$$
\begin{aligned}
\langle\varphi_k^{\pm}|\,\sigma\,|\varphi_k^{\pm}\rangle &= (\frac{1}{\sqrt{2}}\langle\varphi_k^0| \mp i\langle\varphi_k^1|)[\sigma(\frac{1}{\sqrt{2}}|\varphi_k^0\rangle \pm i\,|\varphi_k^1\rangle)] \\
&= \frac{1}{2}(\langle\varphi_k^0| \mp i\langle\varphi_k^1|)[\sigma(|\beta\rangle\otimes|\phi_k\rangle \pm i\frac{V-E_k}{\sqrt{1-E_k^2}}|\beta\rangle\otimes|\phi_k\rangle)] \\
&= \frac{1}{2}(\langle\varphi_k^0| \mp i\langle\varphi_k^1|)\sigma[(|\beta\rangle\otimes\sigma|\phi_k\rangle \pm i\frac{V-E_k}{\sqrt{1-E_k^2}}|\beta\rangle\otimes|\phi_k\rangle)]
\end{aligned}
$$

As V is a real operator and $A|\psi\rangle = \langle\psi|A^{\dagger}$, $\langle\varphi_0^1|$ expands as follows.

$$
\begin{aligned}
&= \frac{1}{2}(\langle\beta|\otimes\langle\phi_k| \mp i\langle\beta|\otimes\langle\phi_k|\frac{V-E_k}{\sqrt{1-E_k^2}})\sigma[(|\beta\rangle\otimes|\phi_k\rangle \pm i\frac{V-E_k}{\sqrt{1-E_k^2}}|\beta\rangle\otimes|\phi_k\rangle)] \\
&= \frac{1}{2}[((\langle\beta|\otimes\langle\phi_k|)\sigma(|\beta\rangle\otimes|\phi_k\rangle) \pm (\langle\beta|\otimes\langle\phi_k|)\sigma(i\frac{V-E_k}{\sqrt{1-E_k^2}}|\beta\rangle\otimes|\phi_k\rangle) \\
&\mp (i\langle\beta|\otimes\langle\phi_k|\frac{V-E_k}{\sqrt{1-E_k^2}})\sigma(|\beta\rangle\otimes|\phi_k\rangle) - (i\langle\beta|\otimes\langle\phi_k|\frac{V-E_k}{\sqrt{1-E_k^2}})\sigma(i\frac{V-E_k}{\sqrt{1-E_k^2}}|\beta\rangle\otimes|\phi_k\rangle)]
\end{aligned}
$$

As the middle two terms carry opposite signs, they cancel eachother out.

$$
= \frac{1}{2}[((\langle\beta|\otimes\langle\phi_k|)\sigma(|\beta\rangle\otimes|\phi_k\rangle) - (i\langle\beta|\otimes\langle\phi_k|\frac{V-E_k}{\sqrt{1-E_k^2}})\sigma(i\frac{V-E_k}{\sqrt{1-E_k^2}}|\beta\rangle\otimes|\phi_k\rangle)]
$$

The last term of above equation is, in its current form, inconvenient to work with. To create a clearer picture of how this term is built up, we slightly rewrite it. For the sake of simplicity of this section, we propose $\frac{V-E_k}{\sqrt{1-E_k^2}} \equiv A$. Then the above term has the form of

$$
(\langle\varphi_k^0|\,A^{\dagger})\sigma(A\;|\varphi_k^0\rangle) = \langle\varphi_k^0|\,A^{\dagger}\,\sigma\,|\varphi_k^0\rangle\,.
$$

Since A is real and symmetric, $A^{\dagger} = A$ and we simplify to

$$
\langle\varphi_k^0|\,A\sigma A\,|\varphi_k^0\rangle
$$

.

It is unknown how σ acts on $|\varphi_0\rangle$, but if we can rewrite the expression to the form of $\langle\varphi_k^0|\,\sigma A^2\,|\varphi_k^0\rangle$, we will obtain an expression in terms of the expectation value of σ in the basis of the eigenstates of the Hamiltonian. To flip the order of σ, we first use the commutation relation:

$$
[A,B] \equiv AB - BA
$$

which implies

$$
AB \equiv BA - [B,A]. \tag{2.12}
$$

Then,

$$
\langle\varphi_k^0|\,A\sigma A\,|\varphi_k^0\rangle = \langle\varphi_k^0|\,(\sigma A - [\sigma,A])A\,|\varphi_k^0\rangle\,. \tag{2.13}
$$

$$
\begin{aligned}
[\sigma,A] &= \sigma\frac{V-E_k}{\sqrt{1-E_k^2}} - \frac{V-E_k}{\sqrt{1-E_k^2}}\sigma \\
&= \frac{1}{\sqrt{1-E_k^2}}(\sigma V - \sigma E_k - V\sigma + E_k\sigma) \\
&= \frac{[\sigma,V]}{\sqrt{1-E_k^2}} \\
&= \frac{[\sigma,\sum_j |j\rangle\langle j|\otimes P_j]}{\sqrt{1-E_k^2}} \\
&= \frac{\sum_j |j\rangle\langle j|\otimes[\sigma,P_j]}{\sqrt{1-E_k^2}}
\end{aligned}
$$

Since the multi-qubit Pauli operators either commute or anti-commute, we would like to express formula 2.13 in terms of both the commutation and anti commutation relation. Nielsen and Chuang [6] state the following identity:

$$AB = \frac{[A, B] + \{A, B\}}{2}$$

.

Rewriting this identity and substituting it into equation 2.13, we obtain

$$[A, B] = 2AB - \{A, B\}$$

If A and B anticommute, we're left with $[A, B] = 2AB$. Filling in the identities above into equation 2.13, we obtain

$$\left\langle \varphi_k^0 \right| \sigma AA - [\sigma, A]A \left| \varphi_k^0 \right\rangle \tag{2.14}$$

Now we're left with the following two scenarios.

1. σ and V commute, meaning $[\sigma, A]$ is zero and the expression we're left with is

$$\left\langle \varphi_k^0 \right| \sigma AA \left| \varphi_k^0 \right\rangle .$$

   Filling in the original definition of A gives

$$\left\langle \varphi_k^0 \right| \sigma \frac{(V - E_k)^2}{1 - E_k^2} \left| \varphi_k^0 \right\rangle$$

$$= \left\langle \varphi_k^0 \right| \sigma \frac{I - 2EkV + E_k^2}{1 - E_k^2} \left| \varphi_k^0 \right\rangle$$

As $\left\langle \varphi_k^0 \right| V \left| \varphi_k^0 \right\rangle = E_k$,

$$= \left\langle \varphi_k^0 \right| \sigma \frac{I - E_k^2}{1 - E_k^2} \left| \varphi_k^0 \right\rangle$$

$$= \langle \beta | \otimes \langle \phi_0 | (\sigma |\beta\rangle \otimes |\phi_0\rangle)$$

$$= \langle \beta | \otimes \langle \phi_0 | (|\beta\rangle \otimes \sigma |\phi_0\rangle)$$

$$= \langle \beta | \beta \rangle \otimes \langle \phi_0 | \sigma | \phi_0 \rangle$$

For reasons that will become obvious later, we rewrite to the following

$$= \frac{1 - E_k^2}{1 - E_k^2} \langle \phi_0 | \sigma | \phi_0 \rangle$$

2. σ and V anticommute, meaning $\sigma, A = 0$. In equation 2.15, we're left with:

$$\begin{aligned}
&\left\langle\varphi_k^0\right| \sigma AA - [\sigma, A]A \\
&= \left\langle\varphi_k^0\right| \sigma AA - \frac{[\sigma, V]}{\sqrt{1-E_k^2}} A \left|\varphi_k^0\right\rangle \\
&= \left\langle\varphi_k^0\right| \sigma AA - \frac{2\sigma V}{\sqrt{1-E_k^2}} A \left|\varphi_k^0\right\rangle \\
&= \langle\phi_0| \sigma \frac{I - 2E_k V + E_k^2}{1-E_k^2} - \frac{2(V^2 - VE_k)}{1-E_k^2} |\phi_0\rangle \\
&= \langle\phi_0| \sigma \frac{I - 2E_k V + E_k^2 - 2I + 2E_K V}{1-E_k^2} |\phi_0\rangle \\
&= \langle\phi_0| \sigma \frac{-I + E_k^2}{1-E_k^2} |\phi_0\rangle \\
&= -\frac{1-E_k^2}{1-E_k^2} \langle\phi_0| \sigma |\phi_0\rangle
\end{aligned}$$

With these results,

$$\left\langle\varphi_k^\pm\right| \sigma \left|\varphi_k^\pm\right\rangle = \langle\phi_0| \sigma |\phi_0\rangle$$

or, if they anticommute

$$\left\langle\varphi_k^\pm\right| \sigma \left|\varphi_k^\pm\right\rangle = 0$$

So ultimately its still off. The end factor for anticommutation has to be $\frac{-1-E_k^2}{1-E_k^2}$, but I am rather sure that obtaining that with this setup is impossible. I tried assuming that the dagger of A is not the same as A, but a sign change in $A^\dagger$ can't give the right result. I also tried expanding V in the eigenstate of the Ham, but that doesn't lead anywhere either...