Calculation of optical properties of semiconductor nanocrystals in the framework of density functional theory using GPU parallel programming

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At the present time silicon nanocrystals form the basis of modern microelectronics and they are widely used for the diagnosis of biological objects. The problem of modeling at the atomic level is relevant for the design of silicon nanoparticles, which play an important role in creating active optical elements - quantum dots - doped silicon nanocrystals, the optical properties are essentially the next generation of optical storage, optical communication devices, etc [1]. There is a large class of situations where the nanocrystals with high quantum states of electrons population are subjected to the strong driving laser field.

In the present work an effective parallel algorithm is proposed for calculating optical properties of many-electron systems based on the dynamic density functional method [2]. The starting point of the time dependent density functional theory is a system coupled Schrödinger equations for the electron orbitals $\varphi_j(\vec{r},t)$: $i\frac{\partial}{\partial t}\varphi_j(\vec{r},t)=\left[-\frac{\nabla^2}{2m}+\upsilon_{KS}(\vec{r},t)\right]\varphi_j(\vec{r},t)$, где $\upsilon_{KS}(\vec{r},t)=\upsilon(\vec{r},t)+\int d^3\vec{r}\,'\frac{n(\vec{r}\,',t)}{|\vec{r}-\vec{r}\,'|}+\upsilon_{xc}(\vec{r},t)$, is the sum of an external potential $\upsilon(\vec{r},t)$, the Hartree potential and the exchange-correlation potential $\upsilon_{xc}(\vec{r},t)$. In this work adiabatic approximation of the local density is used for $\upsilon_{xc}(\vec{r},t)$. The electron density of the interacting system $n(\vec{r},t)=\sum_{j=1}^{N}\left|\varphi_j(\vec{r},t)\right|^2$ can be defined as the sum of squares of the moduli of the single-particle orbitals filled with N electrons.

As a test for the solutions of the dynamic Kohn-Sham equations, the behavior of the interaction electrons in a spherical quantum dot is investigated. The result of the numerical solution is the Fourier transform of the dipole moment $<e\cdot\vec{r}>=\int e\cdot n(\vec{r},t)\cdot\vec{r}d^3\vec{r}$ of the system, which characterizes the excitation spectrum of interacting electrons in a quantum dot.

It was found that the most effective method for solving dynamic equations is the explicit Runge-Kutta 4th order. The main advantage of this algorithm is that the calculation of the wave function at each grid point can be performed independently, and therefore simultaneously. The Runge-Kutta method requires O (N) operations. After that requires a transfer of values of the wave function at the boundary nodes for systems with distributed memory and at only extension of the blocks on the boundary nodes for a system with shared memory. The developed algorithm has been realized on a GPU cluster. Testing of the algorithm was performed on the device with the maximum number of nodes produced by 30464 graphics cores.

The developed software component showed good scalability in the case of proportional resizing of the problem being solved. It is shown that the most effective solutions for the Schrodinger equation is a temporary method of Runge-Kutta method. The possibility of scaling data circuits on distributed memory systems and describes the implementation of the algorithm on the GPU. It has been demonstrated that the algorithm can be used to determine the spectra of both isolated and interacting silicon nanocrystals (quantum dots).

[1] T.W. Ebbesen, C. Genet, and S. I. Bozhevolnyi, Phys. Today 61, 44 (2008).

[2] E. Runge and E.K.U.Gross. Phys. Rev. Lett. 52, 997 (1984).