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[Physics Letters A](http://dx.doi.org/10.1016/j.physleta.2017.09.001) ••• (••••) •••-•••

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11 Evolicit analytical radio frequency boating formulas for spherically $\frac{11}{12}$ Explicit, analytical radio-frequency heating formulas for spherically $\frac{77}{78}$ 13 symmetric nonneutral plasmas in a Paul trap 13 $\frac{1}{2}$ $\frac{1}{2$ 14 80

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22 ARTICLE INFO ABSTRACT 88

Article history: Received 19 July 2017 Received in revised form 27 August 2017 Accepted 3 September 2017 Available online xxxx Communicated by F. Porcelli *Keywords:* Paul trap

- 33 Radio-frequency heating rates and the state of the 34 Heating formulas and the contract of the co Nonneutral plasmas Radio-frequency heating Heating formulas
- 35 101 Coulomb logarithm

²⁴ Article history: **Explicity analytical heating formulas that predict the heating rates of spherical, one-⁹⁰** 25 91 component nonneutral plasmas stored in a Paul trap as a function of cloud size *S*, particle number *N*, 26 Received in revised form 27 August 2017 **and Paul-trap control parameter q** in the low-temperature regime close to the cloud \rightarrow crystal phase $\frac{92}{1}$ 27 Transition. We find excellent agreement between our analytical heating formulas and detailed, time- 93 28 Communicated by E-Dorselli **1944** dependent molecular-dynamics simulations of the trapped plasmas. We also present the results of our 94 29 95 numerical solutions of a temperature-dependent mean-field equation, which are consistent with our 30 96 numerical simulations and our analytical results. This is the first time that analytical heating formulas 31 97 are presented that predict heating rates with reasonable accuracy, uniformly for all *S*, *N*, and *q*. An 32 September 1918 analytical formula for the Coulomb logarithm in the weak-coupling regime is also presented.
Belis by the weak-coupling region of the weak-coupling regime is also presented.

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1. Introduction

41 The Paul trap $[1,2]$ has long secured its place as an indispens- We define it heating as the cycle-averaged power extracted $\frac{107}{107}$ 42 able tool in many fields of science with applications ranging from the monder the trapel the trap. There are two situations of theoretical 108 43 atomic clocks $[3]$ and quantum computers $[4-6]$ to mass spec- and experimental interest. (A) with the neip of a cooling mecha- $\frac{109}{109}$ 44 trometry [\[7\]](#page--1-0) and particle physics [\[8\].](#page--1-0) Given its long and successful hism, such as buffer-gas cooling [9,18] or laser cooling [12,13], the $\frac{1}{100}$ 45 history, it is surprising that the Paul trap still offers unsolved, fun-plasma may be brought to a stationary state in which the size or $\frac{1}{111}$ 46 damental physics problems. For instance, if *N* ≥ 2 charged particles the ion cloud stays constant, on average, over extended periods of 112 47 are simultaneously stored in a Paul trap, the kinetic energy of the time. (B) Arter the stationary state is reached, the cooling may be $\frac{113}{113}$ 48 particles increases in time, i.e., they exhibit the phenomenon of switched on. From this point on, due to the nominear nature or $\frac{1}{14}$ 49 radio-frequency (rf) heating. Rf heating cannot be switched off. It the particle-particle interactions in the plasma [12,13], the plasma the 50 is a basic physical process that necessarily accompanies the oper-cloud will absorb energy from the ri-trapping held, heat up, and $\frac{1}{16}$ 51 ation of the trap. Surprisingly, although the existence of rf heating expand. As discussed in Sec. 3.4, the heating rates in situations (A) $_{117}$ 52 has been known $[9-11]$ and studied $[12-16]$ for a long time, ex-
 $\frac{100}{2}$ and (B) are different, since this studied with $\frac{100}{2}$ and $\frac{100}{2}$ are different, since in situation (A) the ri-field flas to pro 53 plicit heating formulas, capable of predicting rf heating rates, have the diditional power to counteract the dissipative losses due to the 54 so far not been available. This paper addresses this deficiency. In the inicromotion [2] or the trapped particles. To keep the discus-55 particular, focusing on trapped clouds of charged particles of the ston locused, we concentrate in this letter on situation (A). The sto

64 130 <http://dx.doi.org/10.1016/j.physleta.2017.09.001>

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₃₉ **1. Introduction 1. Introduction 1.8 plasmas consisting of** *N* **charged particles as a function of cloud₁₀₅** $\frac{1}{40}$ size *S* and Paul-trap parameter *q* [\[1,2,13\].](#page--1-0)

We define rf heating as the cycle-averaged power extracted from the rf field of the trap. There are two situations of theoretical and experimental interest. (A) With the help of a cooling mechanism, such as buffer-gas cooling [\[9,18\]](#page--1-0) or laser cooling [\[12,13\],](#page--1-0) the plasma may be brought to a stationary state in which the size of the ion cloud stays constant, on average, over extended periods of time. (B) After the stationary state is reached, the cooling may be switched off. From this point on, due to the nonlinear nature of the particle-particle interactions in the plasma [\[12,13\],](#page--1-0) the plasma cloud will absorb energy from the rf trapping field, heat up, and expand. As discussed in Sec. 3.4 , the heating rates in situations (A) and (B) are different, since in situation (A) the rf field has to provide additional power to counteract the dissipative losses due to the micromotion [\[2\]](#page--1-0) of the trapped particles. To keep the discussion focused, we concentrate in this Letter on situation (A).

56 122 same sign of charge (known as one-component, nonneutral plas- 57 mas $[17]$), we present explicit, analytical heating formulas that sic equations that underlie our theory of if heating. In Sec. 3 we 123 58 predict the heating rates of spherical, one-component, nonneutral present our analytical and numerical methods together with a de-
 59 125 tailed comparison between numerically and analytically computed 60 126 rf heating rates. Excellent agreement between the results of our 61 ^{*} Corresponding author **that is a contract of the contrac** 62 62 **62** *E-mail address: rblumel@wesleyan.edu* (R. Blümel). Cases and the section of the attack of the blumbar of the sec. [3.4,](#page--1-0) our heating formulas may also 128 63 ¹ Present address: IonQ Inc., 4505 Campus Drive, College Park, MD 20740, USA. **be used to obtain an analytical expression for the Coulomb log-** 129 This Letter is organized as follows. In Sec. [2](#page-1-0) we present the basic equations that underlie our theory of rf heating. In Sec. [3](#page-1-0) we present our analytical and numerical methods together with a debe used to obtain an analytical expression for the Coulomb log-

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⁴ appendix, in which we convert our dimensionless quantities and **Example 20** 20 20 20 20 20 20 20 20 20 20 20 20 5 71 *3.1. Molecular dynamics simulations* results to standard SI units.

2. Theory

The starting point of our work is the following set of dimenparticles in a hyperbolic Paul trap [\[16\]](#page--1-0)

$$
\ddot{\vec{r}}_i + \gamma \dot{\vec{r}}_i + [a - 2q \sin(2t)] \begin{pmatrix} x_i \\ y_i \\ -2z_i \end{pmatrix} = \sum_{\substack{j=1 \\ j \neq i}}^N \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|^3}, \quad i = 1, ..., N.
$$
\n(1)

Here $\vec{r}_i = (x_i, y_i, z_i)$ denotes the position vector of particle number *i*, *γ* is the damping constant, *t* is the time, and *a* and *q* are the two dimensionless control parameters of the Paul trap [\[1,2,13\].](#page--1-0) The solutions $\vec{r}_i(t)$ of (1) are best represented as a superposition of a slow, large-amplitude macromotion [\[2\],](#page--1-0) $\dot{R}_i(t) = (X_i(t), Y_i(t), Z_i(t)),$ and a fast, small-amplitude micromotion [\[2\],](#page--1-0) $\vec{\xi}_i(t)$, i.e.,

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\vec{r}_i(t) = \vec{R}_i(t) + \vec{\xi}_i(t),
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\vec{r}_i(t) = \vec{R}_i(t) + \vec{\xi}_i(t),
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\n(2) stable (S < S_c) clouds is illustrated in Fig. 15 in [13].

where, to lowest order,

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\vec{\xi}_{i}(t) = -\frac{q}{2}\sin(2t)\begin{pmatrix} X_{i}(t) \\ Y_{i}(t) \\ -2Z_{i}(t) \end{pmatrix}.
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\vec{\xi}_{i}(t) = -\frac{q}{2}\sin(2t)\begin{pmatrix} X_{i}(t) \\ Y_{i}(t) \\ -2Z_{i}(t) \end{pmatrix}.
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33 $\frac{33}{k-1}$ i=1 $\frac{1}{k-1}$ 99
structure of the solutions of (1), our numerical simulations of (1) 34 100 of a plasma cloud in the stationary state [\[16\],](#page--1-0) the kinetic energy $\frac{35}{25}$ (see see, 5.1) are numerically exact. The damping constant γ in the plasma cloud may be evaluated immediately on the basis $\frac{101}{100}$ (1) plays a dual role. In our numerical simulations we use γ as of the plasma cloud may be evaluated immediately on the basis $\frac{102}{102}$ 37 a convenient way to achieve a spherical, stationary state in which $\frac{O(2)}{2}$. The result is [16] 38 1. Evening behavior are become included by γ , the brief in γ , γ , 39 we may then use the equality between heating and cooling in the $E_{\text{kin}} = \frac{3N}{2} \left(1 + \frac{9}{4} \right) T + \frac{1}{2} q^2 S^2$, (7) 105 (see Sec. 3.1) are numerically exact. The damping constant *γ* in rf heating balances the cooling induced by γ . As shown in [\[16\],](#page--1-0)

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44 Where E is the total cycle-averaged energy of the plasma cloud and μ may use (4) and (7) to compute $H(S, N, q)$ analytically. 45 E_{kin} is its cycle-averaged kinetic energy [16]. Since in this paper our analytical formula for $\gamma(S, N, q)$ is based on the *q* and 111 46 we focus on spherical trapped plasma clouds, and since spherical *N* scaling of the critical gamma, $γ_c(N, q)$, at which the transition 112 $_{47}$ clouds are obtained for the choice $a = q^2/2$ [2,13], we assume this to the crystal occurs [\[21\].](#page--1-0) In [\[21\]](#page--1-0) we found that for a given q, that 48 setting of the parameter a for the remainder of this paper. Spheri- γ_c scales like an iterated-log law in N. In order to reveal the q 114 $_{49}$ cal clouds in the stationary state are conveniently characterized by dependence of γ_c , we performed extensive additional molecular- 115 where *E* is the total cycle-averaged energy of the plasma cloud and *E*_{kin} is its cycle-averaged kinetic energy [\[16\].](#page--1-0) Since in this paper we focus on spherical trapped plasma clouds, and since spherical clouds are obtained for the choice $a = q^2/2$ [\[2,13\],](#page--1-0) we assume this setting of the parameter *a* for the remainder of this paper. Spherical clouds in the stationary state are conveniently characterized by their size,

$$
\sum_{53}^{51} S = \lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \left[\sum_{i=1}^{N} \vec{r}_i^2(k\pi) \right]^{1/2},
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⁵⁶ the micromotion amplitude vanishes. The same states are allowed useful and the same of the same then allowed use to dethe micromotion amplitude vanishes.

58 124 **3. Methods and results**

61 ods for evaluating the heating rate $H = H(S, N, q)$. The numerical the same of 62 results obtained in Section 3.1 provide the target data sets to be where $S_c(N, q)$ is the critical cloud size at $\gamma = \gamma_c$. Since S_c is very a 128 63 matched by our analytical formulas developed in Sec. 3.2. This close to the size $S_{crystal}(N, q)$ of the crystal, we write ⁶⁴ succeeds to an excellent degree of accuracy. In Sec. [3.3,](#page--1-0) we com-
 $\zeta(N, a) = \zeta(N, a) + \sigma(N, a)$ (11) ¹³⁰ 65 pare the results of our molecular-dynamics simulations with the 131 external set of $(1, 4)$, $(2, 4)$, (31) ⁶⁶ solutions of a nonlinear mean-field equation. Excellent agreement where [16]

¹ arithm of weakly coupled one-component nonneutral plasmas in between the rf heating rates obtained by these two qualitatively ⁶⁷ 2 the Paul trap. In Sec. [4](#page--1-0) we discuss our results. We conclude our pa- different numerical methods is obtained. This provides an inde- 68 ³ per in Sec. [5.](#page--1-0) For the convenience of the reader we also provide an pendent check of our molecular-dynamics simulations. between the rf heating rates obtained by these two qualitatively different numerical methods is obtained. This provides an independent check of our molecular-dynamics simulations.

⁷ 2. Theory **2. Theory 1.2 Integral 2.3** Using a 5th-order Runge–Kutta method [\[19\],](#page--1-0) we performed ⁷³ 8 **8 extensive molecular-dynamics simulations [\[20\]](#page--1-0) of (1), extracting** $\frac{74}{3}$ ⁹ The starting point of our work is the following set of dimen-
 F heating rates as discussed in [\[15\]](#page--1-0) directly via computation of 75 ¹⁰ sionless equations of motion that describe the motion of *N* charged dE/dt according to (4) for $N = 50$, 100, 200, and 500 particles and ⁷⁶ 11 77 *q* = 0*.*10, 0.15, 0.20, 0.25, 0.30, and 0.35. The resulting rf heating 12 **rates are shown as a function of cloud size S** as the black data ⁷⁸ ¹³ . \therefore $\left(\begin{array}{c} x_i \\ x_i \end{array} \right)$ $\frac{N}{r_i - r_i}$ points in [Fig. 1.](#page--1-0) While rf heating rates for $q = 0.2$ were already 14 $\vec{r}_i + \gamma \vec{r}_i + [a - 2q \sin(2t)]$ $\vec{y}_i = \sum_{i=1}^{i} \vec{r}_i$, $i = 1, ..., N$. computed and presented in [\[15\],](#page--1-0) the data set displayed in [Fig. 1,](#page--1-0) 80 15 **15 b** $\begin{pmatrix} -2z_i \\ -2i \end{pmatrix}$ $\frac{1}{j-1}$ $\begin{pmatrix} i & -i \\ i & j \end{pmatrix}$ covering six different *q* values, is more extensive than the data 16 **16** 16 **1** $\frac{17}{17}$ are consistent with the rf heating rates $\frac{83}{17}$ 18 **18 18 18 18 18 18 184 184 184 184 19** $\begin{aligned} \n\mathbf{a}_1 &= (x_i, y_i, z_i) \quad \text{denoted the positive number of particles.} \\
\mathbf{b}_2 &= (x_i, y_i, z_i) \quad \text{denoted the positive number of particles.} \\
\mathbf{b}_3 &= (x_i, y_i, z_i) \quad \text{denoted the positive number of particles.} \\
\mathbf{b}_4 &= (x_i, y_i, z_i) \quad \text{denoted the positive number of particles.} \\
\mathbf{b}_5 &= (x_i, y_i, z_i) \quad \text{denoted the positive number of particles.} \\
\mathbf{b}_6 &= (x_i, y_i, z_i) \quad \text{denoted the positive number of particles$ 20 bet i, y is the uall plusted to see the part of all of all the set of eff-most data point in [Fig. 1](#page--1-0) corresponds to S_c). From then on, 86 21 The dimensionless control parameters of the ratio trap [1,2,15]. The the for still smaller clouds, the heating rate decreases with decreasing $\frac{87}{100}$ 22 solutions $f_i(t)$ of (1) are best represented as a superposition of a cloud size, which causes a run-away effect that swiftly takes a sub-23 slow, large-amplitude inactomotion [2], $\kappa_i(t) = (x_i(t), r_i(t), z_i(t))$, critical $(S < S_c)$ cloud into the crystalline state. The non-monotonic ⁸⁹ 24 and a last, small-amplitude incromotion [2], $\xi_i(t)$, i.e., shape of the heating curve responsible for stable $(S > S_c)$ and un-²⁵ $\vec{r} \cdot (t) = \vec{R} \cdot (t) + \vec{\xi} \cdot (t)$ 91
(2) stable $(S < S_c)$ clouds is illustrated in Fig. 15 in [\[13\].](#page--1-0) *dE/dt* according to (4) for *N* = 50, 100, 200, and 500 particles and

27 93 *3.2. Analytical heating formulas*

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of (2) . The result is $[16]$

We may then use the equality between heating and cooling in the
stationary state to compute the rf heating rate according to

$$
E_{\text{kin}} = \frac{3N}{2} \left(1 + \frac{q^2}{4} \right) T + \frac{1}{2} q^2 S^2,
$$
 (7)

41 degree of the micro- and macromotions are uncorre- $\frac{dE}{dr}$ and $\frac{dE}{dr}$ are uncorrewe may write $\gamma = \gamma(S, N, q)$. This way, if $\gamma(S, N, q)$ is known, we too

 $_{50}$ their size, $_{116}$ and $_{216}$ dynamics simulations and established that $_{116}$

$$
\gamma_c(N, q) = C(q) \ln[\ln(N)] - D(q),\tag{8}
$$

where

$$
55 \quad \text{where } \vec{r}_i \text{ is evaluated at multiples of } \pi \text{, where, according to (3),} \qquad C(q) = 1.31 \times q^{4.57}, \quad D(q) = 0.13 \times q^{3.77}. \tag{9}
$$

 $\frac{57}{2}$ termine the complete scaling of γ (*S*, *N*, *q*). We found $\frac{123}{2}$

59
\n60 In this section we present our numerical and analytical meth-
\n61 of the evaluating the heating rate
$$
H = H(S \mid N, q)
$$
. The numerical
\n61 of the evaluating the heating rate $H = H(S \mid N, q)$. The numerical

where $S_c(N, q)$ is the critical cloud size at $\gamma = \gamma_c$. Since S_c is very close to the size $S_{\text{crystal}}(N, q)$ of the crystal, we write

$$
S_c(N,q) = S_{\text{crystal}}(N,q) + \sigma(N,q),\tag{11}
$$

where
$$
[16]
$$

Please cite this article in press as: Y.S. Nam et al., Explicit, analytical radio-frequency heating formulas for spherically symmetric nonneutral plasmas in a Paul trap, Phys. Lett. A (2017), http://dx.doi.org/10.1016/j.physleta.2017.09.001

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