ON PERTURBATION THEORY FOR LARGE QUANTUM SYSTEMS

YU. L. MENTKOVSKIĬ

Institute of Physics, Academy of Sciences, Ukrainian S.S.R.

Submitted to JETP editor January 22, 1960

J. Exptl. Theoret. Phys. (U.S.S.R.) **39**, 317-321 (August, 1960)

A new form of the Van Hove-Hugenholtz perturbation theory expansion is proposed. The series obtained differ from the known ones by the simplicity of the energy denominators; this can be useful, for instance, when evaluating excited states. The derivation of these expansions is also fairly simple.

It is well known that the usual perturbation theory expansions cannot adequately describe systems with a large number of degrees of freedom which occupy a large volume in space. The main cause for this is that the series for such systems contain arbitrarily large powers of the volume.

At the present time this difficulty has already been overcome by various means. One of the different solutions of this problem is the theory proposed by Hugenholtz.[1] Using the formalism developed earlier by Van Hove[2,3] and amplifying his diagram method, Hugenholtz reorganized the series in such a way that the theory now only deals with quantities which are proportional to or independent of the volume. The new series contain, however, energy denominators that are more complicated than usual, which makes their practical application difficult. The energy of a perturbed system is, for instance, expressed in terms of the eigenvalues of the operator*

$$G(z) = (V + V(z - H_0 - G(z))^{-1} V + \ldots)_{id}. \tag{1}$$

Here H_0 is the Hamiltonian of the unperturbed system, V the perturbation energy, and z a complex number.

Equation (1) is essentially an equation for $G(z)$ in the form of an infinite series. The series for other quantities are not in the form of equations, but they contain the same denominators $[z - H_0 - G(z)]^{-1}$.† This fact is particularly inconvenient in those cases where the problem to be solved is such that the series can not be broken off after a few terms, and one must sum (at least a well defined class of diagrams) in all perturbation theory orders. The case of a system with Coulomb interactions is, for instance, such a case.

We propose in the present note a simple derivation of the basic expansions of the Van Hove-Hugenholtz theory,[1-3] which leads to series with unperturbed denominators $(z - H_0)^{-1}$. The series obtained can also be used as the basis of the complete theoretical formalism of the papers mentioned, if this formalism is slightly changed (see the survey article[6]).

*The index id indicates that only the so-called irreducible diagonal diagrams are taken into account when evaluating the matrix elements of the series (see reference 1).

†An exception is the series for the ground state, where the results can be simplified. This, however, is not so very interesting as the same results had been obtained earlier by Goldstone[4] and afterwards (and much more simply) by C. Bloch.[5]

1. DERIVATION OF THE BASIC EXPANSIONS USING OPERATOR TECHNIQUES

We shall consider systems with a continuous (or quasi-continuous) spectrum, the Hamiltonian of which can be split into two parts

$$H = H_0 + V, \tag{2}$$

where V can be considered to be a perturbation. We denote the wave function and eigenvalue of the unperturbed system by $|\alpha\rangle_0$ and ϵ_α. We denote the same quantities for the perturbed system by $|\alpha\rangle$ and E_α. We also introduce the perturbed and the unperturbed resolvents

$$R(z) = (z - H)^{-1}, \qquad D(z) = (z - H_0)^{-1}. \tag{3}$$

In references 3 and 1 it was shown that*

$$|\alpha\rangle_\pm = R_{E_\alpha \pm}[R(z)|\alpha\rangle_0], \qquad E_\alpha = \varepsilon_\alpha + G_\alpha(E_\alpha). \tag{4}$$

The symbol $R_{E_\alpha \pm}$ is defined by the equation

$$R_{E_\alpha \pm} f(z) = \lim_{z \to E_\alpha \pm i0} (z - E_\alpha) f(z), \tag{5}$$

and the function $G_\alpha(E_\alpha)$ is the eigenvalue of the

*The presence of two signs for $|\alpha\rangle$ corresponds to two complex-conjugate functions. This can easily be proved for a wide class of systems (see reference 6).

operator (1) in the point $z = E_\alpha$. It is clear that if $f(z)$ has a pole of the first order in the point $z = E_\alpha$, the limit (5) is uniquely defined and gives the residue of $f(z)$ in that pole. We retain the term "residue" also for the case where the two limits in (5) are different.

We must, according to Eqs. (4) and (5), expand $R(z)|\alpha>_0$ in V so that the factor that is singular at the point $z = E_\alpha$ is explicitly split off. We start from the easily verified formula

$$R(z) = D(z) + D(z)VR(z). \tag{6}$$

By iteration we get from (6) the series

$$R(z) = D(z)\sum_{k=0}^{\infty}(VD(z))^k, \tag{7}$$

which is useful for what follows, but which does not possess the property which we need at $E_\alpha \neq \epsilon_\alpha$. We return thus to (6). One can write any operator P as a sum of a diagonal and a non-diagonal operator (in the $|\alpha>_0$ representation)

$$P = P_d + P_{nd}. \tag{8}$$

We shall arrange the splitting up (8) in such a way that the second term on the right hand side of the expression for the matrix element,

$${}_0\langle\alpha|P|\beta\rangle_0 = P_{d\alpha}\delta(\alpha-\beta) + {}_0\langle\alpha|P_{nd}|\beta\rangle_0 \tag{9}$$

does not contain terms with a factor $\delta(\alpha - \beta)$. Here $P_{d\alpha}$ is the eigenvalue of the operator P_d and $\delta(\alpha - \beta)$ a product of the Kronecker symbol and the Dirac delta-function, if the quantum numbers of the system are partly discrete and partly continuous. In such a split, $(P_{nd})_d = 0$.

For the sake of simplicity we assume for the time being that

$$V_{nd} = V. \tag{10}$$

[The requirement (10) does not reduce the generality, as V_d can always be included in H_0. Practically speaking, however, it is inconvenient and we shall later on drop it.] Taking into account the fact that a product of operators of which only one is non-diagonal is itself a non-diagonal operator, we find the diagonal and the non-diagonal part of (6)

$$R_d = D + D(VR_{nd})_d, \tag{11}$$

$$R_{nd} = DVR_d + D(VR_{nd})_{nd}. \tag{12}$$

Assuming the series so obtained to converge, we solve (12) for R_{nd} by iteration. We get then

$$R_{nd} = K_{nd}R_d, \tag{13}$$

$$K_{nd} = \left\{\sum_{k=1}^{\infty}(DV)^k\right\}_{\nu d}. \tag{14}$$

Here we have put, by definition,

$$(DV\ldots DVDV)_{\nu d} \equiv \{DV\ldots[DV(DV)_{nd}]_{nd}\}_{nd}. \tag{15}$$

By virtue of (11) we get from (13)

$$R_d = D + D(VK_{nd})_d R_d. \tag{16}$$

We introduce the diagonal operator*

$$G(z) \equiv (VK_{nd}(z))_d = \left\{V\sum_{k=1}^{\infty}(D(z)V)^k\right\}_{sd}. \tag{17}$$

The meaning of the index sd is defined by Eq. (15) if the last index nd in that equation is replaced by d. Equation (16) now takes the form

$$R_d = D + DGR_d,$$

from which follows directly one of the basic Van Hove-Hugenholtz formulae[1,2]

$$R_d(z) = (z - H_0 - G(z))^{-1}. \tag{18}$$

For the resolvent we get

$$R(z) = \{1 + K_{nd}(z)\}R_d(z). \tag{19}$$

This is the second important formula of the same authors.

One can easily verify the validity of the relations

$$G^+(z) = G(z^*), \quad R_d^+(z) = R_d(z^*), \tag{20}$$

that follow from the hermiticity of H_0 and V.

Equations (18) and (19) have been obtained by relatively simple means and the denominators in the expansions for $K_{nd}(z)$ and $G(z)$ are in our case the operators $z - H_0$.

One verifies easily that the expansion (19), unlike (7), possesses the property we need and enables us to find in fact the residue (4). Indeed, by virtue of (14) the first factor on the right hand side of the equation

$$R(z)|\alpha\rangle_0 = \{1 + K_{nd}(z)\}|\alpha\rangle_0 R_{d\alpha}(z) \tag{21}$$

can suffer only a finite discontinuity on passing through the real axis. The factor $R_{d\alpha}(z)$, however, has, apart from a discontinuity on some segment of the real axis, also a pole in the point $z = E_\alpha$ [see (18)].

Up to now the derivation has been purely formal in character. For a practical application of the formulae obtained it is necessary to establish the rules for evaluating the matrix elements of operators with indices νd and sd. To understand these rules it is enough to consider an example. Let us assume that we must evaluate the matrix element

*Van Hove had also obtained $G(z)$ in the form (17) by other means. The index sd (simple diagonal) was introduced by Van Hove (private communication).

$$ {}_0\langle\alpha|(VDV)_{\nu d}|\beta\rangle_0 = \int\limits_{(\nu d)} d\alpha_1\, {}_0\langle\alpha|V|\alpha_1\rangle_0 D_{\alpha_1}\, {}_0\langle\alpha_1|V|\beta\rangle_0. \qquad (22) $$

According to (9) and (15), the index νd indicates that if $|\alpha\rangle_0 = |\beta\rangle_0$, the element (22) is evaluated by taking the limit $\alpha \to \beta$ for $\alpha \neq \beta$, while in the integral over α_1 we must exclude a small neighborhood near $|\alpha_1\rangle_0 = |\beta\rangle_0$ and let this excluded neighborhood tend to zero after the integral has been evaluated.

From the very beginning we could have started not from (6) but from the equivalent equation

$$ R = D + RVD; \qquad (6a) $$

and we should then, by analogous considerations, have been led to the equation

$$ R = R_d\{1 + Q_{nd}\}; \qquad (19a) $$

$$ Q_{nd}(z) = \left\{\sum_{k=1}^{\infty} (VD(z))^k\right\}_{\bar{\nu}d}, \qquad (14a) $$

$$ (VDVD\ldots VD)_{\bar{\nu}d} \equiv \{[(VD)_{nd}VD]_{nd}\ldots VD\}_{nd}. \qquad (15a) $$

Using the property $P^+_{nd} = (P^+)_{nd}$ one can verify that

$$ K^+_{nd}(z) = Q_{nd}(z^*). \qquad (23) $$

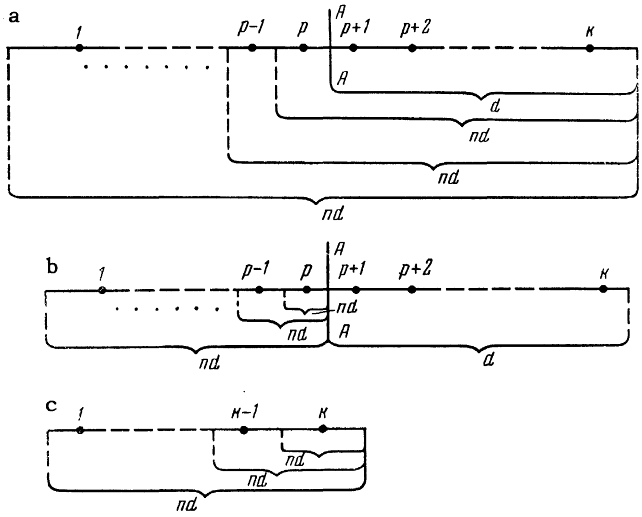
Equation (23) enables us to use Van Hove's method[2] to prove the important inequality

$$ \operatorname{Im} G_\alpha(z) \leqslant 0 \qquad (\operatorname{Im} z > 0). \qquad (24) $$

From the formulae established above we can obtain all basic results of Hugenholtz and Van Hove (see reference 6).

2. DERIVATION USING DIAGRAMS

In order to get rid of arbitrary powers of the volume in the expansions, we must be able to single out the singular factor not only from the resolvent as a whole, but also from its separate parts, which correspond only to diagrams of certain classes. [A method of comparing diagrams with the matrix elements of the operator (7) is described by Hugenholtz.[1]] For instance, it is important to separate the singularity of $R_L(z)$, which is that part of the resolvent obtained when only diagrams without vacuum components (linked clusters) are considered in the matrix elements of the series (7). This part of the resolvent is independent of the volume. The method considered in the foregoing for separating $R_d(z)$ from $R(z)$ cannot be applied immediately in this case. We give therefore a more general method, which is based upon the use of diagrams.



This derivation is essentially already suggested by the preceding arguments and leads also to expansions with simple denominators $z - H_0$. Condition (10) can now be dropped.

An arbitrary Hugenholtz diagram for $R_{nd}(z)$, $R_{Lnd}(z)$, or any other non-diagonal part of the resolvent has been schematically depicted in Fig. a*. Figure a is completely equivalent to Fig. b. In other words, if any diagram is cut by a vertical line AA successively after the first, second, . . . vertex, the diagram to the right of AA will be non-diagonal p-1 times, but the p-th time it will turn out to be diagonal. [Clearly (see Fig. c) this will be the largest diagonal part of the diagram, containing the right hand end.] Combining in one group all terms of the series with the same number p of vertices to the left of the diagonal part, and expanding the group in order of increasing p, we obtain easily not only Eq. (19), but also, for instance, the relation

$$ R_L(z) = \{1 + K_{Lnd}(z)\}\, R_{Ld}(z). \qquad (25) $$

Similarly we obtain also equations of the kind (17), (19a), and so on. In other words, equations which are completely analogous to the equations for $R(z)$ itself are also valid for parts of the resolvent.

We are now already able to reproduce all formulae from the Van Hove-Hugenholtz theory on the basis of the simplified expansions. In conclusion we note that the derivation with the aid of diagrams gives another procedure for evaluating the matrix elements of operators with νd and sd. To evaluate the elements of the operator $K_{nd}(z)$, for in-

*This figure is schematic in that the actual lines between vertices have been replaced by straight line segments, so as to guarantee the generality of our considerations.

stance, we need only take into account diagrams of the type shown in Fig. c.

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[2] L. Van Hove, Physica **21**, 901 (1955).
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Translated by D. ter Haar
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