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THE USE OF THE GREEN FUNCTION METHOD FOR THE SCATTERING OF A PARTICLE ON A SYSTEM OF BOUND PARTICLES

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Abstract: A method for treating elastic and inelastic scattering of a particle on a system of bound particles, using the many-body techniques, is presented. The optical potential model for the elastic scattering is discussed and the way of direct inclusion of the self-consistent incoherent terms is given. Analogous procedure for the inelastic scattering is described.

1. Introduction

Despite the large amount of work done during recent years in the application of Green function method in different domains of quantum physics, a systematic exposition of its use in the scattering theory does not exist. Especially this concerns the scattering of a particle on the system of bound particles. This is, however, one of the most frequent situation which one encounters in atomic and nuclear physics. Thus it seems regrettable, since the calculation techniques for the Green functions are very well developed. The approaches already published are either of purely formal nature[1], and physical approximations are made without neccessary clarifications, or the attention is restricted to the optical potential studies[2] and its use in practice[3].

The aim of this paper is to describe a model for scattering of a particle on the system of bound particles which is close to the reality, and in which the relation between the Green functions and the S-matrix appears in a very simple form. The model consists in the study of the evolution of a bound system and a particle, with the adiabatic inclusion of the full interaction between them, and in the end of the process, after the exclusion of the full interaction, we have again a bound system separated of the rest. This is explained in detail in Chapter 2, where also the non-trivial situation, when the particle is of the same kind as the particles of which the system is composed, is treated. In Chapter 3 we describe the elastic scattering and give the relation to the optical potential. At the same time we propose a method of the evaluation of the T-matrix with the inclusion of the incoherent terms. In Chapter 4 the generalisation of the method applied for elastic scattering to the inelastic processes (excitation and ionization) is given. This generalization can be applied to the cases when the difference in the number of particles in the bound system does not change considerably their excitation spectrum. The analogous formulae as for the optical potential and their modifications are also given. That is done using the two-particle Green function. In Chapter 5 we indicate how this method can be generalized using many-particle Green functions and give some concluding remarks.

2. *General considerations*

Consider the situation in which a particle is scattered on the system of bound particles. Generally, we can study the dynamics of the complete system (projectile plus scatterer) through the transition amplitude defined by

$$S_{\beta\alpha}\left(t'_c, t_c\right) = <\varphi_\beta, t'_c \,|\, e^{-iH\left(t'_c - t_c\right)} \,|\, \varphi_\alpha, t_c> , \tag{1}$$

where t_c and t'_c are the times of the beginning and the end of the collision, respectively, $e^{-iH(t'_c - t_c)}$ is the evolution operator in the Schrödinger representation, and $|\varphi_\alpha, t>$ · $|\varphi_\beta, t>$ represent the evolution of the system before and after collision, respectively. There is no dificulty to remove t_c and t'_c to the infinite past and, correspondingly, to the infinite future. That serves only as a description of the physical situation when before and after the interaction the projectile and the scatterer are well separated. This procedure allows also to avoid the unnecessary complications which arise dealing with the wave packets.

Using the field theoretical language, we can speak of the time development of the scatterer as of the development of the vacuum. By introducing the full interaction between the particles this vacuum becomes a physical vacuum through which the projectile propagates. We shall show that this picture gives a direct relation between the S-matrix and the Green functions, as they are usually defined in the theory of many-particle systems. But, before giving the proof of this relation, we shall explain how one overcomes the difficulties which arise when the extra particle (projectile) is of the same kind as the particles by which the scatterer is built. In order to assure the time development of the bound system to the state of the physical vacuum, the necessary separation of the total Hamiltonian is

$$H = H_0 + H_1 , \qquad (2)$$

where

$$H_0 = \sum_{i=1}^{A+1} T_j + \sum_{i>j}^{A} V_{ij} , \qquad H_1 = \sum_{i=1}^{A} V_{i,A+1} . \qquad (3)$$

It is evident that this separation makes both H_0 and H_1 nonsymmetric. In order to ensure the validity of the exclusion principle, we have to reexamine a procedure by which the proper symmetry of a state is built. Let us also mention that the interaction representation, which is often used in the case of the symmetric separation of the total Hamiltonian, in this case is not applicable.

Since the evolution of non-overlapping wave-packets can be described disregarding the indiscernability of the particles, we have before the collision

$$|\varphi_{\alpha,} t> = e^{-iH_0 t} |\varphi_\alpha> = e^{-iE_\alpha t} |\varphi_\alpha> , \qquad (4)$$

where $|\varphi_\alpha>$ describes n non-ovelapping wave-packets. The function (4) is not properly symmetrized. The function $|\varphi_{\alpha,} t>$ that satisfies the exclusion principle is obtained by postulating

$$|\tilde{\varphi}_{\alpha,} t> = C\mathcal{A}|\varphi_{\alpha,} t> = e^{-iE_\alpha t} |\tilde{\varphi}_\alpha> , \qquad (5)$$

where $\mathcal{A}$ is the antisymmetrization projector, C is the normalization constant and

$$|\tilde{\varphi}_\alpha> = C\mathcal{A}|\varphi_\alpha> . \qquad (6)$$

The antisymmetrization procedure at this point is well adapted for our purpose, since $|\tilde{\varphi}_\alpha>$ can be represented in the second — quantization formalism[4].

The same considerations can be applied to the motion of the system after collision, when the wave — packets are again well separated.

Taking this result into account we write the transition amplitude (1) in the form

$$S_{\beta\alpha}\left(t'_c, t_c\right) = < \tilde{\varphi}_{\beta,} t'_c \,| e^{-iH\left(t'_c - t_c\right)} | \tilde{\varphi}_{\alpha,} t_c > \quad . \tag{7}$$

In the infinite past and infinite future the formula (7) becomes

$$S_{\beta\alpha} = \lim_{\substack{t_c \to -\infty \\ t'_c \to +\infty}} < \tilde{\varphi}_\beta | e^{-H(t'_c - t_c)} | \tilde{\varphi}_\alpha > e^{iE_\beta t'_c - iE_\alpha t_c} \quad . \tag{8}$$

The »lim« in the above formula supposes the average over the phases or the existence of a damping factor, since without that the limes does not exist[5].

For the case of the scattering of n particles on a fixed target consisting of A bound particles (neglecting the recoil) we write

$$| \tilde{\varphi}_\alpha > = \overset{+}{a}_{\alpha_n} \; . \; . \; . \; \overset{+}{a}_{\alpha_1} | A > \quad , \tag{9a}$$

$$| \tilde{\varphi}_\beta > = \overset{+}{a}_{\beta_n} \; . \; . \; . \; \overset{+}{a}_{\beta_1} | A > \quad , \tag{9b}$$

where a_{α_i}, a_{β_i} are the second quantization operators, satisfying the usual fermion anticommutation rules, and

$$H \,| A > \; = E_A \,| A > , \tag{10}$$

i. e., $| A >$ is the ground state of A interacting particles with the ground state energy E_A. We rewrite the formulae (9) in the form

$$| \tilde{\varphi}_\alpha > = \overset{+}{a}_{\alpha_n} \; . \; . \; . \; \overset{+}{a}_{\alpha_1} e^{-iHt} | A > e^{iE_A t} \quad , \tag{11a}$$

$$| \tilde{\varphi}_\beta > = \overset{+}{a}_{\beta_n} \; . \; . \; . \; \overset{+}{a}_{\beta_1} e^{-iHt} | A > e^{iE_A t} \quad . \tag{11b}$$

Defining

$$e_\alpha = E_\alpha - E_A \quad , \quad e_\beta = E_\beta - E_A \quad , \tag{12}$$

and substituting (11) into (8), we get

$$S_{\beta\alpha} = \lim_{\substack{t' \to -\infty \\ t \to +\infty}} \langle A | \widetilde{a}_{\beta_1}(t') \ldots \widetilde{a}_{\beta_n}(t') \widetilde{a}^+_{\alpha_n}(t) \ldots$$

$$\ldots \widetilde{a}^+_{\alpha_1}(t) | A \rangle e^{i(e_\beta t' - e_\alpha t)} \tag{13}$$

where $\widetilde{a}_\alpha(t)$, $\widetilde{a}_\beta(t)$ are operators in the Heisenberg representation, and the subscript »c« is omitted.

Recalling now the definition of the n-particle Green function,

$$G_n(\gamma'_1 t'_1, \ldots \gamma'_n t'_n, \gamma_1 t_1, \ldots \gamma_n t_n) =$$
$$= (-i)^n \langle A | T\{\widetilde{a}_{\gamma'_1}(t'_1) \ldots \widetilde{a}_{\gamma_n}(t'_n) \widetilde{a}^+_{\gamma_n}(t_n) \ldots \widetilde{a}^+_{\gamma_1}(t_1)\} | A \rangle, \tag{14}$$

we see immediately

$$S_{\beta\alpha} = \lim_{\substack{t \to -\infty \\ t' \to +\infty}} i^n G_n(\beta_1 t' \ldots \beta_n t'; \alpha_1 t, \ldots \alpha_n t) e^{i(e_\beta t' - e_\alpha t)}. \tag{15}$$

The transition between (8) and (15) is immediate. This proves our contention, that the expression for the S-matrix, written in a convenient way, leads immediately and almost trivially to the corresponding Green functions.

3. *Elastic scattering*

In order to describe the elastic scattering we note that the states before and after collision, neglecting the recoil of the bound system, can be exactly represented by

$$| i \rangle = a^+_\alpha | A \rangle, \tag{16a}$$

$$| f \rangle = a^+_\beta | A \rangle. \tag{15b}$$

where from it immediately follows

$$S_{\beta\alpha} = \mathrm{i} \lim_{\substack{t \to -\infty \\ t' \to +\infty}} G\left(\beta t'; \alpha t\right) e^{\mathrm{i}\left(e_\beta t' - e_\alpha t\right)} \quad . \tag{17}$$

The notation is the same as in the preceeding chapter. Using the general relation between S and T matrix,

$$S_{\beta\alpha} = \delta_{\beta\alpha} - 2\pi\, \mathrm{i}\, \delta\left(E_\beta - E_\alpha\right) T_{\beta\alpha} \tag{18}$$

and the Dyson equation

$$G = G_0 + G_0\, \Sigma\, G_0 , \tag{19}$$

where G_0 is independent particle Green function and Σ is the non-compact self-energy part of the Green function, one finds

$$T_{\beta\alpha} = \Sigma\left(\beta, \alpha ; \varepsilon_\alpha\right) , \tag{20}$$

where Σ $(\beta, \alpha; E)$ is the Fourier transform of Σ $(\beta t'; \alpha t)$ taken at $E = \varepsilon_\alpha$, i.e. for the value of the single particle energy.

At this stage it is rather simple to see how the elastic scattering process is described as the propagation of particle through the physical vacuum. Recalling that using the Hartree-Fock vacuum, $|A_0>$, the expression for the field theoretical scattering operator is

$$S' = \langle A_0 | S' | A_0 \rangle \left\{ 1 - \mathrm{i} \int d1\, d2\, \Sigma(1,2)\, N\left[\psi^+(1)\, \psi(2)\right] - \right.$$
$$\left. - \mathrm{i} \int d1\, d2\, d3\, d4\, \Gamma(1,2,3,4,)\, N\left[\psi^+(1)\, \psi^+(2)\, \psi(4)\, \psi(3)\right] + \ldots \right\} , \tag{21}$$

where N $[\psi^+(1)\ \psi(2)]$ is the normal product of the one particle operators $\psi(i) = \psi(x_i, t_i)$, and further, making transition to $\{|\alpha>\}$ basis and taking the Fourier transform, we get the expression

$$S_{\beta\alpha} = \langle A_0 | S' | A_0 \rangle \langle A_0 | a_\beta\, S'\, a_\alpha^+ | A_0 \rangle \quad . \tag{22}$$

Since the first factor is just the phase, we can interpret this expression as the mathematical description of the propagation of the particle through the medium with the adiabatic »switching on« of the full interaction. This proofs our assertion.

In practice, one calculates Σ (β, α; E) by the standard diagrammatical techniques[6, 7]. Taking as the one-particle basis the Hartree-Fock one, the first-order contribution to Σ (β, α; E) is

$$\Sigma^{(1)}\left(\beta, \alpha; \varepsilon_{\alpha}\right) = V^{HF}_{\beta\alpha} = \sum \tilde{V}_{\beta\gamma,\alpha\gamma} N_{\gamma} \quad , \tag{23}$$

$$\tilde{V}_{\alpha\beta,\gamma\delta} \equiv V_{\alpha\beta,\gamma\delta} - V_{\alpha\beta,\delta\gamma} . \tag{24}$$

$V_{\alpha\beta,\,\gamma\delta}$ is the non-symmetrized matrix element, and N_{γ} is the fermion occupation number.

This part is included in the potential. The second-order contribution is

$$\Sigma^{(2)}\left(\beta, \alpha, \varepsilon_{\alpha}\right) \sum_{\gamma_1\gamma_2\gamma_3} \frac{V_{\beta\gamma_1,\gamma_1\gamma_2}\,\tilde{V}_{\gamma_2\gamma_3\alpha\gamma_1}}{\varepsilon_{\alpha}+\varepsilon_{\gamma_1}-\varepsilon_{\gamma_2}-\varepsilon_{\gamma_3}+i_{\eta}} \left[N_1(1-N_2)(1-N_3)+(1-N_1)N_2N_3\right] \tag{25}$$

As it is known[2] the equation (18) together with the Dyson equation

$$\Sigma = M + M G_0 \Sigma \tag{26}$$

where M is the compact self-energy part, can be interpreted as the scattering relation

$$T = V + V G_0 T \ , \tag{27}$$

where V or M plays the role of an optical potential. The approximation made in writing optical potential consists in neglecting all the incoherent terms. This definition of the optical potential is consistent with the one used in the multiple scattering theory[8].

Some calculations in atomic physics based on this idea are done[3, 9] for e-H and e-He scattering. There, M is calculated perturbationally up to third and second order, respectively, and then the phase shifts are calculated. But, there is no physical justification, at least for low energies of the incoming particle, which would allow one to neglect the incoherent terms. Therefore, we propose an alternative approach, which consists in calculating M up to a certain order, and then solving (26). This is an infinite partial summation of the perturbation series, and as such should certainly ameliorate the calculation.

If we look at the 2nd (and higher) order contributions, we see that the energy denominators have zeros, and hence the diagram contributions have poles, at the non-perturbed energies. This is an inherent limitation of this series development, analogous in this respect to the Born series in the potential scattering.

4. *Inelastic scattering*

With respect to the use of Green function method, the generalization of the elastic scattering procedure for the inelastic processes is, for a certain class of systems, almost immediate. It is sufficient that the ground state of a considered system, say A^-, containing $(A+1)$ particles can be represented as

$$|\overset{-}{A_0}> = \overset{+}{a}_{\alpha_F} |A> , \tag{28}$$

where $|A>$ is the ground state of A-particle closed shell system, defined as in the previous section. This is valid under the condition that both $|A_0^->$ and $|A>$ could be reasonably well described by a model in which the corresponding single particle states are very nearly, or more generally, for the case where the low-excited states of the A^- system are approximatively given by

$$|\overset{-}{A_n}> = \overset{+}{a}_{\alpha_1} |A> . \tag{29}$$

In reality, this situation is realized in heavy nuclei or in atomic systems where one of the bound electrons has small binding energy. In that case the physical picture which serves as a basis for the description of inelastic processes, is that of the exchange of energy between any two particles during the interaction. In the field theoretical language, one can think about the propagation of two particles through a medium with the adiabatically »swiching on« of the full interaction, which acts between all the particles of the interacting system. We then write

$$|\tilde{\varphi}_\alpha> = \overset{+}{a}_{\alpha_2} |\overset{-}{A_n}> = \overset{+}{a}_{\alpha_2} \overset{+}{a}_{\alpha_1} |A> , \tag{30a}$$

$$|\tilde{\varphi}_\beta> = \overset{+}{a}_{\beta_2} |\overset{-}{A_{n'}}> = \overset{+}{a}_{\beta_2} \overset{+}{a}_{\beta_1} |A> . \tag{30b}$$

Now we can use (15) to get

$$S_{\beta\alpha} = - \lim_{\substack{t \to -\infty \\ t' \to +\infty}} G_2 (\beta_1 t', \beta_2 t' \; ; \; \alpha_1 t, \alpha_2 t) \; e^{i e_\alpha (t' - t)} , \tag{31}$$

where

$$e_\alpha = \varepsilon_{\alpha_1} + \varepsilon_{\alpha_2} = \varepsilon_{\beta_1} + \varepsilon_{\beta_2} = e_\beta \quad (32)$$

Introducing now a Dyson's equation analogous to (19), i. e.

$$G_2 = G\tilde{G} - \mathrm{i}\, G_0 G_0 \Gamma_c G_0 G_0 \ , \quad (33)$$

where

$$G\tilde{G} = G(1,3)\ G(2,4) - G(1,4)\ G(2,3) \ , \quad (34)$$

and Γ_c is the connected vertex part, in a similar way as in obtaining (20), we get

$$T_{\beta_1\beta_2\alpha_1\alpha_2} = \delta_{\beta_1\alpha_1} \Sigma_{\beta_2\alpha_2}(\varepsilon_{\alpha_2}) + \delta_{\beta_2\alpha_2} \Sigma_{\beta_1\alpha_1}(\varepsilon_{\alpha_1}) - \delta_{\beta_1\alpha_2} \Sigma_{\beta_2\alpha_1}(\varepsilon_{\alpha_1}) -$$
$$- \delta_{\beta_2\alpha_1} \Sigma_{\beta_1\alpha_2}(\varepsilon_{\alpha_2}) - 8\pi\ \mathrm{i}\ \Gamma_{nc}(\beta_1 \varepsilon_{\beta_1}, \beta_2 \varepsilon_{\beta_2}\ ;\ \alpha_1 \varepsilon_{\alpha_1}, \alpha_2 \varepsilon_{\alpha_2}) +$$
$$+ \Gamma_c(\beta_1 \varepsilon_{\beta_1}, \beta_2 \varepsilon_{\beta_2}\ ;\ \alpha_1 \varepsilon_{\alpha_1}, \alpha_2 \varepsilon_{\alpha_2}) \ , \quad (35)$$

where Γ_{nc} is the non-compact vertex part. At this stage, by the arguments similar to those used to derive Eq. (22), we obtain

$$S_{\beta\alpha} = \langle A_0 | S' | A_0 \rangle \langle A_0 | a_{\beta_1} a_{\beta_2} S' a^+_{\alpha_2} a^+_{\alpha_1} | A_0 \rangle \ . \quad (36)$$

This justifies our intention to interpret the inelastic processes as a two-particle propagation through the medium. In calculating (35) all the diagrams are taken, except those containing passive loops only (because of the HF vacuum). The exact one-particle Green function G is diagonal in the basis which diagonalizes

$$h^{(1)} = T + M \ , \quad (37)$$

where T is the kinetic energy, and M is the compact self energy operator. Then we can use the Dyson equation

$$G_2 = G\tilde{G} - \mathrm{i}\ GG\,\Gamma\,GG \quad (38)$$

in the same way as before, to obtain

$$T_{\beta_1\beta_2\alpha_1\alpha_2} = \Gamma(\beta_1 \varepsilon_{\beta_1}, \beta_2 \varepsilon_{\beta_2}\ ;\ \alpha_1 \varepsilon_{\alpha_1}, \alpha_2 \varepsilon_{\alpha_2}) \quad (39)$$

Γ is now the compact vertex part, calculated by taking the skeletal diagrams only. The expression (39) is identical with that of Zhivopistsev[1], but only formally. Namely, the first order contributions to M

$$M^{(1)}_{\beta\alpha} = V^{HF}_{\beta\alpha} \tag{40}$$

in Ref.[1] are neglected. Within the accepted model, the relation (39) is an exact one.

The first order contribution to (35) is simply the antisymmetrized interaction

$$T^{(1)}_{\beta_1\beta_2,\alpha_1\alpha_2} = \tilde{V}_{\beta_1\beta_2,\alpha_1\alpha_2} \quad . \tag{41}$$

Using now for convenience the symmetrized variant of the diagrams, we have in 2nd order

a) b)

The contribution of (*a*) is given below as an example:

$$T^{(a)}_{\beta\alpha} = \sum_{\gamma_1\gamma_2} \frac{V_{\beta_1\beta_2,\gamma_1\gamma_2}\tilde{V}_{\gamma_1\gamma_2,\alpha_1\alpha_2}}{E-\varepsilon_{\gamma_1}-\varepsilon_{\gamma_2}+i\eta}\left[N_{\gamma_1}N_{\gamma_2}+(1-N_{\gamma_1})(1-N_{\gamma_2})\right] \quad , \tag{42}$$

where $E = \varepsilon_{\alpha_1} + \varepsilon_{\alpha_2}$ We see that the same restrictions with respect to the singularities produced by zeroes of the energy denominator, as in Eq. (25), apply also in this case. The same is true for the contribution of (*b*), and for those of higher order.

In analogy with the optical potential, which can be considered as an effective one-particle potential describing an overall interaction with the medium, we can define an effective two-particle potential modified by the presence of the medium. The irreducible vertex I (1,2; 3,4) is defined as such a vertex in the skeletal diagram which can not be separated in two parts by cutting only two fermion lines. The vertex satisfies the integral equation,

$$\Gamma(1,2;\ 3,4) = I(1,2;\ 3,4) + \frac{1}{2}\int d5\, d6\, I(1,2;\ 5,6)\, G(5)\, G(6)\, \Gamma(5,6;\ 3,4)\,. \tag{43}$$

This equation can be interpreted as the two-particle scattering equation (27), similarly as it was done in the discussion of the optical model for elastic scattering identifying I (1,2; 3,4) with an effective two-particle potential. As before, this also can be used as the starting point in a more exact calculation in the following way. Calculating $I\,(1,2;\ 3,4)$ perturbationally up to a certain order, we can solve in principle equation (43), obtaining in such a way an infinite resummation of the perturbational development of Γ. In analogy to the modified optical calculations[3,9] one can solve a two-particle Schrödinger equation using $I\,(1,2;\ 3,4)$ as the interaction potential, which would represent an approximation that can be practically handled.

In the framework of this formalism, the ionization processes are a particular case of inelastic processes; it is sufficient to take in the formula (35) the final states of both particles in the continuum.

5. Concluding remarks

We have presented here a systematic method of calculating elastic and inelastic processes in the case of one particle colliding with the system of bound particles of the same kind. The relation between the scattering quantities (S, T-matrices) and the corresponding many-body ones (G, Σ, Γ) was established in the simplest way. We have discussed in detail the relation of the obtained quantities with the intuitive notions about propagation of one or two particles through the medium consisting of a bound system of particles. In such a way we have established a theoretical basis for the systematic investigation of several processes by the many-body techniques.

For more than one particle outside of a complete shell, the presented method can be generalized, but then three- and more-particle Green functions come into the play and the practical calculations become much more difficult.

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GREEN-OVE FUNKCIJE U PROBLEMU RASEJANJA ČESTICE NA SISTEMU ČESTICA U VEZANOM STANJU

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Sadržaj

U osnovi ovog prilaza problemu rasejanja leži veza između n-čestične Green-ove funkcije i S-matrice procesa rasejanja n čestica na vezanom stanju sistema istih takvih čestica (zanemarujući otskok tog sistema). Elastično rasejanje čestice na vezanom sistemu neposredno je opisano jednočestičnom Green-ovom funkcijom. Neelastično rasejanje može se aproksimativno opisati modelom u kome se izdvaja slabo vezana čestica sistema (ako takva postoji), te se posmatra rasejanje dveju čestica kroz medijum koji pretstavlja ostatak vezanog sistema; takav proces opisan je dvočestičnom Green-ovom funkcijom. Na osnovu Dyson-ovih jednačina za ove Green-ove funkcije T-matrica odgovarajućih procesa rasejanja izražava se pomoću Σ i Γ, tj. pomoću self-energetskog dela, odnosno verteksa.

Tim metodom može se tretirati rasejanje elektrona na atomu ili nukleona na jezgru. Problem je sveden na izračunavanje Σ, odnosno Γ, za te fizičke sisteme. Ako je broj čestica u vezanom stanju mali, može se očekivati da će perturbacioni razvoj dati prihvatljiv rezultat.

U opštem slučaju ne može se izbeći beskonačna resumacija dijagrama u aproksimaciji velike (atom), odnosno male (jezgro) gustine. Diskutovan je takođe odnos prema ranijim istraživanjima u ovoj oblasti, a napose pitanje optičkog potencijala i efektivne dvočestične interakcije.