Optical absorption of the Fano model: General case of many resonances and many continua

S. Glutsch
Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und Theoretische Optik, Max-Wien-Platz 1, 07743 Jena, Germany
(Received 26 February 2002; published 5 August 2002)

In this Brief Report we give a brief derivation of the optical absorption of the Fano model in the general case of many resonances coupled to many continua. The calculation is straightforward and is entirely based upon simple matrix algebra. We also show the equivalence of our solution to previous results by Fano and Starace [Phys. Rev. **124**, 1866 (1961)] [Phys. Rev. B **5**, 1773 (1972)].

DOI: 10.1103/PhysRevB.66.075310 PACS number(s): 34.10.+x, 78.20.Bh

I. INTRODUCTION

Fano interference is known as the quantum-mechanical interaction between discrete and continuous states.[1] This universal phenomenon is observed in many different areas of physics. The original paper by Fano[1] gaves explicit results for the case of one resonance interacting with one continuum, one resonance interacting with many continua, and many resonances interacting with one continuum. Later on, Mies,[2] Starace,[3] and Connerade and Lane[4] extended Fano's result to include the case of many resonances interacting with many continua. The paper by Starace expressed the total scattering cross section as a sum of partial cross sections, where each term has the form of Fano's result for many resonances and one continuum.

In nuclear and atomic physics, Fano interference is often described in terms of interaction of open and closed channels. A theoretical framework was developed in a series of papers by Feshbach.[5] Bhatia and Temkin[6] unified the Fano and Feshbach approaches and gave a derivation of Fano's result using the projection-operator formalism. They also included the interaction between discrete resonances, leading to energy-dependent line-shape parameters.

The Fano model[1,3] is exactly solvable, but the calculation, which is based upon an eigenvalue problem, is intricate. Alternative derivations of Fano's result, which are found in the literature, either are no less complicated or do not go as far as the original paper. The use of specific methods of scattering theory, which are less known to the general reader, is contrary to the universality of the subject. In fact, there are cases of Fano interference which cannot be explained in the channel picture with asymptotically free motion. An example is the Coulomb interaction between excitons and continuum states of different minibands in superlattices. In this case, Fano resonances in the optical spectrum were predicted theoretically in 1997,[7] and observed experimentally this year.[8]

In solid-state physics, it is common to derive Fano's result using the method of Green's functions, either by solving a Dyson equation[9,10] or by directly calculating the inverse of a sparse matrix.[11,12] However, in these papers only the simplest case of one resonance interacting with one continuum is considered.

In the present paper we derive a compact formula for the absorption coefficient in the case of many resonances and many continua. The calculation is entirely based upon a simple matrix algebra, uses only a minimum of assumptions, does not invoke scattering theory, and does not require information about the asymptotics of the continuous eigenfunctions. Then we rederive the explicit expressions of Fano and Starace for one resonance interacting with one or more continua, for many resonances interacting with one continuum, and for many resonances interacting with many continua.

II. FANO MODEL

We consider the following model Hamiltonian and transition matrix elements

$$H=\begin{pmatrix} H_0 & V_1 & V_2 & V_3 & \cdots \\ V_1^T & E_1 & 0 & 0 & \cdots \\ V_2^T & 0 & E_2 & 0 & \cdots \\ V_3^T & 0 & 0 & E_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad |M\rangle=\begin{pmatrix} M_0 \\ M_1 \\ M_2 \\ M_3 \\ \vdots \end{pmatrix}. \tag{1}$$

The discrete states are represented by a real symmetric $m \times m$ matrix H_0, and the continuous transitions are modeled by the real energies E_j $(j>0)$. The continuum states are discretized for methodical reasons; later we will let the spacing of the E_j $(j>0)$ go to zero. The coupling between discrete states and continua is given by the real m-dimensional column vectors V_j $(j>0)$ and their transposes V_j^T. The other elements of H are zero, which means that no interaction between different continuum states is considered. Formally, this situation can be achieved by a unitary transformation of the continuum states. In the general case, this is possible only by numerical calculations. The optical transition amplitudes are given by the elements of $|M\rangle$, where M_0 is an m-dimensional real column vector and $M_1, M_2, \ldots$ are real numbers.

In dimensionless units, ignoring prefactors, the optical susceptibility is given by

$$\chi(\omega)=\sum_j \frac{|\langle M|\Phi_j\rangle|^2}{\mathcal{E}_j-(\omega+i\epsilon)}, \tag{2}$$

where $\mathcal{E}_j$ and $|\Phi_j\rangle$ are the eigenvalues and normalized eigenvectors of H, and $\epsilon=+0$ is a positive infinitesimal. [We shall use the term "optical susceptibility" throughout. The result is valid for any spectroscopic quantity, which can be represented in the form of Eq. (2).] The limit $\epsilon\to+0$ is carried out after the continuum limit. A representation of χ, equivalent to Eq. (2), is

$$\chi(\omega)=\langle M|R(\omega)|M\rangle,\quad R(\omega)=[H-(\omega+i\epsilon)]^{-1}. \tag{3}$$

Here $R(\omega)$ is called the resolvent operator, and its diagonal matrix element $\chi(\omega)$ is called a Green's function.[9] The absorption coefficient α is determined by the imaginary part of the optical susceptibility:

$$\alpha(\omega)=\operatorname{Im}\chi(\omega). \tag{4}$$

The elements of the matrix $R(\omega)$ can be found by using the block version of lemma 1 (see the Appendix), and it holds that

$$R_{00}(\omega)=\left[H_0-(\omega+i\epsilon)-\sum_j{}'\ \frac{V_jV_j^T}{E_j-(\omega+i\epsilon)}\right]^{-1},$$

$$R_{j0}(\omega)=-\frac{V_j^TR_{00}(\omega)}{E_j-(\omega+i\epsilon)},$$

$$R_{0k}(\omega)=-\frac{R_{00}(\omega)V_k}{E_k-(\omega+i\epsilon)},\quad j,k>0 \tag{5}$$

$$R_{jk}(\omega)=\frac{\delta_{jk}}{E_j-(\omega+i\epsilon)}+\frac{V_j^TR_{00}(\omega)V_k}{[E_j-(\omega+i\epsilon)][E_k-(\omega+i\epsilon)]},\quad j,k>0,$$

where the prime at the sum means that $j=0$ is excluded from the summation. The optical susceptibility [Eq. (3)], which follows from the elements of $R(\omega)$, is

$$\chi(\omega)=\left[M_0^T-\sum_j{}'\ \frac{M_jV_j^T}{E_j-(\omega+i\epsilon)}\right]R_{00}(\omega)\times\left[M_0-\sum_k{}'\ \frac{V_kM_k}{E_k-(\omega+i\epsilon)}\right]+\sum_j{}'\ \frac{M_j^2}{E_j-(\omega+i\epsilon)}. \tag{6}$$

Result (6) for one resonance was derived by several authors.[9–12]

Now we perform the transition to the continuous limit. Suppose the indices $j=1,\dots,s$ belong to the first continuum, the indices $j=s+1,\dots,2s$ to the second continuum, etc. Then we replace the quantities V_j and M_j by

$$V_j=\frac{\nu^{(\beta)}(E_j)}{\sqrt{D(E_j)}},\quad M_j=\frac{\mu^{(\beta)}(E_j)}{\sqrt{D(E_j)}},$$
$$(\beta-1)s<j\leqslant\beta s,\quad \beta=1,\dots,n, \tag{7}$$

where $D(E_j)$ is the energetic density of states, i.e., the inverse spacing of subsequent energies, and the m-dimensional real vectors $\nu^{(\beta)}$ and $\mu^{(\beta)}$ are continuous functions of E. In the limit $D(E_j)\to\infty$, $s\to\infty$, the sums over j go over into integrals according to

$$\sum_j{}'\ \frac{f[\sqrt{D(E_j)}V_j,\sqrt{D(E_j)}M_j]}{D(E_j)}=\sum_{\beta=1}^{n}\int dE\, f[\nu^{(\beta)}(E),\mu^{(\beta)}(E)]. \tag{8}$$

In the evaluation of expression (6) we encounter the following integrals

$$\sum_{\beta=1}^{n}\int dE\frac{\nu^{(\beta)}(E)\nu^{(\beta)T}(E)}{E-(\omega+i\epsilon)}=F+\frac{1}{2}i\Gamma,$$

$$\sum_{\beta=1}^{n}\int dE\frac{\nu^{(\beta)}(E)\mu^{(\beta)}(E)}{E-(\omega+i\epsilon)}=G+\frac{1}{2}i\Delta, \tag{9}$$

$$\sum_{\beta=1}^{n}\int dE\frac{\mu^{(\beta)2}(E)}{E-(\omega+i\epsilon)}=K+\frac{1}{2}i\Lambda.$$

The quantities F and Γ are real symmetric $m\times m$ matrices, G and Δ are real m-dimensional column vectors, and K and Λ are real numbers. We shall neglect their weak frequency dependence near the resonance and treat them as constants. By virtue of Dirac's identity

$$\frac{1}{E-(\omega+i\epsilon)}=\frac{P}{E-\omega}+i\pi\delta(E-\omega), \tag{10}$$

F, G, and K are given by principal-value integrals and for Γ, Δ, and Λ we have

$$\Gamma=\sum_{\beta=1}^{n}\Gamma^{(\beta)},\quad \Delta=\sum_{\beta=1}^{n}\Delta^{(\beta)},\quad \Lambda=\sum_{\beta=1}^{n}\Lambda^{(\beta)},$$
$$\Gamma^{(\beta)}=2\pi\nu^{(\beta)}\nu^{(\beta)T},\quad \Delta^{(\beta)}=2\pi\nu^{(\beta)}\mu^{(\beta)},$$
$$\Lambda^{(\beta)}=2\pi\mu^{(\beta)2}. \tag{11}$$

With the above definitions, the optical susceptibility [Eq. (6)] becomes

$$\chi(\omega)=\left(M_0-G-\frac{1}{2}i\Delta\right)^T\left[H_0-F-(\omega+i\epsilon)-\frac{1}{2}i\Gamma\right]^{-1}\times\left(M_0-G-\frac{1}{2}i\Delta\right)+K+\frac{1}{2}i\Lambda. \tag{12}$$

In the limit $\omega\to\pm\infty$ the absorption approaches the absorption of the continuum states

$$\alpha(\infty)=\operatorname{Im}\chi(\infty)=\frac{1}{2}\Lambda. \tag{13}$$

With formula (12) we have a compact formulation for the optical susceptibility for the general case of many resonances interacting with many continua. The dimension of the vector space is equal to the number of discrete resonances, independent of the number of continua. Although formulation (12) can easily be used for a numerical calculation of the spectrum, it does not allow one to draw qualitative conclusions about the behavior of the absorption profile. In the following we shall demonstrate how Eq. (12) simplifies in the cases of a single resonance interacting with one or more continua, and of many resonances interacting with one continuum. We also show the equivalence to Starace's result for many resonances and many continua.

III. SINGLE RESONANCE

In the case of a single resonance, the discrete subspace Hamiltonian H_0 is a scalar E_0, and all quantities in Eq. (12) are scalars. In the trivial case $\vec{\nu}=(\nu^{(1)},\ldots,\nu^{(n)})^T=0$, the absorption spectrum consists of a discrete line and, if $\Lambda\neq 0$, a constant background. If $\Gamma\neq 0$ and $\Delta=0$, which means that $\vec{\mu}$ is perpendicular to $\vec{\nu}$, the absorption profile is a Lorentzian with a broadening $\frac{1}{2}\Gamma$. In this case, a constant background, i.e., $\Lambda\neq 0$, is possible only for $n>1$.

Now we consider the case that $\Delta\neq 0$. From the Cauchy-Schwarz inequality

$$\Delta^2\leqslant\Gamma\Lambda, \tag{14}$$

it follows that $\Gamma\neq 0$ and $\Lambda\neq 0$. Introducing the parameters

$$\varepsilon=\frac{\omega-E_0-F}{\frac{1}{2}\Gamma},\quad q=\frac{M_0-G}{\frac{1}{2}\Delta}, \tag{15}$$

the absorption coefficient, normalized to $\alpha(\infty)$, becomes

$$\frac{\alpha(\omega)}{\alpha(\infty)}=\frac{\Delta^2}{\Gamma\Lambda}\frac{(q+\varepsilon)^2}{1+\varepsilon^2}+1-\frac{\Delta^2}{\Gamma\Lambda}. \tag{16}$$

This function is positive and has no zeros for $\Delta^2<\Gamma\Lambda$.

If $\vec{\mu}$ and $\vec{\nu}$ are parallel, then it holds that $\Delta^2=\Gamma\Lambda$. In this case, Eq. (16) simplifies to

$$\frac{\alpha(\omega)}{\alpha(\infty)}=\frac{(q+\varepsilon)^2}{1+\varepsilon^2}. \tag{17}$$

This is the famous result by Fano [Eq. (21) in Ref. 1]. The function (17) is semipositive and has one zero at $\varepsilon=-q$. For interaction with one continuum $(n=1)$, the absorption always drops to zero for one frequency, while for many continua $(n>1)$ this happens only by accident.

IV. MANY RESONANCES AND ONE CONTINUUM

Next we study expression (12) for many resonances and one continuum. To simplify the notation, we replace M_0-G by M_0 and H_0-F by H_0. Furthermore, we ignore the real constant K, which does not contribute to the absorption coefficient. First we consider $\Lambda\neq 0$. Later, we take the limit $\Lambda\to 0$ in the final expression.

Taking into account that $\Gamma=\Delta\Delta^T/\Lambda$, the optical susceptibility, normalized to $\alpha(\infty)$, is

$$\frac{\chi(\omega)}{\alpha(\infty)}=\left(M_0-\frac{1}{2}i\Delta\right)^T\left\{\frac{1}{2}\Lambda[H_0-(\omega+i\epsilon)]-\frac{1}{4}i\Delta\Delta^T\right\}^{-1}\left(M_0-\frac{1}{2}i\Delta\right)+i. \tag{18}$$

The real symmetric matrix H_0 can be diagonalized so that $\tilde{H}_0=\mathrm{diag}(\tilde{E}_{0,1},\ldots,\tilde{E}_{0,m})$. We assume the irreducible case, where $\tilde{E}_{0,1}<\tilde{E}_{0,2}<\cdots<\tilde{E}_{0,m}$ and the transformed vector $\tilde{\Delta}=(\tilde{\Delta}_1,\ldots,\tilde{\Delta}_m)^T$ has all nonzero components. Otherwise, some discrete states are not coupled to the continuum, and the dimension of the problem can be reduced.

To perform the limit $\epsilon\to 0$, we have to investigate the analyticity of the function $\chi(z)$ for complex z near the real axis. From lemma 2 (see the Appendix) it follows that, in the eigensystem of H_0,

$$\det\left[\frac{1}{2}\Lambda(H_0-z)-\frac{1}{4}i\Delta\Delta^T\right]=\left(\frac{\Lambda}{2}\right)^m\prod_{j=1}^{m}(\tilde{E}_{0,j}-z)\left[1-\frac{1}{2}i\sum_{k=1}^{m}\frac{\tilde{\Delta}_k^2/\Lambda}{\tilde{E}_{0,k}-z}\right]. \tag{19}$$

This function is analytic and, as all $\tilde{\Delta}_k$ are assumed nonzero, has no zeros on the real axis. Hence $\chi(z)$ is analytic on a stripe around the real axis, and in Eq. (18) we may replace $\omega+i\epsilon$ with ω.

Then, in order to calculate the imaginary part of expression (18), we apply lemma 3 (see the Appendix) and obtain

$$\frac{\alpha(\omega)}{\alpha(\infty)}=\left|\frac{\det(H_0-\omega-M_0\Delta^T/\Lambda)}{\det(H_0-\omega-\frac{1}{2}i\Delta\Delta^T/\Lambda)}\right|^2. \tag{20}$$

The above expression is a non-trivial generalization of the formula for one resonance and one continuum [Eq. (17)].

We have already seen that the denominator of Eq. (20) has no zeros. For the numerator, by virtue of lemma 2, we find

$$\det\left(H_0-\omega-\frac{M_0\Delta^T}{\Lambda}\right)=\prod_{j=1}^{m}(\tilde{E}_{0,j}-\omega)\left[1-\sum_{k=1}^{m}\frac{\tilde{M}_{0,k}\tilde{\Delta}_k/\Lambda}{\tilde{E}_{0,k}-\omega}\right]. \tag{21}$$

A sufficient condition for m zeros is that either $\tilde{M}_{0,k}\tilde{\Delta}_k>0$ for all k or $\tilde{M}_{0,k}\tilde{\Delta}_k<0$ for all k, in other words, that the individual q-parameters are nonzero and have the same sign.

Inserting the expressions for determinants (19) and (21) into Eq. (20), we obtain

$$\frac{\alpha(\omega)}{\alpha(\infty)}=\frac{\left[1-\sum_{k=1}^{m}\frac{\tilde{M}_{0,k}\tilde{\Delta}_k/\Lambda}{\tilde{E}_{0,k}-\omega}\right]^2}{1+\frac{1}{4}\left[\sum_{k=1}^{m}\frac{\tilde{\Delta}_k^2/\Lambda}{\tilde{E}_{0,k}-\omega}\right]^2}=\cos^2\varphi\left[1-\sum_{k=1}^{m}q_k\tan\varphi_k\right]^2, \tag{22}$$

where

$$\tan\varphi_k = \frac{1}{2}\,\frac{\tilde{\Delta}_k^2/\Lambda}{\tilde{E}_{0,k}-\omega} = \frac{\pi\tilde{\nu}_k^2}{\tilde{E}_{0,k}-\omega}, \qquad \tan\varphi = \sum_{k=0}^{m}\tan\varphi_k,$$

$$q_k = \frac{2\tilde{M}_{0,k}}{\tilde{\Delta}_k} = \frac{\tilde{M}_{0,k}}{\pi\mu\tilde{\nu}_k}. \tag{23}$$

The latter expression is identical to the results by Fano,[1] Mies,[2] and Connerade and Lane.[4]

Now we consider the case that the transition probability of the continuum is zero, which means that $\mu=0$, $\Lambda=0$, and $\Delta=0$. Here, the irreducible case is characterized by $\tilde{\nu}_k\neq 0$ for all k. Furthermore, we assume $M_0\neq 0$, otherwise the absorption coefficient vanishes identically. From Eq. (22), in the limit $\Lambda\to 0$, we obtain

$$\alpha(\omega) = \frac{\left[\displaystyle\sum_{k=1}^{m}\frac{\tilde{M}_{0,k}\sqrt{\pi}\tilde{\nu}_k}{\tilde{E}_{0,k}-\omega}\right]^2}{1+\left[\displaystyle\sum_{k=1}^{m}\frac{\pi\tilde{\nu}_k^2}{\tilde{E}_{0,k}-\omega}\right]^2}. \tag{24}$$

The function $\alpha(\omega)$ approaches zero for $\omega\to\pm\infty$. If all $\tilde{M}_{0,k}\tilde{\nu}_k$ are nonzero and have the same sign, then the absorption coefficient has $m-1$ zeros at finite values of ω. Writing the latter expression in general coordinates and using lemma 2, we find that

$$\alpha(\omega) = \left|\frac{\det(H_0-\omega)-\det(H_0-\omega-M_0^T\sqrt{\pi}\nu^T)}{\det(H_0-\omega-i\sqrt{\pi}\nu\sqrt{\pi}\nu^T)}\right|^2. \tag{25}$$

As Eq. (20), the last expression is free of terms of the form ∞/∞.

V. MANY RESONANCES AND MANY CONTINUA

For many resonances and many continua, the optical absorption can be written as a sum over all continua. From the definitions (11), expression (12), and the proof of lemma 3 it follows that

$$\alpha(\omega) = \mathrm{Im}\,\chi(\omega) = \frac{1}{2}\sum_{\beta=1}^{n}\Lambda^{(\beta)}\left|1-\left(M_0-\frac{1}{2}i\Delta\right)^T \times\left(H_0-\omega-\frac{1}{2}i\Gamma\right)^{-1}\frac{\Delta^{(\beta)}}{\Lambda^{(\beta)}}\right|^2. \tag{26}$$

Again, for notational convenience, we dropped G, F, and K.

As each term under the sum depends on all continua via Δ and Γ, it cannot be brought into form (22). To overcome this problem, we introduce the orthogonal transformation

$$\overline{\nu^{(\beta)}} = \sum_{\beta=1}^{n}U^{\beta'\beta}\nu^{(\beta')}, \qquad \overline{\mu^{(\beta)}} = \sum_{\beta=1}^{n}U^{\beta'\beta}\mu^{(\beta')}. \tag{27}$$

Then we define $\overline{\Gamma^{(\beta)}}$, $\overline{\Delta^{(\beta)}}$, and $\overline{\Lambda^{(\beta)}}$ in analogy to Eq. (11). Because $\overline{\Gamma}=\Gamma$, $\overline{\Delta}=\Delta$ and $\overline{\Lambda}=\Lambda$, the optical susceptibility is invariant under transformation (27), which means that in Eq. (26) we can replace $\Delta^{(\beta)}$ by $\overline{\Delta^{(\beta)}}$ and $\Lambda^{(\beta)}$ by $\overline{\Lambda^{(\beta)}}$.

We now determine the $n\times n$ orthogonal matrix $U(\omega)$ such that

$$\overline{\nu^{(\beta)T}}(\omega)(H_0-\omega)^{-1}\overline{\nu^{(\beta')}}(\omega) = \overline{z^{(\beta)}}(\omega)\,\delta^{\beta\beta'}. \tag{28}$$

While some of the $\overline{z^{(\beta)}}(\omega)$'s have single poles when ω crosses an eigenvalue of H_0, the quantities $\overline{\Gamma^{(\beta)}}$, $\overline{\Delta^{(\beta)}}$, and $\overline{\Lambda^{(\beta)}}$ can be chosen to be continuous functions of ω.

From the series expansion

$$\left(H_0-\omega-\frac{1}{2}i\Gamma\right)^{-1} = (H_0-\omega)^{-1}+(H_0-\omega)^{-1}\frac{1}{2}i\Gamma(H_0-\omega)^{-1}+\cdots \tag{29}$$

and the relation $\overline{\Gamma^{(\beta)}}=\overline{\Delta^{(\beta)}}\,\overline{\Delta^{(\beta)T}}/\overline{\Lambda^{(\beta)}}$, it follows that

$$\overline{\Delta^{(\beta)T}}\left(H_0-\omega-\frac{1}{2}i\Gamma\right)^{-1}\overline{\Delta^{(\beta')}} = \delta^{\beta\beta'}\,\overline{\Delta^{(\beta)}}\left(H_0-\omega-\frac{1}{2}i\overline{\Gamma^{(\beta)}}\right)^{-1}\overline{\Delta^{\beta}}. \tag{30}$$

Going over to the transformed quantities and using relation (30), Eq. (26) goes over into

$$\begin{aligned}\alpha(\omega) &= \frac{1}{2}\sum_{\beta=1}^{n}\overline{\Lambda^{(\beta)}}\left|1-\left(M_0-\frac{1}{2}i\overline{\Delta^{(\beta)}}\right)^T \times\left(H_0-\omega-\frac{1}{2}i\Gamma^{(\beta)}\right)^{-1}\frac{\overline{\Delta^{(\beta)}}}{\overline{\Lambda^{(\beta)}}}\right|^2\\ &= \frac{1}{2}\sum_{\beta=1}^{n}\overline{\Lambda^{(\beta)}}\left|\frac{\det(H_0-\omega-M_0\overline{\Delta^{(\beta)T}}/\overline{\Lambda^{(\beta)}})}{\det\left(H_0-\omega-\frac{1}{2}i\overline{\Delta^{(\beta)}}\,\overline{\Delta^{(\beta)T}}/\overline{\Lambda^{(\beta)}}\right)}\right|^2.\end{aligned} \tag{31}$$

In this expression each of the terms under the sum is of the form of Eq. (22). The latter equation is identical to the formula of Starace, which expressed the total cross section into a sum of partial cross sections.[3]

VI. SUMMARY

In summary, we have given a straightforward derivation for the optical absorption of the Fano model, for the general case of m discrete resonances interacting with n continua. The equivalence to previous results by Fano and Starace is demonstrated.

ACKNOWLEDGMENT

The author is indebted to J.-M. Wagner for useful comments on the paper.

APPENDIX

Lemma 1: Let A be an $n\times n$ matrix with the following structure:

$$A=\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & \cdots & a_{1n}\\ a_{21} & a_{22} & 0 & 0 & \cdots & 0\\ a_{31} & 0 & a_{33} & 0 & \cdots & 0\\ a_{41} & 0 & 0 & a_{44} & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots\\ a_{n1} & 0 & 0 & 0 & \cdots & a_{nn}\end{pmatrix}. \tag{A1}$$

If A is regular, then the elements of the inverse matrix $B=A^{-1}$ are given by

$$b_{11}=\left[a_{11}-\sum_{j=2}^{n}\frac{a_{1j}a_{j1}}{a_{jj}}\right]^{-1},$$

$$b_{1k}=-\frac{b_{11}a_{1k}}{a_{kk}},\quad b_{j1}=-\frac{a_{j1}b_{11}}{a_{jj}}, \tag{A2}$$

$$b_{jk}=\frac{\delta_{jk}}{a_{jj}}+\frac{a_{j1}b_{11}a_{1k}}{a_{jj}a_{kk}},\quad j,k=2,\dots,n.$$

Proof: The inversion of the matrix can be done explicitly by means of the exchange method[13] with pivot elements a_{nn}, $a_{n-1,n-1}$, ... , a_{11}, or by partitioning of A.[14] Alternatively, one can directly verify that $AB=BA=1$.

A block version of lemma 1 is obtained when a_{11} is replaced by an $m\times m$ matrix, the a_{1k} for $k>1$ by m-dimensional row vectors, and the a_{j1} for $j>1$ by m-dimensional column vectors. Then the formula for the inverse matrix remains valid if the elements b_{11}, b_{1k}, and b_{j1} $(j,k>1)$ are interpreted as matrices and vectors.

Lemma 2: For any complex regular $n\times n$ matrix B and complex n-dimensional column vectors u and v it holds that

$$\det(B-uv^T)=(1-u^TB^{-1}v)\det B. \tag{A3}$$

Proof: The left-hand side of the above equation takes the form

$$\begin{aligned}\det(B-uv^T)&=\det(b_1-uv_1,\dots,b_n-uv_n)\\ &=\det(b_1,\dots,b_n)\\ &\quad-\sum_{k=1}^{n}\det(b_1,\dots,b_{k-1},uv_k,b_{k+1},\dots,b_n).\end{aligned} \tag{A4}$$

Here $b_1,\dots,b_n$ are the columns of the matrix B. All other 2^n-n-1 contributions vanish, for example, $\det(uv_1,uv_2,b_3,\dots,b_n)=0$. Expanding each term under the sum into cofactors, we obtain

$$\begin{aligned}&\sum_{k=1}^{n}\det(b_1,\dots,b_{k-1},uv_k,b_{k+1},\dots,b_n)\\ &\quad=\sum_{j=1}^{n}\sum_{k=1}^{n}u_j\overline{B}_{jk}v_k,\end{aligned} \tag{A5}$$

where $\overline{B}_{jk}$ are the minor determinants of B, including the factor $(-1)^{j-k}$. As B is regular, $\overline{B}$ is given by $\overline{B}=B^{-1}\det B$, which proves the proposition.

Lemma 3: Let A be a real symmetric $n\times n$ matrix and x and y real column vectors. Furthermore, we suppose that $A-iyy^T$ is regular. Then it holds that

$$\mathrm{Im}[(x-iy)^T(A-iyy^T)(x-iy)]+1=\left|\frac{\det(A-xy^T)}{\det(A-iyy^T)}\right|^2. \tag{A6}$$

Proof: From lemma 2 it follows that

$$\begin{aligned}\frac{\det(A-xy^T)}{\det(A-iyy^T)}&=\frac{\det[A-iyy^T-(x-iy)y^T]}{\det(A-iyy^T)}\\ &=1-(x-iy)^T(A-iyy^T)^{-1}y.\end{aligned} \tag{A7}$$

Multiplication with its complex conjugate gives

$$\begin{aligned}&\left|\frac{\det(A-xy^T)}{\det(A-iyy^T)}\right|^2\\ &\quad=[1-(x-iy)^T(A-iyy^T)^{-1}y]\\ &\qquad\times[1-y^T(A+iyy^T)^{-1}(x+iy)]\\ &\quad=1+(x-iy)^T(A-iyy^T)^{-1}yy^T\\ &\qquad\times(A+iyy^T)^{-1}(x+iy)-(x-iy)^T(A-iyy^T)^{-1}\\ &\qquad\times y-y^T(A+iyy^T)^{-1}(x+iy)\\ &\quad=1+\mathrm{Im}[(x-iy)^T(A-iyy^T)^{-1}(A+iyy^T)\\ &\qquad\times(A+iyy^T)^{-1}(x+iy)]-\mathrm{Im}[(x-iy)^T\\ &\qquad\times(A-iyy^T)^{-1}2iy]\\ &\quad=1+\mathrm{Im}[(x-iy)^T(A-iyy^T)^{-1}(x-iy)].\end{aligned} \tag{A8}$$

[1] U. Fano, Phys. Rev. **124**, 1866 (1961).
[2] F. H. Mies, Phys. Rev. **175**, 164 (1968).
[3] A. F. Starace, Phys. Rev. B **5**, 1773 (1972).
[4] J.-P. Connerade and A. M. Lane, Rep. Prog. Phys. **51**, 1439 (1988).
[5] H. Feshbach, Ann. Phys. (N.Y.) **5**, 357 (1958); **19**, 287 (1962); **43**, 410 (1967).
[6] A. K. Bhatia and A. Temkin, Phys. Rev. A **29**, 1895 (1984).
[7] S. Glutsch, P. Lefebvre, and D. S. Chemla, Phys. Rev. B **55**, 15786 (1997).

[8] D. Meinhold, K. Leo, N. A. Fromer, D. S. Chemla, S. Glutsch, F. Bechstedt, and K. Köhler, Phys. Rev. B **65**, 161307 (2002).
[9] A. Shibatani and Y. Toyozawa, J. Phys. Soc. Jpn. **25**, 335 (1968).
[10] K. Cho, Phys. Status Solidi B **54**, 583 (1972).
[11] M. Wagner and J. Vàsquez-Màrquez, J. Phys. A **21**, 4347 (1988).
[12] S. Glutsch, in *Festkörperprobleme/Advances in Solid State Physics* edited by R. Helbig (Vieweg, Braunschweig, 1998), Vol. 37, p. 151.
[13] H. Rutishauser, in *Lectures on Numerical Mathematics*, edited by M. Gutknecht (Birkhäuser, Boston, 1990).
[14] G. Hadley, *Linear Algebra* (Addison-Wesley, Reading, MA, 1980).