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# Application of the Maximum Algorithm to the Lipkin Model

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Lipkin constructed a many-Fermion system which, despite the simplicity of its Hamiltonian, exhibits features of complex systems. Application of the maximum algorithm is attempted in order to find the ground-state level. Numerical computations suggest that eigenstates of a particular parity transformation introduced by Lipkin have many advantages. Coupling of two models provides a means of studying the maximum method in the product space generated by the two subsystems.

## 1. INTRODUCTION

Approximation methods in quantum mechanics usually suffer from lack of accuracy. As far as computations of the ground-state level are concerned, criteria of convergence are not ready at hand. This problem arises especially when the effect of truncations is not sufficiently understood.

This difficulty motivated H. Lipkin to construct a many-body system which is accessible to exact diagonalization, although its dynamical properties are in no respect trivial. For example, collective excitations can occur. While Lipkin tested the accuracy of perturbation and Hartree–Fock calculations, a further algorithm is provided by the maximum method.

The first section briefly reviews the notions introduced by Lipkin. The second gives a short account of the maximum principle. The third section deals with applications of this calculus to the ground-state band of the Lipkin model. The final section gives an example concerning the product space of two Lipkin systems.



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## 2. THE LIPKIN MODEL

We ascribe to a Fermion two possible states

$$|+\rangle \text{ and } |-\rangle$$

which are assumed by hypothesis to span the complete state space. We then define three operators $j_z, j_+$, and $j_-$ as follows:

$$\begin{aligned} j_z|+\rangle &= \tfrac{1}{2}|+\rangle, \qquad j_+|+\rangle = 0 \\ j_z|-\rangle &= -\tfrac{1}{2}|-\rangle, \qquad j_+|-\rangle = |+\rangle \\ j_- &= j_+^\dagger \end{aligned} \tag{2.1}$$

Given $N$ identical Fermions, these one-body operators can easily be generalized:

$$\begin{aligned} \mathfrak{J}_z &= \sum_{p=1}^{N} j_{zp}, \qquad \mathfrak{J}_+ = \sum_{p=1}^{N} j_{+p} \\ \mathfrak{J}_- &= \mathfrak{J}_+^\dagger \end{aligned} \tag{2.2}$$

The three operators $\mathfrak{J}_z$, $\mathfrak{J}_+$, and $\mathfrak{J}_-$ obey the canonical angular-momentum commutation relations (Lipkin et al, 1965)

$$\begin{aligned} [\mathfrak{J}_z, \mathfrak{J}_+] &= \mathfrak{J}_+, \qquad [\mathfrak{J}_z, \mathfrak{J}_-] = -\mathfrak{J}_- \\ [\mathfrak{J}_+, \mathfrak{J}_-] &= 2\mathfrak{J}_z \end{aligned} \tag{2.3}$$

On account of identities (2.3) the three observables

$$\mathfrak{J}_x = \frac{1}{2}(\mathfrak{J}_+ + \mathfrak{J}_-), \qquad \mathfrak{J}_y = \frac{1}{2i}(\mathfrak{J}_+ - \mathfrak{J}_-), \qquad \mathfrak{J}_z \tag{2.4}$$

are called quasispin operators. They form the components of angular momentum in an abstract three-dimensional quasispin space.

The ideas presented so far have much in common with isospin (Lipkin, 1966).

The interaction Hamiltonian between the particles of the Lipkin model is defined (Lipkin et al., 1965) as

$$\begin{aligned} H &= \mathfrak{J}_z + V(\mathfrak{J}_+^2 + \mathfrak{J}_-^2) \\ &= \mathfrak{J}_z + 2V(\mathfrak{J}_x^2 - \mathfrak{J}_y^2) \end{aligned} \tag{2.5}$$

$V$ denotes a perturbation parameter. In case $V=0$ the eigenstates of $H$ are just the $N$-particle determinants, and their energy is one-half the number of particles in the plus state minus those in the minus state.

But even in the general case, i.e., $V$ different from zero, the square of quasispin

$$\mathfrak{J}^2=\mathfrak{J}_x^2+\mathfrak{J}_y^2+\mathfrak{J}_z^2 \tag{2.6}$$

is a conserved quantity. For even particle number $N$, $J$ must always be integral while $J$ is half-integral for odd $N$ (Lipkin et al., 1965).

An $N$-particle Lipkin model contains $2^N$ base states (Lipkin et al., 1965). The highest quasispin that can occur is $J=N/2$. This means that $J$ bands are usually degenerate (Lipkin et al., 1965). However, there is but one band belonging to $J=N/2$ which we call the ground-state band according to Lipkin et al. (1965).

An immediate consequence of definition (2.5) in the case of integral $J$ is the splitting of the total $J$-band into an $H$-invariant subspace containing only even eigenvalues $M$ of $J_z$ and the complementary space of odd $M$ (Lipkin et al., 1965).

A closer look at the symmetry properties of $H$ reveals that the energies of the Lipkin model are symmetric with respect to zero. They occur pairwise, $E$ and $-E$ (Lipkin et al., 1965). In order to understand this feature let us introduce the following rotation in quasispin space:

$$L=\exp\left[\frac{i\pi}{2^{1/2}}(\mathfrak{J}_x+\mathfrak{J}_y)\right] \tag{2.7}$$

$L$ performs a 180° rotation about the 45° axis in the $x,y$ plane. Its effect is summarized by the following equations:

$$\begin{aligned} L\mathfrak{J}_xL^{-1}&=\mathfrak{J}_y \\ L\mathfrak{J}_yL^{-1}&=\mathfrak{J}_x \\ L\mathfrak{J}_zL^{-1}&=-\mathfrak{J}_z \end{aligned} \tag{2.8}$$

This proves our assertion since

$$LHL^{-1}=-H \tag{2.9}$$

and to each state of energy $E$ there corresponds a state of energy $-E$ (Lipkin et al., 1965). The dimensionality of an integral $J$ band being odd, we conclude that $E=0$ is an eigenvalue of $H$.

## 3. THE MAXIMUM PRINCIPLE

This section describes the eigenvalue computation scheme which we will apply to the ground-state band of the Lipkin model in order to obtain its ground-state energy.

Let $|x\rangle$ be a normalized state vector and

$$\langle H\rangle_x \equiv \langle x|Hx\rangle \tag{3.1}$$

its expectation value.

Its square variance is defined as

$$\psi_H(|x\rangle) \equiv \langle H^2\rangle_x - (\langle H\rangle_x)^2 \tag{3.2}$$

We further assume $|x\rangle$ has nonvanishing components of the maximum and minimum eigenvalues $E_{\max}$ and $E_{\min}$ of $H$. Surely, then, $\psi_H$ is positive and we can define the sequence

$$|x_{k+1}\rangle = \frac{H|x_k\rangle - \langle H\rangle_{xk}|x_k\rangle}{[\psi_H(|x_k\rangle)]^{1/2}} \tag{3.3}$$

recursively starting from $|x_0\rangle = |x\rangle$.

Evidently $|x_{k+1}\rangle$ is the unit vector perpendicular to $|x_k\rangle$ in the two-space spanned by $|x_k\rangle$ and $H|x_k\rangle$. The expression (3.3) cannot become singular because of the maximum principle (Textor, 1978) which states that $\psi_H$ is a monotonically ascending function:

$$\begin{aligned}\psi_H(|x_0\rangle) &\leqslant \psi_H(|x_1\rangle) \leqslant \cdots \\ &\leqslant \psi_H(|x_k\rangle) \leqslant \psi_H(|x_{k+1}\rangle) \leqslant \cdots \\ &\leqslant \lim_{k\to\infty} \psi_H(|x_k\rangle)\end{aligned} \tag{3.4}$$

Calling the space generated by $|x_k\rangle$ and $|x_{k+1}\rangle$ $\Gamma_k$ the maximum principle has the more precise form

$$\psi_H(|x_k\rangle) = \psi_H(|x_{k+1}\rangle)$$

if and only if $\Gamma_k$ is invariant under $H$. The sequence of subspaces $\Gamma_k$ converges to a $H$-invariant space $\Gamma$ for $k\to\infty$. The eigenvalues of $H$ on $\Gamma$ are $E_{\max}$ and $E_{\min}$ (Textor, 1978).

## 4. CALCULATION OF THE GROUND-STATE ENERGY

We are now going to apply the maximum algorithm to the ground-state band of the Lipkin model. Before selecting a particular $|x_0\rangle$ let us fix the notation. By means of the orthogonal projection

$$P_k = |x_k\rangle\langle x_k| + |x_{k+1}\rangle\langle x_{k+1}|$$

the Hamiltonian $H$ can be projected onto $\Gamma_k$:

$$h_k := P_k H P_k$$

Its eigenvalues are

$$e_k^{\pm} = \tfrac{1}{2}\left(\langle H\rangle_{x_k} + \langle H\rangle_{x_{k+1}}\right) \pm \left[\psi_H(|x_k\rangle) + \tfrac{1}{4}\left(\langle H\rangle_{x_k} - \langle H\rangle_{x_{k+1}}\right)^2\right]^{1/2} \quad (4.1)$$

We can then prove the limit condition (Textor, 1978)

$$\lim_{k\to\infty} e_k^{+} = E_{\max}, \qquad \lim_{k\to\infty} e_k^{-} = E_{\min} \quad (4.2)$$

In the case of the Lipkin model we remember that $E_{\max}$ and $E_{\min}$ are symmetric with respect to zero. The question arises whether the same symmetry can be achieved for the projected eigenvalues $e_k^{+}, e_k^{-}$. If the quasispin $J$ of the ground-state band is integral we assert that $|x_0\rangle$ should be an eigenstate of the operator $L$, equation (2.7).

If $J$ is integral the spin representation of the rotation group in quasispin space is single-valued, i.e., $L^2 = 1$. This is the characteristic of a parity operator since $L$ is also unitary. We therefore call $L$ the Lipkin parity operator. The ground-state band can be subdivided into orthocomplementary spaces of even or odd Lipkin parity.

If $|x_0\rangle$ has got a definite parity its energy expectation value vanishes. We note that

$$\langle Lx_0|H|Lx_0\rangle = \langle H\rangle_{x_0}$$

which using (2.9) leads to the result

$$\langle Lx_0|H|Lx_0\rangle = \langle x_0|LHL^{-1}|x_0\rangle = -\langle H\rangle_{x_0}$$

Hence

$$\langle H\rangle_{x_0} = 0 \quad (4.3)$$

Through consecutive application of (3.3), equation (4.3) leads to the subsequent straightforward result.

If $|x_0\rangle$ is selected to be a parity eigenstate, all $|x_k\rangle$ have well-defined parity, and they also obey equation (4.3)

$$\langle H\rangle_{x_k}=0, \qquad \forall k \tag{4.4}$$

The assertion is obtained by use of (4.1)

$$e_k^{\pm}=\pm\left[\psi_H(|x_k\rangle)\right]^{1/2} \tag{4.5}$$

Not only are the iterated eigenvalues symmetric with respect to zero, they also form a monotonic sequence. This follows from direct inspection of (3.4). However, monotony is not necessarily maintained for arbitrary $|x_0\rangle$.

Parity eigenstates are actually easy to construct. In the ground-state band there is $M=0$, as can be derived from (2.8). For $M\neq 0$ there are the two linear combinations

$$|\psi_M^{\pm}\rangle := 2^{-1/2}(|M\rangle \pm i^M|-M\rangle) \tag{4.6}$$

Hint: (2.8) can be rewritten in the form

$$L\mathfrak{J}_+L^{-1}=i\mathfrak{J}_-, \qquad L\mathfrak{J}_-L^{-1}=-i\mathfrak{J}_+ \tag{4.7}$$

Remembering that the even $M$ band is by itself $H$ invariant as well as the odd one the two cases are considered separately.

The model calculations were carried out with the example of a 100-particle model, i.e., $J=50$ for the ground-state band. The perturbation parameter of (2.5) was set to $V=10.5$. Figure 1 illustrates the iteration scheme for the two trial vectors

(a) $M=0$

(b) $|x_0\rangle=2^{-1/2}(|J\rangle+|-J\rangle)$

The eigenvalue plot in case (a) is almost horizontal. This contrasts sharply with case (b), in which the curves show an appreciable slope. An interpretation ready at hand is the occurrence of a strong perturbation. For small $V$ the spectrum of $H$ would resemble that of $\mathfrak{J}_z$, and trial vector (b) would be favored much more than (a). In the numerical example of Figure 1, however, a small variance in $\mathfrak{J}_z$ coincides with large variance in $H$.

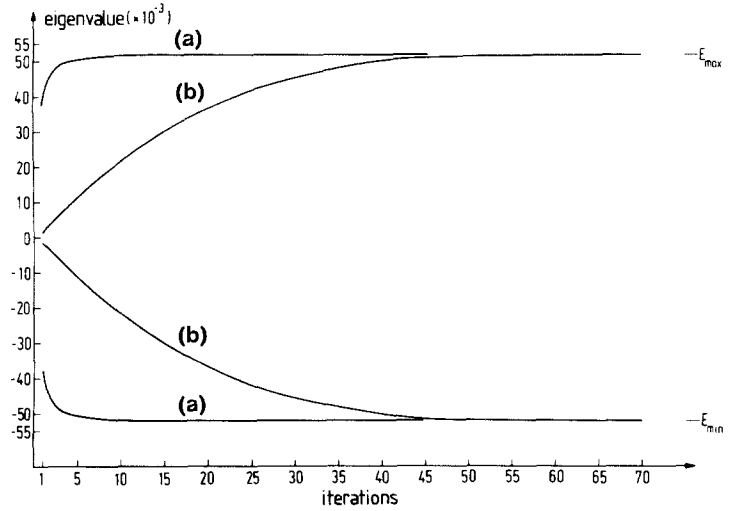


**Fig. 1.** Comparison of two trial states for the even $M$ band.

Thus having understood the situation for even $M$, let us now turn our attention to the odd band. The ansatz

$$|x_{0c}\rangle = 2^{-1/2}(|1\rangle + i|-1\rangle) \tag{4.8}$$

will be used. From (4.6) we know it has good parity, and $\mathfrak{J}_z$ variance was chosen minimal in analogy to Fig. 1. [The index $c$ of (4.8) means complex]. The states $|x_{0c}\rangle$ and $M=0$ behave much the same (see Figure 2).

There remains one striking puzzle. Although $H$ is a real matrix we were led to complex computations. Nevertheless it seems inevitable, as can be recognized by restriction to real phases. Take for comparison

$$|x_{0r}\rangle = 2^{-1/2}(|1\rangle + |-1\rangle) \tag{4.9}$$

The trial state (4.9) is, of course, permitted in applying the maximum algorithm. The plot of Figure 2 demonstrates that it suffers from many disadvantages. While the $e_k^+$ curves coincide for the real and complex situations we notice a fundamental difference in the $e_k^-$ sequences. The symmetry (4.5) is broken, and the $e_k^-$ plot converges so slowly that the actual convergence to the correct limit $E_{\min}$ is not evident from the scaling chosen for Figure 2. The $e_k^-$ are not even monotonic although fluctuations occur only in higher decimals and can roughly be neglected.

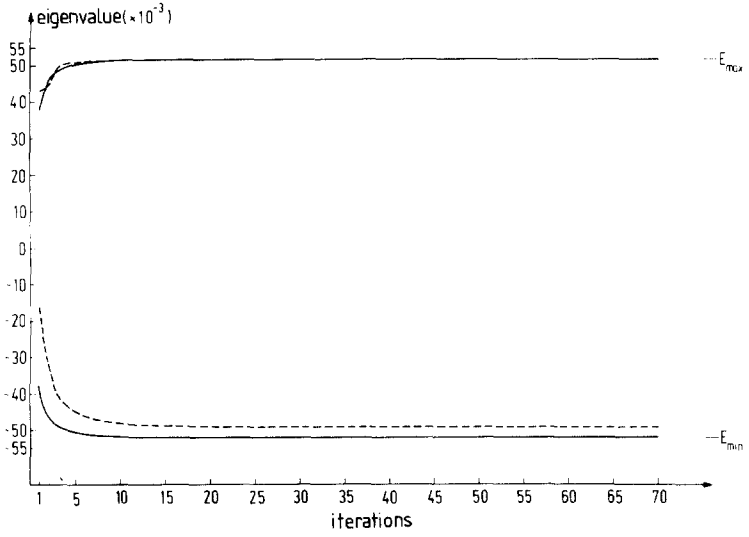


**Fig. 2.** The odd $M$ band. The drawn-out line denotes the complex trial vector, the dashed line denotes the real one.

## 5. COUPLING OF TWO SYSTEMS

The Lipkin model can be regarded from a somewhat different point of view. Instead of selecting a single $J$ band the full system can be decomposed into two subsystems. For instance a model of 100 particles consists of two halves with 50 particles each. The respective ground-state band has got $J=25$. The product space $J\otimes J$ ($J=25$) is the state space of the coupled system.

Let us now set up the interaction in this picture. Starting from the one-particle operators

$$\begin{aligned} \mathfrak{J}_{z\mathrm{I}} &= \sum_{p=1}^{50} j_{zp}, & \mathfrak{J}_{z\mathrm{II}} &= \sum_{p=51}^{100} j_{zp} \\ \mathfrak{J}_{+\mathrm{I}} &= \sum_{p=1}^{50} j_{+p}, & \mathfrak{J}_{+\mathrm{II}} &= \sum_{p=51}^{100} j_{+p} \\ \mathfrak{J}_{-\mathrm{I}} &= \mathfrak{J}_{+\mathrm{I}}^{\dagger}, & \mathfrak{J}_{-\mathrm{II}} &= \mathfrak{J}_{+\mathrm{II}}^{\dagger} \end{aligned} \tag{5.1}$$

$H$ contains the three contributions

$$H = H_{\mathrm{I}} + H_{\mathrm{II}} + H_{\mathrm{int}} \tag{5.2}$$

with the abbreviations

$$H_{\mathrm{I}}=\mathfrak{J}_{z\mathrm{I}}+V(\mathfrak{J}^2_{+\mathrm{I}}+\mathfrak{J}^2_{-\mathrm{I}})$$
$$H_{\mathrm{II}}=\mathfrak{J}_{z\mathrm{II}}+V(\mathfrak{J}^2_{+\mathrm{II}}+\mathfrak{J}^2_{-\mathrm{II}}) \tag{5.3}$$
$$H_{\mathrm{int}}=2V(\mathfrak{J}_{+\mathrm{I}}\mathfrak{J}_{+\mathrm{II}}+\mathfrak{J}_{-\mathrm{I}}\mathfrak{J}_{-\mathrm{II}})$$

In the language of perturbation theory $H_{\mathrm{I}}$ and $H_{\mathrm{II}}$ represent two noninteracting systems whose eigenstates are supposed to be known while $H_{\mathrm{int}}$ is the perturbation Hamiltonian. We are not pursuing perturbation calculations here but we are rather interested in applying the maximum method. We therefore need not know any details about the spectrum of the subsystems as the maximum algorithm allows us to choose a starting vector $M_{\mathrm{I}}\otimes M_{\mathrm{II}}$, which denotes an eigenstate of $\mathfrak{J}_{z\mathrm{I}}\otimes\mathfrak{J}_{z\mathrm{II}}$.

In principle we have to face a $51\times 51$ problem, which can be simplified by symmetry considerations. Restricting our attention to the even $M$-band of the 100-particle system it is clear that either both $M_{\mathrm{I}}$ and $M_{\mathrm{II}}$ are even or both must be odd. It can be shown furthermore that the symmetric space generated by the symmetrized states

$$|M_{\mathrm{I}}M_{\mathrm{II}}\rangle+|M_{\mathrm{II}}M_{\mathrm{I}}\rangle$$

and its antisymmetric complement

$$|M_{\mathrm{I}}M_{\mathrm{II}}\rangle-|M_{\mathrm{II}}M_{\mathrm{I}}\rangle$$

are $H$ invariant.

*Proof.* The product states are decomposed into eigenstates of total quasispin $j$:

$$|M_{\mathrm{I}}M_{\mathrm{II}}\rangle=\sum_j C(J,J,M_{\mathrm{I}},M_{\mathrm{II}},j,M)|jM\rangle \tag{5.4}$$
$$M=M_{\mathrm{I}}+M_{\mathrm{II}}$$

Remember the exchange identity

$$C(J,J,M_{\mathrm{I}},M_{\mathrm{II}},j,M)=(-1)^{2J-j}C(J,J,M_{\mathrm{II}},M_{\mathrm{I}},j,M) \tag{5.5}$$

it is immediate that the symmetric space $U_{\mathrm{sym}}$ contains the even $j$'s

$$U_{\mathrm{sym}}=\bigoplus_{j\ \mathrm{even}} U_j \tag{5.6}$$

while the antisymmetric space comprises the odd $j$ bands of the product space. This implies $H$ invariance of $U_{\text{sym}}$. If our trial state is an element of $U_{\text{sym}}$ then it is possible to compute the ground-state energy. The ground-state band of the total 100-particle system has got even $j$.

We select the start vector

$$M_{\text{I}} = M_{\text{II}} = 0$$

(a) both $M_{\text{I}}$ and $M_{\text{II}}$ are even;
(b) it is an element of $U_{\text{sym}}$;
(c) its $\mathfrak{J}_z$ variance is minimal;
(d) it has got a well-defined parity.

The sequences $e_k^{\pm}$ are plotted in Figure 3. They proceed in analogy to Figure 1.

Since total quasispin $\mathfrak{J} = \mathfrak{J}_{\text{I}} + \mathfrak{J}_{\text{II}}$ is conserved one may wonder that the convergence properties of our start vector are so good although it does not have a good total quasispin $j$. Spin projection before applying the maximum method does not seem necessary.

In order to estimate the influence of the various $j$ contributions on the above trial vector let us look at the plot of the averaging function

$$I(|x_k\rangle) = \left(\langle \mathfrak{J}^2 \rangle_{x_k} + \tfrac{1}{4}\right)^{1/2} - \tfrac{1}{2}$$

in Figure 3.

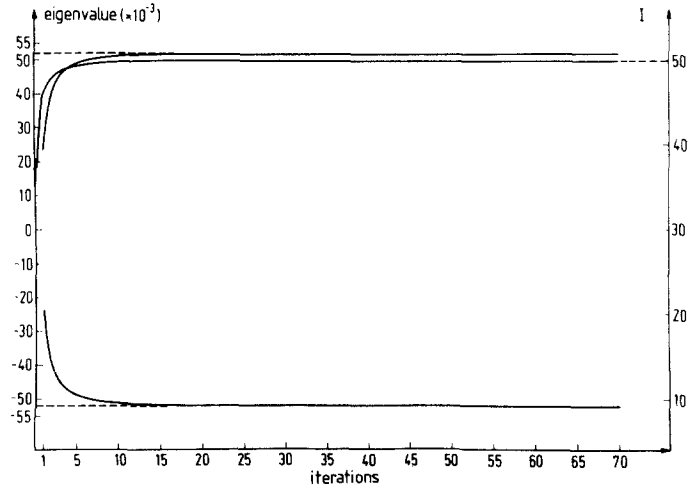


**Fig. 3.** Iteration scheme for the Hamiltonian (5.2); iterations versus energy (left axis) and quasispin (right axis).

Clearly if $|x_k\rangle$ were an eigenstate of total quasispin the function $I$ would assume the respective $j$ value. In general $I$ is some average of the $j$'s that occur, and $I$ converges to $j=2J=50$, the quasispin of the ground-state band in the total system. An interesting fact is revealed by Figure 3; the correct $j$ symmetry is achieved much faster by the maximum algorithm than the exact location of the ground-state energy. This is a strong argument in favor of the method since it means that the calculus establishes the correct symmetry all by itself.

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