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Self-Consistent Treatment of the Pauli Operator in the Brueckner-Hartree-Fock Approach

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Brueckner-Hartree-Fock (BHF) equations are derived including the correction due to treating the Pauli operator in the HF basis instead of the single oscillator basis, both for standard BHF and for a variational calculation. Calculations were done with an approximate energy denominator. The correction effects for ^{16}O are significant: about a 10% decrease in total binding energy, 12–30% decreases in single-particle energies, and up to 20% decrease in the peak of the charge-density distribution.

1. INTRODUCTION

For several years the Hartree-Fock[1-5] (HF) and Brueckner-Hartree-Fock[6-8] (BHF) approaches have been applied with some success in nuclear physics in an attempt to understand ground-state properties of nuclei, such as total binding energies, root-mean-square radii, and static multipole moments. The structure of the ground-state rotational band in nuclei has been reproduced within the framework of an angular momentum projected HF[9] or Hartree-Fock-Bogoliubov[10] theory. However HF and BHF calculations employing forces derived from the basic nucleon-nucleon interaction have been unable to reproduce the charge distribution of nuclei. They produced too high a density in the center of the nucleus and failed to reproduce the nearly constant density inside as indicated by electron scattering data.[11]

Recently this situation has been changed by dropping the requirement that the two-body force be "realistic." Several calculations have reproduced charge distributions by using effective density-dependent forces.[12-15] These forces are derived by solving the Bethe-Goldstone equation in nuclear matter for a special Fermi momentum:

$$k_F = (\tfrac{3}{2}\pi^2\rho)^{1/3} . \tag{1}$$

One finds an effective density-dependent force by transforming the nucleon-nucleon matrix elements from momentum representation into r space and by parametrizing the dependence on the Fermi momentum k_F with the help of the local density approximation.[6] To improve the force one adjusts the short-range part of this effective interaction by fitting the total binding energy per particle and the average density in nuclear matter. Such a calculation is phenomenological in the sense that a reasonable answer for the binding energy of nuclei is guaranteed by the adjustment of the force, but it leads to some insight into the nature of the effective interaction. It avoids the primary purpose of Brueckner theory however, namely the attempt to completely describe the macroscopic properties of nuclear matter and nuclei starting from the basic nucleon-nucleon interaction.

Here we want to treat the effective density dependence of the nucleon-nucleon interaction in finite nuclei microscopically: This is done by taking into account the dependence of the Pauli operator on the self-consistent single-particle states within a Brueckner-Hartree-Fock (BHF) calculation. We coin the name *Pauli-Brueckner-Hartree-Fock* (PBHF) calculation for this procedure because the name BHF is associated with the work of Davies and collaborators[7] and others[8] who treat the Pauli operator in the oscillator representation.

2. DERIVATION OF EQUATIONS

We introduce for the transformation from the oscillator basis $|a\rangle, |b\rangle, |c\rangle \cdots$ to the self-consistent single-particle states $|i\rangle, |k\rangle, |l\rangle, |m\rangle, |n\rangle \cdots$ the notation:

$$|i\rangle = \sum_a |a\rangle A_{ai} . \tag{2}$$

The total energy of the nucleus is given in first-order Brueckner approximation by:

$$\langle H\rangle = \sum_{ab} \langle a|t|b\rangle \sum_{i<F} A^*_{ai} A_{bi} + \tfrac{1}{2} \sum_{abcd} \sum_{ik<F} \langle ac|G(W_{ik})|bd\rangle A^*_{ai} A_{bi} A^*_{ck} A_{dk} . \tag{3}$$

Here $G(W_{ik})$ is the Brueckner reaction matrix for the starting energy $W_{ik} = \epsilon_i + \epsilon_k < 0$ calculated with the self-consistent Pauli operator Q,

$$G = V + V \frac{Q}{W - H} G . \tag{4}$$

Since conventionally the reaction matrix is calculated in the oscillator representation using the oscillator propagator $Q_0/(W_0-H_0)$, the correction to the self-consistent propagator is made using the equation:

$$G = G_0 + G_0\left(\frac{Q}{W-H} - \frac{Q_0}{W_0-H_0}\right) G \,. \tag{5}$$

The above equation in this form is very difficult to use, so we make a few approximations on it. First, our main aim in this paper is to study the effect of the self-consistent Q rather than Q_0; we, therefore, neglect the variation of G with respect to the starting energy W and replace W by W_0. We cannot, however, replace H by H_0 because H_0 does not commute with Q. Secondly, since $H-H_0$ should be small, we write

$$\frac{Q}{W_0-H} \simeq Q\frac{1}{W_0-H_0}Q + Q\frac{1}{W_0-H_0}(H-H_0)\frac{1}{W_0-H_0}Q \,. \tag{6}$$

The first iteration of Eq. (5) gives,

$$G \simeq G_0 + G_0\left(Q\frac{1}{W_0-H_0}Q - \frac{Q_0}{W_0-H_0}\right)G_0 + G_0 Q\frac{1}{W_0-H_0}(H-H_0)\frac{1}{W_0-H_0}Q\,G_0 \,. \tag{7}$$

The third term on the right-hand side of the above equation contains the Hamiltonian H for the unoccupied states. The "correct" choice of H is as yet unknown. This makes the estimation of these terms ambiguous; for this reason we do not include them here in our paper, and hope that their contribution will be small. We, therefore, get

$$G \approx G_0 + G_0\left[Q\frac{1}{W_0-H_0}Q - \frac{Q_0}{W_0-H_0}\right]G_0 \,. \tag{7'}$$

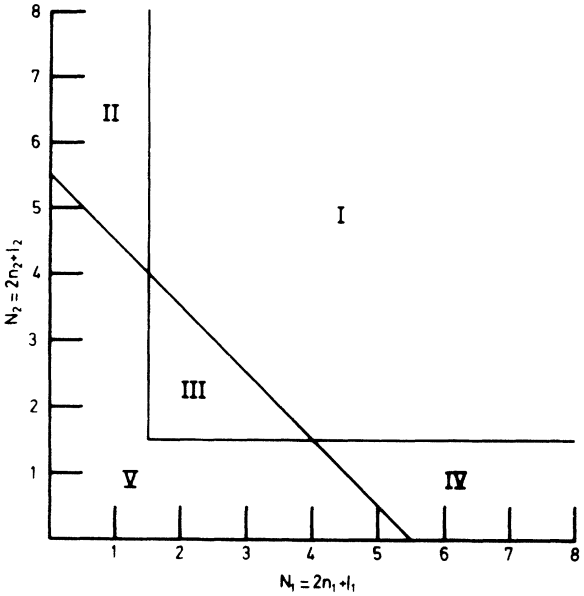

FIG. 1. "Eden-Emery" and oscillator Pauli operator for ^{16}O. The "Eden-Emery"-Pauli operator is equal to unity for $N_1+N_2>5$ (areas I, II, and IV). The Pauli operator in the oscillator basis is unity for N_1 and $N_2 \geq 2$ (areas I and III). The Pauli operator Q_0-Q_{EE} for the strip correction in Eq. (11) is equal to -1 in area I, to $+1$ in area III, and to -1 in area IV.

The two-particle intermediate states are defined by an harmonic-oscillator spectrum $h_{\rm osc}(2p)$ with a single-particle energy shift of $-C$. By introducing Eq. (7′) into the total energy (3) one finds:

$$\begin{aligned}\langle H\rangle = &\sum_{ab}(\langle a|t|b\rangle \sum_{i<F} A^*_{ai}A_{bi}) + \tfrac{1}{2}\sum_{abcd}\sum_{ik<F}\langle ac|G_0(W_{oik})|bd\rangle A^*_{ai}A_{bi}A^*_{ck}A_{dk} \\ &+ \tfrac{1}{2}\sum_{abcd}\sum_{ik<F}\sum_{efgh e'f'}\langle ac|G_0(W_{oik})|e'f'\rangle(\delta_{e';e} - \sum_{r'<F}A_{e'r'}A^*_{er'})(\delta_{f';f} - \sum_{s'<F}A_{f's'}A^*_{fs'}) \\ &\times (W_{oik}-\epsilon_e-\epsilon_f)^{-1}(\delta_{e;g} - \sum_{r<F}A_{er}A^*_{gr})(\delta_{f;h} - \sum_{s<F}A_{fs}A^*_{hs})\langle gh|G_0(W_{oik})|bd\rangle A^*_{ai}A_{bi}A^*_{ck}A_{dk} \\ &- \tfrac{1}{2}\sum_{abcd}\sum_{ik<F}\sum_{ef>F_0}\langle ac|G_0(W_{oik})|ef\rangle(W_{oik}-\epsilon_e-\epsilon_f)^{-1}\langle ef|G_0(W_{oik})|bd\rangle A^*_{ai}A_{bi}A^*_{ck}A_{dk} \,. \end{aligned} \tag{8}$$

The symbol $i<F$ restricts a sum over the self-consistent states to the single-particle levels below the Fermi surface, while $e>F_0$ requires the sum over oscillator basis states to be above the oscillator or shell-model Fermi surface F_0. The oscillator energies ϵ_e, ϵ_f include the shift $-C$.

Finally we replace the energy denominator in Eq. (8) by a constant, $\Delta = \langle W_{oik} - \epsilon_e - \epsilon_f\rangle$. This amounts to replacing (W_0-H_0) in Eq. (7′) by Δ, and is definitely a very rough approximation, but should be good enough for an order-of-magnitude estimate. Since most of the correction of G over G_0 in Eq. (7′) will come from the low-lying excited states in a narrow energy range, and for higher states we will have

$Q = Q_0 = 1$. Under these approximations the variational problem

$$\delta(\langle H\rangle - \sum_i \epsilon_i \langle i|i\rangle) = 0 \tag{9}$$

yields the following Pauli-Brueckner-Hartree-Fock (PBHF) equations:

$$\sum_b h_{ab} A_{bi} = \epsilon_i A_{ai}\,, \tag{10}$$

$$\begin{aligned} h_{ab} = \frac{\partial\langle H\rangle}{\partial \rho_{ab}} &= \langle a|t|b\rangle + \sum_{cd}\langle ac|G_0(W_0)|bd\rangle \rho_{dc} + (1/\Delta)\sum_{cd}\sum_{efgh}\langle ac|G_0(W_0)|ef\rangle(\delta_{f;h}-\rho_{fh}) \\ &\times(\delta_{e;g}-\rho_{eg})\langle gh|G_0(W_0)|bd\rangle\rho_{dc} - (1/\Delta)\sum_{cd}\sum_{ef>F_0}\langle ac|G_0(W_0)|ef\rangle\langle ef|G_0(W_0)|bd\rangle\rho_{dc} \\ &- (1/\Delta)\sum_{cd}\sum_{efgh}\langle gc|G_0(W_0)|bf\rangle(\delta_{f;h}-\rho_{fh})\langle ah|G_0(W_0)|ed\rangle\rho_{dc}\rho_{eg} \\ &+ \sum_{k<F}\sum_{cd}\langle ac|G_0(W_0)|bd\rangle A^*_{ck}A_{dk}\sum_{gehf}\langle ge\left|\frac{\partial G_0}{\partial W_0}\right|hf\rangle A^*_{gk}A_{hk}\rho_{fe}\,, \end{aligned} \tag{11}$$

where we have introduced an average starting energy $W_0 \simeq \langle W_{oik}\rangle$ after the variation.

The density matrix ρ_{dc} is defined in the following way

$$\rho_{dc} = \sum_{s<F} A^*_{cs}A_{ds}\,.$$

The last two terms of the Eq. (11) come from the variation of $G(W, Q)$ with respect to density, namely:

$$\frac{\partial G}{\partial \rho} = \frac{\partial G}{\partial Q}\frac{\partial Q}{\partial \rho} + \frac{\partial G}{\partial W}\frac{\partial W}{\partial \rho}\,. \tag{12}$$

It can be shown[14, 15] that the second term on the right-hand side in the above equation is equivalent to the inclusion of the occupation probabilities.[7] This effect has been studied by Baranger and coworkers[7] and is not treated here for the reasons discussed right after Eq. (5). Hence the numerical results presented in this paper do not take into account the last term of Eq. (11).

In Eq. (11) we are making two improvements over previous Brueckner-Hartree-Fock calculations.[7]

(1) We are treating the Pauli operator self-consistently and are not employing its oscillator representation.

(2) We are allowing for the presence of the Pauli rearrangement term [this is the first term on the right-hand side of Eq. (12)].

3. RESULTS

The Brueckner matrix $G_0(W)$ was calculated[16, 8] by starting with the Eden-Emery[17] approximation for the Pauli operator. The Yale potential[18] was used. In a second step the Eden-Emery reaction matrix G_{EE} was corrected for the difference between the "Eden-Emery"-Pauli operator and the oscillator Pauli operator (see Fig. 1) using the equation:

$$G_0(W) = G_{EE}(W) + G_{EE}(W)\left(\frac{Q_0}{e_0} - \frac{Q_{EE}}{e_0}\right)G_0(W)\,. \tag{13}$$

The effect of these corrections has been previously studied.[16, 19] For ^{16}O the Pauli operator Q_{EE} is equal to unity for $N_1 + N_2 > 5$ and zero otherwise where $N_i = 2n_i + l_i$. All states $N_1 + N_2 \leq 12$ have been taken into account for the solution of the Bethe-Goldstone equation

$$G_{EE}(W) = V + V\frac{Q_{EE}}{e_0}G_{EE}(W) \tag{14}$$

and for the strip correction Eq. (13). The calculations were done with modified versions of the BGOLAP and TGEN codes which were written by Dr. M. R. Patterson of Oak Ridge National Laboratory. A check of truncation effects was done by taking only states for which $N_1 + N_2 \leq 8$. The average starting energy $W = -78$ MeV has been chosen as the weighted average of twice the self-consistent occupied single-particle states calculated without variation of the Pauli operator ($Q = Q_0$). The single-particle level shift C has been fixed to lower the *sd* shell to approximately zero energy ($C = \frac{7}{2}\hbar\omega = 46.5$ MeV). To estimate the average energy denominator $\Delta = W - \langle \epsilon_e + \epsilon_f\rangle$ one assumes that the *sd* shell is contributing the major part and therefore, for this case

$$\Delta \approx W = -78 \text{ MeV}\,. \tag{15}$$

To check the sensitivity of the Pauli-correction

TABLE I. Neutron and proton single-particle levels (in MeV), binding energy per nucleon, and mass and charge radii taking into account the finite size of the proton, resulting from BHF, PBHF (without Pauli rearrangement term), and PBHF (with rearrangement) calculations for ^{16}O. The single-particle energy shift $C=46.5$ MeV and results are shown for $2n_i+l_i \leq 4$ and 6.

	$2n_i+l_i \leq 4$			$2n_i+l_i \leq 6$			
^{16}O	BHF	PBHF (without rearr.)	PBHF (with rearr.)	BHF	PBHF (without rearr.)	PBHF (with rearr.)	Exp. data
			Proton levels				
$0s_{1/2}$	−49.47	−47.37	−42.99	−50.60	−46.91	−40.94	−40 ± 8
$0p_{3/2}$	−20.52	−19.98	−18.75	−20.98	−19.97	−18.02	−18.4
$0p_{1/2}$	−15.50	−15.05	−13.54	−15.55	−14.88	−12.56	−12.1
			Neutron levels				
$0s_{1/2}$	−52.92	−50.76	−46.13	−54.05	−50.26	−43.99	···
$0p_{3/2}$	−23.44	−22.86	−21.51	−23.94	−22.85	−20.71	−21.9
$0p_{1/2}$	−18.81	−18.33	−16.70	−18.87	−18.14	−15.64	−15.7
B/A (MeV)	−5.21	−4.86	−4.88	−5.36	−4.85	−4.89	−7.98
$\langle r_m^2\rangle^{1/2}$ (fm)	2.37	2.38	2.43	2.36	2.39	2.48	
$\langle r_c^2\rangle^{1/2}$ (fm)	2.51	2.52	2.57	2.50	2.54	2.62	2.6 ± 0.1

effect to differences in the average energy denominator the case for which $C=56.5$ MeV, and therefore $W=-58$ MeV, was also calculated.

Results for ^{16}O are summarized in Tables I and II. To see the convergence of Eq. (11) with the number of oscillator states, all the results are presented first with the basis $N_i \leq 4$ and then with $N_i \leq 6$. From here on the basis referred to corresponds to the basis used for the calculation of Eq. (11) and not for solving the G_0 matrix. It can be seen that truncation effects are small. The differences between the $N_i \leq 4$ and $N_i \leq 6$ single-particle energies, total binding energies, and root-mean-square radii are less than a few percent, indicating that $N_i \leq 6$ is a sufficiently large space. As should be expected, lowering the excited-state spectrum ($C=56.5$ MeV vs $C=46.5$ MeV) increased the total BHF binding energy from −5.36 MeV/nucleon to −9.01 MeV/nucleon. (The $\hbar\omega=13.29$ MeV corresponds to the rms charge radius of 2.77 fm in oscillator basis including the finite size of the proton.) However the effect we are trying to study is the Pauli correction. For $C=46.5$ and 56.5 MeV the total binding energies changed by 9 and 15%, respectively, when the BHF results were compared with the PBHF results with Pauli rearrangement. Although taking an average energy denominator is a severe approximation it can be concluded reasonably that a 10% effect is present. Also it was discovered that all of this change was concentrated in the term resulting from an improvement of the Pauli operator within the framework of standard BHF calculations; the contribution to the total binding energy from the Pauli rearrange-

TABLE II. Results for $C=56.5$ MeV. Refer to Table I for a description.

	$2n_i+l_i \leq 4$			$2n_i+l_i \leq 6$		
^{16}O	BHF	PBHF (without rearr.)	PBHF (with rearr.)	BHF	PBHF (without rearr.)	PBHF (with rearr.)
			Proton levels			
$0s_{1/2}$	−64.12	−58.12	−51.19	−67.41	−57.27	−47.58
$0p_{3/2}$	−28.04	−26.55	−24.68	−29.60	−26.71	−23.55
$0p_{1/2}$	−21.44	−20.41	−18.22	−21.82	−19.98	−16.40
			Neutron levels			
$0s_{1/2}$	−67.81	−61.67	−54.39	−71.17	−60.78	−50.65
$0p_{3/2}$	−31.19	−29.60	−27.56	−32.88	−29.78	−26.36
$0p_{1/2}$	−24.95	−23.86	−21.51	−25.42	−23.43	−19.60
B/A (MeV)	−8.65	−7.76	−7.78	−9.01	−7.56	−7.67
$\langle r_m^2\rangle^{1/2}$ (fm)	2.24	2.28	2.34	2.18	2.27	2.38
$\langle r_c^2\rangle^{1/2}$ (fm)	2.39	2.43	2.48	2.33	2.41	2.52

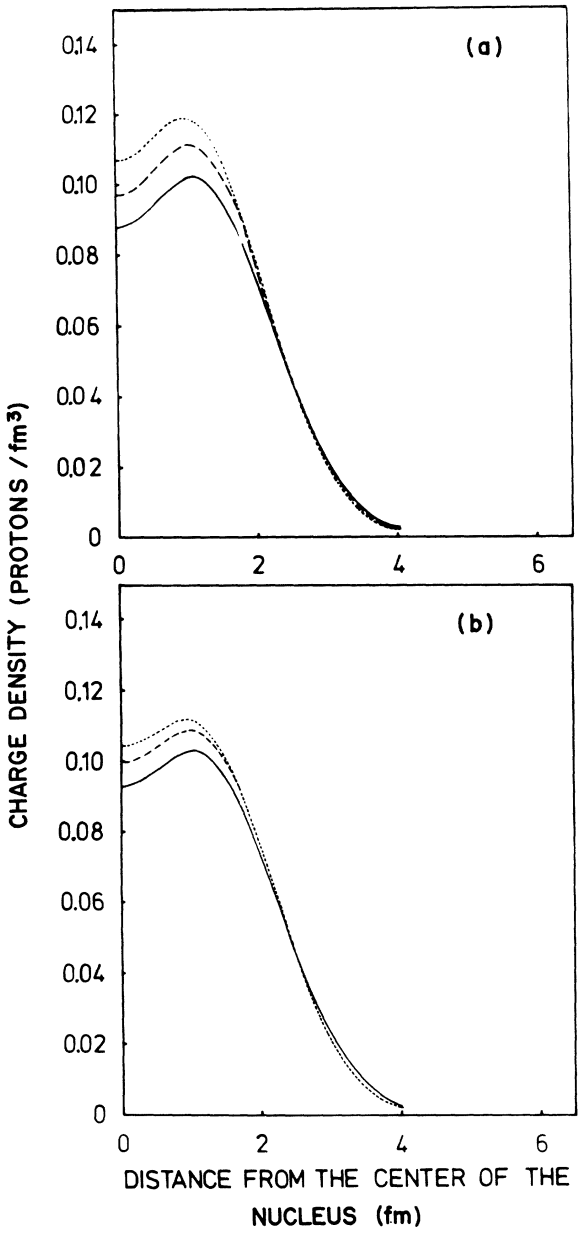

FIG. 2. (a), (b) Charge distributions for ^{16}O with $C = 46.5$ MeV. (a) gives results for $N_i \leq 6$ and (b) for $N_i \leq 4$. The dotted lines are for BHF, the dashed lines for PBHF (without Pauli rearrangement), and the solid lines for PBHF (with rearrangement), respectively. The distributions are normalized to protons per fm^3.

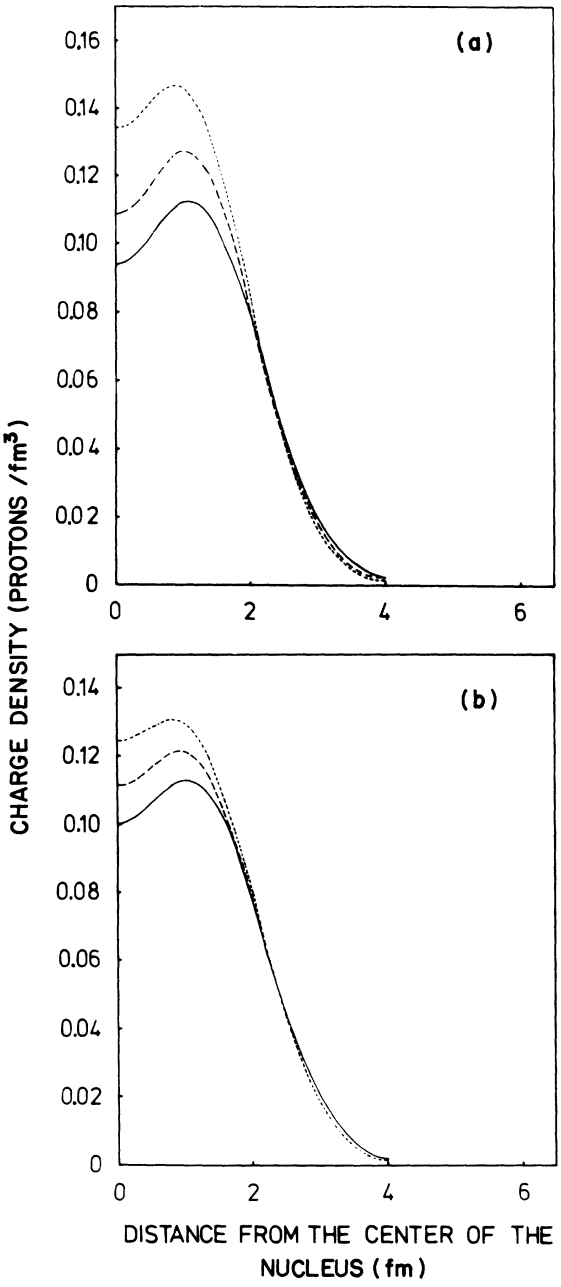

FIG. 3. (a), (b) Charge distributions for ^{16}O with $C = 56.5$ MeV. See Fig. 2 for description.

ment term was negligible. However, this term played a significant role in the decrease in magnitude of the single-particle energies and increase in the rms radii. The rms radius increased by about 5–8% and the single-particle energies decreased in magnitude by about 12–30%. The agreement with experiment for $C = 46.5$ MeV is surprisingly good for everything except the total binding energy, as shown in Table I.

Figures 2 and 3 demonstrate the reduction in the central density resulting from PBHF calculations, both with and without the Pauli rearrangement, when compared with BHF results. For $C = 46.5$ MeV and $N_i \leq 6$ the reduction of the peak density

was about 7% for PBHF without rearrangement and 14% with rearrangement, while for $C = 56.5$ the reduction was about 14 and 23%, respectively. The actual magnitude of this reduction is not important in the present calculation; what is important is that it has been shown that most of the improvements attained by the phenomenological density-dependent BHF calculations over standard BHF can also be reproduced by a more correct microscopic treatment of the Pauli operator.

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