JOURNAL OF MATHEMATICAL PHYSICS **47**, 022109 (2006)

Upper and lower bounds for an eigenvalue associated with a positive eigenvector

Amaury Mouchet[a)]

Laboratoire de Mathématiques et de Physique Théorique (CNRS UMR 6083), Université François Rabelais Avenue Monge, Parc de Grandmont 37200 Tours, France

(Received 28 October 2005; accepted 14 December 2005; published online 28 February 2006)

When an eigenvector of a semibounded operator is positive, we show that a remarkably simple argument allows to obtain upper and lower bounds for its associated eigenvalue. This theorem is a substantial generalization of Barta-type inequalities and can be applied to non-necessarily purely quadratic Hamiltonians. An application for a magnetic Hamiltonian is given and the case of a discrete Schrödinger operator is also discussed. It is shown how this approach leads to some explicit bounds on the ground-state energy of a system made of an arbitrary number of attractive Coulombian particles. © *2006 American Institute of Physics.*
[DOI: 10.1063/1.2168124]

I. INTRODUCTION

In most situations, the principal eigenvalue of a semibounded operator cannot be obtained explicitly whereas it plays a crucial role in physics: the smallest vibration frequency of an elastic system, the fundamental mode of an electromagnetic cavity, the ground-state energy of a quantum system with a finite number of degrees of freedom, the energy of the vacuum in a quantum field theory, the equilibrium state at zero temperature in statistical physics, etc. There are actually very few ways—which are usually specific to a restricted class of systems[1]—to obtain accurate approximations of an eigenvalue with a rigorous control on the errors and a reasonable amount of numerical computations. For instance, in a typical Dirichlet-Laplacian problem defined for an open connected set $\mathcal{Q}\subset\mathbb{R}^d$; $d\in\mathbb{N}$; Barta's inequalities (Barta, 1937) allow to bound to the lowest eigenvalue e_0: The determination of a lower (respectively, upper) bound requires the finding of the absolute minimum (respectively, maximum) of a smooth function defined on $\mathcal{Q}$. Compared to the general and traditional methods like the Rayleigh-Schrödinger perturbative series and the Rayleigh-Ritz or Temple variational methods, an advantage of Barta's approach is not only to naturally provide both an upper and a lower bound, but also does not involve the calculation of any integral. Therefore, generalizations of Barta's inequalities can lead to interesting spectral information. This generalization has been carried out in two directions:

(i) For Laplacian operators acting on square integrable functions defined on a Riemannian manifold (for a recent work on this subject, see Bessa and Montenegro, 2004).

(ii) For Schrödinger operators of the form $-\Delta+V$ acting on square integrable functions defined on an open set of $\mathbb{R}^d$ (Barnsley, 1978; Baumgartner, 1979; Thirring, 1979; Crandall and Reno, 1982; Schmutz, 1985) or more generally second order elliptic operators (Protter and Weinberger, 1966; Berestycki *et al.*, 1994; Harrell II, 2005).

[a)]mouchet@phys.univ-tours.fr

[1]Finding lower bounds for the smallest eigenvalue of a typical Hamiltonian is far more difficult than finding upper bounds. For successful attempts, see for instance the moment method proposed by Handy and Bessis, 1985, the Riccati-Padé method proposed in Fernández *et al.*, 1989 and the lower bounds obtained for few-body systems by Benslama *et al.*, 1998.

In both cases, the proofs of Barta's inequalities involve the use of a Kato-type inequality and therefore rely extensively on the somehow specific properties of the purely quadratic differential operator. In this paper, we propose a significant extension of Barta's inequalities that will rely on the properties of one eigenvector only. More precisely, with a remarkably simple argument, we will show that we can obtain upper and lower bounds for the eigenvalue e_0 associated with the eigenvector Φ_0 of an operator, under the only hypothesis that Φ_0 is real and non-negative. This result includes cases (i) and (ii) because the Krein-Rutman theorem guarantees the positivity of Φ_0 (Reed and Simon, 1978a, Sec. XIII.12) for the smallest eigenvalue e_0,[2] but also applies for a much wider class of operators including the following.

(iii) the Schrödinger operators involving a magnetic field, e.g., the hydrogen atom in a Zeeman configuration;

(iv) discrete Hamiltonians, e.g., the one occurring in the Harper model;[3]

(v) some integral or pseudodifferentiable operators, e.g., the Klein-Gordon or spinless Salpeter Hamiltonians.

The next section fixes the notations, proves the main general results (theorems 1 and 2). Section III shows how the original argument given in Sec. II actually embraces and generalizes the Barta-type inequalities that have been already obtained in the literature and furnishes guidelines to numerically improve the bounds on e_0. Sections IV and V provide two applications in the differentiable case (many-body problem) and in the discrete case, respectively.

II. BOUNDING THE PRINCIPAL EIGENVALUE WITH THE LOCAL ENERGY

A. General inequalities

In the following, $\mathcal{Q}$ will be a locally compact space endowed with a positive Radon measure μ. $\langle\psi|\varphi\rangle$ will denote the scalar product between two elements ψ and φ belonging to the Hilbert space of the square integrable complex functions $\mathsf{L}^2(\mathcal{Q},\mu)$,

$$\langle\psi|\varphi\rangle = \int_{\mathcal{Q}} \bar{\psi}(q)\varphi(q)\mathrm{d}\mu(q).$$

$\mathsf{D}(H)$ will denote the domain of the operator H acting on $\mathsf{L}^2(\mathcal{Q},\mathrm{d}\mu)$. The crucial hypothesis on H is the following.

Hypothesis 1: The operator H is symmetric and has one real eigenvector $\Phi_0 \in \mathsf{D}(H)$ *such that* $\Phi_0 \geqslant 0$ (*almost everywhere with respect to* μ) *on* $\mathcal{Q}$.

If e_0 stands for the eigenvalue of H associated with Φ_0, the symmetry of H implies that, for all $\varphi \in \mathsf{D}(H)$, we have $\langle\Phi_0|(H-e_0)\varphi\rangle=0$ that is

$$\forall\,\varphi \in \mathsf{D}(H), \quad \int_{\mathcal{Q}} \overline{\Phi_0}(q)(H-e_0)\varphi(q)\mathrm{d}\mu(q) = 0.$$

Taking the real part of the integral, we can see that the support of $q\mapsto\mathrm{Re}[\overline{\Phi_0}(q)(H-e_0)\varphi(q)]$ either is empty, either contains two disjoints open sets $\mathcal{Q}_\pm$ such that $\mathrm{Re}(\overline{\Phi_0}(H-e_0)\varphi) \gtrless 0$ and $\mu(\mathcal{Q}_\pm)>0$. The hypothesis of positivity of Φ_0 implies that on $\mathcal{Q}_\pm$, we have $\mathrm{Re}[(H-e_0)\varphi]\gtrless 0$. The last results motivates the following definition.

Definition 1 (*local energy*)*: For any* φ *in* $\mathsf{D}(H)$, *the* local energy *is the function* $E_\varphi : \mathcal{Q} \to \bar{\mathbb{R}}$ *defined by*

[2]The positivity of Φ_0 is also required for the traditional proofs of Barta's inequalities; this explains why, in case (i) and (ii), they concern the lowest eigenvalue only.

[3]After the first version of this paper was written, the author became aware of the paper by Barnsley and Duffin, 1980 where a similar argument as the one presented here was proposed (Theorem 7) for the bounds on an eigenvalue of a finite matrix.

$$E_\varphi(q) = \frac{\mathrm{Re}(H\varphi(q))}{\mathrm{Re}(\varphi(q))}. \tag{1}$$

Therefore from what precedes, we have obtained the main theorem.

Theorem 1: *For any symmetric operator H on $\mathsf{L}^2(\mathcal{Q},\mu)$ having an eigenvalue e_0 whose corresponding eigenfunction is non-negative almost everywhere on $\mathcal{Q}$, we have*

$$\forall \varphi \in \mathsf{D}(H) \text{ such that } \mathrm{Re}(\varphi) \geqslant 0, \quad \inf_{\mathcal{Q}}(E_\varphi) \leqslant e_0 \leqslant \sup_{\mathcal{Q}}(E_\varphi). \tag{2}$$

Actually, for a nonsymmetric operator K, we can keep working with its adjoint K^* and easily generalize the above argument.

Theorem 2: *Let K being an operator on $\mathsf{L}^2(\mathcal{Q},\mu)$ having an eigenvalue k_0 whose corresponding eigenfunction is real and non-negative almost everywhere on $\mathcal{Q}$, we have $\forall\varphi \in \mathsf{D}(K^*)$ such that $\varphi > 0$,*

$$\inf_{\mathcal{Q}}\left[\frac{\mathrm{Re}(K^*\varphi)}{\varphi}\right] \leqslant \mathrm{Re}(k_0) \leqslant \sup_{\mathcal{Q}}\left[\frac{\mathrm{Re}(K^*\varphi)}{\varphi}\right], \tag{3a}$$

$$\inf_{\mathcal{Q}}\left[-\frac{\mathrm{Im}(K^*\varphi)}{\varphi}\right] \leqslant \mathrm{Im}(k_0) \leqslant \sup_{\mathcal{Q}}\left[-\frac{\mathrm{Im}(K^*\varphi)}{\varphi}\right]. \tag{3b}$$

This generalization may be of physical relevance. There are some models (e.g., the so-called "kicked" systems, or quantized maps) where the dynamics are described "stroboscobically", i.e., implemented by a unitary operator (the Floquet evolution operator) that cannot be constructed from a smooth Hamiltonian. However, we will not consider this possibility here, and up to the end of this paper, H will denote a symmetric operator.

B. Optimization strategy

Since generally, the eigenfunction Φ_0 is not known exactly, it will be approximated with the help of test functions that belong to a trial space $\mathsf{T}(H) \subset \mathsf{D}(H)$, very much like the variational method. Since we want a test function to mimic Φ_0 at best, we will restrict $\mathsf{T}(H)$ to functions that respect the *a priori* known properties of Φ_0: its positivity, its boundary conditions and its symmetries if there are any. For each test function the error on e_0 is controlled by inequalities (2). Therefore, the strategy for obtaining reasonable approximations is clear: First, we must choose or construct φ to eliminate all the singularities of the local energy in order to work with a bounded function and second, perturb the test function in the neighborhood of the absolute minimum (respectively, maximum) of the local energy in order to increase (respectively, decrease) its value. For practical and numerical computations, this perturbation will be implemented by constructing a diffeomorphism $\Lambda \to \mathsf{T}(H), \lambda \mapsto \varphi_\lambda$ from a finite dimensional differentiable real manifold Λ of control parameters λ and the optimized bounds for e_0 will be

$$\sup_{\Lambda}\inf_{\mathcal{Q}}(E_{\varphi_\lambda}) \leqslant e_0 \leqslant \inf_{\Lambda}\sup_{\mathcal{Q}}(E_{\varphi_\lambda}). \tag{4}$$

III. INEQUALITIES IN THE DIFFERENTIABLE CASE: OLD AND NEW

A. General considerations

When H is a local differential operator, i.e., involves a finite number of derivatives in an appropriate representation (for instance in position or in momentum representation), one can therefore construct an algorithm that does not require any integration but differential calculus only. In an analytic and in a numerical perspective, this may be a significant advantage on the perturbative or variational methods even though it is immediate to see[4] that the upper bound given by (2) is always larger than $\langle\varphi|H\varphi\rangle/\langle\varphi|\varphi\rangle$. The global analysis appears only through the determination of the singularities and the *absolute* extrema of the local energy that may have bifurcated when the control parameter λ varies smoothly. For a Schrödinger operator, the possible singularities of the potential on $\bar{\mathcal{Q}}$ like a Coulombian divergence or an unbounded behavior at infinite distances may furnish a strong guideline for constructing relevant test functions (see Sec. III D below). We have given in Mouchet, 2005, some heuristic and numerical arguments to show how this strategy can be fruitful. In the present paper, the main focus will concern rigorous results and will explain how some of them can be obtained with great simplicity even for systems as complex as those involved in the many-body problem.

B. Case (i) Barta's inequalities

They immediately appear as a particular case of Theorem 1.

Theorem 3 (Barta, 1937): *Let $\mathcal{Q}$ be a connected bounded Riemannian manifold endowed with the metric g and H, the opposite of the Laplacian Δ_g acting on the functions in $\mathsf{L}^2(\mathcal{Q},\mu)$ that satisfy Dirichlet boundary conditions on the boundary $\partial\mathcal{Q}$. The lowest eigenvalue e_0 of H is such that, for all positive $\varphi\in\mathcal{C}^2(\mathcal{Q})$,*

$$\inf_{\mathcal{Q}}\left(-\frac{\Delta_g\varphi}{\varphi}\right)\leqslant e_0\leqslant\sup_{\mathcal{Q}}\left(-\frac{\Delta_g\varphi}{\varphi}\right). \tag{5}$$

Proof: It follows directly from Theorem 1, with the local energy given by $E_\varphi=-\Delta_g\varphi/\varphi$: The spectrum of H is discrete and the Krein-Rutman theorem assures that Hypothesis 1 is fulfilled for e_0 being the lowest (and simple) eigenvalue. ∎

Remark 1: The Dirichlet boundary conditions are not essential and can be replaced by any other type of boundary conditions provided that Hypothesis 1 remains fulfilled. However, as explained in Sec. II B, *for obtaining interesting bounds on e_0 extending $\mathsf{T}(H)$ to test functions that do not fulfill the boundary conditions (as proposed by Duffin, 1947) seems not appropriate.*

C. Case (ii) Duffin-Barnsley-Thirring inequalities

Extensions of Barta's inequalities for Schrödinger operators have been obtained partially by Duffin (Duffin, 1947) and Barnsley (Barnsley, 1978) (for the lower bound only) and completely (lower and upper bound) by Thirring (Thirring, 1979) using Kato's inequalities (see also Schmutz, 1985).

Theorem 4 (Duffin, 1947; Barnsley, 1978; Thirring, 1979): *Let $H=-\Delta+V$ be a Schrödinger operator acting on $\mathsf{L}^2(\mathbb{R}^d)$ having an eigenvalue below the essential spectrum. Then the lowest eigenvalue e_0 of H is such that for any strictly positive $\varphi\in\mathsf{D}(H)$,*

$$\inf_{\mathbb{R}^d}\left(V-\frac{\Delta\varphi}{\varphi}\right)\leqslant e_0\leqslant\sup_{\mathbb{R}^d}\left(V-\frac{\Delta\varphi}{\varphi}\right). \tag{6}$$

The proof is similar to the one presented above with the local energy being now $E_\varphi=V-\Delta\varphi/\varphi$. This argument has the advantage on the existing ones that it does not involve the specific properties of the Laplacian and can be immediately transposed to the larger class of the differential operators (not necessarily of second order) that fulfill Hypothesis 1.

D. Case (iii) magnetic Schrödinger operators

In the presence of a magnetic field, Schrödinger operators take the form $H=(\mathrm{i}\partial_q+A(q))^2+V(q)$ with $A:\mathcal{Q}\to\mathbb{R}^d$ being a smooth magnetic potential vector and $V:\mathcal{Q}\to\mathbb{R}$ a smooth scalar

[4]For each positive φ, it follows from $\langle\varphi|H\varphi\rangle=\mathrm{Re}[\langle\varphi|H\varphi\rangle]=\int_{\mathcal{Q}}\varphi(q)\mathrm{Re}[H\varphi(q)]\mathrm{d}\mu(q)=\int_{\mathcal{Q}}\varphi^2(q)E_\varphi(q)\mathrm{d}\mu(q)\leqslant\langle\varphi|\varphi\rangle\sup_{\mathcal{Q}}(E_\varphi(q))$.

potential. The Krein-Rutman theorem may not apply whereas there still exists a non-negative real eigenfunction (e_0 may be not simple nor the lowest eigenvalue) (Helffer *et al.*, 1999).

In the particular case of the hydrogen atom in a constant and uniform magnetic field, Hypothesis 1 is fulfilled for all values of the magnetic field (Avron *et al.*, 1977; Avron *et al.*, 1978) and indeed concerns the lowest eigenvalue. Therefore Theorem 1 applies and furnishes relevant analytical bounds that can be improved numerically as shown in (Mouchet, 2005).

Proposition 1: The smallest eigenvalue e_0 of the (3d-)Zeeman Hamiltonian

$$H = \frac{1}{2}\left(-i\vec{\nabla} + \frac{1}{2}\vec{r}\times\vec{B}\right)^2 - \frac{1}{r} \tag{7}$$

is such that

$$\forall B \geqslant 0, \quad e_0 \leqslant -1/2 + B/2. \tag{8}$$

Proof: In cylindrical coordinates $(\rho,\ \theta,\ z)$ where the magnetic field is $\vec{B}=B\vec{u}_z$, the test function of the form $\varphi=\exp(-\sqrt{\rho^2+z^2}-B\rho^2/4)$ is constructed, according to the strategy explained in Sec. II B, in order to respect the rotational invariance of the ground state (Avron *et al.*, 1977) and eliminate both singularities at $r\to 0$ and at $\rho\to\infty$. Indeed such a choice leads straightforwardly to the bounded local energy

$$E_\varphi = -1/2 + B/2 - \frac{\rho^2 B}{2\sqrt{\rho^2+z^2}}. \tag{9}$$

The upper bound follows. ■

IV. APPLICATION TO THE MANY-BODY PROBLEM

A. Expression of the local energy in terms of two-body functions

We will consider in this section a N-body nonrelativistic bosonic system in d dimensions; $(d,N)\in(\mathbb{N}\backslash\{0,1\})^2$; whose Hamiltonian is given by

$$\tilde{H} = \sum_{i=0}^{N-1} -\frac{1}{2m_i}\Delta_i + V(\vec{r}_0,\ \dots,\vec{r}_{N-1}) \tag{10}$$

acting on $\mathsf{L}^2(\mathbb{R}^{Nd})$, endowed with the canonical Lebesgue measure, and where $\forall i\in\{0,\dots,N-1\}$, $\vec{r}_i\in\mathbb{R}^d$. Δ_i is the Laplacian in the $\vec{r}_i$ variables and $m_i\in\mathbb{R}^+\backslash\{0\}$ the mass of the ith particle. The spinless bosons interact only by the two-body radial potentials $v_{ij}=v_{ji}:\mathbb{R}\to\mathbb{R}$, i.e., V is given by

$$V = \sum_{\substack{i,j=0\\ i<j}}^{N-1} v_{ij}(r_{ij}), \tag{11}$$

where $r_{ij}=r_{ji}=\|\vec{r}_j-\vec{r}_i\|$. Once the center of mass is removed, the Hamiltonian $\tilde{H}$ leads to a reduced Hamiltonian H acting on $\mathsf{L}^2(\mathbb{R}^{(N-1)d})$ [see for instance Sec. XI.5 of (Reed and Simon, 1978b)] and we will suppose in the following that H has at least one eigenvector.[5] Therefore, Hypothesis 1 is fulfilled for e_0 being the lowest (and simple) eigenvalue. A natural choice for test functions is to consider factorized ones of the form

[5]Physically, this can be achieved with a confining external potential (a "trap" is currently used in experiments involving cold atoms). Formally, this can be obtained in the limit of one mass, say m_0, being much larger than the others. The external potential appears to be the $v_{0,i}$'s, created by such an infinitely massive motionless device. It will trap the remaining $N-1$ particles in some bounded states if the $v_{0,i}$'s increase sufficiently rapidly with the $r_{0,i}$'s.

$$\varphi(\vec{r}_0, \ldots, \vec{r}_{N-1}) = \prod_{\substack{i,j=0\\ i<j}}^{N-1} \phi_{ij}(r_{ij}), \tag{12}$$

where $\phi_{ij} \in \mathsf{L}^2(\mathbb{R}^+)$ and $\phi_{ji} = \phi_{ij} > 0$. One can check easily that the total momentum of such a test function vanishes. The corresponding local energy (1) is given by

$$E_\varphi(q_N) = \sum_{\substack{i,j=0\\ i<j}}^{N-1} \left[\frac{-1}{2m_{ij}\phi_{ij}(r_{ij})} \left(\phi''_{ij}(r_{ij}) + \frac{d-1}{r_{ij}} \phi'_{ij}(r_{ij}) \right) + v_{ij}(r_{ij}) \right] - \sum_{(\widehat{j,i,k})} \frac{1}{m_i} S'_{ij}(r_{ij}) S'_{ik}(r_{ik}) \cos(\widehat{j,i,k}), \tag{13}$$

where $q_N \in \mathcal{Q}_N = \mathbb{R}^{(N-1)d}$ stands for the $(N-1)d$ relative coordinates $(\vec{r}_1 - \vec{r}_0, \ldots, \vec{r}_{N-1} - \vec{r}_0)$, m_{ij} for the reduced masses $m_i m_j / (m_i + m_j)$, S'_{ij} is the derivative of $S_{ij} = \ln(\phi_{ij})$. The last sum involves all the $N(N-1)(N-2)/2$ angles $(\widehat{j,i,k})$ between $\vec{r}_j - \vec{r}_i$ and $\vec{r}_k - \vec{r}_i$ that can be formed with all the triangles made of three distinct particles.

Whenever each v_{ij} allows for a two-body bounded state, we can choose ϕ_{ij} to be the eigenvector of $-(2m_{ij})^{-1}\Delta + v_{ij}$ having the smallest eigenvalue $\epsilon_{ij}^{(2)}$. Moreover, if $v_{ij}(r)$ is bounded when $r \to \infty$, from an elementary semiclassical analysis [see for instance (Maslov and Fedoriuk, 1981)] it follows that S'_{ij} is also bounded since asymptotically we have $S'_{ij}(r) \sim_{r\to\infty} -\sqrt{2m_{ij}[v_{ij}(r) - \epsilon_{ij}^{(2)}]}$. It follows that the local energy is also bounded and finite lower and upper bounds on e_0 can be found. For instance, directly from expression (13), we have the following.

Proposition 2: If, for all $(i,j) \in \{0, \ldots, N-1\}^2$, $i \neq j$, $v_{ij}(r)$ *is bounded when* $r \to \infty$ *and* $-(2m_{ij})^{-1}\Delta + v_{ij}$ *has a smallest eigenvalue* $\epsilon_{ij}^{(2)}$ *obtained for* $\phi_{ij} = \exp S_{ij}$, *then the smallest eigenvalue* e_0 *of the N-body Hamiltonian in the center-of-mass frame is bounded by*

$$\sum_{\substack{i,j=0\\ i<j}}^{N-1} \epsilon_{ij}^{(2)} - \frac{s^2}{2m} N(N-1)(N-2) \leq e_0 \leq \sum_{\substack{i,j=0\\ i<j}}^{N-1} \epsilon_{ij}^{(2)} + \frac{s^2}{2m} N(N-1)(N-2), \tag{14}$$

where $m = \min_i m_i$ *and* $s = \max_{i,j} \sup_{\mathbb{R}^+} |S'_{ij}|$.

For potentials that are relevant in physics [see for instance the effective power-law potentials of the form $v_{ij}(r) = \mathrm{sign}(\beta) r^\beta$; $\beta \in \mathbb{R}$; between massive quarks as studied by Benslama *et al.*, 1998], the analytic form of the two-body eigenvector is not known in general and some numerical computations are required to obtain the absolute maximum and minimum of the local energy (13).

B. The local energy for a general Coulombian problem

When N is large, the estimation (14) is quite rough, in particular it does not take into account the constraints between the several angles. More precise results are obtained for the Coulombian problem where $v_{ij}(r) = e_{ij}/r$ with $e_{ij} \in \mathbb{R}$ and $d > 1$. In that case, provided a bounded state exists and that we keep the test function (12) in $\mathsf{L}^2(\mathbb{R}^{(N-1)d})$, we choose a constant derivative $S'_{ij} = 2e_{ij}m_{ij}/(d-1)$ in order to get rid of the Coulombian singularities of V. We obtain a bounded local energy given by

$$E_\varphi(q_N) = \sum_{\substack{i,j=0\\ i<j}}^{N-1} - \frac{2m_{ij}e_{ij}^2}{(d-1)^2} - \frac{4}{(d-1)^2} \sum_{(\widehat{j,i,k})} \frac{m_{ij}m_{ik}e_{ij}e_{ik}}{m_i} \cos(\widehat{j,i,k}). \tag{15}$$

C. Identical purely attractive Coulombian particles

The case where all the N particles are identical and attract each other, i.e., when $\forall (i,j) \in \{0, \ldots, N-1\}^2$, $i \neq j$, $m_i = 1$ and $e_{ij} = -1$, has been extensively studied in the literature, in particular the asymptotic behavior of e_0 with large N may have some dramatic consequences on the thermodynamical limit (Fisher and Ruelle, 1966; Lenard and Dyson, 1967; Lévy-Leblond, 1969; Lieb, 2005). The local energy method allows to obtain in a much simpler way energy bounds that are comparable to those already obtained by other methods. Actually, (15) simplifies to

$$E_\varphi(q_N) = -\frac{1}{(d-1)^2}\left[\tfrac{1}{2}N(N-1) + F_N(q_N)\right] \tag{16}$$

with $F_2 \equiv 0$ and for $N \geqslant 3$,

$$F_N(q_N) = \sum_{\widehat{(j,i,k)}} \cos(\widehat{j,i,k}). \tag{17}$$

The angular function F_N depends only on the geometrical configuration of the N vertices $(\vec{r}_0, \ldots, \vec{r}_{N-1})$, i.e., it is invariant under the group of Euclidean isometries and the scale invariance of the Coulombian interaction makes it invariant under dilations as well.

Lemma 1: $\inf_{\mathcal{Q}_3} F_3 = 1$ *is obtained when the three points are aligned.* $\sup_{\mathcal{Q}_3} F_3 = 3/2$ *is obtained when the three points make an equilateral triangle.*

Proof: The extrema of F_3 correspond to the extrema of the function defined by $(\theta_0, \theta_1, \theta_2) \mapsto \cos\theta_0 + \cos\theta_1 + \cos\theta_2$ under the constraint $\theta_0 + \theta_1 + \theta_2 = \pi$ for $(\theta_0, \theta_1, \theta_2)$ being the three angles $(\widehat{1,0,2})$, $(\widehat{0,1,2})$, $(\widehat{0,2,1})$, respectively. The Lagrange multiplier method leads to the determination of the extrema of the function $[0;\pi]^3 \to \mathbb{R}$ defined by $(\theta_0, \theta_1, \theta_2) \mapsto \cos\theta_0 + \cos\theta_1 + \cos\theta_2 + l(\theta_0 + \theta_1 + \theta_2 - \pi)$; $l \in \mathbb{R}$. We immediately obtain that the extremal points are located at $(\theta_0, \theta_1, \theta_2) = (\pi/3, \pi/3, \pi/3)$ and $(\theta_0, \theta_1, \theta_2) = (0, 0, \pi)$ together with the solutions that are obtained by circular permutations. It is easy to check that the first solution provides an absolute maximum for F_3 and the second ones an absolute minimum. ■

An immediate consequence of the preceding lemma is the following.

Proposition 3: The lowest energy e_0 of $N \geqslant 2$ identical attractive Coulombian spinless particles in $d > 1$ dimensions is such that

$$e_0 \leqslant -\frac{1}{(d-1)^2}\frac{1}{6}N(N-1)(N+1) \tag{18}$$

when the individual masses equal to unity and the attractive potential is $-1/r$.

Proof: The sum on the angles that defines F_N in (17) can be written as a sum of $N(N-1)(N-2)/6$ F_3-terms calculated for all the triangles that belong to the N-uplet made of the N vertices. Since, from Lemma 1 the absolute minimum of F_3 is obtained for a flat configuration, when all the N points are aligned all the F_3-terms reach their absolute minimum simultaneously and the absolute minimum of F_N is obtained. We have

Lemma 2: $\inf_{\mathcal{Q}_N} F_N = \frac{1}{6}N(N-1)(N-2)$ *is obtained when all the N points are aligned.*

The upper bound (18) follows from (16). ■

More generally, for a given N-uplet (i.e., a set of exactly N points), clustering the sum (17) in M-uplets $(N \geqslant M \geqslant 3)$ allows to find bounds on F_N from bounds on F_M. Indeed, we can write

$$F_N(q_N) = \sum_{q_M} \frac{(M-3)!\,(N-M)!}{(N-3)!} F_M(q_M), \tag{19}$$

where the sum is taken on all the M-uplets, labeled by the coordinates q_M, that belong to the given N-uplet. This sum involves exactly $N!/(M!(N-M)!)$ terms and we have, therefore,

Lemma 3: $\forall (N,M) \in \mathbb{N}^2$ *such that* $N \geqslant M \geqslant 3$,

$$\sup_{\mathcal{Q}_N} F_N \leqslant \frac{N(N-1)(N-2)}{M(M-1)(M-2)} \sup_{\mathcal{Q}_M} F_M. \tag{20}$$

For a given N, $\sup_{\mathcal{Q}_N} F_N$ is not known exactly but the ordered sequence

$$\frac{\sup_{\mathcal{Q}_N} F_N}{N(N-1)(N-2)} \leqslant \frac{\sup_{\mathcal{Q}_{N-1}} F_{N-1}}{(N-1)(N-2)(N-3)} \leqslant \cdots \leqslant \frac{\sup_{\mathcal{Q}_M} F_M}{M(M-1)(M-2)} \leqslant \cdots \leqslant \frac{\sup_{\mathcal{Q}_3} F_3}{3.2.1} = \frac{1}{4} \tag{21}$$

shows that in order to improve the lower bounds on (16), we must try to find $\sup_{\mathcal{Q}_M} F_M$ with M being the largest as possible. However, when considering identity (19) for $N=4$ and $M=3$ together with Lemma 1 we have the following.

Lemma 4: $\sup_{\mathcal{Q}_4} F_4=6$ *is obtained when the four points make a regular tetrahedron.*

Then $\sup_{\mathcal{Q}_4} F_4/(4.3.2)=\sup_{\mathcal{Q}_3} F_3/(3.2.1)=1/4$ and no better estimate is obtained when considering $M=4$ rather than $M=3$. Numerical investigations lead to the following conjectures.

Conjecture 1: (C_5) *When* $d=3$,

$$\sup_{\mathcal{Q}_5} F_5 = \frac{9}{2} + \frac{6(h_0+1)}{\sqrt{h_0^2+\frac{1}{3}}} - \frac{1}{h_0^2+\frac{1}{3}} \simeq 14.591\,594$$

with

$$6h_0 = 1 + \sqrt{-1+\sqrt[3]{7+4\sqrt{3}}+\frac{1}{\sqrt[3]{7+4\sqrt{3}}}} + \sqrt{-2-\sqrt[3]{7+4\sqrt{3}}-\frac{1}{\sqrt[3]{7+4\sqrt{3}}}+8\frac{1}{\sqrt{-1+(7+4\sqrt{3})^{1/3}+(7+4\sqrt{3})^{-1/3}}}} \tag{22}$$

is obtained when the five points make two mirror-symmetric tetrahedrons sharing one common equilateral basis, their other faces being six isosceles identical triangles.

Remark 2: The only free parameter of the specific configuration can be chosen to be the height h of one tetrahedron (the length of the edges of the common equilateral basis being fixed to one). The maximum of $h \mapsto F_5$ *is reached for* h_0 *being the greatest solution of* $9h^4-6h^3+3h^2-2h+1/3$ *that is precisely given by* (22).

Remark 3: The pyramidal configurations with a squared basis leads to a local maximum that gives $F_5=15/2+5\sqrt{2} \simeq 14.57$.

Conjecture 2: (C_6) *When* $d=3$, $\sup_{\mathcal{Q}_6} F_6=12(1+\sqrt{2})$ *is obtained when the six points make a regular octahedron.*

Conjecture 3: (C_8) *When* $d=3$,

$$\sup_{\mathcal{Q}_8} F_8 = 16\left[\frac{4}{5}+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{5}}+\frac{4(1+\sqrt{2})}{\sqrt{5}\sqrt{5+4\sqrt{2}}}+\frac{3+2\sqrt{2}}{\sqrt{5+4\sqrt{2}}}-\frac{1}{5+4\sqrt{2}}\right] \simeq 79.501$$

is obtained when the eight points make two identical squares (whose edges have length one) lying in two parallel planes separated by a distance $h=\sqrt{1+2\sqrt{2}}/2$. *The axis joining the centers of the two squares is perpendicular to the squares and the two squares are twisted one from the other by a relative angle of* $\pi/4$.

Remark 4: The cube corresponds to $F_8=8(3\sqrt{2}+\sqrt{3}+3/2+\sqrt{6}) \simeq 79.393$.

Conjecture 4: (C_∞) *When* $d=3$ *and* $N \to \infty$, *the configuration that maximizes* F_N *corresponds to N points uniformly distributed on a sphere and* $\sup_{\mathcal{Q}_N} F_N \sim \frac{2}{9}N^3+o(N^3)$.

Remark 5: The ambiguity of distributing N points uniformly on a sphere (Saff and Kuijlaars, 1997 and references therein) vanishes for large N as far as a uniform density is obtained. Assuming such a uniform density, the continuous limit of F_N/N^3 *is a triple integral on the sphere than can be computed exactly to* $2/9$.

The upper bound (18) for $d=3$ is slightly above the one obtained by Lévy-Leblond, 1969, Eq. (17), p. 807, namely $-(5/8)^2N(N-1)^2/8$, and the numerical estimate $-0.0542N(N-1)^2$ by Basdevant *et al.*, 1990, Eq. (16), p. 63. For the lower bounds, from Lemmas 1 or 4, we have obtained the following.

Proposition 4: The lowest energy e_0 of $N \geqslant 2$ identical attractive Coulombian spinless particles in $d > 1$ dimensions is such that

$$-\frac{1}{(d-1)^2}\frac{1}{4}N^2(N-1) \leqslant e_0 \tag{23}$$

when the individual masses equal to unity and the attractive potential is $-1/r$.

The same result has been obtained for $d=3$ by Basdevant *et al.*, 1990, Eq. (11), p. 62 and is slightly better than $-N(N-1)^2/8$ given by Lévy-Leblond, 1969 Eq. (13), p. 807. For $N \geqslant M \geqslant 4$, this lower bound can be improved to

$$-\frac{1}{(d-1)^2}N(N-1)\left(\frac{1}{2}+\alpha_M(N-2)\right) \leqslant e_0 \tag{24}$$

with

$$\alpha_M = \frac{\sup_{\mathcal{Q}_M} F_M}{M(M-1)(M-2)} \leqslant \frac{1}{4}. \tag{25}$$

If conjecture (C_5) [respectively (C_6), (C_8), and (C_∞)] is correct we get, when $d=3$, $\alpha_5 \simeq 0.2432$ (respectively, $\alpha_6 \simeq 0.2414$, $\alpha_8 \simeq 0.2366$, and $\alpha_\infty \sim 2/9$) and the lower bounds are, therefore, improved.

Some numerical investigations, in particular a systematic comparison with the lower bounds obtained with variational methods in (Benslama *et al.*, 1998) for $N=3$ and $N=4$ Coulombian particles will be given elsewhere (Mouchet, 2006).

V. APPLICATION TO DISCRETE HAMILTONIANS

Where $q \in \mathbb{Z}^d$; $d \in \mathbb{N}$; the discretized analog of a local differential operator corresponds to a Hamiltonian that couples at most a finite number of basis vectors (e.g., the nearest neighbors on the lattice $\mathbb{Z}^d$). For instance, when $d=1$, it can be seen as a Hermitian band matrix (finite or infinite) of finite half-width in an appropriate basis. Possibly with renumbering the q's, on $\ell^2(\mathbb{Z}^d)$ H has the form:

$$(H\varphi)_q = \sum_{\substack{\nu \in \mathbb{Z}^d \\ |\nu|_\infty \leqslant N_b}} H_{q,q+\nu}\varphi_{q+\nu}, \tag{26}$$

where $N_b \in \mathbb{N}$, $\forall (q,q') \in \mathbb{Z}^d \times \mathbb{Z}^d$, $H_{q',q} = \bar{H}_{q,q'} \in \mathbb{C}$ and $|\nu|_\infty$ stands for $\max(|\nu_1|,\ldots,|\nu_d|)$. φ will be taken as a discrete set of real strictly positive numbers, and the local energy $E_\varphi(q)$ is computed, for a given q, with elementary algebraic operations whose number is finite and all the smaller than N_b are small: its value at a given q depends on $(2N_b)^d+1$ components of φ at most. Under hypothesis 1,[6] if, say, for a given test vector φ, the absolute maximum of E_φ occurs only at a unique finite q_m, one can immediately improve the upper bound by a finite amount, for instance just by varying φ_{q_m} only, until $E_\varphi(q_m)$ is not an absolute maximum anymore. Only $(2N_b)^d+1$ values of the local energy will be affected by the variation of just one component of φ. One can see easily that this approach leads to a wide variety of algorithms where a sequence of optimization steps is constructed; each step involves a number of optimization parameters and functions that is usually much smaller [of order $(2N_b)^d$ or less] than the dimension of the original matrix.

Discrete Schrödinger operators are important particular cases of Hamiltonians (26) with $N_b = 1$. They are relevant models for the description of quantum (quasi-) particles evolving in periodic crystals. For $d=1$, they can be written as

[6]We have seen at the end of Sec. II A that the symmetry hypothesis can be relaxed.

$$(H\varphi)_q = -\varphi_{q+1} - \varphi_{q-1} + V(q)\varphi_q, \tag{27}$$

where the potential V is a real bounded function on $\mathbb{Z}$. By possibly subtracting a constant positive real number to V, the bounded operator $-H$ can be made positive and ergodic: First, for any positive and non-identically vanishing φ and φ' in $\ell^2(\mathbb{Z})$, $-H\varphi$ remains positive. Second, $\langle\varphi'|(-H)^{|q'-q|}\varphi\rangle = \varphi'_{q'}\varphi_q + (\text{positive terms}) \neq 0$ for any given pair of strictly positive components $\varphi'_{q'}$ and φ_q with $q' \neq q$. [In the marginal case where φ and φ' both vanish everywhere but on the same point, we have $\langle\varphi'|(-H)\varphi\rangle) \neq 0$. Therefore Theorem XIII.43 of (Reed and Simon, 1978a) applies: if H has indeed one eigenvalue, hypothesis 1 is fulfilled for e_0 being the smallest eigenvalue of H. In that case, inequalities (2) takes the following form:

Proposition 5: When the discrete Schrödinger operator (27) *admits at least one eigenvalue and when V is bounded*, *then the smallest eigenvalue* e_0 *is such that*, $\forall\varphi \in \ell^2(\mathbb{Z})$ *such that* $\varphi > 0$,

$$\inf_{q\in\mathbb{Z}}\left(-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} + V(q)\right) \leqslant e_0 \leqslant \sup_{q\in\mathbb{Z}}\left(-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} + V(q)\right). \tag{28}$$

When V is actually a N-periodic real function, the spectral problem (see Reed and Simon, 1978a for instance) leads to the search of complex series $(u_q)_{q\in\mathbb{Z}}$ such that

$$\forall\,\eta = (\eta_1,\eta_2) \in [0;1[^2 \quad \begin{cases} -u_{q+1} - u_{q-1} + V(q+\eta_2)u_q = e(\eta)u_q, \\ u_{q+N} = e^{i2\pi\eta_1}u_q. \end{cases} \tag{29}$$

The spectrum of H is the bounded set $\sigma(H) = \{e(\eta)\,|\,\eta \in [0;1[^2\} \subset \mathbb{R}$. It is given by the reunion for all η's of the N eigenvalues of finite $N\times N$ Hermitian matrices $H^{(\eta)}$ obtained after transforming (29) with the one-to-one mapping $u_q \mapsto u_q \exp(-i2\pi q\eta_1/N)$. As far as positive solutions of (29) are concerned, we will take $\eta_1 = 0$ and will look for the smallest eigenvalue $e_0(\eta_2)$ of

$$H^{(0,\eta_2)} = \begin{pmatrix} V(\eta_2) & -1 & 0 & \cdots & 0 & -1 \\ -1 & V(1+\eta_2) & -1 & 0 & \cdots & 0 \\ 0 & -1 & V(2+\eta_2) & -1 & \cdots & \cdots \\ 0 & \cdots & \cdots & & \cdots & \cdots \\ -1 & 0 & \cdots & 0 & -1 & V(N-1+\eta_2) \end{pmatrix}. \tag{30}$$

Remark 6: The (rational) Harper model (Harper, 1955b; Harper, 1955a) [*also called the almost Mathieu equation (Bellissard and Simon, 1982)*] *corresponds to* $V(q) = -V_0\cos(2\pi qM/N)$ *where* $V_0 > 0$, (M,N) *being strictly positive coprimes integers. For a given N and M*, $\sigma(H)$ *appears to be made of N bands. The union of these bands for each rational number M/N between 0 and 1 produces the so-called Hofstadter butterfly (Hofstadter, 1976).*

We are therefore able to produce two nontrivial bounds on the lowest eigenvalue $e_0(\eta_2)$ without any diagonalization:

Proposition 6: When V is N-periodic, $\forall\eta_2 \in [0;1[$, *the smallest eigenvalue* $e_0(\eta_2)$ *of* (30) *is such that* $\forall\varphi \in (\mathbb{R}^+\backslash\{0\})^N$,

$$\min_{q\in\{0,\ldots,N-1\}}\left(-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} + V(q+\eta_2)\right) \leqslant e_0(\eta_2) \tag{31a}$$

and

$$e_0(\eta_2) \leqslant \max_{q\in\{0,\ldots,N-1\}}\left(-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} + V(q+\eta_2)\right) \tag{31b}$$

(the indices labeling the components of φ *are taken modulo N).*

Therefore, we can bound the bottom of the Hofstadter butterfly with the help of any test function.

Corollary 1: For the rational Harper Hamiltonian

$$H\varphi_q = -\varphi_{q+1} - \varphi_{q-1} - V_0 \cos\left(2\pi q \frac{M}{N}\right)\varphi_q, \tag{32}$$

we have $\forall \varphi \in (\mathbb{R}^+ \backslash \{0\})^N$

$$\min_{q\in\{0,\ldots,N-1\}} \left[-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} - V_0 \cos\left(2\pi q \frac{M}{N}\right) \right] \leqslant \inf[\sigma(H)] \tag{33a}$$

and

$$\inf[\sigma(H)] \leqslant \max_{q\in\{0,\ldots,N-1\}} \left[-\frac{\varphi_{q+1}+\varphi_{q-1}}{\varphi_q} - V_0 \cos\left(2\pi q \frac{M}{N}\right) \right]. \tag{33b}$$

Proof: In the Harper model, for each rational number M/N, the lowest eigenvalue is obtained for $\eta=(0,0)$. It is a direct application of Reed and Simon, 1978a, Theorem XIII.89(e) and thus inequalities (33) follow directly from (31). ■

Choosing for φ, at first guess, semiclassical approximations (i.e., corresponding to large N) constructed from Mathieu functions are therefore expected to provide numerical reasonable bounds.

VI. CONCLUSION

It has been shown on various examples how theorem 1 can be used to obtain rigorous estimates on the principal value of any symmetric operator. Its simplicity, its low cost in computations and its wide domain of applications make the method presented in this article a powerful tool for controlling bounds. In many situations, it provides nontrivial complementary information to those obtained by traditional or more system-dependent methods. Unfortunately, this paper does not extend the method to fermionic systems (see for instance, Sigal, 1995 and references therein) where the spatial wave function of the ground state has generically nontrivial nodes (Ceperley, 1991) that cannot be known *a priori* even with some considerations on symmetries.

This paper presents some clues for further developments of optimization algorithms. However it remains an open question whether such algorithms really bear the potential of an efficient treatment and will overcome the possible difficulties one may face in realistic problems.

ACKNOWLEDGMENTS

The author thanks Laurent Véron for a critical reading of the paper, Evans Harrell for fruitful discussions, Saïd Ilias for providing useful knowledge on references on the generalizations of Barta's inequalities, Emmanuel Lesigne for attracting my attention to the paper by Saff and Kuijlaars, 1997 and Michel Caffarel for the paper by Ceperley, 1991. The author is also grateful to the Laboratoire Kastler Brossel for its warm hospitality.

Avron, J., Herbst, I., and Simon, B., "The Zeeman effect revisted," Phys. Lett. **62A**(4), 214–216. (1977).

Avron, J., Herbst, I., and Simon, B., "Schrödinger operators with magnetic fields. I. General interactions," Duke Math. J. **45**(4), 847–883 (1978).

Barnsley, M. F., "Lower bounds for quantum mechanical energy levels," J. Phys. A **11**(1), 55–68 (1978).

Barnsley, M. F. and Duffin, R. J., "Bounds for the *r*th characteristic frequency of a beaded string or an electrical filter," Proc. Natl. Acad. Sci. U.S.A. **77**(6), 3120–3124 (1980).

Barta, J., "Sur la vibration fondamentale d'une membrane," C. R. Acad. Sci. **204**(7), 472–473 (1937) (in French).

Basdevant, J. L., Martin, A., and Richard, J. M., "Improved bounds on many-body Hamiltonians. I. Self-gravitating bosons," Nucl. Phys. B **343**(1), 60–68 (1990).

Baumgartner, B., "A class of lower bounds for Hamiltonian operators," J. Phys. A **12**(4), 459–467 (1979).

Bellissard, J. and Simon, B., "Cantor spectrum for the almost Mathieu equation," J. Funct. Anal. **48**, 408–419 (1982).

Benslama, A., Metatla, A., Bachkhaznadji, A., Zouzou, S. R., Krikeb, A., Basdevant, J. L., Richard, J. M., and Wu, T. T., "Optimized lower bound for four-body Hamiltonians," Few-Body Syst. **24**(1), 39–54 (1998).

Berestycki, H. and Nirenberg, L., "The principal eigenvalue and maximum principle for second-order elliptic operators in general domains," Commun. Pure Appl. Math. **47**(1), 47–92 (1994).

Bessa, G. P. and Montenegro, J. F., "An extension of Barta's theorem and geometric applications," arXiv: math-ph/0308099 (2004).

Ceperley, D. M., "Fermion nodes," J. Stat. Phys. **63**(5/6), 1237–1267 (1991).

Crandall, R. E. and Reno, M. H., "Ground state energy bounds for potentials $\|x\|^\nu$," J. Math. Phys. **23**(1), 64–70 (1982); **23**, 1737 (1982).

Duffin, R. J., "Lower bounds for eigenvalues," Phys. Rev. **71**, 827–828 (1947).

Fernández, F. M., Ma, Q., and Tipping, R. H., "Eigenvalues fo the Schrödinger equation via the Riccati-Padé method," Phys. Rev. A **40**(11), 6149–6153 (1989).

Fisher, M. E. and Ruelle, D., "The stability of many-particle systems," J. Math. Phys. **7**(2), 260–270 (1966).

Handy, C. R. and Bessis, D., "Rapidly convergent lower bounds for the Schrödinger-equation ground-state energy," Phys. Rev. Lett. **55**(9), 931–934 (1985).

Harper, P. G., "Single band motion of conduction electrons in a uniform magnetic field," Proc. R. Soc. London, Ser. A **68**, 879–892 (1955a).

Harper, P. G., "The general motion of conduction electrons in a uniform magnetic field, with application to the diamagnetism of metals," Proc. R. Soc. London, Ser. A **68**, 874–878 (1955b).

Harrell II, E. M., "Geometric lower bounds for the spectrum of elliptic PDEs with Dirichlet conditions in part" (unpublished).

Helffer, B., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., and Owen, M. P., "Nodal sets for groundstates of Schrödinger operators with zero magnetic fields in a non simply connected domain," Commun. Math. Phys. **202**, 629–649 (1999).

Hofstadter, D. R., "Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields," Phys. Rev. B **14**(6), 2239–2249 (1976).

Lenard, A. and Dyson, F. J., "Stability of matter. I," J. Math. Phys. **8**(3), 423–434 (1967).

Lévy-Leblond, J. M., "Nonsaturation of gravitational forces," J. Math. Phys. **10**(5), 806–812 (1969).

Lieb, E. H., *The Stability of Matter: From Atoms to Stars*, 4th ed. (Springer-Verlag, Berlin, 2005).

Maslov, V. P. and Fedoriuk, M. V., *Semi-Classical Approximation in Quantum Mechanics*, Mathematical Physics and Applied Mathematics, Vol. 7 (D. Reidel, Dordrecht, 1981).

Mouchet, A., "Bounding the ground-state energy of a many-body system with the differential method," Nucl. Phys. A **765**, 319–341 (2006).

Mouchet, A., "A differential method for bounding the ground state energy," J. Phys. A **38**, 1039–1047 (2005).

Protter, M. H. and Weinberger, H. W., "On the spectrum of general second order operators," Bull. Am. Math. Soc. **72**, 251–255 (1966).

Reed, M. and Simon, B., *Analysis of Operators*, Methods of modern mathematical physics, Vol. 4 (Academic, New York, 1978a).

Reed, M. and Simon, B., *Scattering theory*, Methods of modern mathematical physics, Vol. 3 (Academic, New York, 1978b).

Saff, E. B. and Kuijlaars, A. B., "Distributing many points on a sphere," Math. Intell. **19**(1), 5–11 (1997).

Schmutz, M., "The factorization method and ground state energy bounds," Phys. Lett. **108A**(4), 195–196 (1985).

Sigal, I. M., *Lectures on large Coulomb systems, mathematical quantum theory. II. Schödinger operators*, CRM Proceedings and Lecture Notes, Vol. 8 (Amer. Math. Soc., Providence, RI, 1995), pp. 73–107.

Thirring, W., *Quantum Mechanics of Atoms and Molecules*, A Course in mathematical physics, Vol. 3 (Springer-Verlag, New York, 1979).