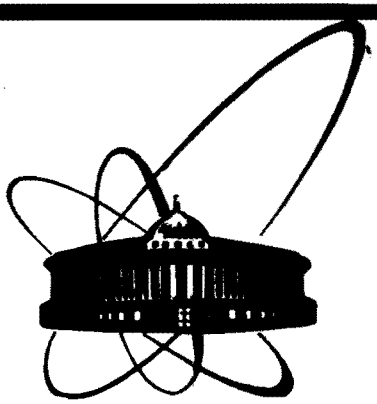

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M.Znojil

PERTURBATION EXPANSIONS GENERATED BY AN APPROXIMATE PROPAGATOR

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1. INTRODUCTION

Numerical solution of the general Schroedinger equation

$$H|\psi> = E|\psi>, \qquad (1.1)$$

is a more or less standard procedure. Indeed, the various variational techniques lead often to very good estimates of the binding energies, while the wavefunctions $|\psi>$ are usually generated by means of the so-called inversion iterations [1].

In the perturbation theory, a close connection with the latter technique may also be noticed. Indeed, both the inverse iterations and perturbation algorithms of the various kinds [2] stem from a common idea - repeated multiplication of some trial wavefunction $|0>$ by an approximate resolvent

$$R = (E_0 - T)^{-1} . \qquad (1.2)$$

Here, E_0 is an approximate energy and T denotes the exact or approximate Hamiltonian in the former or latter context, respectively.

In the present paper, we shall deal with the perturbation theory, noticing that its current forms use only a very restricted class of the approximate Hamiltonians T. To the best of our knowledge, only our recent papers [3] may be quoted as an attempt to build up the perturbation series from the resolvents (1.2) with the non-diagonal (namely, band-matrix) structure of the auxiliary operator T.

In the present text, we intend to complement Ref. [3] by an alternative methodical proposal, based not on a band-matrix generalisation of T, but rather on a similar band- or, in general, invertible-matrix assumption imposed on the propagator (1.2) itself.

Our present main idea is quite straightforward. We assume that the approximate resolvent (1.2) is given to us in an arbitrary form with an available inversion 1/R. Then, the reconstructed operator T,

$$T = E_0 - R^{-1}, \qquad (1.3)$$

and the related decomposition of the Hamiltonian H = T + V become a good starting point for the perturbative considerations.

In more detail, we shall assume that the difference V=H-T-U becomes an almost negligible operator, at worst after its modification via some mean field U,

$$V - U = \lambda H_1 = \text{small}(\lambda \ll 1), \quad H = H_0 + \lambda H_1. \tag{1.4}$$

The auxiliary field U will be chosen here in the separable form of rank p,

$$U = PUP, \quad P = \sum_{m=1}^{p} |0^{[m]}><0^{[m]}|, \tag{1.5}$$

for the sake of definitness.

2. THE ZERO-ORDER EQUATION

In general, we may assume that the input propagator (1.2) and energy estimate E_0 represent a good approximation for more than one state. Thus, we shall consider some s states in (1.1),

$$H|\psi^{[i]}> = E^{[i]}|\psi^{[i]}>, \quad i = 1,2,\ldots,s \tag{2.1}$$

and put s=p for the sake of simplicity.

The assumption of smallness of the "selfconsistently modified" perturbation V - U implies immediately the natural perturbation ansatz

$$|\psi^{[i]}> = |\psi^{[i]}_{\{N\}}> + O(\lambda^{N+1}), \quad E^{[i]} = E^{[i]}_{\{N\}} + O(\lambda^{N+1}), \tag{2.2}$$

with the power-series approximants

$$|\psi^{[i]}_{\{N\}}> = \sum_{k=0}^{N} |\psi^{[i]}_k> \lambda^k \qquad E^{[i]}_{\{N\}} = E_0 + \sum_{k=1}^{N} E^{[i]}_k \lambda^k . \tag{2.3}$$

In combination with (1.4), this should lead to the complete perturbation prescription in principle.

In the limit $\lambda \to 0$, we obtain the so-called "unperturbed equation"

$$H_0|\psi_0^{[i]}> = E_0|\psi_0^{[i]}>, \quad i = 1, 2, \ldots, p \tag{2.4}$$

which may be given also the form of a definition

$$|\psi_0^{[i]}> = RPUP|\psi_0^{[i]}> \tag{2.5}$$

due to our knowledge of the resolvent (1.2) and $H_0 = T+U$.

Now, we are permitted to assume that the pxp - dimensional normalisation matrix

$$W_k^{[i,j]} = <0^{[i]}|\psi_k^{[j]}>, \quad i,j = 1,2,\ldots,p \tag{2.6}$$

with k = 0 is regular, det $W_0 \neq 0$ (otherwise, we should choose a better set $|0>$), and require that the P-projection of eq. (2.5) does not lead to contradictions, i.e.,

$$\sum_{k=1}^{p} <0^{[i]}|R|0^{[k]}><0^{[k]}|U|0^{[j]}> = \delta_{i,j}, \quad i,j = 1,2,\ldots,p \tag{2.7}$$

This is an important equation and defines in fact an optimal auxiliary operator U as an inverse of the matrix PRP.

The first part of our considerations may be summarised. We have found that an arbitrary choice of the resolvent R and energy E_0 becomes compatible with the zero-order equation (2.4) (converts it into an identity), provided only that we define the auxiliary field U by eq. (2.7). In this way, our assumption of smallness acquires a "selfconsistent" character: our input matrix E should generate a small perturbation H-T-U via eqs. (1.3) and (2.7).

3. THE FIRST ORDER CORRECTIONS

Up to the first order in the small variable λ , the insertion of the ansatz (2.2) in our Schroedinger eq. (2.1) gives the identically satisfied zero-order equation accompanied by the p requirements

$$(T + PUP - E_0)|\psi_1^{[i]}> + (V - PUP - E_1^{[i]})|\psi_0^{[i]}> = 0, \quad i = 1,2,\ldots,p. \tag{3.1}$$

Their re-multiplication by R gives the definition similar to (2.5),

$$|\psi_1^{[i]}> = RPUP|\psi_1^{[i]}> + R(V - PUP - E_1^{[i]})|\psi_0^{[i]}>. \tag{3.2}$$

Nevertheless, in contrast to the zero-order case, the P-projection of (3.2) becomes a nontrivial requirement

$$W_1^{[j,i]} = W_1^{[j,i]} + (0^{[j]}|R(V-E_1^{[i]})|\psi_o^{[i]}> - W_o^{[j,i]}, \qquad j,i = 1,2,\ldots,p \tag{3.3}$$

where the first-order normalisation matrices drop out but the rest acquires a structure of a homogeneous linear set of equations

$$\sum_{n=1}^{p} (M^{[m,n]} - \epsilon S^{[m,n]})x^{[n]} = 0, \quad m = 1,2,\ldots,p \tag{3.4}$$

where $\epsilon = E_1^{[i]}$, $x^{[n]} = W_o^{[n,i]}$ and

$$M^{[m,n]} = <\rho^{[m]}|V|\rho^{[n]}> - <0^{[m]}|U|0^{[n]}>$$

$$S^{[m,n]} = <\rho^{[m]}|\rho^{[n]}>, \quad |\rho^{[m]}> = R\sum_{k=1}^{p}|0^{[k]}><0^{[k]}|U|0^{[m]}>. \tag{3.5}$$

Thus, we may conclude that the first-order perturbation form (3.2) of our Schroedinger equation leaves the corrections $|\psi_1^{[i]}>$ free again. At the same time, it fixes the "old" wavefunction corrections $|\psi_o^{[i]}>$ and also the new energies $E_1^{[i]}$, $i = 1,2,\ldots,p$. The corresponding generalised eigenvalue problem (3.4) must be solved numerically, in a way which parallels precisely the degenerate perturbation theory of the Rayleigh-Schroedinger (RS) type [2].

4. THE HIGH-ORDER CORRECTIONS

4.1. The Simplified Notation

In the above text, a use of the square-bracketed superscript indices of the pxp - dimensional matrices is not always necessary. In what follows, we shall indicate a matrix character of such quantities by the bra and ket symbols and drop the superscripts. Thus, the definitions (1.5) or (2.6) acquire the simple matrix form

$$P = |0><0| \qquad <0|\psi_k> = <W_k>, \tag{4.1}$$

etc. Also the p-plets of energies will be arranged in the pxp-dimensional and diagonal matrices $<E_k>$ from now on.

The new notation enables us to re-write our Schroedinger eq. (2.1) in the simple matrix form

$$H|\psi> = |\psi><E>. \tag{4.2}$$

Also an insertion of the power-series ansatz (2.2) - (2.3) becomes simplified. Besides the k = 0 and k = 1 equations ((2.4) and (3.1), respectively), the general perturbation requirement

$$|\psi_k^{[i]}> = RPUP|\psi_k^{[i]}> + R|r_{k-1}^{[i]}>, \tag{4.3}$$

will become expressible in the matrix form

$$|\psi_k> = |\rho><W_k> + R|r_{k-1}>$$
$$|r_{k-1}> = (V - PUP)|\psi_{k-1}> - \sum_{m=1}^{k}|\psi_{k-m}><E_m>, \tag{4.4}$$

containing eqs. (3.2) or even (2.5) as its simpliest special cases.

4.2. The Renormalisation Ambiguity of the Recurrences

We may treat eq. (4.4) as a definition of its left-hand side as well as a recurrent specification of $<E_k>$ and $<W_{k-1}>$. In the latter interpretation, it is sufficient to consider only the P-projection of eq. (4.4),

$$<W_{k-1}> = <0|RV|\psi_{k-1}> - \sum_{m=1}^{k}<0|R|\psi_{k-m}><E_m>. \tag{4.5}$$

For a clear understanding of the structure of eq. (4.5), let us fix now the perturbation order $k > 1$ and denote $R|r_{k-2}> = |b>$. This enables us to introduce the matrix $<Z>$ defined by the formula

$$<\rho|\rho><W_o><Z> = <\rho|V|b> - <\rho|b><E_1> - \sum_{m=2}^{k-1}<\rho|\psi_{k-m}><E_m> \tag{4.6}$$

and independent of both the unknown quantities $<W_{k-1}>$ and $<E_k>$. With its use, our eq. (4.5) (multiplied by $<U>$ from the left, combined with its k = 1 predecessor (3.3) and divided by the common and regular matrix coefficient $<\rho|\rho><W_o>$) acquires a highly symmetric form of a pxp - dimensional equation

$$<Z> = <E_k> + <A><E_1> - <E_1><A> \tag{4.7}$$

for the unknown matrix elements of $\langle E_k \rangle$ and $\langle W_{k-1} \rangle = \langle W_o \rangle \langle A \rangle$.

An explicit, element-by-element transcription of eq.(4.7),

$$\begin{pmatrix} Z^{[1,1]}, & Z^{[1,2]}, & \dots, & Z^{[1,p]} \\ Z^{[p,1]}, & \dots, & & Z^{[p,p]} \end{pmatrix} = \begin{pmatrix} E_k^{[1]}, 0, \dots, 0 \\ \dots \\ 0, 0, \dots, 0, E_k^{[p]} \end{pmatrix} \tag{4.8}$$

$$\begin{pmatrix} 0, e_{21} A^{[1,2]}, e_{31} A^{[1,3]}, \dots, e_{p1} A^{[1,p]} \\ e_{1p} A^{[p,1]}, \dots, e_{p-1p} A^{[p,p-1]}, 0 \end{pmatrix}$$

with $e_{ij} = E_1^{[i]} - E_1^{[j]}$ demonstrates clearly that the energies coincide with the diagonal elements of $\langle Z \rangle$, while the diagonal matrix elements of the normalisations $\langle A \rangle$ remain entirely free. In a way known from the degenerate RS perturbation theory, these p free parameters $A^{[i,i]}$ reflect an ambiguity of the perturbation recurrences and may be fixed by a suitable normalisation requirement.

5. AN ILLUSTRATION

The main condition of applicability of our preceding construction lies in a simultaneous availability of the propagator (matrix R) and its inversion (matrix T). With the simplest nontrivial choice of p = 1, such a situation may be illustrated on the simple one- or three-dimensional anharmonic oscillator example

$$H = p^2 + g_1 r^2 + g_2 r^4, \tag{5.1}$$

where, in the light of its recent fixed-point (FP) analysis [4], we may start from certain FP auxiliary sequence

$$f_k = f_k^{(FP)}(M), \quad k = M, M+1, \dots \tag{5.2}$$

of the 2x2 - dimensional matrices, and define both T = T(M) and R = R(M) non-numerically [5].

In general, there are two essentially different types of such a construction - we may require a band-matrix structure of T(M) or R(M). The former case has been considered elsewhere [3]. The latter requirement is more suitable in the present context:

(a) The band-matrix structure of R simplifies the perturbative prescriptions, preserving the number of the RS intermediate-state summations.

(b) The general matrix structure of T fits better its reconstructed character in the present methodical framework.

We shall refer here to [3-5] for the technicalities, and will pay attention to the numerical results only. Thus, we shall use the sequence (5.2) with M = 5 (a relatively low FP precision), M = 10 (a reliable FP approximation) and M = ∞ (exact limit, no FP approximation). The resulting propagator

Table 1.

The ground-state deviations $D = (E - E_{exact}) \times 10^3$ *as a function of the perturbation order* N *and trimming parameter* t, *with* $E_o = 6.0$

N_{MRS}	1	2	3	4
t				
13	39.35	-5.24	0.56	-0.009
12	39.36	-5.24	0.56	-0.008
11	39.37	-5.24	0.56	-0.009
10	39.37	-5.24	0.56	-0.009
9	39.35	-5.24	0.56	-0.008
8	39.52	-5.25	0.56	-0.007
7	40.74	-5.32	0.60	-0.006
6	44.70	-5.55	0.84	-0.010
5	50.97	-5.93	1.29	-0.015
4	49.84	-6.01	0.88	-0.008
3	44.29	-6.13	0.90	-0.046
2	234.83	-9.18	177.47	- 129.09
1	1410.62	+1883.41	7951.75	+ 25814.99
0	5617.82	-19589.89	77898.28	-384287.35

Table 2.

An extension of Table 1 to the higher N, *with* E_o= 7.0

N^t	5	4	3
1	170.41	165.83	166.74
2	-38.51	-38.56	-40.29
3	6.30	5.89	6.76
4	0.65	0.51	0.42
5	-0.53	-0.63	-0.35
6	0.20	0.21	0.27
7	0.20	-0.01	0.53
8	-0.01	-0.01	0.32
9	0.02	0.01	2.01
10	0.0005	0.0005	2.61

Table 3.

An extension of Table 2 to the second excited state, with t = 10 *and* E_o= 23.0

N	1	2	3	4	5	6	7	8	9	10
D	-134.	-62.	-26.	-9.4	2.7	7.2	21.	28.	77.	104.

Table 4.

An E_o *- dependence of the first excited-state energies* $E = E^{(N)}$ *for* t = 10 *and* M = 10

$E^{(0)}$	$E^{(9)}$	$E^{(10)}$
12.6	13.153 336	13.155 116
12.8	13.156 817	13.156 807
13.0	13.156 808	13.156 799
13.2	13.156 807	13.156 800
13.4	13.156 816	13.156 808
13.6	13.156 780	13.156 806
13.8	13.156 689	13.157 471

Table 5.

An irrelevance of removal of the FP and trimming approximations from the fourth row of Table 4

t	∞	10	∞	10
M	∞	∞	10	10
N				
0	13.200 000	13.200 000	13.200 000	13.200 000
1	13.154 922	13.155 530	13.155 620	13.155 680
2	13.156 847	13.156 817	13.157 220	13.157 230
3	13.156 775	13.156 784	13.157 027	13.157 024
4	13.156 777	13.156 782	13.156 949	13.156 942
5	13.156 777	13.156 782	13.156 898	13.156 890
6	13.156 777	13.156 782	13.156 863	13.156 856
7	13.156 777	13.156 782	13.156 839	13.156 833
8	13.156 777	13.156 782	13.156 823	13.156 817
9	13.156 777	13.156 782	13.156 812	13.156 807
10	13.156 777	13.156 782	13.156 803	13.156 800

R will be permitted to contain 2t+1 nonzero diagonals (with T = H for $t \to \infty$ in principle). We shall also fix $g_1 = g_2 = 1$ in (5.1) and restrict our attention to the first three s-wave bound states with energies E_{exact} = 4.648 8127, 13. 156 800 and 23.297 442 [6].

Our sample of results is summarised in the Tables. The introductory one (Table 1) displays the negligibility of errors in the first four perturbation approximations ($N \leq 4$) for the decreasing trimming parameter $t \geq 6$ and fixed E_o = 6.0. The errors remain small even for $t \geq 3$ while the $t < 3$ cases become quickly divergent.

Table 6.

The ground-state deviation $D'=(E - E_{exact})\times 10^5$ *as a function of the FP precision* M *and parameters* N, t *and* E_0

	F		5.00			6.00	
	M	5	10	∞	5	10	∞
t	N						
6	1	499	574	579	4229	4429	4470
	2	239	-11	-11	-268	-556	-555
	3	210	4	21	264	58	84
	4	181	1	1	180	-1	-1
3	1	492	493	494	4234	4427	4429
	2	329	-19	19	328	-613	-613
	3	204	5	9	243	82	90
	4	176	1	1	137	5	9
2	1		13192	13171	18967	23466	23483
	2		-1325	-1326	1620	-3917	-3918
	3		8157	8766	1088	15905	17747
	4		-5506	-5729	187	-12582	-12909

Table 2 contains similar results for E = 7.0 and up to N = 10. We may notice that the t = 3 item starts also to diverge at N ≈ 7.

In the forthcoming three Tables, an excited-state analogue of the same type of behaviour is documented. An asymptotic deterioration of convergence is shown to take place there

at t = 10 and N = 7 (Table 3), giving still the fairly good results for N = M = t = 10 and variable E_0 (Table 4). An introduction of the FP approximation may even improve the overall convergence pattern and quality of the approximants (Table 5).

A use of a less precise propagator R is illustrated by the choice of M = 5 here. Similarly, our final Table 7 uses a modified form of the input (6.2) (we omit the details here) and demonstrates a validity of the same conclusions.

We may summarise that our choice of the free parameters (within reasonable bounds) does not lead to a significant deterioration of precision. Thus, our R-input perturbation prescription should be tested on the more realistic problems in the future. A work in this direction is in progress [7].

Table 7.

A sample of the influence of a modified FP formula

FP modification		A		B	
N	M	5	10	5	10
1		4353	4423	4228	4431
2		-228	-556	-268	-556
3		308	57	264	58
4		229	0.5	181	-0.7

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Зноил М. E4-87-667

Теория возмущений, порожденная приблизительным пропагатором

Конструкция связанных состояний в виде ряда теории возмущений обобщается на случей, когда известен приближенный но, вообще, не диагональный пропагатор R. Не пользуясь стандартной РШ /Рэлея - Шредингера/ диагонализацией R, ряд теории возмущений построен при помощи вспомогательной pxp матрицы взаимодействия U типа Хартри - Фока. Полученные формулы обобщают вырожденную теорию возмущений РШ. Численно, формализм с p=1 проиллюстрирован на примере ангармонического осциллятора. Хорошая сходимость получилась для различных выборов R.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1987

Znojil M. E4-87-667

Perturbation Expansions Generated by an Approximate Propagator

Starting from a knowledge of an approximate propagator R at some trial energy guess E_0, a new perturbative prescription for a p-plet of bound states and of their energies is proposed. It generalizes the Rayleigh-Schroedinger (RS) degenerate perturbation theory to the nondiagonal operators R (eliminates a RS need of their diagonalisation) and defines an approximate Hamiltonian T by mere inversion. The deviation V of T from the exact Hamiltonian H is assumed small only after a subtraction of a further auxiliary Hartree-Fock-like separable "selfconsistent" potential U of rank p. The convergence is illustrated numerically on the anharmonic oscillator example.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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