and U. Rau² ¹ Institut für Photovoltaik, Universität Stuttgart, Pfaffenwaldring 47, 70569 Stuttgart, Germany ² IEK5-Photovoltaik, Forschungszentrum Jülich, 52425 Jülich, Germany Received: 29 August 2011 / Accepted: 29 February 2012

The AiiDA-Spirit plugin for automated spin-dynamics simulations and multi-scale modelling based on first-principles calculations Philipp Rüßmann¹, Jordi Ribas Sobreviela,^{1,2} Moritz Sallermann,^{1,3} Markus Hoffmann,¹ Florian Rhiem,⁴ and Stefan Blugel¹ ¹ Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, ...

Green function at finite temperature) and the self-energy $\Sigma(k; z)$ can be introduced as usual: $z \pm \Sigma(k; z) = G(k; z)^{-1}$ (11) Next we discuss the analytical structure of the Green function and the self energy. It can be seen from (10) that the Fourier transform of the Green function has the general form $G(z) = \sum_i \frac{c_i}{z - \epsilon_i}$; where the ϵ_i are ...

Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany; Abstract We analyze the finite lifetimes of the topologically protected electrons in the surface state of Bi_2Te_3 and Bi_2Se_3 due to elastic scattering off surface vacancies and as a function of energy. The scattering

that the self-energy has a spectral representation similar to that of the Green function: $G(z) = 1 + \sum_r S_r S_r^\dagger / (z - \epsilon_r)$; (22) where the ϵ_r are poles located on the real axis (they are zeros of the Green function). By contrast with the Green function, the self-energy may have a ...

In the beginning the Green functions were calculated mostly by using the spectral representation (8). This is easy for the imaginary part of the Green function because according to (9) the imaginary part of the denominator leads to a delta function so that only values contribute which are in the range for which the Green function is needed.

and the spin flip terms yields $\langle T^j T^k \rangle = JS$, so that all three contributions from the scalar product $JS \sim S$ add up to $\langle T^j T^j \rangle = J^2 S(S+1) + O(J^3)$ using the optical theorem. In second order in J , we just find a constant contribution similar to a residual potential scattering term.

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