Modified Thomson problem

Jerzy Cioslowski
Institute of Physics, University of Szczecin, Wielkopolska 15, 70-451 Szczecin, Poland
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The modified Thomson problem, which concerns an assembly of N particles mutually interacting through a Coulombic potential and subject to a Coulombic-harmonic confinement, is introduced. For sufficiently strong confinement strengths M, properties of its solutions (such as the energy and the particle positions at the minimum, and the corresponding zero-point vibrational energy) are accurately estimated by expressions dependent on only a few quantities pertaining to the original Thomson problem [such as the energy $E_{\mathrm{Th}}(N)$] and the reduced confinement strength $\xi = \frac{NM}{E_{\mathrm{Th}}(N)}$. For $N \leq 12$, this regime of the perturbed Thomson problem persists for all non-negative values of ξ. On the other hand, the perturbed spherical Coulomb crystal regime emerges for $\xi < \xi_{\mathrm{crit}}(N)$ and larger numbers of particles. For $13 \leq N \leq 22$, the transition that delineates these two regimes is due to the existence of two energy minima, the crystal-like one becoming global for sufficiently weak confinements. For $N \geq 23$, the transition involves a catastrophe brought about by the vanishing of one of the Hessian matrix eigenvalues, the value of $\xi_{\mathrm{crit}}(N)$ being related to the magnitude of radial instability in the corresponding solution of the original Thomson problem.

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I. INTRODUCTION

The celebrated Thomson problem [1] concerns determining the optimum arrangement of N equally charged particles confined to a sphere with a unit radius that interact through a Coulombic potential, i.e., finding the global minimum $E_{\mathrm{Th}} \equiv E_{\mathrm{Th}}(N)$ of

$$V_{\mathrm{Th}}(N) = \sum_{i>j=1}^{N} r_{ij}^{-1} \tag{1}$$

with respect to $\{\vec{r}_i\} \equiv \{\vec{r}_i(N)\}$, subject to the constraint of

$$\forall_i \, r_i = 1. \tag{2}$$

Although no general solution of the Thomson problem is known at present, significant inroads into understanding of the large-N asymptotics of E_{Th} (and also of analogous expressions arising from other power-law potentials) have been made [2,3]. Energy minima that are believed to be global have been published for all $N \leq 400$ and also for some larger numbers of particles [4].

The significance of the Thomson problem stems from not only its mathematical appeal but also its relevance to various physical systems. In particular, its solutions are employed in the construction of an accurate model of spherical Coulomb crystals [5]. However, the two-dimensional nature of the Thomson problem renders its use inappropriate in instances where radial motions are important, e.g., in estimation of the zero-point vibrational energies of particles interacting with spherically symmetrical external potentials.

In this paper, we introduce a modified Thomson problem that offers a connection between its original counterpart and the concept of a spherical Coulomb crystal. Solutions of this problem are well-defined global minima on $3N$-dimensional potential-energy hypersurfaces that are associated with positive-semidefinite Hessians. As such, they are ideally suited as building blocks from which more complicated systems can be readily assembled.

II. MODIFIED THOMSON PROBLEM

A spherical Coulomb crystal constitutes an equilibrium configuration of N particles interacting through the potential [5–8]

$$V_{\mathrm{SCC}}(N) = \frac{2}{3} \sum_{i>j=1}^{N} r_{ij}^{-1} + \frac{N}{3} \sum_{i=1}^{N} r_i^2. \tag{3}$$

Such assemblies of particles are encountered in a surprisingly wide array of physical problems [9–11].

In order to devise a mathematical model that allows for a continuous interpolation between the Thomson problem and spherical Coulomb crystal limits, one has to augment $V_{\mathrm{Th}}(N)$ with a term that assures asymptotic confinement to the surface of a unit sphere and reduces to a (scaled) harmonic potential for large and vanishing confinement strengths, respectively. This objective is accomplished by considering a spherical Coulomb crystal with $N+M$ particles and then partitioning the potential energy $V_{\mathrm{SCC}}(N+M)$ into the contribution due to interactions among M particles and the remainder $\frac{2}{3} V(N,M) + \frac{N}{3} \sum_{i=1}^{N} r_i^2$. At the limit of the M particles confined to the origin of the coordinate system, $V(N,M)$ becomes

$$V_{\mathrm{MTh}}(N,M) = \sum_{i>j=1}^{N} r_{ij}^{-1} + M \sum_{i=1}^{N} \left(r_i^{-1} + \frac{1}{2} r_i^2 \right). \tag{4}$$

It can be easily shown [see Eqs. (8) and (17) in Secs. II A and II B of this paper] that $V_{\mathrm{MTh}}(N,M)$ indeed conforms to the aforementioned limits.

Potential-energy expression (4) defines the modified Thomson problem that differs from its original counterpart by the addition of the Coulombic-harmonic confinement term with M acting as the confinement strength. Its solution corresponds to finding the global minimum $E_{\mathrm{MTh}} \equiv E_{\mathrm{MTh}}(N,M)$ of $V_{\mathrm{MTh}}(N,M)$ with respect to $\{\vec{r}_i\} \equiv \{\vec{r}_i(N,M)\}$.

A. Large-M limit and the upper bound to $E_{\mathrm{MTh}}(N,M)$

At the limit of $M \to \infty$, the Coulombic-harmonic confinement term constraints the particles to the surface of a unit sphere, which implies vanishing relaxation of the particle positions from those pertaining to the original Thomson problem. Consequently, since any configuration of particles possesses potential energy greater or equal to that corresponding to the global minimum, setting

$$\forall_i \, r_i = R \tag{5}$$

affords an upper bound $\tilde{E}_{\mathrm{MTh}}(N,M)$ to $E_{\mathrm{MTh}}(N,M)$ that is asymptotically exact. Inserting Eq. (5) into Eq. (4) produces

$$\begin{aligned} E_{\mathrm{MTh}}(N,M) &\leq \tilde{E}_{\mathrm{MTh}}(N,M) \\ &= \min_R \left(\frac{E_{\mathrm{Th}} + NM}{R} + \frac{NM}{2} R^2 \right) \\ &= \frac{3}{2} E_{\mathrm{Th}} \, \xi^{1/3} (1+\xi)^{2/3}, \end{aligned} \tag{6}$$

where

$$\xi \equiv \xi(N,M) = \frac{NM}{E_{\mathrm{Th}}} \tag{7}$$

is the reduced confinement strength. The respective minimum is attained at

$$R \equiv R(N,M) = \xi^{-1/3} (1+\xi)^{1/3}. \tag{8}$$

For large M, $\tilde{E}_{\mathrm{MTh}}(N,M)$ tends to $(1+\frac{3}{2}\xi)E_{\mathrm{Th}}$, which, as expected, equals the sum of E_{Th} and $\frac{3}{2}NM$, the latter term being simply the confinement energy of N particles located at the surface of a unit sphere.

Inspection of the data produced by extensive energy minimizations (commencing for each N with the solution of the original Thomson problem and involving a series of quadratic searches with exact Hessian diagonalizations and inversions for gradually decreasing values of M) reveals that the bound given by Eq. (6) is remarkably tight (see Fig. 1). The energy difference $\Delta E_{\mathrm{MTh}} \equiv \Delta E_{\mathrm{MTh}}(N,M) = E_{\mathrm{MTh}}(N,M) - \tilde{E}_{\mathrm{MTh}}(N,M)$ arises from the particle-position relaxation, the displacements possessing both radial (parallel to the vectors $\{\vec{r}_i\}$) and angular (perpendicular to $\{\vec{r}_i\}$) components. An accurate approximation to ΔE_{MTh} is readily derived by analyzing the leading term in the Hessian $\mathbf{H}_{\mathrm{MTh}}(N,M)$ at the minimum.

The Hessian $\mathbf{H}_{\mathrm{MTh}}(N,M)$ is given by the sum of the pairwise-interaction contribution $\mathbf{H}_{\mathrm{pair}}(N,M)$ and the contribution $M\mathbf{H}_{\mathrm{conf}}(N,M)$ due to the confinement term,

$$\mathbf{H}_{\mathrm{MTh}}(N,M) = \mathbf{H}_{\mathrm{pair}}(N,M) + M\mathbf{H}_{\mathrm{conf}}(N,M). \tag{9}$$

The matrix $\mathbf{H}_{\mathrm{conf}}(N,M)$ has the eigenvalues of $\{1+2r_i^{-3}, 1-r_i^{-3}, 1-r_i^{-3}\}$. Thus, for each i, there is a pair of degenerate eigenvalues that correspond to eigenvectors perpendicular to $\{\vec{r}_i\}$ and a single eigenvalue associated with the parallel eigenvector. Application of the similarity transformation that diagonalizes $\mathbf{H}_{\mathrm{conf}}(N,M)$ to Eq. (9) yields

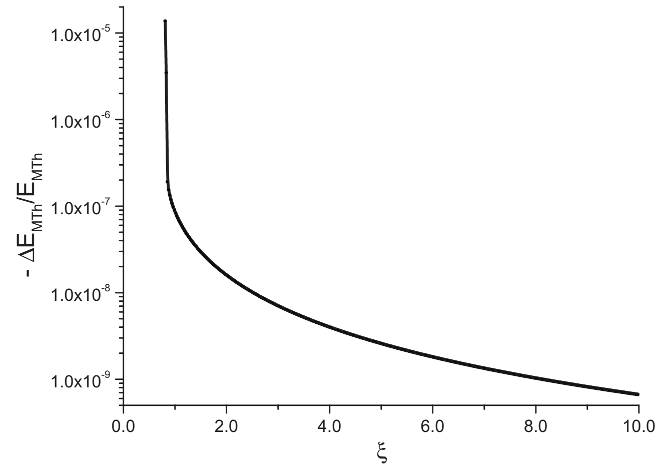

FIG. 1. The dependence of the relative error of upper bound (6) on ξ for $N=100$.

$$\tilde{\mathbf{H}}_{\mathrm{MTh}}(N,M) = \tilde{\mathbf{H}}_{\mathrm{pair}}(N,M) + M\tilde{\mathbf{H}}_{\mathrm{conf}}(N,M), \tag{10}$$

where the eigenvalues of $\tilde{\mathbf{H}}_{\mathrm{MTh}}(N,M)$ are the same as those of $\mathbf{H}_{\mathrm{MTh}}(N,M)$.

Since solving the original Thomson problem implies finding the optimum angular particle positions, the energy gradient at the point given by constraint (5) possesses only the radial components. At the $M \to \infty$ limit, the respective block of $\tilde{\mathbf{H}}_{\mathrm{MTh}}(N,M)$ is dominated by the $M\tilde{\mathbf{H}}_{\mathrm{conf}}(N,M)$ diagonal contribution with the N-tuply degenerated eigenvalues of $M(1+2R^{-3})$. Consequently, by virtue of the quadratic approximation (according to which the relaxation energy equals one-half of the product of the transposed energy gradient, the inverse of the energy Hessian, and the energy gradient),

$$\Delta E_{\mathrm{MTh}} \approx -\frac{1}{2} M^{-1} (1+2R^{-3})^{-1} \sum_{i=1}^{N} \left(\frac{\partial E_{\mathrm{MTh}}}{\partial r_i} \right)^2 \tag{11}$$

and

$$\Delta r_i \equiv \Delta r_i(N,M) \approx -M^{-1}(1+2R^{-3})^{-1} \frac{\partial E_{\mathrm{MTh}}}{\partial r_i}. \tag{12}$$

The energy derivatives that enter Eqs. (11) and (12) are given by

$$\frac{\partial E_{\mathrm{MTh}}}{\partial r_i} = -\frac{E_{\mathrm{Th}}}{N} R^{-2} \gamma_i, \tag{13}$$

where

$$\gamma_i \equiv \gamma_i(N) = -1 + \frac{N}{2E_{\mathrm{Th}}} \sum_{j \neq i}^{N} r_{ij}^{-1} \tag{14}$$

measures the deviation of the ith particle contribution to E_{Th} from its mean value, the interparticle distances $\{r_{ij}\}$ referring to the original N-particle Thomson problem.

Combining Eqs. (5), (7), and (11)–(14) affords

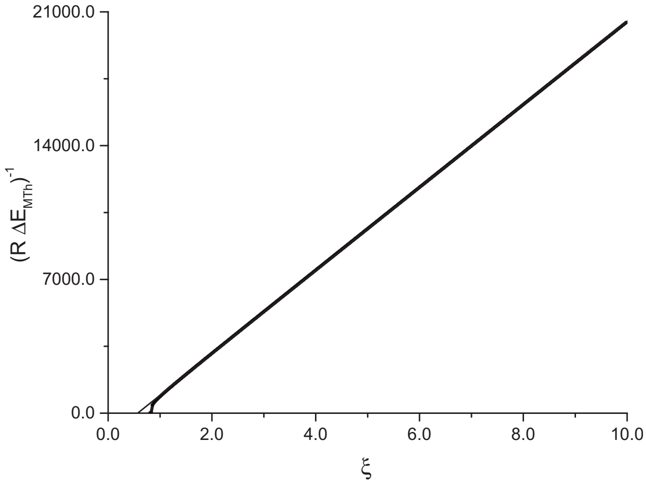

FIG. 2. The dependence of $(R\Delta E_{\mathrm{MTh}})^{-1}$ on ξ for $N=100$. The thin straight line has the theoretical slope of 2164.2.

$$\Delta E_{\mathrm{MTh}} \approx -\frac{E_{\mathrm{Th}}}{2N} R^{-1}(1+3\xi)^{-1} \sum_{i=1}^{N} \gamma_i^2 \tag{15}$$

and

$$\Delta r_i \approx R(1+3\xi)^{-1}\gamma_i. \tag{16}$$

Accordingly, one expects the plots of $(R\Delta E_{\mathrm{MTh}})^{-1}$ and $\frac{R}{\Delta r_i}$ vs ξ to be straight lines with the slopes of $\frac{6N}{E_{\mathrm{Th}}}(\sum_{i=1}^{N}\gamma_i^2)^{-1}$ and $3\gamma_i^{-1}$, respectively. Inspection of Figs. 2 and 3 confirms this theoretical prediction. One should note that the particle-position relaxation is absent in highly symmetrical cases (i.e., for $N=2$, 3, 4, 6, 8, 12, and 24) where all the members of the set $\{\gamma_i\}$ equal zero.

B. $M=0$ limit and the transition to a spherical Coulomb crystal

As revealed by the scaling $\vec{r}_i=(\frac{N}{M})^{1/3}\vec{r}_i'$ that brings Eq. (4) into

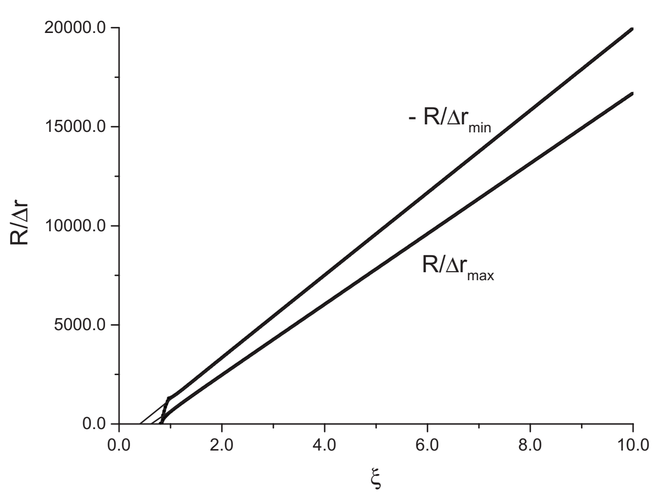

FIG. 3. The dependences of $-\frac{R}{\Delta r_{\mathrm{min}}}$ and $\frac{R}{\Delta r_{\mathrm{max}}}$ on ξ for $N=100$. The thin straight lines have the theoretical slopes of 2074.9 and 1775.3, respectively.

$$V_{\mathrm{MTh}}(N,M) = \frac{3}{2}\left(\frac{M}{N}\right)^{1/3} \times \left(\frac{2}{3}\sum_{i>j=1}^{N} r_{ij}'^{-1} + \frac{N}{3}\sum_{i=1}^{N} r_i'^2 + \frac{2M}{3}\sum_{i=1}^{N} r_i'^{-1}\right), \tag{17}$$

the modified Thomson problem is also a modified spherical Coulomb crystal problem. In other words, solving the modified Thomson problem for $M=0$ is equivalent to finding the particle positions of the respective spherical Coulomb crystal. This observation implies the existence of two regimes, namely, that of the large-M perturbed Thomson problem solutions characterized by single "thick-shell" particle configurations and that of the small-M perturbed spherical Coulomb crystals, which are known to possess multishell structures for all $N>12$ [5–8]. The transition between these two regimes can be due to either a catastrophe involving radial instability precipitated by a vanishing Hessian eigenvalue or the existence of two distinct minima, each associated with one regime, that become equienergetic for some value of M.

Indeed, numerical data, such as those displayed in Figs. 1–3, clearly demonstrate the presence of a transition that is accompanied by sudden departures of the computed ΔE_{MTh}, and the most negative and positive radial displacements (Δr_{min} and Δr_{max}) from their estimates provided by Eqs. (15) and (16). One should note that the validity of these estimates throughout the entire perturbed Thomson problem regime implies insensitivity of the Hessian matrix eigenvalues to the radial particle-position relaxation and a negligible contribution of its angular counterpart.

Neglecting the effect of the radial relaxation on the Hessian eigenvalues allows for a simple scaling argument that yields

$$\mathbf{H}_{\mathrm{pair}}(N,M) = \xi(1+\xi)^{-1}\mathbf{H}_{\mathrm{Th}}(N), \tag{18}$$

where $\mathbf{H}_{\mathrm{Th}}(N)$ is the Hessian matrix of the original N-particle Thomson problem. Consequently, the eigenvalues $\{\epsilon_i\}\equiv\{\epsilon_i(N,M)\}$ of $\mathbf{H}_{\mathrm{MTh}}(N,M)$ are found to behave approximately like $\{\frac{\xi\chi_i^{\parallel}+M(1+3\xi)}{1+\xi}, \frac{\xi\chi_i^{\perp 1}+M}{1+\xi}, \frac{\xi\chi_i^{\perp 2}+M}{1+\xi}\}$, where $\{\chi_i^{\parallel}\}\equiv\{\chi_i^{\parallel}(N)\}$, $\{\chi_i^{\perp 1}\}\equiv\{\chi_i^{\perp 1}(N)\}$, and $\{\chi_i^{\perp 2}\}\equiv\{\chi_i^{\perp 2}(N)\}$ are the respective eigenvalues of the radial and angular blocks of $\tilde{\mathbf{H}}_{\mathrm{Th}}(N)$ [which is related to $\mathbf{H}_{\mathrm{Th}}(N)$ through the similarity transformation mentioned in Sec. II A]. By virtue of the first-order perturbation theory, $\{\chi_i^{\parallel}\}$ equal the diagonal elements of the radial block of $\tilde{\mathbf{H}}_{\mathrm{Th}}(N)$.

The above considerations provide a simple estimate of $\xi_{\mathrm{crit}}\equiv\xi_{\mathrm{crit}}(N)$ at which the transition of the first type occurs, i.e., the value of ξ at which the smallest eigenvalue of the radial block of $\tilde{\mathbf{H}}_{\mathrm{MTh}}(N,M)$ vanishes, obliterating the radial stability of the thick-shell particle configuration that persists throughout the perturbed Thomson problem regime. Let

$$\eta \equiv \eta(N) = \min_i \left(1 + \frac{N\chi_i^{\parallel}}{E_{\mathrm{Th}}}\right). \tag{19}$$

Setting $\min_i \frac{\xi\chi_i^{\parallel}+M(1+3\xi)}{1+\xi}$ to zero readily yields $\xi_{\mathrm{crit}}=-\eta/3$. The dependence of η on N is displayed in Fig. 4. The values of η

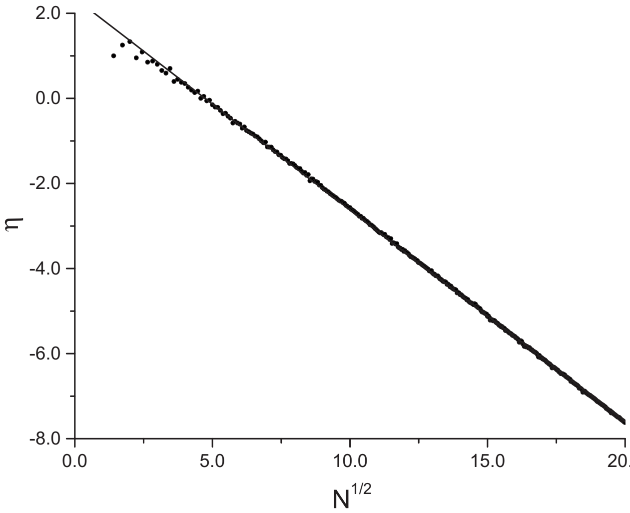

FIG. 4. The dependence of the minimum eigenvalue η on $N^{1/2}$ for $2 \leq N \leq 400$. The straight line is given by the least-squares fit of $\eta = 2.355 \pm 7 - 0.4978 \pm 5\, N^{1/2}$.

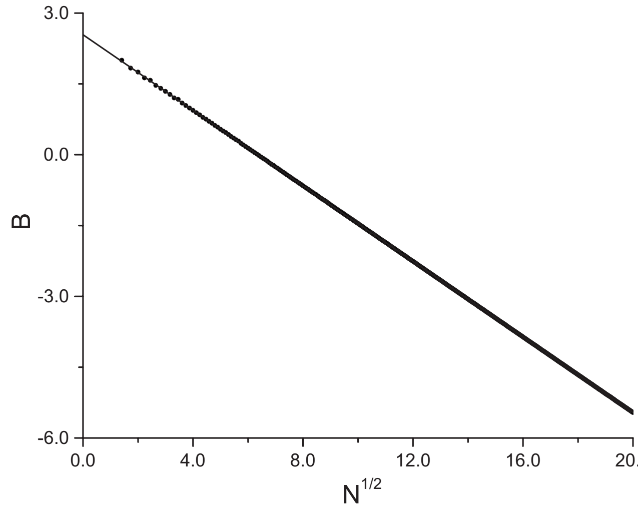

FIG. 5. The dependence of the parameter B on $N^{1/2}$ for $2 \leq N \leq 400$. The straight line is given by the least-squares fit of $B = 2.5423 \pm 4 - 0.400\,09 \pm 2\, N^{1/2}$.

correlate well with $N^{1/2}$, although considerable scatter is present, especially for smaller values of N. They are found to be positive for all $N < 23$, implying that the solutions of the modified Thomson problem with fewer than 23 particles undergo transitions of the second type that do not involve catastrophe due to radial instability.

C. Zero-point vibrational energy

Being global minima, solutions of the modified Thomson problem are associated with positive-semidefinite Hessians and thus well-defined zero-point vibrational energies,

$$\varepsilon_{\mathrm{MTh}}(N,M) = \frac{1}{2} \sum_{i=1}^{3N} \epsilon_i^{1/2}, \tag{20}$$

knowledge of which allows for estimation of vibrational properties of complex systems that can be approximated by assemblies of particle configurations individually minimizing $V_{\mathrm{MTh}}(N,M)$. Upon neglect of the particle-position relaxation discussed in Sec. II B of this paper, $\varepsilon_{\mathrm{MTh}}(N,M)$ can be readily calculated by replacing the exact values of $\{\epsilon_i\}$ with those of the set $\{\frac{\xi \chi_i^{\parallel} + M(1+3\xi)}{1+\xi}, \frac{\xi \chi_i^{\perp 1} + M}{1+\xi}, \frac{\xi \chi_i^{\perp 2} + M}{1+\xi}\}$, which yields

$$\begin{aligned} \varepsilon_{\mathrm{MTh}}(N,M) &= \frac{1}{2}\left(\frac{\xi}{1+\xi}\right)^{1/2} \sum_{i=1}^{N} \left\{ \left[\chi_i^{\parallel} + \frac{E_{\mathrm{Th}}}{N}(1+3\xi) \right]^{1/2} \right. \\ &\quad \left. + \left(\chi_i^{\perp 1} + \frac{E_{\mathrm{Th}}}{N} \right)^{1/2} + \left(\chi_i^{\perp 2} + \frac{E_{\mathrm{Th}}}{N} \right)^{1/2} \right\} \\ &= N \left(\frac{3M}{2} \right)^{1/2} F(\xi). \end{aligned} \tag{21}$$

The function $F(\xi) \equiv F(N,\xi)$ that enters the above equation possesses the large-ξ asymptotics of

$$F(\xi) = \sqrt{\frac{\xi}{2+2\xi}} \left(1 + \frac{A}{\sqrt{3}} \xi^{-1/2} + \frac{B}{6} \xi^{-1} + \cdots \right), \tag{22}$$

where

$$A \equiv A(N) = \frac{1}{N} \sum_{i=1}^{N} \left[\left(1 + \frac{N}{E_{\mathrm{Th}}} \chi_i^{\perp 1} \right)^{1/2} + \left(1 + \frac{N}{E_{\mathrm{Th}}} \chi_i^{\perp 2} \right)^{1/2} \right] \tag{23}$$

and

$$B \equiv B(N) = 1 + \frac{1}{E_{\mathrm{Th}}} \sum_{i=1}^{N} \chi_i^{\parallel}. \tag{24}$$

Computation of B involves evaluating the trace of the radial block of $\mathbf{H}_{\mathrm{Th}}(N)$. After some straightforward algebra, one obtains

$$B = \frac{5}{2} - \frac{2}{E_{\mathrm{Th}}} \sum_{i>j=1}^{N} r_{ij}^{-3}, \tag{25}$$

where the interparticle distances $\{r_{ij}\}$ refer to the original N-particle Thomson problem. Upon employing the results of Kuijlaars and Saff [2] for the sum of reciprocal cubes of the interparticle distances, the leading asymptotics of B are readily recovered as

$$\begin{aligned} \lim_{N\to\infty} \frac{B}{N^{1/2}} &= -(32\pi^3)^{-1/2}\, 3^{1/4}\, \zeta\left(\frac{3}{2},0\right) \left[\zeta\left(\frac{3}{2},\frac{2}{3}\right) - \zeta\left(\frac{3}{2},\frac{1}{3}\right) \right] \\ &\approx -0.399\,256, \end{aligned} \tag{26}$$

where $\zeta(s,a)$ is the generalized Riemann zeta function. The plot of B vs $N^{1/2}$ (Fig. 5) is in a remarkable agreement with this result, the slope closely matching the theoretical prediction and the deviation of the intercept from $\frac{5}{2}$ being due to higher-order terms in the large-N asymptotics of the pertinent sums. On the other hand, although A is found to scale like

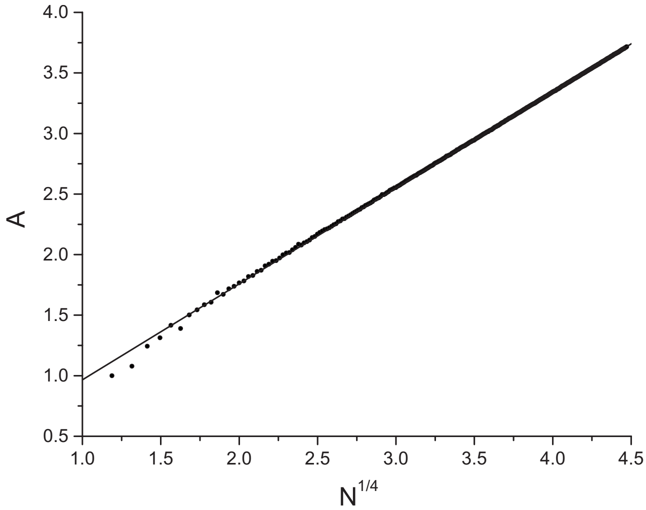

FIG. 6. The dependence of the parameter A on $N^{1/4}$ for $2 \leq N \leq 400$. The straight line is given by the least-squares fit of $A = 0.174 \pm 3 + 0.7925 \pm 8\, N^{1/4}$.

$N^{1/4}$ (Fig. 6), no closed-form expression analogous to Eq. (26) can be easily obtained.

In the highly symmetrical cases that are devoid of the particle-position relaxation, Eq. (21) is exact. In particular,

$$F(2,\xi) = \frac{2+\sqrt{3+3\xi}+\sqrt{1+3\xi}}{2\sqrt{6+6\xi}}, \tag{27}$$

$$F(3,\xi) = \frac{1+\sqrt{3+3\xi}+\sqrt{10+12\xi+4\sqrt{6+15\xi}}}{3\sqrt{6+6\xi}}, \tag{28}$$

and

$$F(4,\xi) = \frac{2\sqrt{3}+2\sqrt{3+3\xi}+3\sqrt{10+12\xi+4\sqrt{6+14\xi}}}{8\sqrt{6+6\xi}}. \tag{29}$$

Interestingly, upon appropriate scaling and shifting, the plots of $F(2,\xi)$, $F(3,\xi)$, and $F(4,\xi)$ match very closely. This observation suggests the existence of a universal (although approximate) scaling of the form

$$F(\xi) = \frac{1}{\sqrt{2}} + \left(F_{\max} - \frac{1}{\sqrt{2}}\right)\Phi[\lambda(\xi - \xi_{\max})], \tag{30}$$

where $F(\xi)$ is the exact (i.e., including the particle-position relaxation) function calculated from $\varepsilon_{\mathrm{MTh}}(N,M)$ according to Eq. (21), $F_{\max} \equiv F_{\max}(N)$ is the value of $F(\xi)$ at the maximum of $\xi_{\max} \equiv \xi_{\max}(N)$, and

$$\lambda \equiv \lambda(N) = 3A^{-2}(\sqrt{2}F_{\max} - 1)^2 \tag{31}$$

is the scaling factor that yields the large-t asymptotics of

$$\Phi(t) = t^{-1/2} + Ct^{-1} + \cdots. \tag{32}$$

Examination of over 47 000 points computed for $2 \leq N \leq 400$ and various values of M that lie within the perturbed Thomson problem regime confirms the approximate validity of Eq. (30) (Fig. 7). When the simplest closed-form universal function

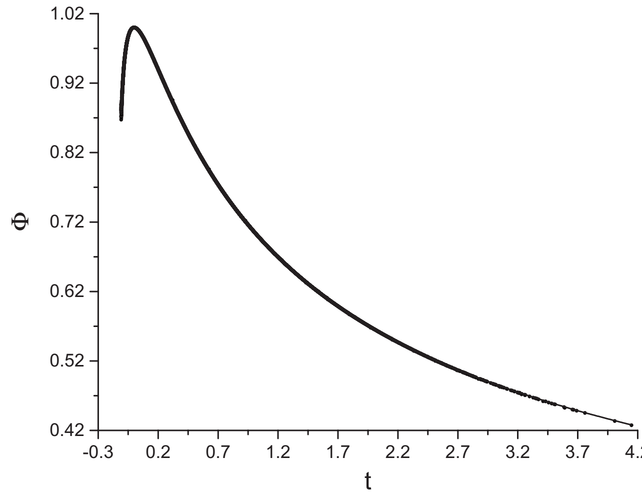

FIG. 7. The approximate universality of the dependence of $\Phi(t) = [F(\xi) - \frac{1}{\sqrt{2}}]/(F_{\max} - \frac{1}{\sqrt{2}})$ on $t = \lambda(\xi - \xi_{\max})$. The solid line corresponds to the function $\Phi(t)$ given by Eq. (33).

$$\Phi(t) = \frac{1+\sqrt{3}}{2}\,\frac{2+\sqrt{1+2(2+\sqrt{3})t}-\sqrt{3+2(2+\sqrt{3})t}}{\sqrt{3+2(2+\sqrt{3})t}}, \tag{33}$$

derived from $F(2,\xi)$ and scaling (30), is employed, the rms errors in the estimates of the exact $F(\xi)$ amount to 1.4×10^{-3} (for $t<0$), 3.9×10^{-4} (for $t>0$), and 5.3×10^{-4} (for all values of t). The corresponding maximum errors equal 8.2×10^{-3} (for $t<0$) and 6.2×10^{-4} (for $t>0$) [note that the values of $F(t)$ are close to unity]. This excellent accuracy of the predictions afforded by scaling expressions (30) and (33) is somewhat surprising in light of the rather large scatter in the values of C (Fig. 8) computed according to the equation

$$C \equiv C(N) = (2A^2)^{-1}(B-3)(\sqrt{2}F_{\max} - 1) \tag{34}$$

that follows from Eq. (30) and asymptotics (22) and (32).

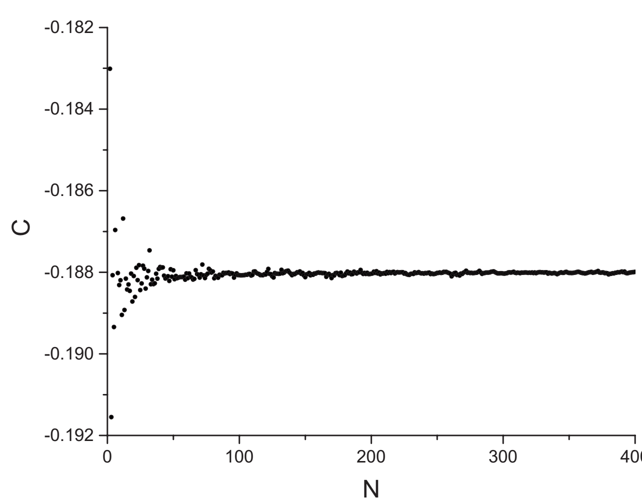

FIG. 8. The dependence of the parameter C on N for $2 \leq N \leq 400$.

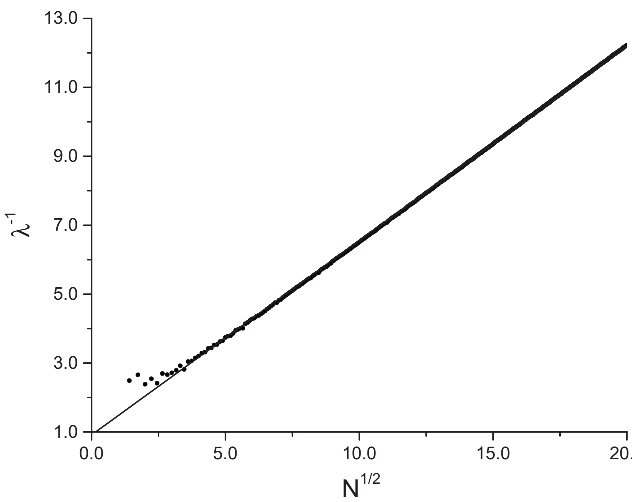

FIG. 9. The dependence of the reciprocal scaling factor λ^{-1} on $N^{1/2}$ for $2 \leq N \leq 400$. The straight line is given by the least-squares fit of $\lambda^{-1} = 0.91 \pm 1 + 0.5635 \pm 8\, N^{1/2}$.

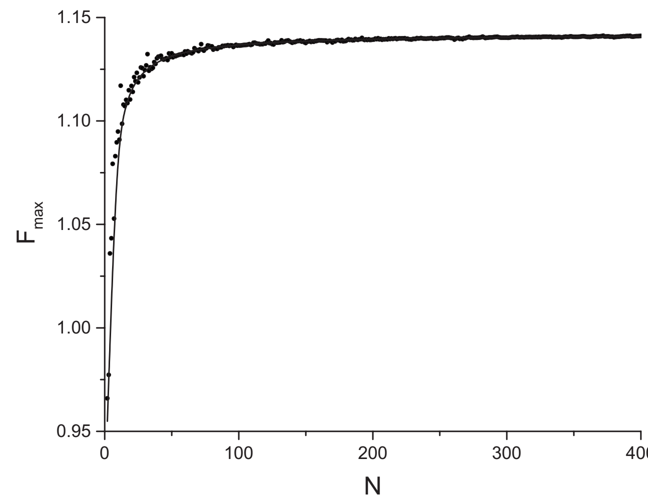

FIG. 11. The dependence of the maximum magnitude $F_{\max}$ on N for $2 \leq N \leq 400$. The solid line is given by the least-squares fit of $F_{\max} = (0.57 \pm 3 + 1.16 \pm 8\, N)/(1 + 1.01 \pm 7\, N)$.

For sufficiently large values of N, the scaling parameters λ, $\xi_{\max}$, and $F_{\max}$ follow simple power laws with λ^{-1} and $\xi_{\max}$ scaling like $N^{1/2}$, and $F_{\max}$ tending to a constant (Figs. 9–11), which implies universal dependence of $N^{-1}M^{-1/2}\varepsilon_{\mathrm{MTh}}(N,M)$ on $MN^{-3/2}$ [compare Eqs. (7), (21), and (30), together with the large-N asymptotics of $N^{-2}E_{\mathrm{Th}} \to 1/2$]. Interestingly, since ξ_{crit} also scales asymptotically like $N^{1/2}$, one expects the transition between the perturbed Thomson problem and the perturbed spherical Coulomb crystal regimes to occur at an N-independent t_{crit} as $N \to \infty$. Inspection of Fig. 12 confirms this prediction.

III. CONCLUSIONS

The modified Thomson problem, which concerns an assembly of N particles mutually interacting through a Coulombic potential and subject to a Coulombic-harmonic confinement, provides a formalism for a continuous interpolation between the original Thomson problem and that of a spherical Coulomb crystal. For sufficiently strong confinements, its solutions possess properties that are readily estimated with approximate (yet accurate) expressions involving only the reduced confinement strength ξ and a few quantities pertaining to the original Thomson problem. In particular, a tight upper bound to the energy is found to depend only on its Thomson problem counterpart E_{Th} and ξ, the next-order correction requiring just one additional parameter. Similarly, an accurate first-order correction to the positions of particles at the global energy minimum is entirely determined by ξ and their energy contributions to E_{Th}. Even more interestingly, the corresponding zero-point vibrational energy follows very closely an approximate scaling law that employs three N-dependent parameters $\lambda(N)$, $\xi_{\max}(N)$, and $F_{\max}(N)$.

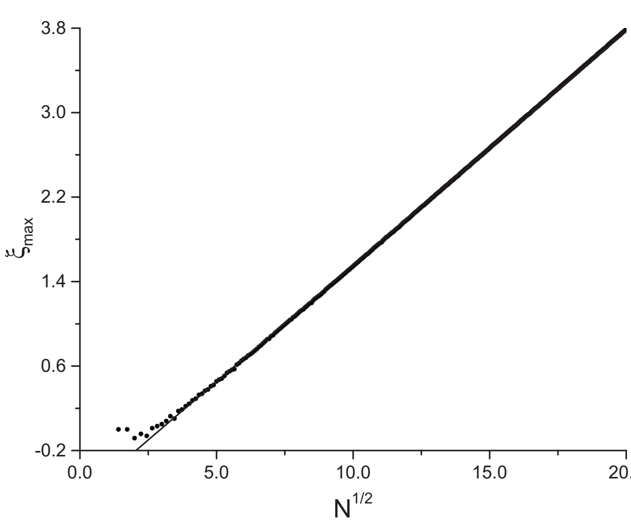

FIG. 10. The dependence of the maximum position $\xi_{\max}$ on $N^{1/2}$ for $2 \leq N \leq 400$. The straight line is given by the least-squares fit of $\xi_{\max} = -0.653 \pm 4 + 0.2213 \pm 3\, N^{1/2}$.

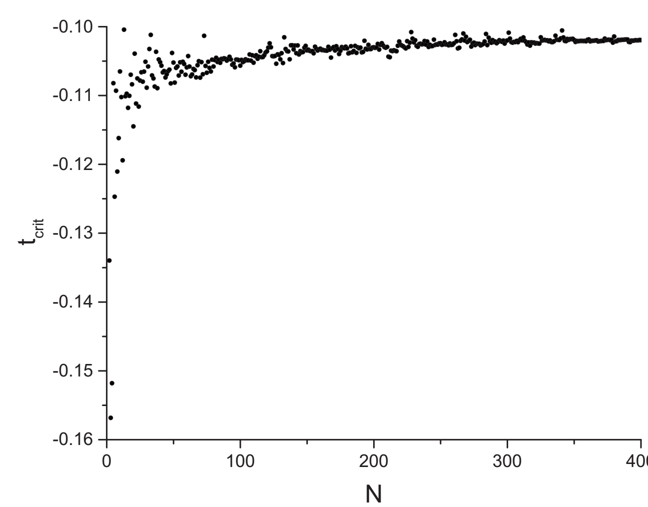

FIG. 12. The dependence of the critical parameter t_{crit} on N for $2 \leq N \leq 400$.

For $N \leq 12$, this regime of the perturbed Thomsonproblem persists for all non-negative values of ξ. On the other hand, the perturbed spherical Coulomb crystal regime emerges for $\xi < \xi_{\mathrm{crit}}(N)$ and larger numbers of particles. For $13 \leq N \leq 22$, the transition that delineates these two regimes is due to the existence of two energy minima, the crystal-like one becoming global for sufficiently weak confinements. For $N \geq 23$, the transition involves a catastrophe brought about by the vanishing of one of the Hessian matrix eigenvalues, the value of $\xi_{\mathrm{crit}}(N)$ being related to the magnitude of radial instability in the corresponding solution of the original Thomson problem. In this case, the thick-shell perturbed Thomson problem energy minimum simply ceases to exist for $\xi < \xi_{\mathrm{crit}}(N)$.

The parameters $\xi_{\mathrm{crit}}(N)$, $\lambda(N)$, $\xi_{\max}(N)$, and $F_{\max}(N)$, which depend solely on the particle-position vectors that solve the original N-particle Thomson problem, follow simple power laws at the limit of $N \to \infty$. At that limit, $t = N^{-3/2} M$ (where M is the confinement strength) becomes the quantity controlling the vibrational properties, the transition between the two regimes occurring at $t_{\mathrm{crit}} \approx -0.1$.

Thanks to its capability of interrelating the particles on the sphere and the spherical Coulomb crystal models, the modified Thomson problem affords particle configurations that are bound to find numerous applications as building blocks in approximate theories dealing with electrostatically interacting particles subject to confining external potentials. Further work along these lines is currently in progress.

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