Spherical many-center scattering systems

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High-symmetric systems of a large number of scatterers located at a sphere of radius R (the R sphere) are considered. A method of constructing such systems with point symmetries of crystalline lattices which is based on the projection of atomic shells onto the R sphere is proposed. In this way one can obtain the R sphere with the number of scatterers tending to infinity. By choosing potentials of separate centers one finds that such a system is closest to a spherically symmetric one. In this case the solution of scattering is uniquely characterized by a certain value of the orbital quantum number l. Specific shape resonances, geometric resonances, which can exist in many-center systems only in narrow energetic intervals and are destroyed as a potential becomes stronger, are examined. [S1050-2947(99)07109-7]

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I. INTRODUCTION

The discovery of fullerenes has stimulated the development of the investigations of various types of exotic structures including speculative constructions of a large number of atoms. The achievements of nanotechnology allow us to hope that some kinds of these constructions can be realized. However, even though some constructions are unstable and cannot exist in reality, the analysis of them can be useful both from the theoretical and practical points of view if it enables us to discover new properties of many-atom systems or generalize some theoretical propositions.

The purpose of this paper is to develop a scheme of constructing hypothetical spherical many-atom systems and study their properties appearing in the electron scattering from these systems. We consider systems of many atoms located at a sphere of some radius that are, in a sense, similar to fullerenes. The basic question is how much the scattering from such systems can be close to the scattering from spherically symmetric potentials and what principal differences there are between these types of scattering. In addition, below specific quasistationary states (geometric shape resonances), which are characteristic for high-symmetric many-center systems and expected to be most strongly pronounced in objects under consideration, are investigated.

II. MANY-CHANNEL SCATTERING FROM A MANY-CENTER SYSTEM

Let us consider a system of a large number of scatterers, whose centers are located at a sphere of radius R. We assume that the potential describing the interaction between the scattered electron and the system is equal to zero outside the system. In this case electronic states with certain values of quantum numbers l and m are eigenstates of an asymptotic Hamiltonian, and it is possible to say about L channels through which the electron can approach and move off from the system [$L \equiv (l,m)$ is a combined quantum number]. Then, as is well known, solutions of the stationary Schrödinger equation can be represented as

$$\Psi_L(E,\mathbf{r}) = h_l^-(kr)Y_L(\Omega) + \sum_{L'} S_{LL'} h_{l'}^+(kr)Y_{L'}(\Omega) \quad (r>R), \tag{1}$$

where $h_l^{\pm}(kr)$ are spherical Hankel functions, $Y_L(\Omega)$ are real spherical harmonics, $S_{LL'}$ are elements of the S matrix, $k=\sqrt{E}$, E is the energy of the scattered electron, and r is a distance from the electron to the sphere center. Equation (1) describes the situation when the electron approaches the system through a certain input L channel and moves off through a system of many output L' channels. It is the fact that distinguishes the scattering by many-center systems from the scattering by a spherically symmetric potential for which it is characteristic that the electron approaches and moves off from the system through the same channel. The main problem to be solved below is to construct a many-center system so that the scattering by it is most close to the scattering by a spherically symmetric potential. More exactly, we try to find a system for which the scattering is one channel, at least in some finite energetic interval.

Beforehand we shall write a few general relations that will be useful later on. System of solutions (1) can be transformed to more symmetric form in which there are some input channels and, moreover, the flows incoming and outgoing in every channel are equal to each other. Obviously, the question is a basis set of solutions in which the S matrix is diagonal. In this case

$$\Psi_\lambda = \sum_L q_{\lambda L}\Psi_L = \sum_L q_{\lambda L}[h_l^-(kr) + \exp(2i\eta_\lambda)h_l^+(kr)]Y_L(\Omega), \tag{2}$$

where the index λ numbers linearly independent solutions, η_λ are eigenphases of the system, and $q_{\lambda L}$ are elements of a matrix diagonalizing the S matrix.

Further one can pass to the most symmetric expression for Ψ_λ, where summands describing incoming and outgoing waves are identical. To this end we redefine coefficients and require that the function Ψ_λ is real

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$$\Psi_\lambda = \sum_L d_{\lambda L}[\exp(-i\eta_\lambda)h_l^-(kr) + \exp(i\eta_\lambda)h_l^+(kr)]Y_L(\Omega)$$

$$= (\Psi_\lambda^- + \Psi_\lambda^+)/2 = \mathrm{Re}\,\Psi_\lambda^+ . \quad (3)$$

Here $\Psi_\lambda^+ = (\Psi_\lambda^-)^* = \Sigma_L d_{\lambda L}\exp(i\eta_\lambda)h_l^+(kr)Y_L(\Omega)$ is the solution of the Schrödinger equation for a system with sources [1]. It is proportional to the many-center Jost solution [1]. The coefficients $d_{\lambda L}$ are real and satisfy the condition

$$\sum_L d_{\lambda L}d_{\mu L} = \delta_{\lambda\mu} \quad (4)$$

that provides the orthonormalizing of the functions from Eq. (3)

$$\int \Psi_\lambda(k,\mathbf{r})\Psi_\mu(k',\mathbf{r})dV = [\pi/(2k^2)]\delta_{\lambda\mu}\delta(k-k').$$

It is easy to show that as $r\to\infty$ the solutions Ψ_λ^+ for the system of sources due to the properties of $h_l^\pm$ take the form

$$\Psi_\lambda^+ = [\exp(ikr + i\eta_\lambda)/(ikr)]A_\lambda(\mathbf{n}),$$

where $A_\lambda(\mathbf{n}) = \Sigma_L(\mp i)^l d_{\lambda L}Y_L(\Omega)$ are some effective spherical harmonics describing the angular dependence of the total wave emitted by the system of sources.

The coefficients $d_{\lambda L}$ are uniquely determined by the potential of a concrete system and depend on the energy of the scattered electron. As $k\to 0$ only one of these coefficients remains nonzero: $d_{\lambda L}\to\delta_{LL_\lambda}$, where L_λ is the quantum number characterizing approximately the solution Ψ_λ at small k values. In this case $A_\lambda(\mathbf{n}) = (\mp i)^{l_\lambda}Y_{L_\lambda}(\Omega)$ and the phases η_λ behave as phases for spherical objects: $\eta_\lambda \sim k^{2l_\lambda+1}$. Thus at $k\to 0$ the scattering from any finite many-center system becomes one-channel and is similar to the scattering from a spherically symmetric potential. However, as k increases, the situation changes and some channels become connected with Ψ_λ. The larger the system, the more channels one must to take into account. In real calculations at finite k values one should consider channels with $l \leqslant kR$.

If a system has no point symmetry, all such channels mix in each solution. In the case of systems with a point symmetry the whole set of the channels is divided into subsets corresponding to the irreducible representations of the symmetry group. In particular, in the case of the cubic symmetry (the symmetry group O_h) in a_{1g} solutions only channels with $l = 0,4,6,\ldots,$ remain mixed. Due to this sequence of the numbers one of the a_{1g} solutions can be imitated by the one-channel representation with $l=0$ up to comparatively large k values ($k<4/R$). For the highest point symmetry, icosahedral symmetry (the group Y_h), in the identical representation a_g the channels with $l = 0,6,\ldots,$ mix, and a system with this symmetry (e.g., the molecule C_{12}) is still more similar to spherically symmetric one.

Thus, high-symmetric systems at small energies are not distinguished significantly from spherically symmetric ones in the scattering processes. This general conclusion is, of course, well known, and some details adduced above are necessary for us only to approach our problems. The first of them is to determine the conditions under which a many-center system is not distinguished from spherically symmetric ones *at arbitrary energies*. It is natural to expect that the most satisfying these conditions is a system of scattering centers located at a sphere. As long as we are interested in symmetry properties of the Schrödinger equation solutions rather than concrete potentials of scattering centers, it is worth to consider models within which the arrangement of centers is reproduced exactly but potentials can be reproduced roughly. The simplest such model is a system of point scatterers (PSs). We shall attempt to find how many PSs to choose and how to locate them in order for the scattering from the system to be most close to the scattering from a spherically symmetric potential? A system of PSs allows us to find this on an analytical level.

It should be reminded that an isolated PS is uniquely characterized by only the parameter α (see, e.g., Ref. [2]). Near the scatterer the real wave function can be represented as

$$\Psi = \mathrm{const}\times[1/r - \alpha] + O(r),$$

which can be considered as the determination of the α parameter. If $\alpha>0$, the PS has a single bound s state (in a frame of reference related to this PS) with the energy $E = -\alpha^2/2$. For a system of N point scatterers there are N orthonormalized solutions with nonzero phases η [2]. Sources in PS system can emit only s waves. The Ψ_λ^+ solution for a system of sources centered at PSs can be written for arbitrary $\mathbf{r}$ values (both inside and outside the system) as

$$\Psi_\lambda^+ = \exp(i\eta_\lambda)\sum_j b_{\lambda j}h_0^+(k|\mathbf{r}-\mathbf{r}_j|), \quad (5)$$

where $\mathbf{r}_j$ are coordinates of PSs and $b_{\lambda j}$ are amplitudes of s waves emitted by the sources. Using the known h_0^+ reexpansion formula

$$h_0^+(k|\mathbf{r}-\mathbf{r}'|)$$

$$= 4\pi\sum_L j_l(kr')Y_L(\Omega')h_l^+(kr)Y_L(\Omega) \quad (r'<r) \quad (6)$$

[$j_l(kR)$ are spherical Bessel functions], we get the one-center expansion of Ψ_λ^+ written about the sphere center

$$\Psi_\lambda^+ = \exp(i\eta_\lambda)\sum_L d_{\lambda L}h_l^+(kr)Y_L(\Omega) \quad (r>R) \quad (7)$$

in which

$$d_{\lambda L} = 4\pi j_l(kR)\sum_j b_{\lambda j}Y_L(\mathbf{n}_j). \quad (8)$$

From these equations it follows that some s wave, emitted by a source, in the frame of reference related to the sphere center is an aggregate of L waves emitted into channels with all l values ($l = 0,1,\ldots,\infty$). Such waves in channels are characterized by the amplitudes $d_{\lambda L}$. Notice also that the phase η_λ is common for all s waves emitted by the sources and L waves in channels, i.e., the sources are coherent. Only due to the superposition of waves emitted by various sources

can one attain that a wave in channel with a certain l value vanishes. It is possible if for this l value $d_{\lambda L} \sim \Sigma_j b_{\lambda j} Y_L(\mathbf{n}_j) = 0$. [Effects conditioned by the vanishing of the factor $j_l(kR)$ will be considered in Sec. IV.] Thus, changing amplitudes $b_{\lambda j}$ of s waves of sources (through changing parameters α_j), one can pick up a set of $b_{\lambda j}$ so that a wave in a certain L channel vanishes. Moreover, for a finite number of PSs it is possible to eliminate waves simultaneously from a finite number of channels. In order that the scattering from a system is strictly one channel, one must eliminate waves from all channels except one. It is clear, that at arbitrary energies it is possible only for a system of the *infinite* number of scatterers.

In our approach it is easy to determine what distribution of amplitudes in an infinite system of sources provides the strictly one-channel scattering. From Eq. (8) it follows that if scatterers are distributed at the sphere uniformly and amplitudes $b_{\lambda j} \rightarrow b Y_{L_\lambda}(\mathbf{n}_j)$ where b is a constant, then $d_{\lambda L} = 4\pi j_l(kR) \int b Y_{L_\lambda}(\Omega) Y_L(\Omega) d\Omega = \delta_{L L_\lambda} 4\pi b j_l(kR)$. Hence, an infinite system of PSs located uniformly at the sphere and emitting s waves whose amplitudes are proportional to some spherical harmonic $Y_L(\Omega)$ with a given L value, generates a total wave with the same L value at arbitrary energies.

Here we want to emphasize a fact important from point of view of the methodology. If in a system at $r > R$ there is an only wave with a certain L value and $l \neq 0$, it signifies that the system being in this state is surrounded by the centrifugal barrier with the same l. (It follows immediately from the fact that such a wave is the solution of the Schrödinger equation with the corresponding centrifugal barrier.) Because we have obtained our L wave via the superposition of $l = 0$ waves, every of which is not related to any centrifugal barriers we may affirm that the centrifugal barrier surrounding the system is an *interference effect*. In this case it is the *destructive interference* of waves from various centers that leads to the suppression of the total wave in a region adjacent to the system. This point of view on the nature of centrifugal barriers is indeed less formal than one adduced in standard textbooks, and it is constructive for the analysis of one-electron quasistationary states in many-center systems (see Ref. [3] and Sec. IV of this paper).

Above we studied the way of obtaining one-channel solutions at arbitrary energies and have shown that it is possible only in case of model systems of the infinite number of scatterers. However, for finite preassigned energies the situation is essentially simpler. If an energetic region under consideration is limited by a maximum value $E_{\max}$, then in the total solution we can ignore waves in channels with $l \gg k_{\max} R$, and even for a finite system it is possible to realize the one-channel scattering to a high precision. (Here we consider not a complete set of solutions involving all the scattering channels, but only solutions with nonzero scattering phases appearing in quantities observed experimentally, e.g., in the cross section for scattering, etc.) Obviously, the more scatterers in a system, the larger the region of energies where one can realize the one-channel scattering. In the next section we consider a practical way of constructing systems for which it is possible to get the one-channel scattering to any preassigned precision.

III. ONE-CHANNEL SCATTERING FROM A MANY-CENTER SYSTEM

At the beginning of the previous section we already considered examples of high-symmetric systems the scattering from which at small nonzero energies is close to one-channel. The octahedral and icosahedral arrangements of scatterers were in question. A system of the minimum number of scatterers with the octahedral symmetry is the system of six identical centers located at apexes of an octahedron. If scatterers are point, in this case there are six solutions Ψ_λ^+ with nonzero scattering phases: one a_{1g} solution, three t_{1u} solutions, and two e_g solutions. At small k values these solutions, as stated above, can be classified by means of the orbital quantum number l. Below we shall need information what l values are represented in one-center expansions of the solutions about the point symmetry center in the case of the O_h group. This information (see, e.g., Ref. [4]) is collected in Table I. From it follows particularly that in the a_{1g} solution expansion there are summands with $l = 0$, 4, and so on. At $k \rightarrow 0$ it should retain in the expansions only a summand with the minimal l value ($l = l_1$). Thus, at $k \rightarrow 0$ the a_{1g} solution contains only a term with $l_1 = 0$, the t_{1u} solution with $l_1 = 1$, and the e_g solution with $l_1 = 2$. The size of an energetic region where one can restrict oneself to the first summand depends on the second l value ($l = l_2$) in the expansions. In particular, for the a_{1g} solution $l_2 = 4$, and the region of the one-channel scattering is restricted by the value $k_{\max} < 4/R$.

In the case of icosahedral symmetry the minimum system is a system of twelve PSs located at apexes of an icosahedron [Fig. 1(a)]. As mentioned above, for solutions of the a_g type in such a system the one-channel scattering region with $l = 0$ is restricted by the value $k_{\max} < 6/R$.

Now we go over to the consideration of systems consisting of large number of PSs for which the one-channel scattering region is bigger than for the above instances. Proceeding from the reasons stated in Sec. II we shall study systems of scatterers located at a sphere of radius R. In order that the situation is closer to real we do not fix the R value but assume that it depends on the number of scatterers. We hold fixed the minimum distance d between scatterers and accept it to be equal to 1 a.u. which is equal in order to internuclear distances in real compounds. Under such conditions, as the number of scatterers increases, the sphere radius increases too.

For the system of six PSs located at apexes of an octahedron $R = 0.7071$ a.u., and for the system of twelve PSs located at apexes of an icosahedron $R = 0.9511$ a.u. In these small systems the amplitudes of the s waves emitted by sources are the same for all PSs within a given solution ($b_{\lambda j} = \text{const}$) that provides the high symmetry and leads to a certain similarity between these systems and spherically symmetric ones. While constructing systems of a larger number of PSs one should keep, of course, the point symmetry of the arrangement of scatterers to be high. [Here we do not consider the variant with no symmetry when amplitudes $b_{\lambda j}$ of all PSs may be quite different. It should be noted that the analysis of even the simplest two-PS system (see, e.g., Ref. [3]) shows that it is advisable for our aim to build a system, keeping its symmetry to be high enough]. It is well-known that the highest point symmetry is icosahedral and, hence, we

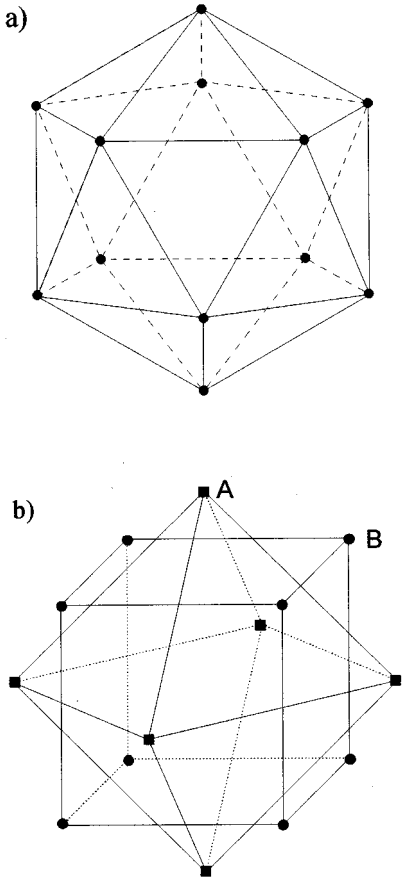

FIG. 1. Systems of point scatterers with the icosahedral (a) and octahedral (b) symmetries. The upper system contains 12 identical scatterers located at apexes of an icosahedron. The lower system contains 14 scatterers disposed at a sphere including six scatterers located at apexes of an octahedron (marked by ■, the subsystem *A*) and eight scatterers located at apexes of a cube (marked by ●, the subsystem *B*).

should build large systems with this symmetry. However, to do it is a complicated thing. It is essentially simpler to build large systems with the octahedral symmetry, and here we choose this symmetry.

Below we act as follows. We take a face-centered cubic lattice, then choose one of its atoms as central and consider atomic shells around this atom. Every atomic shell is a certain set of atoms with the octahedral symmetry. Angular coordinates of atoms from different shells, generally speaking, are not the same, and we have, thus, an infinite variety of sets of angular coordinates. Let us describe around our central atom a sphere of radius R (the R shells), then project centers of atoms from various atomic shells onto this sphere preserving angular coordinates of atoms, and place point scatterers at corresponding points of the R sphere. (Projections of some atoms from different shells can be coincident, and then atoms whose projections do not add new points at the R sphere should be excepted from the consideration.) As a result we obtain the desired system of scattering centers located at R sphere, with the octahedral symmetry and with the centers number that we can choose according to our judgment. The radius of R sphere is determined finally so that the nearest PS distance is 1 a.u.

TABLE I. The decomposition of the space of the functions Y_L with l fixed into subspaces corresponding to the irreducible representations of the O_h group.

l	Irreducible representations
0	a_{1g}
1	t_{1u}
2	e_g+t_{2g}
3	$a_{2u}+t_{1u}+t_{2u}$
4	$a_{1g}+e_g+t_{1g}+t_{2g}$
5	$e_u+t_{2u}+2t_{1u}$
6	$a_{1g}+a_{2g}+e_g+2t_{1g}+t_{2g}$

If the radius of R sphere does not change, we can consider a pure theoretical problem of proceeding to the limit of a spherically symmetric system. Our construction supposes that the number of points on a sphere of fixed radius can be infinite, and in this case the points are uniformly distributed on the sphere. It follows from the fact that in the direction of any ray outgoing from the central atom of the initial crystalline lattice there are atoms whose centers are situated at this ray. If the number of atomic shells projected onto the R sphere increases, we sooner or later reach the first sphere with one of these atoms, and the corresponding point appears on the R sphere. Obviously, by increasing the number of atomic shells projected, in the limit we can fill the sphere completely.

In this section, however, we do not consider systems of very large numbers of scatterers and restrict ourselves to comparatively small systems which, nevertheless, are sufficient to show the tendencies appearing as the systems increase. More exactly, we consider only a system obtained by projecting the two first atomic shells from the face-centered cubic lattice. The first shell coincides in fact with the system of six PSs already considered above. The second shell consists of eight scatterers located at the apexes of a cube. The projection of these shells onto the R sphere gives us two subsystems A and B containing six and eight PSs, respectively [Fig. 1(b)]. The symmetry operations from the O_h group transfer into each other point scatterers either from the subsystem A or from the subsystem B. The radius of the R sphere providing the value $d=1$ a.u. is equal to 1.0877 a.u. which is somewhat greater than in the case of the icosahedron [Fig. 1(a)]. From the fact that the system is divided into the two subsystems it follows that parameters α_j of scatterers and wave amplitudes b_j of sources from different subsystems can be different. This freedom allows us to choose the parameters so that the solutions of scattering from our system are most close to spherically symmetric ones.

The total number of PSs (and also of the solutions with nonzero phases) in our system is equal to 14. All the solutions are distributed over the irreducible representations so: $2a_{1g}+a_{2u}+e_g+2t_{1u}+t_{2g}$. When associating these solutions at $k\to 0$ with certain l values it should be taken into account that if some representation occurs twice in such a distribution then for the scattering system there exist two different orthonormalized solutions. One of them is characterized by the first value of l, and the other by the second value from a set corresponding to a given representation (see Table I). Thus, in our case the a_{1g} solutions are classified by

values $l=0$ and 4, a_{2u} by $l=3$, e_g by $l=2$, t_{1u} by $l=1$ and 3, and t_{2g} by $l=2$. We can see that in case of the total system there is the $l=4$ solution which is absent in solution sets for the separate subsystems (for the A subsystem $l\leqslant 2$, and for the B subsystem $l\leqslant 3$).

However, the presence of the two subsystems does not lead automatically to additional vanishing of some summands in one-center expansions of the solutions for the total system. In particular, in the both a_{1g} solutions of the system there are summands with $l=0$ and $l=4$ existing in the expansions for the subsystems too. But at small k the contributions of these summands to both the a_{1g} solutions are different. In the first solution, also as in the solutions for the separate subsystems, the $l=0$ summand is dominant, and the $l=4$ one is comparatively small. The situation in the second solution is inverse. In this case our task is to find such a system whose solutions are closer to spherically symmetric ones than for the separate subsystems. For example, for the first a_{1g} solution with dominant $l=0$ summand it is required to find a form in which the $l=4$ summand is absent completely. The presence of the two subsystems with independent parameters α enables such solutions to be constructed.

To fit properly the parameters we turn to the problem of determining wave amplitudes b_j for the system. In our case there are only two different amplitudes b_j: b_A characterizes sources in the A subsystem, and b_B in the B subsystem. To determine concrete values of these amplitudes we use equations of matching of solutions (5) and the ''inner'' solutions for separate point scatterers $\psi_j=p_j(|\mathbf{r}-\mathbf{r}_j|^{-1}-\alpha_j),\mathbf{r}\to\mathbf{r}_j$, where p_j are coefficients depending on the energy (see, e.g., Ref. [2]). The matching procedure includes the power series expansion of solution (5) and the equality of the corresponding terms in Eq. (5) and in the ''inner'' solutions. As a result for the a_{1g} solutions we get the pair of coupled equations

$$b_A[4\sin(kr_{13}+\eta)/r_{13}+\sin(2kR+\eta)/(2R)+k\cos\eta+\alpha_A\sin\eta]+b_B[4\sin(kr_{12}+\eta)/r_{12}+4\sin(kr_{14}+\eta)/r_{14}]=0,$$

$$b_A[3\sin(kr_{12}+\eta)/r_{12}+3\sin(kr_{14}+\eta)/r_{14}]+b_B[3\sin(kr_{24}+\eta)/r_{24}+3\sin(kr_{25}+\eta)/r_{25}+\sin(2kR+\eta)/(2R)$$
$$+k\cos\eta+\alpha_B\sin\eta]=0. \tag{9}$$

Here $r_{12}=0.9194R$, $r_{13}=1.4142R$, $r_{14}=1.7761R$, $r_{24}=1.1547R$, $r_{25}=1.6330R$ are different distances between the scatterers. The written system of equations allows us to find the phases η and the relation between the amplitudes b_A and b_B. To determine these amplitudes completely it is necessary also to use the normalizing condition (4).

The next step is the analysis of the one-center expansion of the a_{1g} solution about the sphere center written in the form

$$\Psi_\lambda^+=[6b_{\lambda A}+8b_{\lambda B}]j_0(kR)h_0^+(kr)+[6b_{\lambda A}\phi_4(\Omega_1)+8b_{\lambda B}\phi_4(\Omega_2)]j_4(kR)h_4^+(kr)\phi_4(\Omega)$$
$$+[6b_{\lambda A}\phi_6(\Omega_1)+8b_{\lambda B}\phi_6(\Omega_2)]j_6(kR)h_6^+(kr)\phi_6(\Omega)+\cdots\quad(r>R), \tag{10}$$

where $\phi_l(\Omega)$ are cubic harmonics corresponding to the a_{1g} solution. Their values at the centers of the A subsystem are $\phi_4(\Omega_1)=0.6464,\phi_6(\Omega_1)=0.3596$, and at the centers of the B subsystem $\phi_4(\Omega_2)=-0.4309,\phi_6(\Omega_2)=0.6393$. In order that the $l=4$ summand in Eq. (10) becomes zero at some energy it is sufficient, for example, to fix the α_A quantity and, by varying the α_B quantity, find its proper value. In particular, at $k=2.0$ and $\alpha_A=5$ we get $\alpha_B=4.55$. In this case the amplitudes take the following (non-normalized) values: for the first solution $(\lambda=1)b_A=1,b_B=1.128$ which provides the vanishing of the $l=4$ summand, for the second solution $(\lambda=2)b_A=1,b_B=-0.75$ which leads to the vanishing of the $l=0$ summand. It should be noted that the amplitudes b depend on the energy, and in our example the summands indicated do not become zero at $k\neq 2.0$ although they remain small enough (smaller than for the separate subsystems) in a wide interval of E. Also such a relation between the summands with l_1 and l_2 takes place, as a rule, in the case of any values of α_A and α_B close enough to each other. Only if one of the parameters becomes large in modulus (>100), this relation becomes similar to that for the separate subsystems.

The result obtained is, of course, not unexpected. It can be easily extended to larger systems. We affirm that by varying parameters α one can attain that the solution for a finite system of PSs approaches a spherically symmetric solution. The more scatterers in a system, the nearer these solutions each other. Already for the considered system of 14 PSs with the octahedral symmetry we have obtained the effect typical for icosahedral systems—the absence of the $l=4$ summand in the solution with the dominant $l=0$ summand. As the number of scatterers increases, one can sequentially eliminate the summands with $l=6,8$ and so on, increasing in this way the l_2 quantity up to any preassigned value. In the next section we consider a specific phenomenon appearing in many-center systems for which the l_2 value is large.

IV. GEOMETRIC SHAPE RESONANCES IN A SPHERICAL MANY-CENTER SYSTEM

In high-symmetric systems there may exist one-electron quasistationary states (shape resonances) of a peculiar kind discovered in Ref. [5]. These states are distinguished by a specific behavior as the potential of a system intensifies, and they occur only in narrow energetic intervals determined by the geometric size of the system. In contrast to usual (hybridized) shape resonances which shift smoothly into the discrete spectrum when the potential becomes stronger, the geometric resonances are destroyed under such conditions. The higher

the symmetry of the system, the more strongly pronounced these resonances are. In Ref. [5] the resonances in a system of eight identical PSs located at apexes of a cube were examined. Later on such resonances were discovered also in real many-atom systems. In particular, in Ref. [6] these resonances were investigated for the compounds $LiBiS_2$ and $NaBiS_2$.

The reasons of the existence of geometric resonances can be shown easily by considering point scatterers for which simple analytical expressions can be written. Let us again turn to Eqs. (7) and (8). In the previous section we examined the vanishing of coefficients $d_{\lambda L}$ caused by sums $\Sigma_j b_{\lambda j} Y_L(\mathbf{n}_j)$. Now we consider an effect related to the vanishing of the function $j_l(kR)$. In particular, in the case of the a_{1g} solution in octahedral systems, behaving at small k as the s solution, the second summand, as repeatedly mentioned above, is the $l=4$ term. However, in the energetic domain where $kR \approx \pi$ the $l=0$ summand vanishes because here the function $j_0(kR)$ is close to zero. Under such conditions the $l=4$ summand becomes dominant. Thus, when k increases from zero to $2\pi/R$ the a_{1g} solution turns from the s solution into the g solution and conversely. In a narrow energetic interval including the value $k^2=(\pi/R)^2$ the system is in the g state and surrounded by the high centrifugal barrier with $l=4$. If one-center potentials of the system (parameters α_j for the PS system) are fitted properly, in this energetic interval there exists a strongly pronounced shape resonance with $l=4$. If the potentials intensify, the resonance is destroyed because its energy shifts into a domain where the $l=0$ summand again becomes dominant in Ψ^+. At these energies the barrierless s channel becomes connected to the system and the scattered electron goes to infinity through this channel without delay. Since such resonances exist in narrow energetic intervals determined by the geometric size of the system they appear in, they are called geometric resonances.

The behavior of geometric resonances, their dependence on the potential, is described visually by means of the motion of the corresponding poles of the S matrix in the complex k or E plane. It is known that the real coordinate of the S-matrix pole corresponds to the resonance energy and the imaginary coordinate to the lifetime of the resonant state (see, e.g., Ref. [7]). The nearer the pole to the real axis, the more long-lived the state and more strongly pronounced the corresponding peak in the cross section for the elastic electron scattering from a system. For hybridized resonances it is characteristic that when a potential intensifies a pole approaches the real axis monotonically. At $k \to 0$ the imaginary coordinate of such a pole is conjugate with its real coordinate by the relation $\mathrm{Im}\, k_{\mathrm{res}} \sim (\mathrm{Re}\, k_{\mathrm{res}})^{2l}$. The behavior of poles in the case of geometric resonances is quite different. When a potential intensifies, the pole at first approaches the real axis and then moves away. For a system of PSs located at the R sphere the point of the maximum approach is determined by the equation $j_l(kR)=0$ with the minimum $l(=l_1)$ for the irreducible representation corresponding to the resonant state. If this state is the a_{1g} state, then $l_1=0$ and the maximum approach point is $k \approx \pi/R$.

The degree of the proximity of a pole to the real axis depends on the l_2 value for the one-center expansion of Ψ^+. For the system of eight PSs located at apexes of a cube $l_2=4$, for the system of twelve PSs located at apexes of an icosahedron $l_2=6$, and in the second case a pole approaches the real axis significantly nearer than in the first. It is caused by different penetrability of the $l=4$ and $l=6$ centrifugal barriers. For the system of 14 PSs considered in the previous section one can also obtain the solution with $l_2=6$. Trajectories of the S-matrix poles corresponding to the geometric a_{1g} resonances in the systems of 8 and 14 PSs with $d=1$ a.u. are shown in Fig. 2. In the case of 8 PSs the point of the maximum proximity to the real axis is $k_0=3.522-i0.0592$, and in the case of 14 PSs $k_0=2.886-i0.000823$. In the same figure the trajectory of the S-matrix pole corresponding to the hybridized resonance with $l_2=4$ (the second a_{1g} solution) in the system of 14 PSs is presented for the comparison. (In all calculations performed for the system of 14 PSs the parameters α_j were accepted to be identical: $\alpha_A \equiv \alpha_B$.)

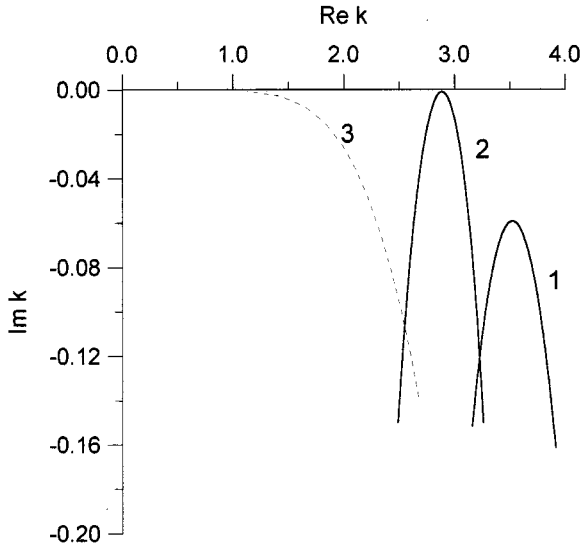

FIG. 2. Trajectories of the S-matrix poles corresponding to geometric (1,2) and hybridized (3) shape resonances in systems of point scatterers with the nearest-neighbor distance $d=1$ a.u. Curve 1 corresponds to a system of eight scatterers located at apexes of a cube, and curves 2,3 correspond to the system of 14 scatterers shown in Fig. 1(b).

It is clear that by increasing the number of PSs at the R sphere and, respectively, the l_2 value one can achieve an essential proximity of a pole to the real axis. Then the corresponding geometric resonance is almost not distinguished from a state of the discrete spectrum. One may assume that, if such systems can be realized, the geometric resonances with superlarge lifetimes can be used for the creation of traps for free electrons. As long as characteristics of geometric resonances significantly depend on the symmetry of the atomic arrangement and any breakdown of the symmetry deteriorates the conditions of the existence of the resonances, the traps can be controlled by distorting them by means of external fields. A detailed consideration of this problem will be published.

V. CONCLUSIONS

For a system of large number of scatterers located at a sphere one can obtain the solutions of scattering which are

close to the solutions for spherically symmetric potentials. By fitting potentials of separate centers it is possible to attain that in a given interval of energies the wave function of the scattered electron outside the system is described, to a high precision, by a term with a certain value of the orbital quantum number l. In the one-center expansion of the wave function about the point symmetry center one can neglect all other terms corresponding to other l values. The degree of this approximation depends on the number of scatterers.

In such systems there may exist geometric shape resonances with large lifetimes increasing if systems increase. These specific states can be used for creating traps for free electrons.

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