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Application of many-body perturbation theory to the investigation of energy spectra of atoms and ions with open shells

ABSTRACT

Un till now accurate calculations of energy spectra of many-electron atoms have usually been carried out using the superposition-of-configurations method or the multi-configurational Hartree-Fock approach. Perturbation theory (PT) has been applied to relatively simple systems with few electrons outside closed shells. This is explained by the absence of a well developed PT in the case of quasi-degenerate states as well as by considerable computational difficulties. In this paper, an efficient PT is described, which is suitable for atoms with several open shells. The carbon isoelectronic sequence is considered as an example of the application of the method.

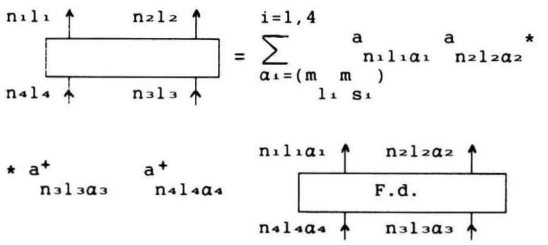
DESCRIPTION

Merkelis et al. (1986) proposed the original graphical method for constructing a stationary PT series, when its spin-angular part is expressed in terms of irreducible tensorial products of electron creation and annihilation operators (a^+ and a).

The diagrams employed represent (Fig. 1) sums of Feynman diagrams (F.d.) over one-electron magnetic quantum numbers.

Using this method, expressions for H_{eff} in second order of PT have been obtained for the case of an extended model space (Lindgren and Morrison, 1982). The computer programmes to generate radial and spin-angular parts of matrix elements of H_{eff} have been worked out for two open shells $(n_1l_1)^{N_1}(n_2l_2)^{N_2}$.

Fig. 1



RESULTS

Energy spectra in the carbon isoelectronic sequence were calculated to illustrate the application of the method and the use of the developed programmes. The energy levels of the configurations $1s^22s^22p^2$, $1s^22p^4$ and $1s^22s2p^3$ were calculated. The united basis of one-electron functions, found in the Hermitian potential, proposed by Morrison (1972), was used. The first order relativistic corrections were taken into account in the Breit-Pauli approximation. The energy levels of the configurations considered were calculated in an extended model space. The calculations were carried out for C I, O III, Ne V, P X, Ca XV and Fe XXI. Table I contains the energy values for P X (second column: this work; third: multi-configurational Hartree-Fock calculations due to Froese Fischer and Saha (1985); fourth: multiconfigurational Dirac-Fock calculations due to Cheng, Kim and Desclaux (1979); fifth: experiment of Kasyanov, Kononov, Korobkin, Koshelev and Serov (1973) and the sixth column: Hartree-Fock calculations using the potential proposed by Morrison (1972)). σ_M denotes the root-mean-square deviation.

Table 1. The energy levels (in cm^{-1}) of the configurations $1s^22s^22p^2$, $1s^22s2p^3$ and $1s^22p^4$ in P X.

	this work	theo.[a]	theo.[b]	exp.[c]	HF[d]
$1s^22s^22p^2$					
$^3P_0$	0	0	0	0	0
$^3P_1$	3588	3679	3685	3681	3598
$^3P_2$	9170	9044	9024	9033	9187
$^1D_2$	59336	61397	62393	59679	62310
$^1S_0$	119670	120399	116287	119963	116322
σ_M	215	770	2046		2010
$1s^22s2p^3$					
$^5S_2$	167896	166526	154918	167730	153285
$^3D_2$	321786	326886	325592	323195	324561
$^3D_1$	321859	327099	325762	323405	324646
$^1D_3$	322273	326930	325605	323222	325055
$^3P_0$	378772	383719	381358	379932	380874
$^3P_1$	378934	383697	381474	379907	381052
$^3P_2$	379258	383915	381691	380139	381378
$^1D_2$	483808	492937	499680	484741	502163
$^3S_1$	490401	498368	502137	490584	506970
$^1P_1$	540767	550518	555441	541968	558447
σ_M	1035	5351	8522		10309
$1s^22p^4$					
$^3P_2$	739889		754251	742605	754932
$^3P_1$	746184		760585	749020	761151
$^3P_0$	748665		762938	751420	763667
$^1D_2$	789179		812516	793057	813909
$^1S_0$	898734		922664	902341	927807
σ_M	3196		15451		17507

[a] Froese Fischer and Saha (1985)
[b] Cheng et al. (1979)
[c] Kasyanov et al. (1973)
[d] HF with Morrison potential

The analysis of the calculations shows that our approach leads to the most accurate results for the ions Ne V, P X, and Ca XV. For C I and O III it is necessary to take higher orders in the Coulomb interaction into account, whereas for Fe XXI one has to account for the correlation corresponding to relativistic operators. Let us notice that correlation effects considerably lowers the upper levels of the ground and excited configurations.

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