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ITERATIVE CALCULATION OF ELECTRON WAVE FUNCTIONS IN QUANTUM NANOCLUSTERS

Электронның өзіндік функцияларын жаңа тиімді жолмен есептеп шығару ұсынылған. Үлкен көлемді реттелмеген нанокластерде кванттық сәттер зерттелген. Бұл үшін ретсіз қоспалы потенциалды Андерсонның моделі қолданылды. Электрондардың спектрі мен толқындық функциялары Ланцоштың итерациялық тәсілін қолдану арқылы есептеліп шығарылған. Бұл тәсілдің көлемі 100 Å электроникада эксперименталдық жағдайға жақындаудың мүмкіндігі дәлелденген.

Предлагается новое эффективное вычисление собственных функций электрона. Изучены квантовые состояния в неупорядоченных нанокластерах большого размера. Для расчетов используется модель Андерсона с хаотическим примесным потенциалом. Вычисление спектра и волновых функций электронов проводится методом итераций Ланцоша. Показано, что этот метод позволяет приблизиться к экспериментальной ситуации в наноэлектронике с реальными размерами кластеров до 100 Å.

1. Introduction

The investigation of the conductivity of an electronic system of very small sizes corresponding to the dimensions of nanodevices belongs to the very heard of the modern condensed matter physics. The classical Drude theory of the electronic transport was built on the idea of free electrons scattered by positive ions located in sites of a metallic lattice. A crucial point of this approach was the mean free path, the average length an electron flies before it encounters a lattice ion. Therefore, the electron conductivity should be proportional to the mean free path, according to the classical theory of metals. This was established experimentally as being too large, i.e. around 100nm, meaning two orders of magnitude larger than the lattice constant. The wave character of an electron causes the electron to diffract from an ideal nanocrystal. Actually, the resistance appears only when electrons scatter form imperfections in a crystal, such as impurities, lattice shifts, dislocations, declinations etc. Since there is no perfect ideal crystal in the nature, the experimentalists mostly deal with the disordered samples. The main consequence is: the more the imperfections, the smaller the mean free path and the lower the conductivity. The question arises: will any increase in the degree of the lattice disorder lead to just a decrease of the mean free path and thus to a lower electronic conductivity? A half century ago P.Anderson has discovered that beyond a critical amount of disorder of impurity potential the diffusive motion of the electrons not only reduced, it can come to a complete stopping [1]. The electron becomes trapped by the disorder and the conductivity may vanish to zero. This is due to effects of quantum localization, resulting from the enhanced backscattering provided that the motion of the electron is phase-coherent (the phase of the wave function is preserved). This is a key concept for a metal-insulator transition, based on the quantum interference phenomena. The critical amount of potential disorder, at which the extended wave functions become suddenly localized, is called the critical disorder. Thus, the one-electron states in the presence of a random impurity potential can be localized in a finite range of space at the critical point of the metal-insulator transition.

The metal insulator transition is of particular interest from the viewpoint of studying the spatial structure of the wave functions and the statistical properties of the energy spectrum of the electrons. It was found that the correlations between the amplitudes of wave functions exactly at the critical point possess the uni-

versal properties [2]. In other words, the statistics of the eigenstates calculated for finite sizes of nanoclusters can be extrapolated to those in the thermodynamic limit. At the same time the behaviour of the electron states exactly at the critical point of the transition is neither localizes, nor delocalized, it is essentially multifractal [3]. To gain knowledge about the multifractal nature of the critical wave functions one need to explore a precise structure of the eigenstates which is possible only by the exact numerical calculations. That is why it is important to investigate the nature of eigensolutions by using direct large-scale computer diagonalization. The Lanczos algorithm is one of the most effective computational tools for searching for few extreme eigenvalues and corresponding eigenvectors of large sparse Hermitian matrices [4]. It has been successfully applied to many problems in atomic, molecular and condensed matter physics, where it is required to gain information about low-lying excitations in a spectrum close to the ground state. In many applications the matrices are sparse due to various constraints, for example, a limited connectivity and a short-range coupling. Practically, the number of non-zero matrix elements is often proportional to the dimension of the matrix N rather than to N^2.

2. Iteration scheme

One of the common models used for describing electron transport properties in disordered systems close to the transition is the Anderson model oflocalization. The Hamiltonian of the model defined on a three-dimensional lattice is given by the operator

$$H = \sum_i \varepsilon_i |i><i| + I \sum_{i,j \neq i} |i><j|, \qquad \text{Eq. (1)}$$

where $|i>$ ($<i$) is the creation (annihilation) operator of an electron at a lattice site n, and m labels the neighbour sites to the site n. The on-site energies ε_i are random variables uniformly distributed within an interval of width W, such that W parameterizes the disorder. The second term corresponds to the hopping processes between the neighbour sites in the lattice. The transfer integral t can be set to unity ($t = 1$). The metal-insulator transition in the band centre, $E = 0$, occurs at the disorder $W = W$c ≈ 16.4. This value of W is called critical disorder. The sparse structure of the matrix A corresponding to the Hamiltonian H makes the Lanczos method the most suitable for solving the eigenvalue problem $H\psi_n = E\psi_n$ of large systems. For instance, the number of non-zero off-diagonal elements per line equals six in a simple cubic lattice of linear size L.Indeed, this speeds up substantially the most time-consuming part of the implementation, namely the matrix–vector multiplications. A single matrix–vector product needs computer time proportional to $N = L^3$.

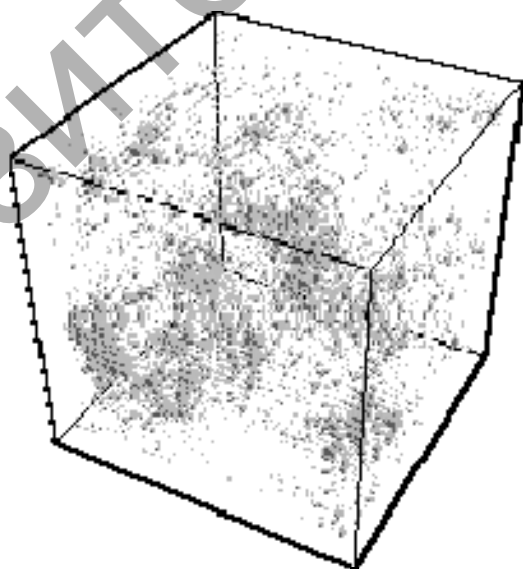

Fig. 1. Illustration of the spatial distribution of the amplitude squares of the wave function of the electronic quantum state in the middle of the Anderson model (Eq. 1). The disorder W is chosen to be exactly at the critical point of the metal-insulator transition. The linear size of the cubic nanocluster is $L = 100$. The intensity is proportional the amplitude squared. The sizes of tiny cubes correspond to the electron density at certain coordinate. One can clearly observe the multifractal structure of the electron wave function spread over the whole nanocluster

In addition, by applying the helical boundary conditions instead of the traditionally used periodic boundary conditions, as in [2], it is possible to eliminate several expensive loops of the program. Another advanced optimization is to reorganize the position of the co-diagonals, so that some of them go beyond the borders of the original square matrix A, becoming a continuation of other co-diagonals. This leads to a rectangular matrix of size $(L^2 + N)$ N. All of the off-diagonal matrix entries are presented in the form of six co-diagonals with the same length N parallel to the main diagonal and horizontally shifted from it by the distances $-L^2$; $-L$; -1; 1; L; L^2, respectively. This restructuring of the matrix A does not change the components of the resulting matrix–vector product. In fact, it allows to avoid the procedure of 'look-up' of the table-given positions of the A-matrix elements, which are usually necessary for the standard Lanczos diagonalization of the Anderson Hamiltonian [1, 3]. As a consequence, the memory requirements are also markedly diminished. Thus, instead of storing the initial structure of the matrix in the main processor memory, one needs only the fast random-number generator in order to create repeatedly the same set of diagonal elements for each matrix-vector multiplication. The convergence process to the eigensolutions was controlled by determining the upper limit of the user-specified tolerance, meaning that the norm of the matrix $(H\psi_n - E\psi_n)$ should be much more less that the minimal scale of the problem.

It is known [4] that due to the floating point arithmetic, which leads to round-off errors, the Lanczos vectors lose their global orthogonality. Therefore, after the recursions finish the size M of the tri-diagonal matrix (transfer matrix [4]) after approaches should be at least $M = 2{,}2/N$. The figure 1 shows the number of iterations as a function of energy of the electron inside of the model spectrum. The above-mentioned size M is required in order to detect the pairs of eigenvalues and the corresponding eigenvectors with absolute precision less than 10^{-9} in the internal part of the spectrum, where the density of states is maximal. Closer to the energy band edge the optimal value of M drastically decreases. Stability of the modified Lanczos-like algorithm has been tested in a wide range of the system size L ranging from 5 to 100. There is a specific property of the spectrum of disordered systems at criticality, which turns to be important and helpful for the converging procedure.

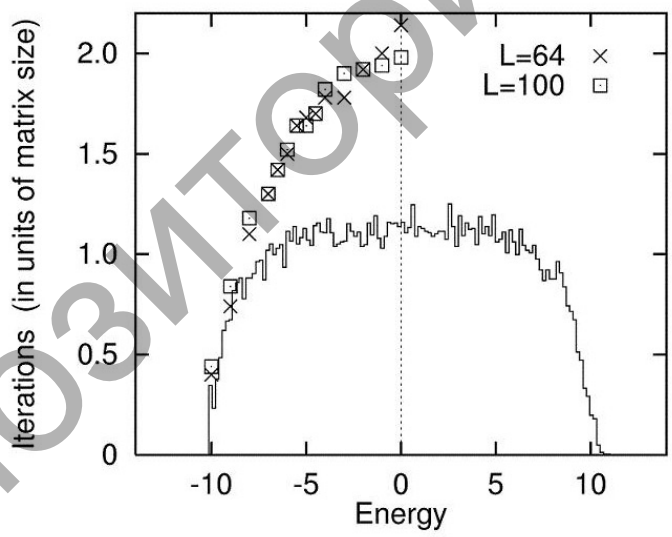

Fig. 2. The number of iterations (ratio M/N) as a function of energy E. M and N is size of the transfer-matrix and of the initial matrix, respectively. The result is for an eigenpair with the highest achievable accuracy at the disorder $W = 16.4$ for different cube sizes L.The mobility edge is exactly at the band centre of the nanocluster. The spectral density of states shown by the step line defines the band boundaries

It is a strong quantum-mechanical level repulsion that decreases the probability to find two eigenvalues close to each other by decreasing the spacing between them. This property facilitates not only the speed of the iterations, but also the bisection algorithm for finding the eigenvalues of the TM-matrix. The latter becomes more time-consuming, when one needs to calculate a relatively large part of the spectrum (more than 10 % of all of the eigenvalues). In this case the performance has been further improved by parallelizing the bisection algorithm for consequent energy sub-intervals. By varying the disorder W apart from the critical value, we have checked that the size of the transfer-matrix should be slightly larger in order to reach the desirable accuracy of the eigenvalues in a given part of the spectrum.

3. Critical statistics

One can numerically study statistical properties of fluctuations in electron spectra of 3D disordered systems. The nearest-neighbour level spacing distribution, the two-point correlation function and the form-factor have been shown with high precision to exhibit size-independence at the critical point of the Anderson transition. With increasing the size of the system they scale towards the corresponding results of the RMT below the critical disorder ($W < Wc$), and to the Poisson distribution above the critical value ($W > Wc$). As a result, in the thermodynamic limit only three universal statistics exist, including the critical statistics precisely at the transition. In the metallic phase, the range of validity of the Wigner-Dyson statistics extends to the infinite energy, because the Thouless conductance diverges for large L.In the insulating phase, the Poisson limit is expected to apply since the statistics is a consequence of the superposition of the contributions from many independent localization volumes.

In the case when time-reversal symmetry is preserved one can compare P(s) in the metallic regime for periodic and Dirichlet boundary conditions. We have found that it is important to distinct between the Wigner surmises and the results of the RMT, in order to extract the weak-localization corrections. It is consistent with our results to assume that the level statistics depends on the boundary conditions, not only in the metallic regime, but also at the critical point, since at $W = Wc$ the localization length diverges. The influence of the broken time-reversal symmetry on the critical level statistics is also essential. In the Aharonov-Bohm geometry we found a family of scale-invariant level statistics, which are controlled only by the AB-flux. By increasing the flux, the level spacing distribution shows a crossover from the critical orthogonal to the critical unitary form, so called COE-CUE crossover.

Analogous study can be performed for investigating the crossover between the critical orthogonal (COE) and the critical symplectic ensembles (CSE). In this case, the controlling parameter is the strength of the spin-orbit coupling characteristic of the broken rotational symmetry. The COE-CSE transition in the regime of the strongest spin-orbit coupling has been discussed in the literature. We have calculated the dependence of the level number variance on its mean value in a given energy interval in the metallic regime. The number variance undergoes a smooth crossover from the Wigner-Dyson theory for small energy to the diffusive regime for large energy, which is governed by the single parameter. Interestingly, in higher dimensions, $d > 3$, when the diffusive approximation breaks down, the number variance should reveal a new behaviour regime governed by an additional spatial scale. All this represents a collection of the most important spectral statistical measures at criticality exploited for the numerical-scaling evaluation. They indicate the presence of the new class of statistical ensembles inherent to the disordered-induced metal-insulator transitions.

This means there exist three generic situations for a given basic symmetry. Although occupying an intermediate position, these `critical' ensembles are essentially different from both the standard Wigner ensembles and the Poisson ensemble of completely uncorrelated variables. A disordered system in the thermodynamic limit can be prescribed to only one of these three ensemble classes. The fact that the spectrum of a disordered system has the properties of a critical ensemble obviously signalizes that the system undergoes the transition between the metallic and insulating regime. By other words, the spectral critical statistics play role of an adequate precursor of the localization transition. Similarly to the ergodic regime, depending on fundamental symmetry the system at criticality falls into one of the classes: Critical Orthogonal, Critical Unitary and Critical Symplectic. The description of the Anderson transition in terms of the spectral statistical quantities peculiar to the new critical classes implies relevance and significance for other physical problems, where crossover between the two limits of non-integrable and exactly solvable models is accompanied by a critical phenomenon [2]. For example, an analogue to the Anderson transition in nonlinear physics called the dynamical localization allows the semi-classical description of integrability-to-chaos transition.

The localization of the wave functions in the momentum space gives rise to the Anderson-type transition in the ballistic domain. One should notice that the universality of the critical level statistics implies the independence on the system size and on the type of disorder model. In addition, they should be invariant with respect to the type of the underlying lattice and to the energy. On the other hand, the level statistics at the Anderson transition is shown to be sensitive to the basic symmetry. It depends also on the type of boundary conditions and on the shape of a sample (aspect ratio). Dependence on the dimensionality of the system is an additional important issue, which deserves separate investigation. It is found that in the four-dimensional systems the critical level statistics at the localization transition tends towards the Poisson limit, while the numerical studies performed for $2 < d < 3$, e.g. on the bifractal structure with $d = 2{,}58$, demonstrate that P(s) scales closer to the Wigner-Dyson distribution.

4. Discussions

After employing various successful optimizations it was possible to compute not only the extreme eigenvalues in the tails of the density of states, but also the interior of the spectrum of disordered lattices of large size $N = 100\times100\times100$. The maximal dimensions of the matrices from previous diagonalization studies [1–3] have been exceeded by more than two orders of magnitude. The spectral fluctuations represented in terms of the level spacing distribution and the two-level correlation function exhibit scale-invariant behaviour. Moreover, they proved to be independent of the type of boundary conditions, provided that it belongs to a given topology. We have verified that for sufficiently large sizes one does not need to average over different random systems with the same disorder W. This is due to the ergodicity principle, which establishes equivalence between averaging over an ensemble of many systems and averaging over the energy of a single system. We have also succeeded in determining several eigenstates of unprecedented matrix sizes of million-by-million very close to the centre of the spectrum by partly using the conventional version of the restarted Lanczos solver with reorthogonalization [4].

This was performed on a single-processor workstation Alpha UNIX within a period of few days (10000 CPU-seconds). We have investigated the probability distribution of the local amplitudes of the wave functions and the energy dependence of their mutual correlations at the transition. It is interesting to notice that the achieved scale of disordered Hamiltonians becomes now comparable with typical realistic sizes of quantum dots and quantum wires in many experimental situations, although the Anderson model of localization does not take electron–electron interactions into account. We have also applied similar optimization techniques for diagonalizing the Hubbard model, where in addition to the disorder a few spinless fermions can interact if they are on the nearest-neighbouring lattice sites (short-range coupling). The sparseness of the matrix of the Hubbard model is, however, less advantageous compared to the non-interacting models.

5. Conclusions

An implementation of an advanced numerical algorithm for solutions of eigenvalue problems which appear in modelling electronic properties of quantum disordered nanoclusters is considered. I study the electron wave states at the localization transition caused by a chaotic impurity potential on the basis of the Anderson lattice model. The calculation of the internal part of the electron spectrum and the corresponding wave functions for very huge and sparse Hamiltonian matrices of sizes up to million-by-million is performed by the Lanczos type method especially developed for explore the statistical properties of energy levels and eigenfunction amplitudes. It is known that the correlations of eigenvalues are decoupled from the correlations of the eigenfunctions only in 'pure' Gaussian ensembles. Besides, in the crossover regime between different universality classes the long-range spatial wave function correlations do not vanish in contrast to the 'pure' limiting symmetry cases. As to the mobility edge, the spectral correlations in the crossover regime should generally be considered in close relation with the eigenfunctions correlations. One might expect that the multifractal properties of the critical wave functions undergo a smooth transition between the 'pure' critical ensembles. Exploring these issues, as well as investigating the statistical properties in higher dimensions is a challenging problem left for the future.

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