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Anticorrelation and an exact wave function in an exactly solvable model

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The concept of correlation between two parts of the total Hamiltonian is used to obtain information about the eigenfunction of a total Hamiltonian. Using a solvable model it is shown that the present formulation gives an energetically good wave function.

I. INTRODUCTION

One of the interesting problems in many-body physics has been to study the various correlations. The importance of the correlation coefficients for the electronic wave functions was first brought out by Kutzelnigg and his collaborators.[1] They had studied the correlation of the position of the electrons. At one time it was thought that the more negative the correlation coefficient the better would be the approximate many-body wave functions. If this had been true for all many-body wave functions, then one would have obtained a prescription for obtaining a good wave function. It has now been conclusively shown by King and Rothstein,[2] using an exactly solvable model, that the requirements of minimum energy and most negative correlation coefficients are usually not compatible.

Since it is possible to define other kinds of correlations apart from the correlation of the position of electrons, it is worthwhile to explore this possibility to obtain information about the goodness of the many-body wave function. A new formulation in this direction can be carried out by noting that in some other branches of many-body physics[3] the concept of correlation between two operators of the system has played a significant role.

The purpose of the present note is to present a formulation based on the concept of correlation between two parts of the Hamiltonian to obtain an energetically good wave function. We present this formulation in the next section and apply it to the exactly solvable models in Sec. III. Concluding remarks are presented in Sec. IV.

II. FORMULATION

Let H be the exact Hamiltonian of the system satisfying the exact eigenvalue equation

$$H\Psi=E\Psi \ . \tag{1}$$

We now split the Hamiltonian H into two parts, H_0 and V where V is the part which arises due to the correlations in the Hamiltonian. Then Eq. (1) becomes

$$(H_0+V)\Psi=E\Psi \ , \tag{2}$$

which immediately gives

$$E=\langle H_0\rangle+\langle V\rangle \ , \tag{3}$$

where the angle bracket sign $\langle\ \rangle$ denotes the expectation value of the enclosed operator with respect to Ψ.

We next multiply the left-hand side of Eq. (2) by V to obtain

$$(VH_0+V^2)\Psi=EV\Psi \ . \tag{4}$$

Rewriting Eq. (4) in the form of matrix element with respect to Ψ and using Eq. (3) we get

$$\frac{\langle VH_0\rangle-\langle V\rangle\langle H_0\rangle}{\langle V^2\rangle-\langle V\rangle^2}=-1 \ . \tag{5}$$

By multiplying Eq. (2) from left by H_0 and carrying through the same steps we can also derive the following relation:

$$\frac{\langle H_0V\rangle-\langle H_0\rangle\langle V\rangle}{\langle H_0^2\rangle-\langle H_0\rangle^2}=-1 \ . \tag{6}$$

From Eqs. (5) and (6) we see that the expectation value of the product of $(V-\langle V\rangle)$ with $(H_0-\langle H_0\rangle)$ divided by the mean-square deviation of H_0 or V using the exact wave function is -1.

We can also calculate the value of the correlation coefficient ρ given by the expression[4]

$$\rho=\frac{\langle VH_0\rangle-\langle V\rangle\langle H_0\rangle}{[(\langle H_0^2\rangle-\langle H_0\rangle^2)(\langle V^2\rangle-\langle V\rangle^2)]^{1/2}} \ . \tag{7}$$

Assuming H_0 to be Hermitian, we find, using expressions (5) and (6), that $\rho=-1$ which implies that there is complete anticorrelation between V and H_0 for the exact wave function.

A very general result of the type (5) or (6) can be derived for an arbitrary operator A belonging to the same Hilbert space as the Hamiltonian H by noting that the expectation value $\langle A\rangle$ and $\langle H-A\rangle$ have the same variance. This arbitrariness is taken care of in the present case by splitting the Hamiltonian specifically into two parts H_0, V, as mentioned in the beginning of this section, where H_0 represents the single-particle part of the Hamiltonian and V the rest of it.

We would now like to apply these expressions to find an exact wave function for solvable models.

III. SOLVABLE MODELS

The Hamiltonian H of the solvable model is given by[2]

$$H=-\tfrac{1}{2}\nabla_1^2-\tfrac{1}{2}\nabla_2^2+\tfrac{1}{2}k_1(r_1^2+r_2^2)-\tfrac{1}{2}k_2r_{12}^2\ . \tag{8}$$

By using the center of mass $\bar{R}=1/\sqrt{2}(\bar{r}_1+\bar{r}_2)$ and the relative coordinate $\bar{r}=1/\sqrt{2}(\bar{r}_1-\bar{r}_2)$ it is transformed[2] to a sum of two oscillator Hamiltonians $H(\bar{R})$ and $H(\bar{r})$. Further, since in the trial wave function exact eigenfunction of $H(\bar{R})$ is used and since there is complete symmetry between x,y,z directions, it is sufficient to consider the following Hamiltonian H:

$$H=-\frac{1}{2}\frac{\partial^2}{\partial X^2}+kX^2+\alpha X^2\ , \tag{9}$$

with

$$H_0=-\frac{1}{2}\frac{\partial^2}{\partial X^2}+kX^2 \tag{10a}$$

and

$$V=\alpha X^2\ . \tag{10b}$$

For the trial wave function ϕ we write

$$\phi=N\exp(-\tfrac{1}{2}\beta X^2)\ , \tag{11}$$

where N is the normalization constant and β is the unknown parameter. It is now a simple matter to calculate the various matrix elements of Sec. II and we find that

$$\frac{\langle\phi\,|\,VH_0\,|\,\phi\rangle-\langle\phi\,|\,V\,|\,\phi\rangle\langle\phi\,|\,H_0\,|\,\phi\rangle}{\langle\phi\,|\,V^2\,|\,\phi\rangle-\langle\phi\,|\,V\,|\,\phi\rangle^2}=\frac{2k-\beta^2}{2\alpha}\ .$$

According to Eq. (5), ϕ will be the exact wave function provided the right-hand side of Eq. (12) is -1. This gives us $\beta=2(k+\alpha)$. This is also the energetically best wave function for the Hamiltonian given by Eq. (9). This clearly demonstrates that the concept of correlation can be used to obtain energetically good wave functions.

We next consider another example using the solvable model of Lipkin, Meshkov, and Glick.[5] This model has been very useful in studying various approximations for a many-body system. Using quasispin operators, this Hamiltonian is given by[5]

$$H=J_z+\tfrac{1}{2}(J_+^2+J_-^2)\ . \tag{12}$$

For such a Hamiltonian it is obvious that $H_0=J_z$ and $V=\frac{1}{2}(J_+^2+J_-^2)$. The trial ground-state wave function for a two-body system is written as

$$\phi=\cos\theta\,|\,1-1\,|\,\rangle+\sin\theta\,|\,1\,1\rangle\ , \tag{13}$$

where $|\,jm\rangle$ represent the eigenfunctions of J^2,J_z.

Using angular momentum algebra it is easy to see that

$$\frac{\langle\phi\,|\,H_0V\,|\,\phi\rangle-\langle\phi\,|\,H_0\,|\,\phi\rangle\langle\phi\,|\,V\,|\,\phi\rangle}{\langle\phi\,|\,V^2\,|\,\phi\rangle-\langle\phi\,|\,V\,|\,\phi\rangle^2}=\tan 2\theta\ . \tag{14}$$

Expression (5) then tells us that ϕ will be the exact ground state if $\tan 2\theta=-1$ which gives $\theta=-\pi/8$. By actual diagonalization of the Hamiltonian given by expression (12) we see that this is indeed the correct solution of the problem.

IV. CONCLUDING REMARKS

It can be shown easily that the same value of the parameter β or θ is obtained for the solvable models discussed in Sec. III if we use Eq. (6). Since the mean-square deviation of V seems to be easier to calculate, in practice Eq. (5) seems to be simpler than Eq. (6). Also we can easily calculate the correlation coefficient ρ between H_0 and V and show that it is -1. Therefore the solvable models conclusively show that anticorrelation between H_0 and V can be used to obtain energetically good wave functions. Further it is interesting to note that for the solvable models one could also calculate the value of the parameter β or θ by minimizing the quantity $(1+g)^2$. This quantity, for example, for the second solvable model is $(1+\tan 2\theta)^2$. Minimizing it with respect to θ we get the same value as we had obtained earlier using Eq. (5). We should also mention here that for the unsolved problems the present formulation, namely relations (5) and (6), tell us that the trial wave functions which one chooses must be such that it gives maximum anticorrelation between V and H_0. We conclude this note by saying that, in the light of the results obtained for the solvable models, the present formulation provides one more way of obtaining approximate many-body wave functions which are also energetically good wave functions.

[1]W. Kutzelnigg, G. Del Re, and G. Berthier, Phys. Rev. 172, 49 (1968). F. W. King and S. M. Rothstein, Phys. Rev. A 21, 1376 (1980). Also see the other references cited at the end of this article.

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[5]H. J. Lipkin, N. Meshkov, and A. J. Glick, Nucl. Phys. 62, 188 (1965).