Gershgorin radii as natural bounds for the correlation energies

A. Odriazola[a1]

[1]School of Electrical, Computer, and Energy Engineering, Arizona State University, Tempe, AZ 85287, USA

We investigate yet another direct link between linear algebra and electronic structure theory by exploring the usefulness of the Gershgorin theorem in the estimation of the correlation energies of many-particle systems.

The calculation of the eigenvalues of arbitrary matrices is a routine activity in today's science. However, it is a fundamentally complex problem and, in most cases, a very demanding one from the computational point of view. Therefore, to obtain good estimates of the eigenvalues is of vital importance.

In this work we investigate another direct link between linear algebra and electronic structure theory by exploring the usefulness of the Gershgorin theorem [1] in the estimation of the correlation energies E_c of many-particle systems. We focus on a particular class of systems, two-dimensional quantum dots (2DQDs), and perform extensive numerical calculations. We find that, indeed, the Gershgorin radii $R_{\rm G}$ constitute *natural* bounds for the correlation energies though – unfortunately – very loose bounds.

The Gershgorin theorem

The most crude estimate of the eigenvalues of a matrix A is given by the inequality $\rho(A) \leq ||A||$, where $\rho(A) = \max|\lambda| \;\; with \;\; \lambda \in \sigma(A)$, is known as the spectral radius of A. This estimate, although useful in many cases, is not very accurate in terms of the location of the eigenvalues of A. Gersgorin's theorem goes further in this direction. Let us recall:

Theorem 1 *Let $A = a_{i,j}$ be an arbitrary $n \times n$ matrix and let us define the disks $\mathcal{D}_i$ by $\mathcal{D}_i = \{z \in \mathbb{C} : |z - a_{i,i}| \leq r_i\}$, where $r_i = \sum_{i \neq j} |a_{i,j}|$ with $1 \leq i \leq n$. Then*

$$\lambda \in \bigcup_{i=1}^{n} \mathcal{D}_i \tag{1}$$

for every eigenvalue λ of A. Furthermore, if S is the union set of m disks which are disjoint from the other $n - m$ disks, then S contains exactly m eigenvalues of A.

Now, let us analyze the structure of the Full Configuration Interaction (FCI) matrix but taking into account the definition of the correlation energy $E_c = E_{\rm gs} - E_{\rm HF}$. That is, the difference between the total ground-state energy and the Hartree-Fock energy. Fig. 1 shows its general structure. Note that the matrix is Hermitian, therefore only the upper triangle is shown.

It is easy to realize that if (i) we use a Hartree-Fock basis, $|\Phi_0\rangle = |{\rm HF}\rangle$, and (ii) we apply the Gershgorin Theorem to the first eigenvalue of the FCI matrix (See Fig. 1), then we can associate the correlation energy E_c to the first Gershgorin radius. That is

$$\begin{array}{c} \\ \langle\Phi_0| \\ \langle S| \\ \langle D| \\ \langle T| \\ \vdots \end{array} \begin{array}{c} \begin{array}{ccccc} |\Phi_0\rangle & |S\rangle & |D\rangle & |T\rangle & \dots \end{array} \\ \begin{pmatrix} E_0 & \mathbf{0} & \int \Phi_0 \hat{H} D & \mathbf{0} & \dots \\ & \int S \hat{H} S & \int S \hat{H} D & \int S \hat{H} T & \dots \\ & & \int D \hat{H} D & \int D \hat{H} T & \dots \\ & & & \int T \hat{H} T & \dots \\ & & & & \ddots \end{pmatrix} \end{array}$$

Figure 1: Structure of the full-CI matrix. Singly, doubly, triply, and highly excited determinants are denoted as $|S\rangle$, $|D\rangle$, $|T\rangle$, etc.

$$|E_c| < \sum_{j=1}^{{\rm Dim}(D)} D_{1,j}, \tag{2}$$

where we use the shorthand notation D and ${\rm Dim}(D)$ to denote the submatrix $\int \Phi_0 \hat{H} D$ and its dimension, respectively. The sum in Eq. (2) runs over all elements of the submatrix D. Let us recall that, in a scheme of FCI, there is no mixture of HF with excitations higher than $|D\rangle$, which means that the higher excitation sectors ($|T\rangle$, $|Q\rangle$, etc), contain only null elements.

According to Eq. (2), the (first) Gershgorin radius is a *natural* (mathematical) bound for the (ground-state) correlation energy. However, it cannot be said – a priori – how *tight* this bound is. Therefore, our next steps are 1) to study how the Gershgorin radii depends on the perameters defining our system and, 2) to determine under which conditions – if any – they provide useful estimates of the correlation energies.

Numerical results

In order to evaluate the quality of the above bounds, we consider a concrete model system. We compute the correlation energy and the first Gershgorin radius, R_G, of two-dimensional parabolic quantum dots with different number of electrons and different confinements strengths. For the calculation of $R_{\rm G}$, we use our own implementation of a truncated CI scheme (up to the singles-and-doubles excitation level) [2].

The starting point is the Hartree-Fock solution of the problem. Then a basis of functions made up from (i) the Hartree-Fock state, $|{\rm HF}\rangle$, (ii) one-particle one-hole (1p1h) excitations, that is $|\sigma\mu\rangle = e^{\dagger}_{\sigma} e_{\mu} |{\rm HF}\rangle$,

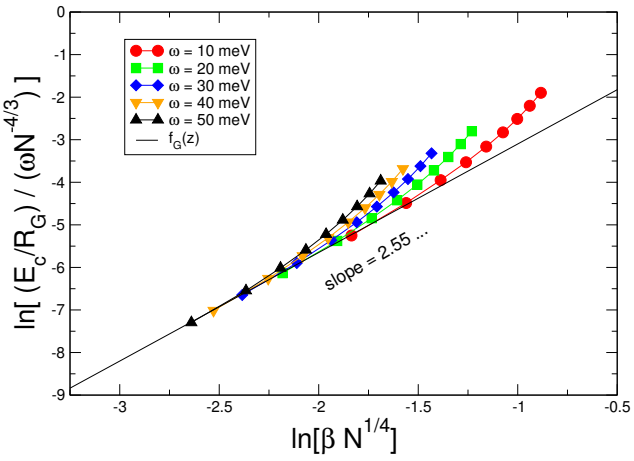

Figure 2: An *approximate* scaling relation of the ratio $E_c/R_{\rm G}$ as a function of $z = \beta N^{1/4}$ (see main text). The deviations observed for large-N systems are a consequence of the basis truncation at double-excitations level.

and (iii) two-particle two-hole (2p2h) excitations, i.e. $|\sigma\rho,\mu\lambda\rangle = e^\dagger_\sigma e^\dagger_\rho e_\mu e_\lambda|{\rm HF}\rangle$; is used in order to diagonalize the Hamiltonian. Note that $e(e^\dagger)$ are the annihilation (creation) operators while $\sigma < \rho$ are single-particle states above the Fermi level, and $\mu < \lambda$ are states below the Fermi level. The explicit matrix elements are given in Ref. [2].

We computed values of $R_{\rm G}$ of QDs with $N = 2, 6, 12, 20, 30, 42, 56, 72$ and 90 electrons, and confinement strengths $\hbar\omega = 10, 20, 30, 40$ and 50 meV. GaAs parameters for the electron efective mass ($m = 0.067\ m_0$) and dielectric constant ($\epsilon = 12.8$) were used in the calculations. Notice that all the systems considered here are closed-shell quantum dots with ground-state angular momentum and spin quantum numbers $L = S = 0$. As a reference, we also compute values of E_c based on an accurate Variational Monte Carlo (VMC) approach [3, 4].

We compared the VMC-based reference values of E_c to the corresponding Gershgorin radii and we found similar qualitative trends, i.e., in a logarithmic scale, the values of both E_c and $R_{\rm G}$ show a linear dependence on the particle number. In the case of $R_{\rm G}$, we observe a deviation from the linear behavior in the large-N region. Such deviations can be explained as the effects of the truncation of the basis in our CI scheme. The main difference, however, is quantitative: $R_{\rm G}$ being about three orders of magnitude larger than the corresponding values of E_c. This numerical difference makes $R_{\rm G}$ useless in terms of chemical accuracy.

Even though the Gershgorin radii do not constitute reasonably tight bounds for the correlation energies of the systems considered, we show that both magnitudes may be related by some kind of *scaling law* of the type reported in previous works [2]. To this end, we assume a relation of the form

$$\frac{E_c}{R_{\rm G}} \sim (\hbar\omega)^{\alpha_R} N^{\beta_R} f_{\rm G}(z), \tag{3}$$

where α_R and β_R are numerical constants, and $z = \beta N^{1/4}$ is the interaction coupling parameter ($\beta \propto (\hbar\omega)^{-1/2}$ being the ratio between the Coulomb energy and the harmonic confinement) [2].

From our numerical data we find that, in a logarithmic scale, the scaled ratio E_c/R_G is a linear function of z:

$$\ln\left(\frac{E_c/R_G}{\hbar\omega N^{4/3}}\right) \approx a\ln(z) + b, \tag{4}$$

where $a = 2.55$ and $b = 0.55$ are obtained from a fit to the small-N systems (see Fig. 2). The expression in Eq. (4), after some algebra, can be written in a compact form $E_c = K\ R_{\rm G}$, where the coefficient K is a function of N and $\hbar\omega$:

$$K(\hbar\omega, N) = e^b\ (\hbar\omega)^{\frac{2-a}{2}}\ N^{\frac{3a-16}{12}}. \tag{5}$$

The scaling law shown in Fig. 2 was found "empirically", and a rigorous proof of this relation is yet to be found. However, improved values of all numerical parameters can be achieved by including larger data sets.

Conclusions

Our results imply that, (i) in the first approximation the first Gershgorin radius does not provide a tight enough bound for the correlation energy of 2DQDs, but (ii) both quantities can be numerically related by means of scaling law. These conclusions apply only to a particular class of systems (2DQDs) and the situation can differ in different systems. This possibility, in our opinion, is what makes the problem worth exploring: the promise of finding – with a highly parallelizable recipe – good estimates of the eigenvalues without diagonalising the matrix, even when the so-called chemical accuracy requires this bounds to be extremely sharp.

Notes

a. Email: aodriazo@asu.edu (On leave: *mere association*)

References

[1] S. Gerschgorin, Über die Abgrenzung der Eigenwerte einer Matrix, *Izv. Akad. Nauk. USSR Otd. Fiz.-Mat. Nauk (in German),* **6** (1931) 749

[2] A. Odriazola, A. Delgado and A. Gonzalez, *Phys. Rev. B,* **78** (2008) 205320

[3] A. Harju, *J. Low Temp. Physics,* **140** (2005) 181

[4] A. Odriazola, *Scaling Approaches to Quantum Many-Body Problems,* Tampere University of Technology. Publication Vol. 1525 (2017)