

Group theory used to improve the efficiency of transfer-matrix computations

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Transfer-matrix methodology is frequently used to deal with elastic scattering problems that require a solution of Schrödinger or homogeneous Maxwell equations in the continuous part of their spectra. As predicted by group theory, the basic states used for the expansion of the solutions can be separated into independent sets, thus enabling the scattering problem to be solved with a drastically improved efficiency. Depending on the peculiar symmetry in the problem, the basic states can present pairs of “conjugate sets,” whose associated characters are complex conjugate of each other. When the potential energy takes strict real values, the transfer matrices corresponding to these conjugate sets have well-defined relationships that enable the transfer matrices of both conjugate sets to be computed from a single propagation step. This results in a further reduction of up to 50% of the total computation time. This paper presents the way group theory can be used systematically to improve the efficiency of transfer-matrix computations. In a first part, the basic states are separated into independent sets. Relationships between the transfer matrices corresponding to conjugate sets are then derived. The theory is finally illustrated by a simulation of electronic scattering by a C_{60} molecule in a projection configuration. [S1063-651X(99)06912-3]

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I. INTRODUCTION

Linear systems of differential equations are frequently encountered in theoretical physics. Such equations indeed appear when dealing with the Schrödinger equation in quantum mechanics or with the Maxwell equations in electromagnetism. A useful property that appears in these situations is the additivity of solutions. When an analytic solution is not obtainable, several numerical techniques exist to deal with these equations in the energy or frequency continuum.

The Green's-function formalism is one of these techniques. In addition to many other applications, this real-space approach provided excellent simulations of the scanning tunneling microscope (STM) [1], calculations of field intensity maps around fullerene molecules trapped in a STM junction [2] and more recently simulations of the Fresnel projection microscope [3]. Although the application of this formalism is not sensitive to the orientation and relative position of the constitutive parts of the physical system, excessive storage requirements are encountered when they cannot be kept localized in space.

The transfer-matrix methodology [4–9] comes as a useful alternative to the Green's-function formalism, since the storage space requirements are significantly reduced. To apply this methodology, the physical system considered should be located between two separate boundaries. Given basic states used for the wave function expansion, the transfer matrices contain, for each state incident on one boundary of the system, the amplitudes of the corresponding transmitted and reflected states. The method basically depends on the additivity property of solutions, and requires (in its basic formulation) the numerical propagation of basic states from one boundary to the other. Since the main part of the computation time is

spent in this propagation step, any way to reduce the number of basic states to treat simultaneously or bypass the propagation step should be considered.

By applying group theory, any symmetry assumed in the problem can be exploited to split the basic states used for the expansion of the solutions into independent sets. This separation enables the scattering problem to be solved by considering these sets separately, thus drastically reducing both the required storage space and computation time (also see Ref. [10] for taking advantage of C_n symmetry within the Green's-function formalism). Depending on the peculiar symmetry in the problem, the basic states can present pairs of so-called “conjugate sets,” whose associated characters are complex conjugates of each other. When the potential energy is real valued, the complex conjugate of the solutions computed with a given set of basic states provides new solutions in its conjugate set. The transfer matrices corresponding to this conjugate set can be derived from these new solutions, thus enabling one to bypass the construction of intermediate solutions by a time-consuming numerical propagation. Since a single propagation step is required to derive the transfer matrices of two sets of basic states, considering these conjugate sets results in a reduction of up to 50% of the total computation time.

The objective of this paper is to show how group theory can be used systematically to improve the efficiency of a transfer-matrix computation, by enabling a reduction of the basic states to consider them simultaneously, and taking advantage of conjugate sets. The subdivision of the basic states into independent sets by application of group theory is presented in Sec. II. The technique, enabling the computation of the corresponding transfer matrices by a numerical propagation step or by consideration of conjugate sets, is presented in Sec. III. In Sec. IV, the theory is illustrated by a simulation of electronic diffraction by a C_{60} molecule in a projection configuration.

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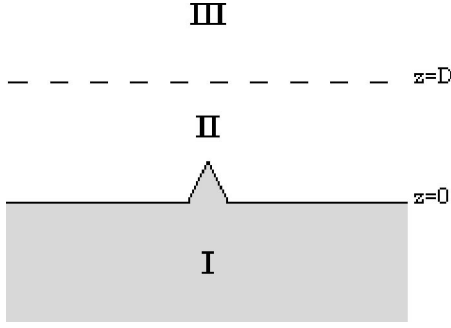


FIG. 1. Configuration of the three regions involved with scattering. These regions are referred to as region I ($z \leq 0$), region II ($0 \leq z \leq D$), and region III ($z \geq D$). Region II is the only diffusive part of the system.

II. CONSTRUCTION OF INDEPENDENT SETS OF BASIC STATES

Let us consider scattering in a physical system made of three adjacent regions, and let us assume the intermediate region to be the only diffusive part. The scanning tunneling microscope [6,11] and the Fresnel projection microscope [12] provide examples of such situations. Let us refer to the intermediate region as ‘‘region II,’’ and the two other regions as ‘‘region I’’ and ‘‘region III.’’ Let z be a coordinate axis oriented from region I to region III, so that region II corresponds to the interval $0 \leq z \leq D$. This situation is depicted in Fig. 1.

At this point, we should make the choice of simple basic states to expand the wave function in all regions. Let us write these basic states $\{\Psi_j\}$. In the context of a transfer-matrix computation, they usually take the form

$$\Psi_j(\mathbf{r}) = \langle \mathbf{r} | \Psi_j \rangle = \Phi_j(z) \psi_j(\rho), \quad (1)$$

where $\mathbf{r} = (\rho, z)$.

Any symmetry in the physical problem can be used to separate these states $\{\Psi_j\}$ into independent sets $\{\Psi_{j[k]}\}$, where k stands for the set of basic states associated with a given representation of the symmetry. These independent sets are obtained by projection of the basic states $\{\Psi_j\}$ on the various inequivalent irreducible representations of the symmetry. If g is the order of the symmetry group, \hat{R} the symmetry operator, and $\chi_k(\hat{R})$ the character associated with the operator \hat{R} in the k th inequivalent irreducible representation, the projection is achieved according to

$$\begin{aligned} \Psi_{j[k]} &= [P^k] \Psi_j \\ &= \frac{1}{g} \sum_{\hat{R}} [\chi_k^*(\hat{R}) \hat{R}] \Psi_j. \end{aligned} \quad (2)$$

Due to the orthogonality of the lines in the character table, these projections represent the symmetry in the following sense:

$$\langle \mathbf{r} | \hat{R} | \Psi_{j[k]} \rangle = \chi_k(\hat{R}) \langle \mathbf{r} | \Psi_{j[k]} \rangle, \quad (3)$$

TABLE I. Character table corresponding to a C_n symmetry. The notations k and ω_k stand for the number of the n inequivalent irreducible representations and $\omega_k = e^{ik(2\pi/n)}$, respectively.

k	E	C_n	C_n^2	\dots	C_n^{n-1}
0	1	1	1	\dots	1
1	1	ω_1	ω_1^2	\dots	ω_1^{n-1}
\vdots					
$n-1$	1	ω_{n-1}^1	ω_{n-1}^2	\dots	ω_{n-1}^{n-1}

and the initial set of basic states $\{\Psi_j\}$ is split into independent sets that are representative of the symmetry.

Table I gives the character table relevant to a C_n symmetry (z being an n -fold axis). When the physical system is characterized by this symmetry, the projection is achieved according to

$$\Psi_{j[k]} = \frac{1}{n} \sum_i [\omega_k^{-i} \hat{C}_n^i] \Psi_j, \quad (4)$$

with $\omega_k = e^{ik(2\pi/n)}$ and $\hat{C}_n^0 \equiv \hat{E}$.

A set of basic states is ‘‘conjugate’’ to a given set $\{\Psi_{j[k]}\}$ if the characters associated with these two sets are complex conjugates of each other. In the case of C_n symmetry, this situation is encountered with the sets numbered by k and $n-k$. Since $\omega_{n-k} = \omega_{-k}$, we refer conventionally to the two conjugate sets by $\{\Psi_{j[k]}\}$ and $\{\Psi_{j[-k]}\}$. Except for the set characterized by $k=0$ (for which the notation A is relevant) and the set characterized by $k=n/2$ (for which the notation B is relevant when n is even), each set is conjugate to another set and all pairs of conjugate sets are gathered in the character table under the notation E .

III. COMPUTATION OF THE TRANSFER MATRICES

A. Objective

Let us now distinguish the basic states by writing them $\Psi_{j[k]}^{I,\pm}$ or $\Psi_{j[k]}^{III,\pm}$ according to whether they describe the wave function in region I or III. The sign \pm stands for the direction of propagation relative to the z axis. In the context of a scattering problem, we are interested in computing the transmitted and reflected parts of the wave functions corresponding to a single incoming basic state $\Psi_{j[k]}^{I,+}$ in region I or $\Psi_{j[k]}^{III,-}$ in region III. Since the basic states are separated according to the symmetry of the Hamiltonian, the expansion of these solutions will imply a single set k of basic states. The coefficients of this expansion corresponding to the transmitted and reflected parts of the solutions are stored, respectively, in the two transfer matrices $\mathbf{t}_{[k]}^{++}$ and $\mathbf{t}_{[k]}^{-+}$ when the incident state $\Psi_{j[k]}^{I,+}$ belongs to region I and the two transfer matrices $\mathbf{t}_{[k]}^{--}$ and $\mathbf{t}_{[k]}^{+-}$ when the incident state $\Psi_{j[k]}^{III,-}$ belongs to region III.

The solutions we aim to construct can be written in the following forms:

$$(\dots, \Psi_{j[k]}^+, \dots) = \begin{cases} (\dots, \Psi_{j[k]}^{I,+}, \dots) + (\dots, \Psi_{i[k]}^{I,-}, \dots) \mathbf{t}_{[k]}^{-+} & \text{for } z \leq 0 \\ (\dots, \Psi_{i[k]}^{III,+}, \dots) \mathbf{t}_{[k]}^{++} & \text{for } z > D, \end{cases} \quad (5)$$

$$(\dots, \Psi_{j[k]}^-, \dots) = \begin{cases} (\dots, \Psi_{i[k]}^{I,-}, \dots) \mathbf{t}_{[k]}^{- -} & \text{for } z \leq 0 \\ (\dots, \Psi_{j[k]}^{III,-}, \dots) + (\dots, \Psi_{i[k]}^{III,+}, \dots) \mathbf{t}_{[k]}^{+-} & \text{for } z \geq D. \end{cases} \quad (6)$$

B. Construction from solutions provided by numerical propagation

The usual way to derive the solutions given in Eqs. (5) and (6) consists of constructing intermediate solutions and operating an appropriate combination. The intermediate so-

lutions are obtained by considering a single outgoing state ($\Psi_{j[k]}^{III,+}$ in region III or $\Psi_{j[k]}^{I,-}$ in region I), propagating it to the opposite side of region II, and expanding the solution along incident and reflected basic states. The following set of solutions is then obtained:

$$(\dots, \bar{\Psi}_{j[k]}^+, \dots) = \begin{cases} (\dots, \Psi_{i[k]}^{I,+}, \dots) \mathbf{A}_{[k]}^+ + (\dots, \Psi_{i[k]}^{I,-}, \dots) \mathbf{B}_{[k]}^+ & \text{for } z \leq 0 \\ (\dots, \Psi_{j[k]}^{III,+}, \dots) & \text{for } z \geq D, \end{cases} \quad (7)$$

$$(\dots, \bar{\Psi}_{j[k]}^-, \dots) = \begin{cases} (\dots, \Psi_{j[k]}^{I,-}, \dots) & \text{for } z \leq 0 \\ (\dots, \Psi_{i[k]}^{III,-}, \dots) \mathbf{A}_{[k]}^- + (\dots, \Psi_{i[k]}^{III,+}, \dots) \mathbf{B}_{[k]}^- & \text{for } z \geq D, \end{cases} \quad (8)$$

where the two matrices $\mathbf{A}_{[k]}^+$ and $\mathbf{A}_{[k]}^-$ contain the coefficients of the expansion corresponding to the incident part of the solutions, and $\mathbf{B}_{[k]}^+$ and $\mathbf{B}_{[k]}^-$ contain those corresponding to the reflected part.

Once the construction of these intermediate solutions is completed, it is straightforward to derive those given in Eqs. (5) and (6). The four transfer matrices describing these solutions are indeed given by

$$\mathbf{t}_{[k]}^{++} = \mathbf{A}_{[k]}^+{}^{-1}, \quad (9)$$

$$\mathbf{t}_{[k]}^{-+} = \mathbf{B}_{[k]}^+ \mathbf{A}_{[k]}^+{}^{-1}, \quad (10)$$

$$\mathbf{t}_{[k]}^{--} = \mathbf{A}_{[k]}^-{}^{-1}, \quad (11)$$

$$\mathbf{t}_{[k]}^{+-} = \mathbf{B}_{[k]}^- \mathbf{A}_{[k]}^-{}^{-1}. \quad (12)$$

An efficient technique to control the numerical instabilities encountered in the computation of these transfer matrices is presented in Refs. [13–15]. A generalization of this formalism to deal with nonsquare transfer matrices is given in Ref. [16]. While this way of computing the transfer matrices reveals efficient (with the extensions of Refs. [13,16]), the derivation of the intermediate solutions (7) and (8) is by far the most time-consuming part of the technique. It is the reason for now presenting an alternative method.

C. Construction from solutions provided by a conjugate set

Let us assume the scattering problem to be solved for a given set k of basic states (by the previously given method). The idea we are going to develop is the following: when the potential energy takes strict real values, taking the complex conjugate of these solutions provides another set of solu-

tions, which can be used as intermediate solutions for deriving transfer matrices corresponding to the conjugate set $-k$. This enables to bypass the time-consuming construction of the intermediate solutions given in Eqs. (7) and (8). When the potential energy takes strict real values, the wave function $\Psi(\mathbf{r})$ is the only complex-valued quantity in the Schrödinger equation $-(\hbar^2/2m)\nabla^2\Psi(\mathbf{r}) + V(\mathbf{r})\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$, so its complex conjugate $\Psi^*(\mathbf{r})$ is also a solution of this equation.

The key point is that the complex conjugate of a solution described in a given set k of basic states belongs to its conjugate set $-k$. In fact, by considering the complex conjugate of Eq. (3), one finds

$$\langle \mathbf{r} | \hat{R} | \Psi_{j[k]}^* \rangle = \chi_k^*(\hat{R}) \langle \mathbf{r} | \Psi_{j[k]}^* \rangle, \quad (13)$$

with $\langle \mathbf{r} | \Psi_{j[k]}^* \rangle$ standing for $\Psi_{j[k]}^*(\mathbf{r})$. So by considering the complex conjugate of the solutions obtained in a given set of basic states, we straightforwardly obtain solutions in its conjugate set, which can be used for deriving the corresponding transfer matrices.

To establish the relations enabling the derivation of these transfer matrices, let us first relate the basic states in the two conjugate sets by writing

$$\begin{aligned} & (\dots, \Psi_{j[k]}^{I,+*}, \dots, \Psi_{j[k]}^{I,-*}, \dots) \\ &= (\dots, \Psi_{j[-k]}^{I,+}, \dots, \Psi_{j[-k]}^{I,-}, \dots) \begin{pmatrix} \mathbf{U}_I^{++} & \mathbf{U}_I^{-+} \\ \mathbf{U}_I^{+-} & \mathbf{U}_I^{--} \end{pmatrix}, \end{aligned} \quad (14)$$

$$(\dots, \Psi_{j[k]}^{\text{III},+*}, \dots, \Psi_{j[k]}^{\text{III},-*}, \dots) = (\dots, \Psi_{j[-k]}^{\text{III},+}, \dots, \Psi_{j[-k]}^{\text{III},-}, \dots) \begin{pmatrix} \mathbf{U}_{\text{III}}^{++} & \mathbf{U}_{\text{III}}^{-+} \\ \mathbf{U}_{\text{III}}^{+-} & \mathbf{U}_{\text{III}}^{--} \end{pmatrix}. \quad (15)$$

When the basic states are orthonormal, these two relations imply a unitary transformation matrix.

Considering these relations, the complex conjugate of the solutions given in Eqs. (5) and (6) takes the forms

$$(\dots, \Psi_{j[k]}^{+*}, \dots) = \begin{cases} (\dots, \Psi_{j[-k]}^{I,+}, \dots, \Psi_{j[-k]}^{I,-}, \dots) \begin{pmatrix} \mathbf{U}_I^{++} & \mathbf{U}_I^{-+} \\ \mathbf{U}_I^{+-} & \mathbf{U}_I^{--} \end{pmatrix} \begin{pmatrix} \mathbf{I} \\ \overline{\mathbf{t}_{[k]}^{++}} \end{pmatrix} & \text{for } z \leq 0 \\ (\dots, \Psi_{j[-k]}^{\text{III},+}, \dots, \Psi_{j[-k]}^{\text{III},-}, \dots) \begin{pmatrix} \mathbf{U}_{\text{III}}^{++} & \mathbf{U}_{\text{III}}^{-+} \\ \mathbf{U}_{\text{III}}^{+-} & \mathbf{U}_{\text{III}}^{--} \end{pmatrix} \begin{pmatrix} \overline{\mathbf{t}_{[k]}^{++}} \\ \mathbf{0} \end{pmatrix} & \text{for } z \geq D, \end{cases} \quad (16)$$

$$(\dots, \Psi_{j[k]}^{-*}, \dots) = \begin{cases} (\dots, \Psi_{j[-k]}^{I,+}, \dots, \Psi_{j[-k]}^{I,-}, \dots) \begin{pmatrix} \mathbf{U}_I^{++} & \mathbf{U}_I^{-+} \\ \mathbf{U}_I^{+-} & \mathbf{U}_I^{--} \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ \overline{\mathbf{t}_{[k]}^{--}} \end{pmatrix} & \text{for } z \leq 0 \\ (\dots, \Psi_{j[-k]}^{\text{III},+}, \dots, \Psi_{j[-k]}^{\text{III},-}, \dots) \begin{pmatrix} \mathbf{U}_{\text{III}}^{++} & \mathbf{U}_{\text{III}}^{-+} \\ \mathbf{U}_{\text{III}}^{+-} & \mathbf{U}_{\text{III}}^{--} \end{pmatrix} \begin{pmatrix} \overline{\mathbf{t}_{[k]}^{--}} \\ \mathbf{I} \end{pmatrix} & \text{for } z \geq D, \end{cases} \quad (17)$$

where the notations $\overline{\mathbf{t}_{[k]}^{\pm\pm}}$ refer to the complex conjugate of the matrices $\mathbf{t}_{[k]}^{\pm\pm}$.

We can now make combinations of these solutions, i.e., consider the expressions

$$(\dots, \Psi_{j[-k]}^{+}, \dots) = (\dots, \Psi_{j[k]}^{+*}, \dots) \mathbf{M}^{++} + (\dots, \Psi_{j[k]}^{-*}, \dots) \mathbf{M}^{-+}, \quad (18)$$

$$(\dots, \Psi_{j[-k]}^{-}, \dots) = (\dots, \Psi_{j[k]}^{+*}, \dots) \mathbf{M}^{+-} + (\dots, \Psi_{j[k]}^{-*}, \dots) \mathbf{M}^{--}, \quad (19)$$

and choose the four matrices $\mathbf{M}^{\pm\pm}$ in order to obtain the appropriate form:

$$(\dots, \Psi_{j[-k]}^{+}, \dots) = \begin{cases} (\dots, \Psi_{j[-k]}^{I,+}, \dots, \Psi_{j[-k]}^{I,-}, \dots) \begin{pmatrix} \mathbf{I} \\ \mathbf{t}_{[-k]}^{-+} \end{pmatrix} & \text{for } z \leq 0 \\ (\dots, \Psi_{j[-k]}^{\text{III},+}, \dots, \Psi_{j[-k]}^{\text{III},-}, \dots) \begin{pmatrix} \mathbf{t}_{[-k]}^{++} \\ \mathbf{0} \end{pmatrix} & \text{for } z \geq D, \end{cases} \quad (20)$$

$$(\dots, \Psi_{j[-k]}^{-}, \dots) = \begin{cases} (\dots, \Psi_{j[-k]}^{I,+}, \dots, \Psi_{j[-k]}^{I,-}, \dots) \begin{pmatrix} \mathbf{0} \\ \mathbf{t}_{[-k]}^{--} \end{pmatrix} & \text{for } z \leq 0 \\ (\dots, \Psi_{j[-k]}^{\text{III},+}, \dots, \Psi_{j[-k]}^{\text{III},-}, \dots) \begin{pmatrix} \mathbf{t}_{[-k]}^{+-} \\ \mathbf{I} \end{pmatrix} & \text{for } z \geq D. \end{cases} \quad (21)$$

Solving for $\mathbf{M}^{\pm\pm}$ provides the results

$$\mathbf{M}^{++} = \{[\mathbf{U}_I^{-} \overline{\mathbf{t}_{[k]}^{++}} + \mathbf{U}_I^{++}] - [\mathbf{U}_I^{-} \overline{\mathbf{t}_{[k]}^{--}}][\mathbf{U}_{\text{III}}^{--} + \mathbf{U}_{\text{III}}^{+-} \overline{\mathbf{t}_{[k]}^{--}}]^{-1}[\mathbf{U}_{\text{III}}^{+-} \overline{\mathbf{t}_{[k]}^{++}}]\}^{-1}, \quad (22)$$

$$\mathbf{M}^{-+} = -[\mathbf{U}_{\text{III}}^{--} + \mathbf{U}_{\text{III}}^{+-} \overline{\mathbf{t}_{[k]}^{--}}]^{-1}[\mathbf{U}_{\text{III}}^{+-} \overline{\mathbf{t}_{[k]}^{++}}] \mathbf{M}^{++}, \quad (23)$$

$$\mathbf{M}^{--} = \{[\mathbf{U}_{\text{III}}^{+-} \overline{\mathbf{t}_{[k]}^{++}} + \mathbf{U}_{\text{III}}^{--}] - [\mathbf{U}_{\text{III}}^{+-} \overline{\mathbf{t}_{[k]}^{--}}][\mathbf{U}_I^{++} + \mathbf{U}_I^{+-} \overline{\mathbf{t}_{[k]}^{++}}]^{-1}[\mathbf{U}_I^{+-} \overline{\mathbf{t}_{[k]}^{--}}]\}^{-1}, \quad (24)$$

$$\mathbf{M}^{+-} = -[\mathbf{U}_I^{++} + \mathbf{U}_I^{+-} \overline{\mathbf{t}_{[k]}^{++}}]^{-1}[\mathbf{U}_I^{+-} \overline{\mathbf{t}_{[k]}^{--}}] \mathbf{M}^{--}. \quad (25)$$

The coefficients $\mathbf{M}^{\pm\pm}$ of the combinations to consider being known, the transfer matrices $\mathbf{t}_{[-k]}^{\pm\pm}$ corresponding to the conjugate set $-k$ of basic states are obtained from

$$\mathbf{t}_{[-k]}^{++} = [\mathbf{U}_{\text{III}}^{++} \overline{\mathbf{t}_{[k]}^{++}}] \mathbf{M}^{++} + [\mathbf{U}_{\text{III}}^{++} \overline{\mathbf{t}_{[k]}^{--}} + \mathbf{U}_{\text{III}}^{+-}] \mathbf{M}^{-+}, \quad (26)$$

$$\mathbf{t}_{[-k]}^{-+} = [\mathbf{U}_I^{+-} + \mathbf{U}_I^{-} \overline{\mathbf{t}_{[k]}^{++}}] \mathbf{M}^{++} + [\mathbf{U}_I^{-} \overline{\mathbf{t}_{[k]}^{--}}] \mathbf{M}^{-+}, \quad (27)$$

$$\mathbf{t}_{[-k]}^{--} = [\mathbf{U}_I^{-} \overline{\mathbf{t}_{[k]}^{--}}] \mathbf{M}^{--} + [\mathbf{U}_I^{-} \overline{\mathbf{t}_{[k]}^{++}} + \mathbf{U}_I^{+-}] \mathbf{M}^{+-}, \quad (28)$$

$$\mathbf{t}_{[-k]}^{+-} = [\mathbf{U}_{\text{III}}^{+-} + \mathbf{U}_{\text{III}}^{++} \overline{\mathbf{t}_{[k]}^{--}}] \mathbf{M}^{--} + [\mathbf{U}_{\text{III}}^{++} \overline{\mathbf{t}_{[k]}^{++}}] \mathbf{M}^{+-}. \quad (29)$$

Equations (22)–(25) are formulated so that the inversion of matrices with bad condition numbers is avoided. These

matrices are those expressing transmission, i.e., $\mathbf{t}_{[k]}^{++}$ and $\mathbf{t}_{[k]}^{--}$. In fact, the range of their eigenvalues grows exponentially with the distance D (see Ref. [13]). On the other hand, the eigenvalues of the transfer matrices expressing reflection, i.e., $\mathbf{t}_{[k]}^{+-}$ and $\mathbf{t}_{[k]}^{-+}$, remain close to unity, and therefore have better condition numbers. Furthermore, since the eigenvalues of the transfer matrices expressing transmission all decrease exponentially with the distance D , the terms that contain these matrices tend to become negligible compared to the others. These considerations explain for the efficiency of relations (22)–(25).

Computing the transfer matrices of a given set of basic states from those corresponding to its conjugate set requires negligible time, compared to that needed for constructing intermediate solutions like those given in Eqs. (7) and (8) by numerical propagation. In the case of C_n symmetry, there are $(n-1)/2$ pairs of conjugate sets if n is odd and $(n-2)/2$ pairs in the other case. Since a single propagation step is required for two conjugate sets, the computation time turns out to be reduced nearly by a factor 2 when n is large.

IV. APPLICATION TO DIFFRACTION BY A C_{60} MOLECULE

A. Preliminaries

To illustrate this theoretical material, let us simulate electronic field emission from a small conical tip [17] and the scattering of the extracted beam by a C_{60} molecule centered on the tip axis. The extraction field results from a potential bias V established between the metallic support of the tip and a conducting grid located at a distance D . This grid supports the C_{60} molecule, which stands on a pentagonal ring.

Let us assume region I (i.e., the metallic support of the tip) to be a Sommerfeld metal, delimited by the plane $z=0$ and characterized by empirical values of W (work function) and E_F (Fermi energy). If we conventionally set the potential energy in region III (i.e., the region beyond the conducting grid $z \geq D$) to the constant value 0, the potential energy in region I is then $V_{met} = eV - W - E_F$. With these assumptions, region II is the only diffusive part of the problem and, the Schrödinger equation being linear, the problem can be solved within the transfer-matrix methodology.

Due to the conical shape of the tip and the C_{60} molecule standing on a pentagon, the symmetry of the problem is C_{5v} (with z the corresponding symmetry axis). However, since the associated character table only enables the construction of four independent sets of basic states and does not contain any pair of lines with values that are complex conjugates of each other, we take account only of the C_5 symmetry. This symmetry indeed predicts five independent sets of basic states with two pairs of conjugate sets.

B. Wave function expansion

In the general case of C_n symmetry, it is useful to use polar coordinates in the plane normal to the symmetry axis z (i.e., ϕ for the azimuthal angle and ρ for the radial distance to the z axis). By assuming the scattering electron to remain localized inside a cylinder with radius R [18], the wave func-

tion can be expanded along a discrete set of basic states, whose specific forms in regions I and III are given by

$$\Psi_{(m,j)}^{I,\pm}(\mathbf{r}) = e^{\pm i \sqrt{[2m(E-V_{met})/\hbar^2] - k_{m,j}^2} z} \psi_{(m,j)}(\rho, \phi), \quad (30)$$

$$\Psi_{(m,j)}^{III,\pm}(\mathbf{r}) = e^{\pm i \sqrt{(2mE/\hbar^2) - k_{m,j}^2} z} \psi_{(m,j)}(\rho, \phi), \quad (31)$$

with

$$\psi_{(m,j)}(\rho, \phi) = \begin{cases} \frac{J_m(k_{m,j}\rho) e^{im\phi}}{\sqrt{2\pi \int_0^R \rho [J_m(k_{m,j}\rho)]^2 d\rho}} & \text{if } \rho \leq R \\ 0 & \text{otherwise,} \end{cases} \quad (32)$$

where all functions involved in these expressions have a pair of subscripts (m,j) . The radial wave vectors $k_{m,j}$ are solution of $J'_m(k_{m,j}R) = 0$.

C. Consideration of group theory

By application of Eq. (4), the basic states are split into n independent sets of functions $\Psi_{(m,j)[k]}^{I,\pm}$ and $\Psi_{(m,j)[k]}^{III,\pm}$ associated with m subscripts given by $m = k + in$, with i an integer and k ranging from 0 to $n-1$. The conjugate sets are those numbered by k and $n-k$, respectively.

The matrices $\mathbf{U}_I^{\pm\pm}$ and $\mathbf{U}_{III}^{\pm\pm}$ introduced in Sec. III C take the specific forms

$$\begin{pmatrix} \mathbf{U}_I^{++} & \mathbf{U}_I^{-+} \\ \mathbf{U}_I^{+-} & \mathbf{U}_I^{--} \end{pmatrix} = \begin{pmatrix} \mathbf{S}(\mathbf{I} - \mathbf{P}^I) & \mathbf{S}\mathbf{P}^I \\ \mathbf{S}\mathbf{P}^I & \mathbf{S}(\mathbf{I} - \mathbf{P}^I) \end{pmatrix}, \quad (33)$$

$$\begin{pmatrix} \mathbf{U}_{III}^{++} & \mathbf{U}_{III}^{-+} \\ \mathbf{U}_{III}^{+-} & \mathbf{U}_{III}^{--} \end{pmatrix} = \begin{pmatrix} \mathbf{S}(\mathbf{I} - \mathbf{P}^{III}) & \mathbf{S}\mathbf{P}^{III} \\ \mathbf{S}\mathbf{P}^{III} & \mathbf{S}(\mathbf{I} - \mathbf{P}^{III}) \end{pmatrix}, \quad (34)$$

where \mathbf{S} , \mathbf{P}^I , and \mathbf{P}^{III} are diagonal matrices defined by

$$S_{(m',j'),(m,j)} = \begin{cases} (-1)^m & \text{if } (m',j') = (m,j) \\ 0 & \text{otherwise,} \end{cases} \quad (35)$$

$$P_{(m',j'),(m,j)}^I = \begin{cases} 1 & \text{if } (m',j')=(m,j) \text{ and } k_{m,j} \leq \sqrt{\frac{2m}{\hbar^2}(E-V_{met})} \\ 0 & \text{otherwise,} \end{cases} \quad (36)$$

$$P_{(m',j'),(m,j)}^{III} = \begin{cases} 1 & \text{if } (m',j')=(m,j) \text{ and } k_{m,j} \leq \sqrt{\frac{2m}{\hbar^2}E} \\ 0 & \text{otherwise.} \end{cases} \quad (37)$$

The matrix \mathbf{S} characterizes the transformation of the factor $\psi_{(m,j)}(\rho, \phi)$ that appears in the basic states. Its peculiar form is due to the property $J_{-m}(x) = (-1)^m J_m(x)$ of Bessel functions. The two matrices \mathbf{P}^I and \mathbf{P}^{III} characterize the transformation of the other factor $\Phi_{(m,j)}(z)$, by indicating the basic states whose propagation direction is changed in the complex conjugate operation. In this context, the wave vectors $k_{m,j}$ are restricted by the condition $k_{m,j} \leq \sqrt{(2m/\hbar^2)E}$, so one has $\mathbf{P}^{III} = \mathbf{I}$.

D. Propagation equations

To propagate the solutions $\bar{\Psi}_{(m,j)[k]}^+$ and $\bar{\Psi}_{(m,j)[k]}^-$ through region II, we use the expression:

$$\bar{\Psi}_{(m,j)[k]}^\pm = \sum_{m[k],j} \Phi_{(m,j)}(z) \psi_{(m,j)}(\rho, \phi), \quad (38)$$

where the unknown z dependence of the wave function is contained in the coefficients $\Phi_{(m,j)}(z)$ of the expansion, and the sum is restricted to the m subscripts defined by $m = k + in$.

When this expression is substituted in the stationary Schrödinger equation, the wave function expansion coefficients $\Phi_{(m,j)}(z)$ turn out to verify the exact set of coupled equations [19,20]:

$$\frac{d^2 \Phi_{(m,j)}(z)}{dz^2} + \left[\frac{2m}{\hbar^2} E - k_{m,j}^2 - \frac{2m}{\hbar^2} V_0(z) \right] \Phi_{(m,j)}(z) = \sum_q \sum_{j'} M_{m,j}^{q,j'}(z) \Phi_{(m-q,n,j')}(z), \quad (39)$$

where E is the electron energy, and the coupling coefficients $M_{m,j}^{q,j'}(z)$ are defined by the expression

$$M_{m,j}^{q,j'}(z) = \frac{2m}{\hbar^2} \frac{\int_0^R \rho \bar{V}_q(\rho, z) J_m(k_{m,j}\rho) J_{m-q,n}(k_{m-q,n,j'}\rho) d\rho}{\sqrt{\int_0^R \rho [J_m(k_{m,j}\rho)]^2 d\rho} \sqrt{\int_0^R \rho [J_{m-q,n}(k_{m-q,n,j'}\rho)]^2 d\rho}}. \quad (40)$$

In these expressions, $V_0(z)$ and $\bar{V}_q(\rho, z)$ are the coefficients used in the n -fold symmetric potential energy,

$$V(\rho, \phi, z) = V_0(z) + \sum_{q=-\infty}^{+\infty} \bar{V}_q(\rho, z) e^{iqn\phi}, \quad (41)$$

where the choice of $V_0(z)$ is arbitrary but should correspond to the main part of the potential energy for better efficiency. Inspection of Eq. (39) confirms the fact that coupling is restricted to a single set k of basic states, since only basic states with m subscripts separated by an integer multiple of the symmetry axis order n are involved by the sum in the right-hand side.

E. Characterization of the physical system

An electric bias of 40 V and a metal-grid distance of 4 nm are considered. The bulk of the metal is characterized by a Fermi energy of 19.1 eV and a work function of 4.5 eV (values for tungsten). The conical tip has a height and basis

radius of 1 nm, and is represented by a continuous medium with infinite dielectric constant. The atoms of the C_{60} molecule are described by Gaussian electronic distributions that move rigidly around the positive nuclei as the result of the local electric field. The dynamic polarizability of the carbon atoms is chosen according to Ref. [21]. A vertical section of the potential energy distribution in region II is illustrated in Fig. 2. The details of this computation are given in Ref. [22].

F. Results

The current density on the conducting grid $z=D$ was computed by considering a cancellation radius R of 4 nm, and m values ranging from -20 to 20 . The number of basic states corresponding to these parameters is 1403. By taking account of the C_5 symmetry, these basic states are split into five independent sets whose associated m values and number of basic states are given in Table II. The two pairs of conjugate sets correspond to $k=1$ and 4 , respectively, for the first pair and $k=2$ and 3 , respectively, for the second pair, and differ only by the sign of the associated m subscripts.

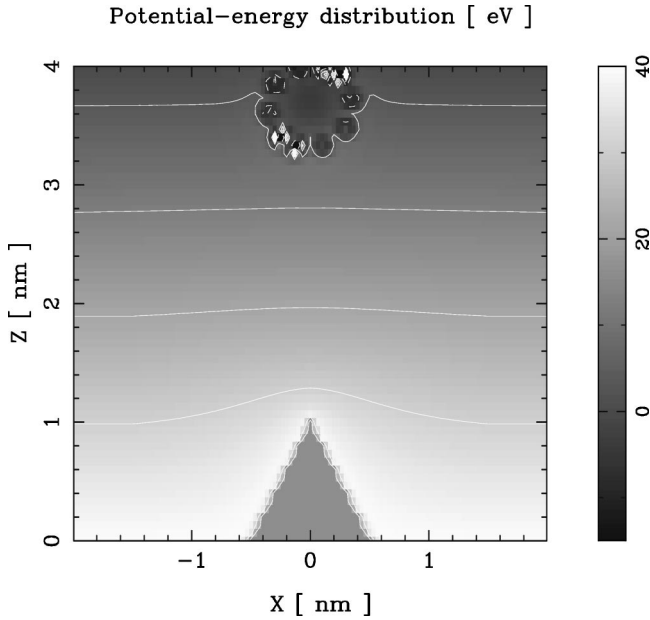


FIG. 2. Potential energy distribution (in eV) in the XZ vertical plane. A 40-V bias is applied over the 4-nm separation between the metallic tip holder surface and the sample supporting grid. This grid supports a C_{60} molecule standing on a pentagonal ring.

The result of the scattering computation is presented in Fig. 3. This figure shows the electronic beam that results from the field-emission process. The variations of intensity in the central part of the figure are related to the atomic structure of the C_{60} molecule, and can be interpreted as a projection of the carbon atoms from the tip apex on the conducting grid. The fivefold symmetry is clearly visible.

The results obtained by considering all basic states simultaneously, the five sets of basic states separately, or taking account of the two pairs of conjugate sets are identical (in short-precision representation). However, there is a significant difference in the storage and time requirements. To quantify this difference, let us refer to the number of basic states to consider simultaneously by nb . To be efficient, the computation of the coupling coefficients requires the storage of an array whose size is typically proportional to nb^3 . The time needed to compute the coupling coefficients and perform all matrix inversions along the distance D is proportional to $DE^{1/2}nb^3$. Since the number nb of basic states to consider simultaneously is reduced approximately by a factor 5 when the independent sets are considered, the storage and time requirements turn out to be reduced by a factor 5^3

TABLE II. List of the m values and number of elements in the five independent sets k of basic states corresponding to a cancellation radius R of 4 nm and an energy $E = eV - W$ of 35.5 eV.

k	m values	Number of basic states
0	-20, -15, -10, -5, 0, 5, 10, 15, 20	305
1	-19, -14, -9, -4, 1, 6, 11, 16	274
2	-18, -13, -8, -3, 2, 7, 12, 17	275
3	-17, -12, -7, -2, 3, 8, 13, 18	275
4	-16, -11, -6, -1, 4, 9, 14, 19	274

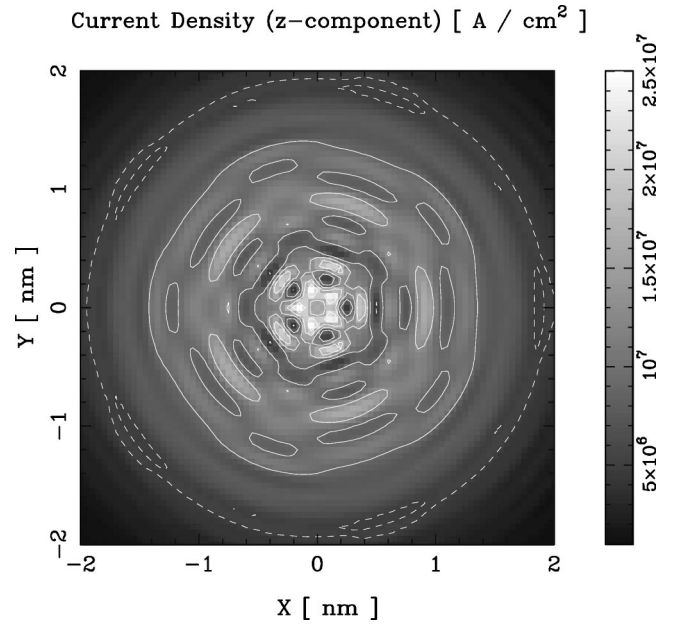


FIG. 3. Current density (in A/cm^2) on the conducting grid. A 40-V bias is applied over the 4-nm separation between the metallic tip holder surface and the sample supporting grid. This grid supports a C_{60} molecule standing on a pentagonal ring.

$=125$. Since there are two pairs of conjugate sets and the potential energy is exclusively real valued, the numerical propagation step can be bypassed for two sets among the five independent sets of basic states. This results in a further reduction of the time requirement by a factor $5/3$.

V. CONCLUSION

Group theory can be used systematically to improve the efficiency of transfer-matrix computations in situations where a given symmetry can be assumed, by enabling a reduction of the basic states to consider simultaneously and taking advantage of conjugate sets. The number of possible subdivisions in the initial set of basic states is given by the number of irreducible inequivalent representations of the symmetry. Since the storage and time requirements are proportional to the cube of the number of basic states to consider simultaneously, the efficiency of the technique is increased approximately by the cube of the achieved subdivisions.

Conjugate sets of basic states appear when the character table contains pairs of lines whose values are complex conjugates of each other. In general, symmetry operators involved with rotations have to be encountered for this situation to occur. When the potential energy is real valued, computing the transfer matrices corresponding to a pair of conjugate sets requires a single propagation step. Since this step is the most time-consuming part of the whole process, the time requirement for this pair of conjugate sets is thus reduced by a factor 2. The time needed to solve the scattering problem can therefore be reduced by another factor close to 2 when the main parts of the independent sets are in pairs of conjugate sets.

This theoretical material was illustrated by a simulation of

electronic diffraction by a C_{60} molecule in a projection configuration. The presence of a fivefold symmetry axis was exploited to split the basic states into five independent sets, among which two pairs of conjugate sets are present. Taking advantage of all techniques presented in this paper enabled the scattering problem to be solved with $5^3 = 125$ less storage space and $5^4/3 \approx 208$ less time.

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