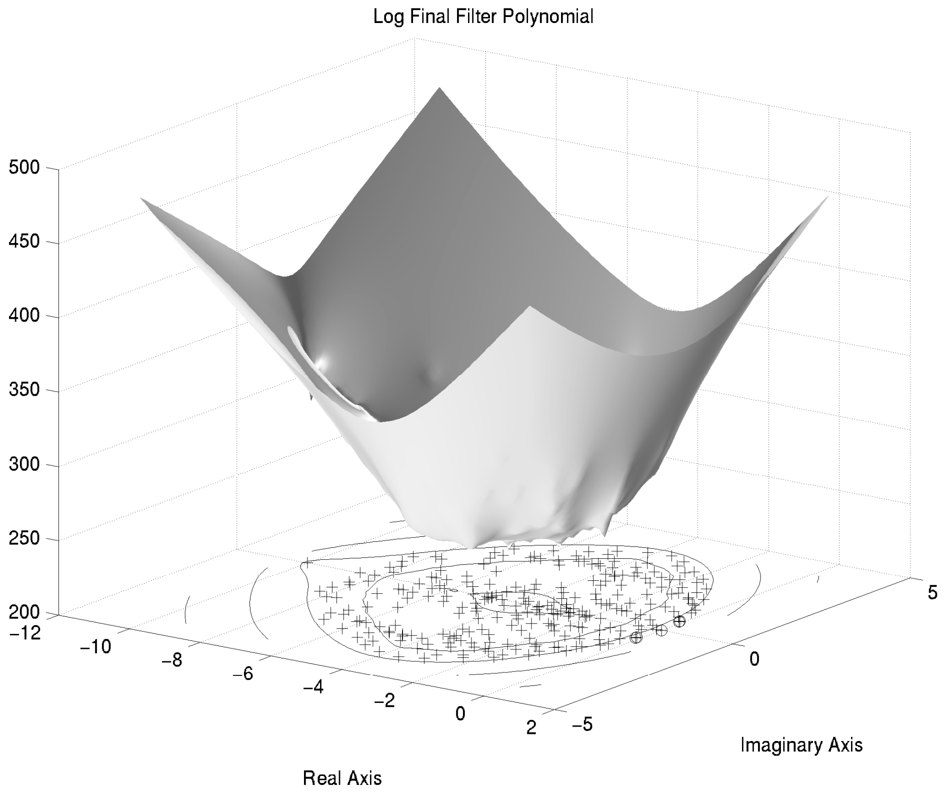

Figure 4.8: Total filter polynomial from an IRA iteration.

degree p polynomial. A sequence of Householder transformations may developed to form a unitary matrix $\mathbf{Q}$ such that $\mathbf{Q}\mathbf{e}_1 = \mathbf{q}_1$ and $\mathbf{H}_m \leftarrow \mathbf{Q}^H \mathbf{H}_m \mathbf{Q}$ is upper Hessenberg. The details which follow standard developments for the Implicitly Shifted QR iteration will be omitted here.

A shift selection strategy that has proved successful in practice and is used as the default in ARPACK is called the "Exact Shift Strategy". In this strategy, one computes $\sigma(\mathbf{H}_m)$ and sorts this into two disjoint sets Ω_w and Ω_u. The k Ritz values in the set Ω_w are regarded as approximations to the "wanted" eigenvalues of $\mathbf{A}$, and the p Ritz values in the set Ω_u are taken as the shifts μ_j. An interesting consequence (in exact arithmetic) is that after Step (a3.4) above, the spectrum of $\mathbf{H}_k$ in Step (a3.6) is $\sigma(\mathbf{H}_k) = \Omega_w$ and the updated starting vector $\mathbf{v}_1$ is a particular linear combination of the k Ritz vectors associated with these Ritz values. In other words, the implicit restarting scheme with exact shifts provides a specific selection of expansion coefficients γ_j for a new starting vector as a linear combination of the current best estimates (the Ritz vectors) for wanted eigenvectors. This implicit scheme costs p rather than the $k+p$ matrix-vector products the explicit scheme would require. Thus the exact shift strategy can be viewed both as a means to damp unwanted components from the starting vector and also as directly forcing the starting vector to be a linear combination of wanted eigenvectors. See [23, 44] for information on the convergence of IRAM and [3, 45] for other possible shift strategies for Hermitian $\mathbf{A}$. The reader is referred to [25, 33] for studies comparing implicit restarting with other schemes.

4.4.2 Block Methods

Implicit restarting can also be used in conjunction with a block Arnoldi method. A block method attempts to use the block Krylov subspace

$$\mathcal{K}_k(\mathbf{A}, \mathbf{U}_1) = \text{Span } \{\mathbf{U}_1, \mathbf{A}\mathbf{U}_1, \mathbf{A}^2\mathbf{U}_1, \ldots, \mathbf{A}^{k-1}\mathbf{U}_1\},$$

where $\mathbf{U}_1$ has b columns, to approximate eigenvalues and eigenvectors. A block Arnoldi reduction uses a subspace drawn from a sequence of subspace iterates. The details associated with implicitly restarting a block Arnoldi reduction are laid out in [4, 24].

Block methods are used for two major reasons. The first one is to aid in reliably determining multiple and/or clustered eigenvalues. Although [26] indicates that an unblocked Arnoldi method coupled with an appropriate deflation strategy may be used to compute multiple and/or clustered eigenvalues, a relatively small convergence tolerance is required to reliably compute clustered eigenvalues. Many problems do not require this much accuracy, and such a criterion can result in unnecessary computation. The second reason for using a block formulation is related to computational efficiency. Often, when a matrix-vector product with $\mathbf{A}$ is very costly, it is possible to compute the action of $\mathbf{A}$ on several vectors at once with roughly the same cost as computing a single matrix-vector product. This can happen, for example, when the