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A PROCEDURE FOR SYSTEMATIC IMPROVEMENTS OF VARIATIONAL METHOD CALCULATIONS OF GROUND EXCITED STATES

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A method is proposed for systematic improvements of variational estimates of energies and wave functions of stationary states in quantum mechanics and field theories. The mean value of the time derivative of any observable should vanish in a true stationary state. The method starts with some trial state and modifies it so that this condition is approximatively satisfied for a selected set of observables. The set can consist of subsequent time derivatives of a particular physical quantity. The state vector obtained in this case corresponds to an approximatively time independent mean value of this quantity. We present a few illustrative examples including the Bardeen—Cooper—Schrieffer ansatz for the ground state of a superconductor, which follows naturally from this approach.

Two approaches are proposed based on differential equations for a motion of the state vector along the steepest descent to the stationary state. They are both unbiased in the sense that they do not require a preliminary selection of a particular set of "relevant" operators.

The former maximizes locally the decrement of $\langle \Psi | H | \Psi \rangle$ and is equivalent to a differential form of the t-expansion used recently by Horn and Weinstein and is suitable for a search of the ground state. The latter maximizes locally the decrement of $\langle \Psi | H^2 | \Psi \rangle - \langle \Psi | H | \Psi \rangle^2$ and is suitable for a search of excited stationary states.

I. INTRODUCTION

In numerous problems of physics, as, e.g. in studying the properties of hadrons, one has to use non-perturbative methods in order to determine the energies and state vectors of stationary states. The variational method is a rather simple and useful procedure but it is usually based on an educated guess of the form of the state vector. In this paper we shall present a method which helps in guessing the form of the state vector to be used in variational method calculations and leads to systematic improvements of the estimates of energies and state vectors of stationary states.

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The method is based on the following simple observation. In a true stationary state $|\Psi_n\rangle$ the expectation value of an observable A is time independent

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Psi_n|A|\Psi_n\rangle = 0. \tag{1}$$

Suppose that we have a trial state $|\Psi_V\rangle$, obtained by a guess or by a "preliminary" minimization, which does not obey the condition (1). We now wish to find a unitary operator U such that the state $|\Psi'\rangle = U|\Psi_V\rangle$ obeys Eq. (1). The operator U is, of course, not unambiguously determined but one of the solutions can be found easily. We write $U = \exp(\mathrm{i}\alpha A)$ and determine the value of the parameter α by minimizing the expectation value of the Hamiltonian. This leads to the condition

$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle\Psi'|H|\Psi'\rangle = \frac{\mathrm{d}}{\mathrm{d}\alpha}\langle\Psi_V|e^{-\mathrm{i}\alpha A}He^{\mathrm{i}\alpha A}|\Psi_V\rangle = 0 \tag{2}$$

This implies

$$\langle\Psi_V|e^{-\mathrm{i}\alpha A}[H,A]e^{\mathrm{i}\alpha A}|\Psi_V\rangle = \langle\Psi'|[H,A]|\Psi'\rangle = 0. \tag{3}$$

The state vector $|\Psi'\rangle$ with the value of α determined form Eq (2) satisfies also the condition ($\hbar = 1$)

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Psi'|A|\Psi'\rangle = \mathrm{i}\langle\Psi'|[H,A]|\Psi'\rangle = 0 \tag{4}$$

which means that the time derivative of the expectation value of A vanishes in the state $|\Psi'\rangle$.

The connection between the vanishing of the time derivative of $\langle\Psi'|A|\Psi'\rangle$ the minimum of $\langle\Psi'(\alpha)|H|\Psi'(\alpha)\rangle$ indicates that in order to improve the variational estimates it is useful to look for states with vanishing time derivatives of expectation values of particular operators.

The preceding formulation of the problem can be generalized in a few ways. Instead of considering a single operator A we can take into account a set of operators $A, B, C, \ldots Z$. We shall show below how one can, starting from the trial state $|\Psi_V\rangle$, arrive at the state $|\Psi\rangle$ in which time derivatives of the expectation values of all the operators $A, B, C, \ldots Z$ vanish simultaneously

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Psi|A|\Psi\rangle = \mathrm{i}\langle\Psi|[H,A]|\Psi\rangle = 0, \frac{\mathrm{d}}{\mathrm{d}t}\langle\Psi|B|\Psi\rangle = \mathrm{i}\langle\Psi|[H,B]|\Psi\rangle = 0, \ldots \tag{5}$$

It will also be shown that such a state $|\Psi\rangle$ is an optimal variational state on a particular subset of the Hilbert space of the problem.

We arrive at particular case of the preceding problem when we want to have the expectation value of an operator $A(t)$ approximately constant over some interval. The time evolution of an operator $A(t)$ in the Heisenberg picture is

$$A(t) = e^{\mathrm{i}Ht}Ae^{-\mathrm{i}Ht} = A + \mathrm{i}t[H,A] + \frac{(\mathrm{i}t)^2}{2!}[H,[H,A]] + \ldots \tag{6}$$

where $A = A(0)$ shows that

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n}A(t)\bigg|_{t=0} = \mathrm{i}^n[H,\ldots[H,A]\ldots.] \tag{7}$$

Requiring that the first $(n-1)$ derivatives of the expectation value of $A(t)$ at $t = 0$ vanish is equivalent to the previous situation with

$$A = A(0),\ B = [H,A(0)],\ C = [H,[H,A(0)]],\ldots \tag{8}$$

Starting with the trial state $|\Psi_V\rangle$ we are then looking for a state $|\Psi\rangle = U|\Psi_V\rangle$ which satisfies the conditions

$$\langle\Psi|[H,A]|\Psi\rangle = 0,\ \langle\Psi|[H,[H,A]]|\Psi\rangle = 0,\ldots \tag{9}$$

Formulating the problem in this way one can make use of the time evolution of the operators if this is available. In fact such a time evolution of operators has recently been studied in a series of papers by Bender, Milton and Sharp [1] in the finite element scheme.

The solutions to these problems will be given in a form of partial differential equations which specify the motion of the state vector in the Hilbert space from the initial state $|\Psi_V\rangle$ to the final state $|\Psi\rangle$ which satisfies Eqs (5) or their special form Eq (9). Sometimes it is intuitively clear which the "important" operators of the problem are, sometimes it is not. In selecting a particular set of operators we are then in a sense biased. Because of that we shall finally study the non-biased approach to the variational calculations of the energies and state vectors of the stationary states. The problem is formulated in the following way. Suppose that the current value of the state vector is given. We want to find the infinitesimal vector $|\delta\Psi\rangle$, orthogonal to $|\Psi\rangle$ (in order not to spoil the normalization) and such that the replacement

$$|\psi\rangle \to |\Psi\rangle + |\delta\Psi\rangle$$

leads to the fastest possible decrease of $\langle\Psi|H|\Psi\rangle$, with $|\delta\Psi\rangle$ of a given norm. We shall obtain the differential eqs. governing the motion of the state $|\Psi\rangle$ in the

Hilbert space. It will turn out that they are a differential version of the t-expansion method which consists in the transformation

$$|\Psi\rangle \to \frac{\exp(-tH)|\Psi\rangle}{\sqrt{\langle\Psi\exp(-2tH)|\Psi\rangle}}$$

studied recently by Horn and Weinstein [2]. The state converges to the ground state of the theory.

We then generalize this procedure by writing down differential eqs. for the motion of a state vector $|\Psi\rangle$ in the Hilbert space along the steepest descent with respect to the quantity $\langle\Psi|H^2|\Psi\rangle - \langle\Psi|H|\Psi\rangle^2$. This quantity has a local minimum at *any* stationary state and the method is thus suitable for the search of excited stationaty states.

The paper is arranged as follows. In Sect. II we describe two simple warm-up examples illustrating the basic idea and proceed in Sect. III to the discussion of the ground state of the *BCS* model. In Sect. IV we present the method leading to states which satisfy simultaneously conditions (5) for a set of operators. Differential equations governing the motion of the state vector in the Hilbert space along the steepest descent of $\langle\Psi|H|\Psi\rangle$ are presented in Section V and similar eqs. corresponding to the steepest descent of $\langle\Psi|H^2|\Psi\rangle - \langle\Psi|H|\Psi\rangle^2$ are derived in Sect. VI. The last section contains comments and conclusions.

II. SIMPLE EXAMPLES

In order to get insight into how the method works and into its biases and limitations we consider first the simplest examples, namely the spin in the external magnetic field. We shall discuss this example in some detail since that will provide also the motivation for ruther discussion of a more general situation.

The spin in the external magnetic field

The simplest choice of the hamiltonian is certainly

$$H = -\sigma_z. \tag{10}$$

Suppose further that the starting value of the spin state corresponds to the spin pointing in the direction given by the unit vector $(\cos\varphi, \sin\varphi, 0)$, $0 < \varphi < \pi/2$:

$$\Psi_v = \frac{1}{\sqrt{2}}\begin{pmatrix}\exp(-i\varphi/2)\\ \exp(i\varphi/2)\end{pmatrix} \tag{11}$$

and select the operator $A = \sigma_y/2$. In this case the variational method consists in minimizing the expectation value

$$E(\alpha) = \langle\Psi_v|\exp(-i\alpha\sigma_y/2)(-\sigma_z)\exp(i\alpha\sigma_y/2)|\Psi_v\rangle \tag{12}$$

A straightforward calculation gives

$$E(\alpha) = -\sin\alpha\cos\varphi. \tag{13}$$

The extremum is reached for $\alpha = \pi/2$. It is intuitively obvious what is going on. The change in the angle α corresponds to the rotation of the spinor around the y-axis and the optimal α is obtained for the spinor $|\Psi\rangle$ shown in Fig. 1. The calculation confirms that. We obtain

$$E(\alpha) = -\sin\alpha\cos\varphi.$$

The extremum is reached for $\alpha = \pi/2$, which corresponds to the rotation of $|\Psi_v\rangle$ around the y axis by the angle $\pi/2$. The radius of the circle in Fig. 1 is equal to $\cos\varphi$ and this is also the reason why the best estimate based on Eq (13) is $E(\alpha = \pi/2) = -\cos\varphi$.

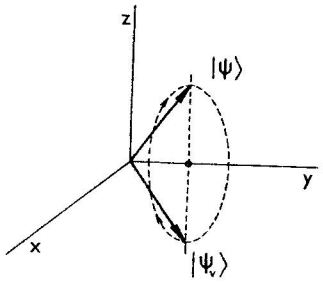

Fig. 1. The rotation around the y-axis heading from $|\Psi_v\rangle$ to $|\Psi\rangle$.

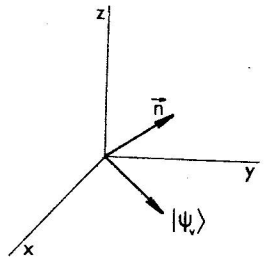

Fig. 2. The axis of rotation $\boldsymbol{n}$ is orthogonal to the plane containing $|\Psi_v\rangle$ and z-axis.

The example shows clearly the limitation of the method. If the operator A is chosen in such a way that the rotation around the "A axis" cannot improve the variational estimate very much, the method will not lead to a significant improvement of the variational estimate.

It is not difficult to improve the method in such a transparent situation as the present example. The simplest possibility is of course to use $|\Psi\rangle$ in Fig. 1 as the starting state vector for a further optimization and select now $A = \sigma_x/2$ as the next operator. The rotation around the x axis performed in the same way as before (around the y-axis) brings immediately the state vector into the ground state.

For application to more complicated situations another procedure seems more promising. We start at the very beginning, considering all the three possible operators σ_x, σ_y, σ_z and try to find their linear combination which rotates the original spinor $|\Psi_v\rangle$ in the fastest way to the true stationary state.

Suppose that the original spinor $|\Psi_\nu\rangle$ "points" in the direction $\boldsymbol{n}_0$ ($\sin\vartheta\cos\varphi$, $\sin\vartheta\sin\varphi$, $\cos\vartheta$) given by the angles ϑ, φ in spherical coordinates. Then

$$|\Psi\rangle_\nu = \begin{pmatrix} \exp(-i\varphi/2)\cos(\vartheta/2) \\ \exp(i\varphi/2)\sin(\vartheta/2) \end{pmatrix}. \tag{14}$$

It is obvious that in order to rotate this spinor into the direction of the z-axis we have to rotate it around the axis orthogonal both to the z-axis and to $\boldsymbol{n}_0$. This axis corresponds to $\boldsymbol{n}(-\sin\varphi, \cos\varphi, 0)$.

We now obtain the same result in a more formal way, which can be later on generalized to less transparent cases. The operator A to be used as in Eq. (2) can be generally written as

$$A = \boldsymbol{n}.\boldsymbol{\sigma} = n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3 \tag{15}$$

where n_1, n_2, n_3 are components of a unit vector. The infinitesimal transformation of $|\Psi_\nu\rangle$ connected with the operator A becomes

$$|\Psi_\nu\rangle \to [1 + i\varepsilon\boldsymbol{n}.\boldsymbol{\sigma}]|\Psi_\nu\rangle .$$

The expectation values of the hamiltonian $H = -\sigma_z$ in the new state is

$$E(\varepsilon) = \langle\Psi_\nu|H|\Psi_\nu\rangle + i\varepsilon\langle\Psi_\nu|[\boldsymbol{n}.\boldsymbol{\sigma}, H]|\Psi_\nu\rangle + 0(\varepsilon^2) \tag{16}$$

We now wish to have a maximal change of the expectation value $E(\varepsilon)$ with a fixed (infinitesimal) value of ε and the fixed unit length of the vector $\boldsymbol{n}$. Inserting Eqs. (14) and (15) into (16) we obtain

$$|\langle\Psi_\nu|[\boldsymbol{n}.\boldsymbol{\sigma}, H]|\Psi_\nu\rangle|^2 = 4\sin^2\vartheta(n_1\sin\varphi - n_2\cos\varphi)^2 \tag{17}$$

The right-hand side of this equation reaches the maximum for $n_1 = -\sin\varphi$, $n_2 = \cos\varphi$, $n_3 = 0$, obtained above as well. The infinitesimal rotation around the axis $\boldsymbol{n}$ changes the angle ϑ in Eq. (14) but not the angle φ. The subsequent optimal infinitesimal rotation is thus again around the $\boldsymbol{n}$ axis, that means that we arrive at the correct result by a single finite rotation around $\boldsymbol{n}$ (see Fig. 2)

$$|\Psi_\nu\rangle \to \exp[i\alpha(\boldsymbol{\sigma}.\boldsymbol{n})]|\Psi_\nu.$$

Before concluding the section we shall very briefly discuss the application of this method to one dimensional problem in quantum mechanics. Suppose we have a hamiltonian H and a trial wave function $\Psi_\nu(x)$. Choosing a hermitian operator A we write the new wave function $\Psi(x)$ in the form

$$\Psi(x) = \exp(i\alpha A)\,\Psi_\nu(x) \tag{18}$$

and determine the optimal value of α from the requirement

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\int \Psi^*(x)\,A\,\Psi(x)\,\mathrm{d}x = i\int \Psi^*(x)[H, A]\,\Psi(x)\,\mathrm{d}x = 0.$$

The condition is equivalent to requiring the local minimum of

$$E(\alpha) = \int \Psi_\nu^*(x)\,e^{-i\alpha A}\,H\,e^{i\alpha A}\,\Psi_\nu(x)\,\mathrm{d}x .$$

The simplest operators which one can use are $A = p = -\mathrm{id}/\mathrm{d}x$ and $B = x$, $C = xp_x + p_x x$. In this case the transformation $\Psi_\nu \to \exp(i\alpha A)\,\Psi_\nu$ corresponds to the shift of the argument of the function $\Psi_\nu(x)$: $\Psi_\nu(x) \to \Psi_\nu(x + \alpha)$. The transformation $\Psi_\nu(x) \to \exp(i\alpha B)\,\Psi_\nu(x)$ corresponds to the shift in the momentum space. The two transformations are usually unnecessary because variational ansätze are chosen in such a way that the expectation values of x and p have correct values. Finally the transformation

$$\Psi_\nu(x) \to \exp[i\alpha(xp + px - 1)]\,\Psi_\nu(x) = \Psi_\nu(\alpha^2 x)$$

corresponds to the conformal transformation. In starting with some $\Psi_\nu(x)$, the transformation $\Psi_\nu(x) \to \exp(i\alpha p)\,\Psi_\nu$ can make the expectation value of the momentum vanish, and subsequent $\exp(i\alpha x)$ causes $\langle x\rangle$ to vanish. In standard situations these two requirements are usually built into the $|\Psi_\nu\rangle$ directly. The transformation using the operator $(xp + px - 1)$ then changes the "width" of the function. This is used, e.g. when we are trying to find the best approximation to the ground state of an anharmonic oscillator by using the functions proportional to $\exp(-x^2/\sigma^2)$ and vary the value of the parameter σ.

It is clear that the variational method for one dimensional problems possesses much more freedom in the choice of the operators than the problem of the spin in the external magnetic field and a more refined strategy has to be formulated. We shall come back briefly to this point in Sect. IV.

III. THE BCS MODEL OF THE GROUND STATE OF THE SUPERCONDUCTOR AND THE USING MODEL

In this section we shall discuss the BCS model of superconductivity [3] and show that the structure of the ground state is obtained in a straightforward way by the method described in Sect. I. To introduce the notation we briefly recapitulate the basic facts.

After the discovery of the mechanism of the Cooper pair creation BCS formulated the model with the effective hamiltonian

$$H = \sum_k 2\,\varepsilon_k b_k^+ b_k + \sum_{kk'} V_{kk'}\,b_{k'}^+\,b_k. \tag{19}$$

Here b_k^+, b_k are the creation and the annihilation operators of the Cooper pairs

$$b_k^+ = c_{k\uparrow}^+ c_{-k\downarrow}^+ \quad b_k = c_{-k\downarrow} c_{k\uparrow}$$

where c_k denote the anticommuting electron operators.

The b's obey the following commutation relations

$$[b_k, b_k^+] = 1 - (n_{k\uparrow} + n_{-k\downarrow})$$
$$\{b_k, b_k^+\} = 1 - (n_{k\uparrow} + n_{-k\downarrow}) + 2n_{k\uparrow}n_{-k\downarrow}$$
$$[b_k, b_{k'}] = 0 \quad \text{for } k \neq k'$$

and

$$b_k^2 = b_k^{+2} = 0$$

where $n_{k\uparrow}$, $n_{k\downarrow}$ are occupation numbers of the corresponding electron states, $n_{k\uparrow} = c_{k\uparrow}^+ c_{k\uparrow}$, etc.

Motivated by the work of Lee, Low and Pines [4] Schrieffer [3] suggested the following ansatz for the ground state of the Hamiltonian in Eq. (19)

$$|\Psi_0\rangle = \prod_k \frac{\exp(g_k b_k^+)}{1+g_k^2}|0\rangle = \prod_k (u_k + v_k b_k^+)|0\rangle = \prod_k (\cos\alpha_k + \sin\alpha_k . b_k^+)|0\rangle \tag{20}$$

where $|0\rangle$ is the state with electronic levels filled up to the Fermi level and with higher levels being empty. In writing Eq. (20) we have used the relation $b_k^{+2} = 0$ and $u_k^2 + v_k^2 = 1$.

It is worth noting that unlike in Eq. (13) Lee et al. used in the study of the polaron unitary operator acting on the perturbative vacuum, which also corresponds to the method discussed in Sect. I.

When using this method we have to decide first which operator is going to play the role of A in Eq. (2). The structure of the BCS Hamiltonian (19) indicates that the operators b_k, b_k^+ should play the crucial role. The simplest possibilities are

$$A_k^{(1)} = b_k^+ b_k,\ A_k^{(2)} = b_k b_k^+,\ A_k^{(3)} = b_k + b_k^+,\ A_k^{(4)} = -\mathrm{i}(b_k^+ - b_k).$$

The operators $A_k^{(1)}$, $A_k^{(2)}$ act trivially on the "perturbative" ground state $|0\rangle$. The unitary operator

$$\exp(\mathrm{i}\alpha_k A_k^{(4)}) = \exp[\alpha_k(b_k^+ - b_k)]$$

acts nontrivially on the vacuum. According to the method of Sect. I we can make the first approximation to the exact ground state by using the ansatz

$$|\Psi_0\rangle = \prod_k \mathrm{e}^{\alpha_k(b_k^+ - b_k)}|0\rangle .$$

Using anticommutation relations for b_k, b_k^+ we can rewrite this expression as

$$|\Psi_0\rangle = \prod_k [\cos\alpha_k + (b_k^+ - b_k)\sin\alpha_k]|0\rangle . \tag{21}$$

This is just the Schrieffer ansatz (20). This demonstrates that the method leads naturally to the correct expression for the approximate ground state of the BCD model.

In fact we could proceed in a more general way and start with a linear combination of operators $A_k^{(3)}$ and $A_k^{(4)}$

$$A_k = \cos\beta A_k^{(3)} + \sin\beta A_k^{(4)} = b_k^+ \mathrm{e}^{-\mathrm{i}\beta} + b_k \mathrm{e}^{\mathrm{i}\beta}.$$

According to the method described in Sect. I we would start with the ansatz

$$|\Psi_0\rangle = \prod_k \exp[\mathrm{i}\alpha_k(b_k^+ \mathrm{e}^{-\mathrm{i}\beta} + b_k \mathrm{e}^{\mathrm{i}\beta})]|0\rangle . \tag{22a}$$

Using the anticommutation relations for b_k, b_k^+ we can rewrite $|\Psi_0\rangle$ in the form

$$|\Psi_0\rangle = \prod_k [\cos\alpha_k + \mathrm{i}(b_k^+ \mathrm{e}^{-\mathrm{i}\beta} + b_k \mathrm{e}^{\mathrm{i}\beta})\sin\alpha_k]|0\rangle . \tag{22b}$$

For $\beta = \pi/2$ this ansatz is completely equivalent to the standard one in Eq. (21), for $\beta \neq \pi/2$ we obtain the nonequivalent representations for the vacuum of the BCS theory. This is connected with the fact that the operator $U = \pi\exp(-\mathrm{i}\beta b_k^+ b_k)$ commutes with the Hamiltonian (19) and this operator induces the transformations

$$Ub^+U^+ = b^+\mathrm{e}^{-\mathrm{i}\beta},\ UbU^+ = b\,\mathrm{e}^{\mathrm{i}\beta} \tag{23}$$

which are just responsible for the transition from (21) to (22).

Abandoning the discussion of the BCS model, let us discuss in a general way, how to improve by one step the estimate of the ground state of a system. Suppose we have a trial state $|\Psi_V\rangle$, a hamiltonian and an operator A. We start with an ansatz

$$|\Psi^{(1)}\rangle = \mathrm{e}^{\mathrm{i}\alpha A}|\Psi_V\rangle$$

and determine $\alpha = \alpha_0$ from the condition

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle_{t=0} = \langle\Psi^{(1)}|\,\mathrm{i}[H, A]|\Psi^{(1)}\rangle = \mathrm{i}\langle\Psi_V|\mathrm{e}^{-\mathrm{i}\alpha A}[H, A]\mathrm{e}^{\mathrm{i}\alpha A}|\Psi_V\rangle = 0 . \tag{24}$$

The next approximation would consist in finding a state $|\Psi^{(2)}\rangle$ which, apart of (24), satisfies also

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle A\rangle_{t=0} = 0 . \tag{25}$$

This can be in principle obtained as

$$|\Psi^{(2)}\rangle = e^{-\beta[H,A]}|\Psi^{(1)}\rangle \tag{26}$$

where β is to be determined from the condition

$$\frac{d^2}{dt^2}\langle A\rangle_{t=0} = \frac{d}{dt}\langle i[H,A]\rangle_{t=0} = -\langle\Psi^{(1)}|e^{\beta[H,A]}[H,[H,A]]e^{-\beta[H,A]}|\psi^{(1)}\rangle = 0. \tag{27}$$

Note that $i[H,A]$ is a hermitian operator and because of that no i appears in the exponents in (27).

The transition from $|\Psi^{(1)}\rangle$ to $|\Psi^{(2)}\rangle$ leaves the condition (24) satisfied since the additional factor $\exp[-\beta[H,A]]$ commutes with $[H,A]$ standing in (24).

The next step would consist in a simultaneous fulfilment of the three conditions

$$\langle\Psi^{(3)}|[H,A]|\Psi^{(3)}\rangle = \\ = -\langle\Psi^{(3)}|[H,[H,A]]|\Psi^{(3)}\rangle = \langle\Psi^{(3)}|[H,[H,[H,A]]]|\Psi^{(3)}\rangle = 0$$

and that cannot be done by the simple procedure described above. For this purpose one has to use a more complicated approach, to be discussed in the next section.

Before concluding this section let us discuss very briefly, by using the same method, the *one-dimensional Ising* model in an *external field.*

After the Jordan—Wigner transformation and transition to the k-space the Hamiltonian of the Ising model in the external magnetic field is given by the following expression [5]

$$H = -2\sum_{k>0}(1+\lambda\cos k)(a_k^+a_k + a_{-k}^+a_{-k}) + 2i\lambda\sum_{k>0}\sin k(a_k^+a_{-k}^+ + a_ka_{-k}).$$

We are using the standard notation, for more detail see, e.g. Ref. 5. The operators a_k, a_k^+ fulfil anticommutative (fermionic) relations and annihilate, resp. create, topological excitations (kinks). Introducing the operators

$$b_k^+ = a_k^+a_{-k}^+ \qquad b_k = a_{-k}a_k$$

describing the creation, resp. annihilations, of kink-antikink pairs, we obtain

$$H = -2\sum_k(1+\lambda\cos k)\,2b_k^+b_k + 2i\lambda\sum_{k>0}\sin k(b_k^+ - b_k). \tag{29}$$

The structure of the Hamiltonian indicates again that the operators b_k^+, b_k play

the important role and it is natural to assume that the first approximation to the ground state has the structure

$$|\Psi_0\rangle = \prod_k \exp[i\alpha_k(b_k^+e^{-i\beta} + b_ke^{i\beta})]|0\rangle \tag{30}$$

identical with Eq. (22). In this situation there is no degeneration of the ground state corresponding to various values of β. This difference with respect to the BCS model is caused by the presence of terms linear in b_k^+, b_k in Eq. (29). By minimizing the expectation value of $\langle\Psi_0|H|\Psi_0\rangle$ with respect to values of α_k we obtain again the correct ground state of the hamiltonian. The similarity between the Ising and the BCS models is not accidental, in the former the ground state is formed by the condensate of kink-antikink pairs [6] in the latter by the condensate of Cooper pairs.

IV. DIFFERENTIAL EQUATIONS FOR THE APPROACH OF THE VARIATIONAL ESTIMATE TO THE STATIONARY STATE

In a general case we would like to find the state which satisfies simultaneously the conditions

$$\begin{aligned}
&\frac{d}{dt}\langle\Psi|A|\Psi\rangle = i\langle\Psi|[H,A]|\Psi\rangle = 0\\
&\frac{d}{dt}\langle\Psi|B|\Psi\rangle = i\langle\Psi|[H,B]|\Psi\rangle = 0\\
&\vdots\\
&\frac{d}{dt}\langle\Psi|Z|\Psi\rangle = i\langle\Psi|[H,Z]|\Psi\rangle = 0
\end{aligned} \tag{31}$$

where $A, B, \ldots Z$ is specified set of operators and all the derivatives are taken at $t = 0$. We were unable to find any method which would permit to write the answer in an explicit form. Instead we have constructed the following procedure which starts with the initial estimate $|\Psi_\nu\rangle$ and then follows the steepest descent path to a stationary state.

We consider the infinitesimal transformation of a current state

$$|\Psi\rangle \to [1 + i(\alpha A + \beta B + \ldots + \omega Z)]|\Psi\rangle \tag{32}$$

where $\alpha, \beta, \ldots \omega$ are infinitesimal parameters. The expectation value of the Hamiltonian in the new state is easy to calculate

$$\begin{aligned}
&E(\alpha,\beta,\ldots,\omega) = \langle\Psi|[1 - i(\alpha A + \ldots + \omega Z)]\\
&H[1 + i(\alpha A + \ldots + \omega Z)]|\Psi\rangle = \langle\Psi|H|\Psi\rangle -\\
&- i\langle\Psi|\alpha[A,H] + \ldots + \omega[Z,H]|\Psi\rangle + 0(\alpha^2,\alpha,\beta,\ldots)
\end{aligned}$$

It follows that

$$\frac{\partial E}{\partial \alpha} = \mathrm{i}\langle \Psi | [H, A] | \Psi \rangle$$
$$\vdots$$
$$\frac{\partial E}{\partial \omega} = \mathrm{i}\langle \Psi | [H, Z] | \Psi \rangle .$$

The right-hand sides give components of the gradient of $E(\alpha, \beta, \ldots, \omega)$ in the space of the parameters $\alpha, \beta, \ldots \omega$. The steepest descent is in the direction exactly opposite to this gradient. Moving along the steepest descent means therefore that the parameters $\alpha, \beta, \ldots \omega$ satisfy the following conditions

$$\begin{aligned} \alpha &= -\varepsilon \frac{\partial E}{\partial \alpha} = -\mathrm{i}\varepsilon \langle \Psi | [H, A] | \Psi \rangle , \\ &\vdots \\ \omega &= -\varepsilon \frac{\partial E}{\partial \omega} = -\mathrm{i}\varepsilon \langle \Psi | [H, Z] | \Psi \rangle \end{aligned} \tag{34}$$

where ε is an infinitesimal quantity. The infinitesimal transformation along the steepest descent becomes

$$[1 + \varepsilon(\langle \Psi | [H, A] | \Psi \rangle A + \ldots + \langle \Psi | [H, Z] | \Psi \rangle Z]. \tag{35}$$

Labelling the trajectory of the vector $|\Psi\rangle$ in the Hilbert space by a parameter τ and denoting ε by $\mathrm{d}\tau$ we obtain from Eq. (35) the differential equation

$$\mathrm{i}\frac{\partial}{\partial \tau} |\Psi_{(\tau)}\rangle = \{\langle \Psi(\tau) | \mathrm{i}[H, A] | \Psi(\tau) \rangle A + \ldots\} |\Psi(\tau)\rangle \tag{36}$$

with the initial condition $|\Psi(\tau = 0)\rangle = |\Psi_V\rangle$.

This non-linear equation formally looks like a Schrödinger eq. with the "Hamiltonian"

$$\mathscr{H} = \langle \Psi(\tau) | \mathrm{i}[H, A] | \Psi(\tau) \rangle A + \ldots + \langle \Psi(\tau) | \mathrm{i}[H, Z] | \Psi(\tau) \rangle Z \tag{37}$$

The resulting state $|\Psi(\tau \to \infty)\rangle$ corresponds to the best approximation to the ground state on the space of functions which can be reached from $|\Psi_V\rangle$ by successive infinitesimal transformation of the form

$$|\Psi\rangle = \prod_k (1 + \mathrm{i}\alpha_k A + \mathrm{i}\beta_k B + \ldots + \mathrm{i}\omega_k Z) |\Psi_V\rangle \tag{38}$$

or

$$|\Psi\rangle = \prod_k \exp(\mathrm{i}\alpha_k A + \mathrm{i}\beta_k B + \ldots + \mathrm{i}\omega_k Z) |\Psi_V\rangle . \tag{39}$$

In a special case when the operators $A, B, \ldots Z$ form an algebra, any element of the sets (38) a (39) can be written in a form $\exp(\mathrm{i}\alpha A + \mathrm{i}\beta B + \ldots)|\Psi_V\rangle$.

On the set of functions (38) the conditions in Eq. (31) correspond to the local minimum of the expectation value of the hamiltonian H.

In order to get an insight into how Eq. (36) works we shall consider a simple example of a spin in the external magnetic field. The hamiltonian is simply $H = -\sigma_Z$, the operators A, B are chosen as $A = \sigma_x$, $B = \sigma_y$ and let the initial state $|\Psi_V\rangle$ correspond to the spin "pointing" in the direction of the x-axis

$$|\Psi_V\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{40}$$

The current state $|\Psi(\tau)\rangle$ is denoted as

$$|\Psi(\tau)\rangle = \begin{pmatrix} a(\tau) \\ b(\tau) \end{pmatrix}. \tag{41}$$

Inserting all that into Eq. (36) we obtain

$$\mathrm{i}\frac{\partial}{\partial \tau} |\Psi(\tau)\rangle = -\{\langle \Psi(\tau) | 2\sigma_x | \Psi(\tau) \rangle \sigma_y - \langle \Psi(\tau) | 2\sigma_y | \Psi(\tau) \rangle \sigma_x\} |\Psi(\tau)\rangle . \tag{42}$$

It can be shown easily that with the initial condition (40) both $a(\tau)$, $b(\tau)$ will remain real during the evolution and the second term on the r.h.s. vanishes. Inserting (41) into (42) we get

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \begin{pmatrix} a \\ b \end{pmatrix} = 4ab \begin{pmatrix} b \\ -a \end{pmatrix}. \tag{43}$$

Because of the normalization we can put

$$\begin{pmatrix} a(\tau) \\ b(\tau) \end{pmatrix} = \begin{pmatrix} \cos \vartheta(\tau)/2 \\ \sin \vartheta(\tau)/2 \end{pmatrix}. \tag{44}$$

After inserting that into Eq. (43) we find

$$\frac{\mathrm{d}\vartheta(\tau)}{\mathrm{d}\tau} = -4 \sin \vartheta(\tau) . \tag{45}$$

The initial condition becomes

$$\vartheta(0) = \frac{\pi}{2}.$$

Making use of the integral

$$\int \frac{dx}{\sin x} = \ln\left|\operatorname{tg}\frac{x}{2}\right|$$

we find the solution of Eq. (45) in the form

$$\vartheta = 2\,\mathrm{atan}\,(e^{-4\tau}) \tag{46}$$

For $\tau \to \infty$ the angle ϑ approaches exponentially zero, which is reasonable also form the physical point of view. The spinor in Eq. (44) corresponds to the "spin direction" along the ray with angles ϑ and $\varphi = 0$ in spherical coordinates and $\vartheta \to 0$ implies that for $\tau \to \infty$ the spinor "points" along the z-axis as expected for the Hamiltonian $H = -\sigma_z$.

The exponential approach to the stationary state for $\tau \to \infty$ is a typical feature of Eq. (36). This is connected with the fact the "Hamiltonian" $\mathscr{H}$ in Eq. (37) approaches zero when the vector $|\Psi(\tau)\rangle$ approaches the stationary state.

Another very simple example illustrating this property of Eq. (36) is provided by a harmonic oscillator for which we take the starting wave function $\Psi_v(x)$ of a correct shape but with a wrong width

$$\Psi_v(x) \sim \exp(-x^2/2a^2).$$

Taking $A = xp + px$, $B = \mathrm{i}[H, A] = 2(p^2 - x^2)$ and inserting it into Eq. (36) shows that a approaches the correct value a_0 exponentially $a \to a_0(1 + \mathrm{const}\, e^{-\tau})$ for $\tau \to \infty$.

The case of an infinite set of operators

It is easy to generalize the argument leading from Eqs. (31) to the differential Eq. (36) for a situation with an infinite set of operators. Suppose that there is a set $\{A(u)\}$ with $u_1 \leqslant u \leqslant u_2$ and we wish to find a state which instead of Eqs. (31) satisfies conditions

$$\frac{d}{dt}\langle\Psi|A(u)|\Psi|\rangle = \mathrm{i}\langle\Psi|[H, A(u)]|\Psi\rangle \text{ for } u_1 \leqslant u \leqslant u_2.$$

Such a state is obtained as an asymptotic solution (for $\tau \to \infty$) of the differential equation which generalizes Eq. (36), namely

$$\mathrm{i}\frac{d|\Psi(\tau)\rangle}{d\tau} = \int \langle\Psi(\tau)|\,\mathrm{i}[H, A(u)]|\Psi(\tau)\rangle\, A(u)\,du\,|\Psi(\tau)\rangle \tag{36b}$$

with the initial condition $|\Psi(\tau = 0)\rangle = |\Psi_v\rangle$.

This may be relevant to the situation when we want to find a state $|\Psi\rangle$ for which the time derivative of the expectation value of an operator $A(t)$ vanishes at any time t within $t_1 \leqslant t \leqslant t_2$.

The differential equation becomes

$$\mathrm{i}\frac{d|\Psi(\tau)\rangle}{d\tau} = \int \langle\Psi(\tau)|\,\mathrm{i}[H, A(t)]|\Psi(\tau)\rangle\, A(t)\,dt\,|\Psi(\tau)\rangle.$$

V. AN UNBIASED EVOLUTION EQUATION FOR A VECTOR IN THE HILBERT SPACE TOWARDS THE GROUND STATE

In the preceding discussion we have been always biased by two factors: the choice of the set of "relevant operators" and the choice of the starting estimate $|\Psi_v\rangle$. There is probably no way how to get rid of the latter bias, but the former can be avoided. We shall now describe a construction of the evolution equation for $|\Psi(\tau)\rangle$ from the condition that the replacement

$$|\Psi(\tau)\rangle \to |\Psi(\tau)\rangle + |\delta\Psi\rangle$$

corresponds to the maximal decrement of the expectation value of the Hamiltonian at fixed $\langle\delta\Psi|\,\delta\Psi\rangle$. We shall perform the construction in two ways. The former is short but rather formal, the latter (described in the appendix) is less formal but more cumbersome.

The expectation value of the Hamiltonian H in the state $|\Psi\rangle = |\Psi(\tau)\rangle$ is written in the standard form

$$E(\Psi) = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\,\Psi\rangle}. \tag{47}$$

Then

$$\frac{\delta_E(\Psi)}{\delta\langle\Psi|} = \frac{1}{\langle\Psi|\,\Psi\rangle}\left[H - \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\,\Psi\rangle}\right]|\Psi\rangle. \tag{48}$$

The right-hand side gives the direction of the gradient of $E(\Psi)$ in the Hilbert space. The steepest descent is just in the opposite direction and the $|\Psi(\tau)\rangle$ should move in this way. Because of that we can write directly the evolution equation

$$\frac{\partial|\Psi(t)\rangle}{\partial\tau} = -\frac{1}{\langle\Psi(\tau)|\,\Psi(\tau)\rangle}\left[H - \frac{\langle\Psi(\tau)|H|\Psi(\tau)\rangle}{\langle\Psi(\tau)|\,\Psi(\tau)\rangle}\right]|\Psi(\tau)\rangle.$$

This equation can be somewhat simplified. When starting from a normalized vector $|\Psi_v\rangle$ the evolution equation will not change the norm of $|\Psi\rangle$ and $\langle\Psi|\,\Psi\rangle = 1$. This follows from the fact that for a normalized $|\Psi\rangle$: $\langle\Psi|\,\Psi\rangle = 1$,

the vector $|\delta\Psi\rangle = [H - \langle\Psi|H|\Psi\rangle]|\Psi\rangle$ is orthogonal to $|\Psi\rangle$. In this situation the evolution equation becomes

$$\frac{\partial|\Psi(\tau)\rangle}{\partial\tau} = -[H - \langle\Psi(\tau)|H|\Psi(\tau)\rangle]|\Psi(\tau)\rangle . \tag{49}$$

The simplest illustration of this equation is again provided by the spin in the external magnetic field. Putting $H = -\sigma_z$ as before and

$$|\Psi(\tau) = \begin{pmatrix} a(\tau) \\ b(\tau) \end{pmatrix}, \quad |\Psi_{(0)}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

we obtain from Eq. (49) ($\dot{a} \equiv da/d\tau$, $\dot{b} = db/d\tau$)

$$\dot{a} = a(1 - a^2 + b^2)$$
$$\dot{b} = b(-1 - a^2 + b^2) .$$

With the initial condition $a(0) = b(0) = 1/\sqrt{2}$ (spin "pointing" in the x-direction) we can see that $a(\tau)$, $b(\tau)$ will remain real during the evolution. It can be immediately seen that $a^2 + b^2 = 1$ implies $a\dot{a} + b\dot{b} = 0$ and the spinor remains normalized. The meaning of the last eq. becomes clear when we make use of $a^2 + b^2 = 1$ and rewrite them into the form

$$\begin{pmatrix} da \\ db \end{pmatrix} = i\,2ab\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} d\tau .$$

This is the infinitesimal rotation of the spinor around the y-axis. With the parametrization $a = \cos\vartheta/2)$, $b = \sin(\vartheta/2)$ we come easily to the equation

$$\frac{d\vartheta}{d\tau} = -2\sin\vartheta \tag{50}$$

and, in the same way as in Sect. IV, we find

$$\vartheta(\tau) = 2\,\mathrm{atan}\,(e^{-2\tau}),$$

which is an exponential approach to the ground state corresponding to $\vartheta = 0$. Eq. (50) shows that we shall reach the ground state starting from any spinor $(\cos\vartheta_0/2, \sin\vartheta_0/2)$ except for $\vartheta_0 = \pi$ which is an excited stationary state. That follows from the fact that the r.h.s. of Eq. (50) is negative for any $\vartheta \neq 0, \pi$.

This example was, of course, rather trivial and we hope to test the usefullness of the method in future in more complicated situations like the BCS model or simple field theoretical models.

A few comments are in order. The unbiased steepest descent method as given by Eq. (49) is closely related to the method of t-expansion proposed recently by Horn and Weinstein [2]. In this approach one writes

$$|\Psi(t)\rangle = \frac{e^{-tH}|\Psi_V\rangle}{\langle\Psi_V|e^{-2tH}|\Psi_V\rangle} . \tag{51}$$

In the limit $t \to \infty$ the vector $|\Psi(t)\rangle$ converges to the ground state of the system. The differential form of Eq. (51) follows from the infinitesimal transformation corresponding to Eq. (51), namely

$$|\Psi(t)\rangle \to |\Psi(t + \Delta t)\rangle = |\Psi(t)\rangle + \delta\Psi|(t)\rangle =$$
$$= \frac{(1 - H\mathrm{d}t)|\Psi(t)\rangle}{\sqrt{\langle\Psi(t)|(1 - 2H\mathrm{d}t)|\Psi(t)\rangle}} = [1 - \mathrm{d}t(H - \langle\Psi(t)|H|\Psi(t)\rangle)]|\Psi(t)\rangle .$$

This leads immediately to Eq. (49). It is also easy to convince oneself by an explicit calculation that Eq. (51) is a solution of Eq. (49).

Note finally that the infinitesimal transformation corresponding to Eq. (51)

$$\Psi(\tau) \to \{1 - [H - \langle\Psi|H|\Psi\rangle]\mathrm{d}\tau\}|\Psi\rangle \tag{52}$$

can be rewritten as

$$|\Psi(\tau)\rangle \to \{1 + iA\,\mathrm{d}\tau\}|\Psi\rangle \tag{53}$$

where A is a hermitian operator

$$A = |\xi(\tau)\rangle\langle\Psi(\tau)| + |\Psi(\tau)\rangle\langle\xi(\tau)|$$

with

$$|\xi(\tau)\rangle = i[H - \langle\Psi|H|\Psi\rangle]|\Psi(\tau)\rangle .$$

As seen from the simple example with the rotating spin and in a general way from Eq. (51), the solution of Eq. (49) leads for $\tau \to \infty$ to the ground state of the theory and the method is thus suitable only for the search of the ground state of a theory. A method suitable for the identification of the excited stationary states will be described in the next section.

VI. EVOLUTION EQUATION LEADING TO EXCITED STATIONARY STATES

The methods described so far lead to the determination of the ground state of the theory. In this section we shall present a method devised for the search of the excited stationary states. The method makes use of the properties of the expectation value of the variance of the energy

$$D \equiv \langle\Psi|H^2|\Psi\rangle - \langle\Psi|H|\Psi\rangle^2 . \tag{54}$$

In any stationary state the variance vanishes and what is more important, D has a local minimum at the stationary state. In this sense the variance D does not prefer in any way the ground state and is democratic with respect to all stationary states. By minimizing D one also minimizes in an unbiased way the time derivatives of all physical quantitaties. This is seen from the inequality

$$|\langle\Psi|[A,H]|\rangle|^2 \leq 4\langle\Psi|A^2|\Psi\rangle D \tag{55}$$

which can be easily derived by procedures used by proofs of uncertainity relations.[1])

In order to test whether minimizing D is a useful method for the determination of the excited stationary states we have made some numerical tests with the anharmonic oscillator, taking the trial wave functions as the superpositions of stationary states of the harmonic oscillator. The results were quite encouraging, but since they are not directly related to the present topic we shall not present them in detail here.

We shall now construct the evolution equation which describes the steepest descent of the state $|\Psi\rangle$ with respect to the variance D.

The steepest descent — or the gradient in the Hilbert space — is given by the expression

$$\frac{\partial}{\partial\langle\Psi|}\left\{\frac{\langle\Psi|H^2|\Psi\rangle}{\langle\Psi|\Psi\rangle}-\frac{\langle\Psi|H|\Psi\rangle^2}{\langle\Psi|\Psi\rangle^2}\right\}=$$

$$=\left\{\frac{H^2}{\langle\Psi|\Psi\rangle}-\frac{\langle\Psi|H^2|\Psi\rangle}{\langle\Psi|\Psi\rangle^2}-\frac{2\langle\Psi|H|\Psi\rangle H}{\langle\Psi|\Psi\rangle^2}+\frac{2\langle\Psi|H|\Psi\rangle^2}{\langle\Psi|\Psi\rangle^3}\right\}|\Psi\rangle .$$

For $\langle\Psi|\Psi\rangle = 1$ the r.h.s. becomes

$$\{H^2-\langle\Psi|H^2|\Psi\rangle-2\langle\Psi|H|\Psi\rangle H+2\langle\Psi|H|\Psi\rangle^2\}|\Psi\rangle$$

which is orthogonal to $|\Psi\rangle$. Because of that we can write the evolution equation in the form

$$\frac{\partial|\Psi(\tau)\rangle}{\partial\tau}=-\{H^2-\langle\Psi|H^2|\Psi\rangle-2\langle\Psi|H|\Psi\rangle H+2\langle\Psi|H|\Psi\rangle^2\}|\Psi\rangle \tag{56}$$

It is easy to convince oneself that Eq. (56) follows from the infinitesimal transformation

$$|\Psi\rangle\to\frac{e^{-(H-\langle\Psi|H|\Psi\rangle)^2 d\tau}|\Psi\rangle}{\langle\Psi|e^{-2(H-\langle\Psi|H|\Psi\rangle)^2 d\tau}|\Psi\rangle^{1/2}}$$

[1]) One starts with the inequality $\langle(A+iuB)\Psi|(A+iuB)\Psi\rangle \geq 0$, u-real; comes to $|\langle\Psi|[A,B]|Y\rangle|^2 \leq 4\langle\Psi|A^2|\Psi\rangle\langle\Psi|B^2|\Psi\rangle$ and puts $B = H-\langle\Psi|H|\Psi\rangle$.

We shall illustrate the properties of this eq. again on the simplest possible system — the spin in the magnetic field. Choosing $H=-\sigma_z$ and the components of the spinor as $\cos(\vartheta/2)$, $\sin(\vartheta/2)$ we obtain from Eq. (56) the following two equations

$$\frac{d}{d\tau}\begin{pmatrix}\cos\frac{\vartheta}{2}\\ \sin\frac{\vartheta}{2}\end{pmatrix}=-2\begin{bmatrix}\cos^2\vartheta-\cos\vartheta, & 0\\ 0, & \cos^2\vartheta+\cos\vartheta\end{bmatrix}\begin{bmatrix}\cos\frac{\vartheta}{2}\\ \sin\frac{\vartheta}{2}\end{bmatrix}$$

The two equations are equivalent and a little manipulation leads to

$$\frac{d\vartheta}{d\tau}=-2\sin 2\vartheta \tag{57}$$

The explicit solutions can be obtained by the same method as above, but only the following point is really important. For $0<\vartheta<\pi/2$ the r.h.s. is negative, which means that ϑ is decreasing and asymptotically reaching the value $v=0$; For $\pi/2<\vartheta<\pi$ the r.h.s. is positive, ϑ is increasing and asymptotically reaches the value $\vartheta=\pi$, which corresponds to a stationary state $\begin{pmatrix}0\\1\end{pmatrix}$. The situation is shown in Fig. 3.

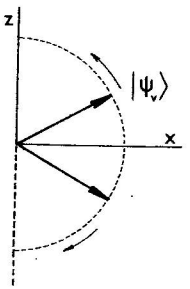

Fig. 3. For $|\Psi_v\rangle$ (above (below)) the x,y plane the state vector $|\Psi\rangle$ rotates to the positive (negative) direction of the z-axis.

The exact solutions are

$$\vartheta=\operatorname{atan} e^{-4(\tau-\tau_0)} \qquad \text{for } 0<\vartheta_0<\frac{\pi}{2}$$

$$\vartheta=\pi-\operatorname{atan} e^{-4(\tau-\tau_0)} \qquad \text{for } \frac{\pi}{2}<\vartheta_0<\pi .$$

One could generalize the previous procedure and derive differential equations corresponding to state vectors moving against the gradients of higher moments

$\mu_n = \langle\Psi|(H - \langle\Psi|H|\Psi\rangle)^n|\Psi\rangle$ and their linear combinations or to functions $f(H - \langle H\rangle)$ which are positive everywhere except for the origin where they vanish, but we shall not elaborate upon that here. We have written down here only the unbiased evolution equation. In some cases it might be, however, simpler to restrict oneself to a subspace given by Eq. (38) of the whole Hilbert space and write the evolution equations only for the motion of the state vector within this subspace. For this purpose we generalize somewheat a procedure leading from Eqs. (31) to Eq. (36) and write

$$D(\alpha, \beta, \ldots) = \langle\Psi|[1 - \mathrm{i}(\alpha A + \beta B + \ldots)]\, H^2 [1 + \mathrm{i}(\alpha A + \beta B + \ldots)]|\Psi\rangle - \langle\Psi|[1 - \mathrm{i}(\alpha A + \beta B + \ldots)]\, H [1 + \mathrm{i}(\alpha A + \beta B + \ldots)]|\Psi\rangle^2 .$$

We find again a gradient of $D(\alpha, \beta, \ldots)$ and write an evolution equation which moves the state $|\Psi\rangle$ exactly against the gradient, that means along the steepest descent. Instead of Eq. (36) we now obtain

$$\mathrm{i}\frac{\partial}{\partial\tau}|\Psi(\tau)\rangle = \{[\langle\Psi(\tau)|\,\mathrm{i}[H^2, A]|\Psi(\tau)\rangle - 2\langle\Psi|H|\Psi\rangle\langle\Psi|\,\mathrm{i}[A, H]|\Psi\rangle]\, A + + (A \to B) + (A \to C) + \ldots\}|\Psi(\tau)\rangle . \tag{58}$$

VIII. COMMENTS AND CONCLUSIONS

In the present paper we have described a few methods for systematic improvements of variational estimates of energies and state vectors of stationary states. Methods discussed in Sections I.—IV. are based on the observation that in a stationary state derivatives of expectation values of (time independent) observables vanish. This condition permits to improve the original estimate $|\Psi_v\rangle$ of the vector of the ground state. Provided that it is — for physical reasons or from intuition — obvious which operator plays the most important role it is rather straightforward to perform the improvement. This happened, e.g., in the case of the BCS model of the superconductor discussed in Sect. III. In other cases when one suspects that more operators are important the procedure is more complicated. In order to reach the state $|\Psi\rangle$ in which time derivatives of expectation values of a set of operators vanish we derived differential equations for the trajectory of the vector in the Hilbert space, starting at $|\Psi_v\rangle$ and asymptotically approaching the desired state $|\Psi\rangle$. For the case when it is impossible to select a set of "important" operators one could follow the unbiased method described in Sect. V. The method of Sect. I. to V. are suitable for the determination of the ground state of the theory. In the most transparent, although not general, way this is seen from the eqs. of motion of the spinors in the illustrative examples. In Sect. VI. we have therefore suggested a method

which is especially suitable for the identification of the stationary states of the theory. The illustrative spin-example shows clearly that the spinor moves to the "closest" stationary state.

We have used the method described in Sect. VI. to calculate a few lowest excited states in simple systems, namely the linear anharmonic oscilator and the $U(1)$ lattice theory on a single plaquette. In both cases the method works in a very satisfactory way. Details of calculations and the results obtained will be described in the forthcoming publication.

It might seem also surprising why we discuss the less general methods when presenting later on more general ones. This is due to our belief that simpler methods are sometimes more useful than general ones. In, using for instance, the general methods of Sects. V. and VI. one has the instruction how the state vector moves in the Hilbert space but prior an actual calculation one has to specify a basis in this space, and for practical reasons this basis has to be finite at any step of the calculation. Practical applications of these methods will not be trivial and sometimes it might be very useful to have a hint at the extected result based on a more simple method.

Let us also point out that our starting point which leads to conditions requiring that time derivatives of expectation values vanish in the stationary state is, in a sense, a special case of the requirement

$$\langle\Psi_n|A(t)|\Psi_k\rangle = \exp[\mathrm{i}(E_n - E_k)t]\langle\Psi_n|A(0)\,\Psi_k\rangle$$

used in numerical computations of energy differences of stationary states n and m. Such a procedure was recently used by Bender et al. [1] in their studies of time evolution of operators by the finite element method. The condition which we used is obtained from the preceding one if $n = k$. It would be interesting to know whether the conditions corresponding to $n \neq k$ could provide a basis for more constrained methods enabling an accurate determination of energies and state vectors of stationary states.

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APPENDIX

We shall outline here a more elementary argument leading to Eq. (49). Let $|\Psi\rangle$ denote the current estimate of a stationary state. We are interested in the infinitesimal transformation

$$|\Psi\rangle \to |\Psi'\rangle = |\Psi\rangle + \varepsilon|\Phi\rangle$$

with $|\Phi\rangle$ being normalized and orthogonal to $|\Psi\rangle$ and such that the decrease of the expectation value of the energy

$$\delta E = \langle\Psi|H|\Psi\rangle - \langle\Psi'|H|\Psi'\rangle$$

would be maximal. Let us decompose both $|\Psi\rangle$ and $|\Phi\rangle$ into the eigenstates of H

$$|\Psi\rangle = \Sigma c_n|n\rangle$$
$$|\Phi\rangle = \Sigma a_n|n\rangle .$$

The requirements given above lead to

$$\Sigma c_n^* a_n = \Sigma c_n a_n^* = 0 \tag{A1}$$

$$\Sigma a_n^* a_n = 1 , \tag{A2}$$

under these conditions we have to find the maximum of

$$\delta E = -\varepsilon \Sigma E_n (c_n^* a_n + c_n a_n^*)$$

with respect to the parameters $\{a_n\}$.

Introducing Lagrange multipliers we are looking for the extremum of the expression

$$\Phi(\{a_n, a_n\}) = \Sigma E_n (c_n^* a_n + c_n a_n^*) - \lambda \Sigma a_n^* a_n - \mu \Sigma (c_n^* a_n + c_n a_n^*) . \tag{A3}$$

Taking derivatives with respect to a_n^* we obtain

$$a_n = \frac{1}{\lambda} E_n c_n - \frac{\mu}{\lambda} c_n .$$

This implies

$$|\Phi\rangle = \frac{1}{\lambda}\{H|\Psi\rangle - \varkappa|\Psi\rangle\} .$$

The conditions (A1), (A2) lead finally to

$$|\Phi\rangle = \text{const}\,[H - \langle\Psi|H|\Psi\rangle]\,|\Psi\rangle ,$$

which leads to Eq. (49).

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ОБ ОДНОМ СПОСОБЕ СИСТЕМАТИЧЕСКОГО УТОЧНЕНИЯ ВАРИАЦИОННОГО МЕТОДА ПРИ ВЫЧИСЛЕНИЯХ ОСНОВНОГО И ВОЗБУЖДЕННЫХ СОСТОЯНИЙ

В работе предложен метод для систематического уточнения вариационных оценок энергий и волновых функций стационарных состояний в квантовой механике и теории поля. Среднее значение производной по времени от любых наблюдаемых в истинно стационарном состоянии должно равняться нулю. Метод сначала продемонстрирован на некоторых пробных состояниях и вариантах, в случае которых это условие приблизительно выполнено для некоторого выбранного набора наблюдаемых. Набор наблюдаемых может состоять из последовательности производных по времени некоторой частной физической величины. Вектор состояний, полученный в этом случае, соответствует приблизительно среднему значению этой величины, которое не зависит от времени. Приведен ряд примеров для иллюстрации метода, в том числе выражение Бардина—Купера—Шиффера для основного состояния сверхпроводника, которое естественным образом следует из использованного метода.

Предложены два подхода, основанные на дифференциальных уравнениях, определяющих движение вектора состояния вдоль наибыстрейшего спуска к стационарному состоянию. Оба метода справедливы в том смысле, что не требуют предварительного выбора частного набора «соответствующих» операторов. Первый локально максимизирует декремент выражения $\langle\Psi|H|\Psi\rangle$ и эквивалентен дифференциальной форме t-разложения, недавно использованной Горном и Вейнштейном и подходящей для исследования основного состояния. Второй подход локально максимизирует декремент выражения $\langle\Psi|H^2|\Psi\rangle - \langle\Psi|H|\Psi\rangle^2$ и является подходящим для исследования возбужденных стационарных состояний.