Theory of the Quantum Breathing Mode in Harmonic Traps and its Use as a Diagnostic Tool

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An analytical expression for the quantum breathing frequency ω_b of harmonically trapped quantum particles with inverse power-law repulsion is derived. It is verified by *ab initio* numerical calculations for electrons confined in a lateral (2D) quantum dot. We show how this relation can be used to express the ground state properties of harmonically trapped quantum particles as functions of the breathing frequency by presenting analytical results for the kinetic, trap, and repulsive energy and for the linear entropy. Measurement of ω_b together with these analytical relations represents a tool to characterize the state of harmonically trapped interacting particles—from the Fermi gas to the Wigner crystal regime.

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Physics is replete with quantum systems of harmonically trapped interacting particles. In addition to a multitude of interesting applications in nanoscience [1–7] and in the area of ultracold gases [8–11], these systems are important from a fundamental perspective of many-body physics. By changing the size of the harmonic trap, a multiparticle system can be investigated over a wide range of states characterized by the coupling parameter λ (described below). The states range from a weakly correlated, quantum gas ($\lambda \ll 1$), to metallic systems ($\lambda \approx 1$), to the highly correlated, classical limit of Wigner crystallization ($\lambda \gg 1$) [12].

Collective modes are an important aspect of the dynamics of harmonically trapped quantum systems. In terms of multipoles, the first two modes are the breathing (monopole) and Kohn (dipole) mode [13]. Because of its strong interaction with laser radiation, the dipole mode has received the most attention so far; an analytical theory exists [13], and it has found important applications in nanoscience [14,15]. The dipole mode has also been shown to dominantly contribute to transport properties of trapped gases and therewith to spectroscopic methods, such as the Coulomb blockade measurements [16].

Comparatively little research has been done involving (non-center-of-mass) breathing and higher-order modes [17–20]; for an animation of the quantum breathing mode (QBM) see Ref. [21]. There exists no comprehensive analytical approach and only recently have practical applications appeared in the field of cold quantum gases [22,23]. In this Letter we analytically and numerically investigate the QBM and show that it can be used as a powerful tool to experimentally and theoretically characterize quantum particles in harmonic traps. Our analysis reveals two main results.

First, an analytical theory of the QBM is developed that is valid for harmonically trapped fermionic and bosonic systems of any particle number and arbitrary dimension, with inverse power-law repulsion between particles. Our theory is tested by comparing it to *ab initio* numerical calculations for the special case of electrons confined in a lateral (2D) quantum dot (QD) [24–26]. Our numerical analysis is based on multiconfiguration time-dependent Hartree-Fock (MCTDHF) calculations, as outlined in Ref. [27]; calculations of the QBM are performed for $N = 2$, 3, 4, and 6 electrons in their ground state. Good agreement between numerical and analytical results is found in the whole range between an ideal quantum gas and Wigner crystallization. We would like to stress that, although numerical verification is done for a lateral QD, our theory applies to trapped gases in general [3–11].

In the second part of the Letter the relation for the QBM is used to show that all properties associated with the ground state can be approximately expressed as analytical functions of the breathing frequency; this enables the QBM to be used as a novel diagnostic tool which is important for electrons in QDs and for dipolar quantum gases. Measurement of the QBM frequency [28], together with these analytical relations, is sufficient to characterize all eigenstate properties of harmonically trapped particles. Experimentally, there exists no other method to measure most of these quantities. This opens a new avenue to investigate fundamental properties of many-body systems as a function of interaction strength—from the weakly to the highly correlated limit.

Some analytical relations, such as the kinetic, trap and repulsive energies, are obtained directly from the QBM relation; these relations are shown to be valid over the range of λ investigated here by comparison with MCTDHF. For all other quantities, the QBM relation is first utilized to replace the exact Hamiltonian with an effective Hamiltonian with quadratic interaction for which an analytical solution of the ground state [29–31] exists. As a result, through the effective Hamiltonian all properties associated with the ground state can be expressed as functions of the QBM frequency. We outline the derivation for general λ; however, analytical results are obtained here with the help of perturbation theory

in λ. The quadratic Hamiltonian has been used in many different contexts including quantum chemistry [32,33], black hole physics [34,35], and the quantum Hall effect [29,36]. However, so far the coupling constant in the quadratic repulsion term had to be chosen qualitatively. By virtue of the QBM relation, an analytical expression for the optimum coupling constant can be obtained for which the eigenstate of the quadratic Hamiltonian is as close as possible to the real eigenstate. The closeness is measured through the expectation values of the potential, kinetic, and total energy operators. This is not a unique measure, but it is shown that other measures, such as the entropy discussed below, lead only to small changes in the coupling constant.

The quadratic Hamiltonian is used here to determine the linear entropy, the knowledge of which is key to determine correlation and entanglement of a quantum many-body system. This is not only important for quantum information science, but recently the notion of entanglement has been successfully employed in the field of condensed matter [37–39] for the analysis of model systems such as spin chains [40], harmonic chains [34,35,41], and has also been proven useful in the description of quantum phase transitions [42–44]. Comparison with MCTDHF results for $N \leq 6$ shows reasonable agreement; qualitatively the numerical results are well reproduced; quantitatively, there is a constant factor of $\lesssim 2$ between the numerical and analytical results, corresponding to a factor $\sqrt{2}$ in the coupling constant.

Our analysis starts with the derivation of an analytical expression for the breathing frequency. For N particles in a harmonic trap of frequency Ω, an analytical expression for the QBM can be obtained from the Heisenberg equation of motion. The Hamiltonian for this system is given by $\hat{H} = \hat{T} + \hat{U} + \lambda\hat{V}$, where $\hat{T}$, $\hat{U}$, and $\lambda\hat{V}$ represent the total kinetic energy, total harmonic trap, and inverse power-law particle interaction potential energy respectively. Here, $\hat{V} = \sum_{i<j}^{N}(\hat{\mathbf{x}}_{ij}^2 + \sigma^2)^{-\alpha/2}$, where $\hat{\mathbf{x}}_{ij} = \hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j$ and the shielding parameter σ accounts for the fact that, in 2D QDs, integration over the wave function of the third (transverse) dimension results in an effective shielding of the Coulomb singularity [1]. Units of energy, length, and time are given by $\hbar\Omega$, l_0, and Ω^{-1}, respectively, where $l_0 = \sqrt{\hbar/m\Omega}$ is the oscillator length with m being the mass of the trapped particles; the transformation of the time-dependent Schrödinger equation (TDSE) in SI units to this new system of units is shown in Ref. [21]. These units are used throughout unless otherwise indicated.

We first express the Hamiltonian in terms of center-of-mass (c.m.) and relative coordinates as $\hat{H} = \hat{H}_{\text{c.m.}} + \hat{H}_{\text{rl}}$, where $\hat{H}_{\text{c.m.}} = \hat{T}_{\text{c.m.}} + \hat{U}_{\text{c.m.}}$ and $\hat{H}_{\text{rl}} = \hat{T}_{\text{rl}} + \hat{U}_{\text{rl}} + \lambda\hat{V}$. Then, starting from the Heisenberg equation of motion for the operator $\hat{S} = 1/2\sum_i(\hat{\mathbf{p}}_i \cdot \hat{\mathbf{x}}_i + \hat{\mathbf{x}}_i \cdot \hat{\mathbf{p}}_i)$ that performs a radial displacement of each coordinate, we obtain an inhomogeneous second-order differential equation in time for $\hat{U}_{\text{rl}}$, similar to that in Ref. [45],

$$\frac{d^2}{dt^2}\hat{U}_{\text{rl}}(t) = -4\hat{U}_{\text{rl}}(t) - (2-\alpha)\lambda\hat{V}(t) + \sum_{i<j}^{N}\frac{\alpha\lambda\sigma^2}{(\hat{\mathbf{x}}_{ij}^2(t) + \sigma^2)^{\alpha/2+1}}. \quad (1)$$

Equation (1) only contains the relative coordinates $\hat{\mathbf{x}}_{ij}$. In the following, we outline the key points of the derivation; for further details see Ref. [21]. We take the expectation value of Eq. (1) with regard to some radially symmetric, weak distortion of an eigenstate of $\hat{H}$ that results in an excitation of the breathing mode. The resulting equation can be re-expressed in a way that the expectation value is taken with regard to the unperturbed eigenstate $|k\rangle$ and in return the Heisenberg space operators are perturbed from $\hat{\mathbf{x}}_i(t)$ to $\hat{\mathbf{x}}_i(t) + \Delta\hat{\mathbf{x}}_i(t)$. The only term that contributes to the perturbation to order $\mathcal{O}(\hat{\mathbf{p}}, \hat{\mathbf{x}}^2)$ is $\Delta\hat{\mathbf{x}}_i(t) = \varepsilon(t)\hat{\mathbf{x}}_i(t)$. Taylor expansion of the expectation value of Eq. (1) results in a second-order ordinary differential equation for $\varepsilon(t)$, with coefficients given by expectation values of the form of $\langle k|h[\hat{\mathbf{x}}(t)]|k\rangle$; h represents an arbitrary function. By using the identity relation $e^{-i\hat{H}t}e^{i\hat{H}t} = \mathbf{1}$, we find that $\langle h[\hat{\mathbf{x}}(t)]\rangle = \langle h[\hat{\mathbf{x}}(t=0)]\rangle = \langle h(\mathbf{x})\rangle$. Because of the time independence of the coefficients, the equation for $\varepsilon(t)$ has a sinusoidal solution with frequency

$$\omega_b^2 = 4 - \frac{\langle\hat{W}\rangle}{2\langle\hat{U}_{\text{rl}}\rangle}, \quad (2)$$

where

$$\hat{W}(t) = \sum_{i<j}^{N}\left[2 - \alpha + \frac{(\alpha+2)\sigma^2}{x_{ij}^2(t) + \sigma^2}\right]\frac{\alpha\lambda x_{ij}^2(t)}{(x_{ij}^2(t) + \sigma^2)^{\alpha/2+1}}. \quad (3)$$

Note that when $\sigma \ll 1$ we have $\langle\hat{W}\rangle \approx \alpha(2-\alpha)\lambda\langle\hat{V}\rangle$. For our calculations we consider the Coulomb case ($\alpha = 1$) for which $\lambda = e^2/4\pi\hbar\epsilon l_0\Omega$, where e is the electron charge and ϵ the permittivity.

The quality of Eq. (2) is assessed by comparison to exact solutions of the TDSE; here, this is done for a 2D QD. N electrons, interacting via the Coulomb potential, are confined by a harmonic trap $\hat{U}$ with frequency Ω. For $N = 2$ it is possible to obtain an exact solution by separating the TDSE into c.m. and difference coordinates [17]. For $N = 2$, 3, 4, and 6 the TDSE is solved by using MCTDHF. All results are compared to those obtained from Eq. (2). Details on MCTDHF and the parameters chosen for the numerical solutions are given in Ref. [21].

The difference between the direct solution of the TDSE and MCTDHF for $N = 2$ in Fig. 1 is below the symbol resolution, validating MCTDHF. Our operator approach is substantiated by the good agreement of Eq. (2) with MCTDHF for all values of N and λ shown in Fig. 1. The good agreement for all numerically investigated cases in combination with the fact that the derivation of Eq. (2) is not limited to small N, indicates that it will also be valid for $N > 6$.

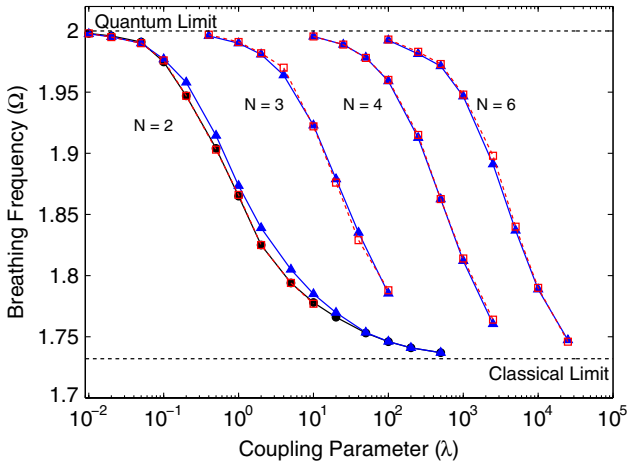

FIG. 1 (color online). Breathing frequency vs electron correlation parameter λ, as determined by the (i) difference coordinate solution of the TDSE (filled circle), (ii) Eq. (2) (filled triangle), and (iii) MCTDHF (opened square) for $N = 2$, 3, 4, and 6. For $N = 3$, 4 and 6 the origin of the curves ($\lambda = 0.02$) have been shifted to make the plot clearer.

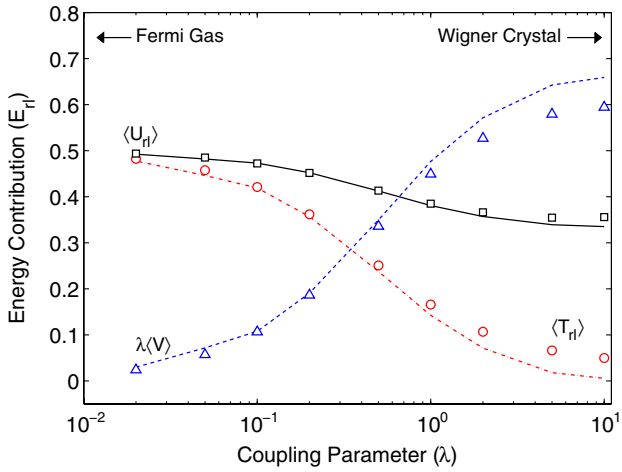

FIG. 2 (color online). $\lambda\langle\hat{V}\rangle/E_{\rm rl}$ (dash), $\langle\hat{T}_{\rm rl}\rangle/E_{\rm rl}$ (dash-dot) and $\langle\hat{U}_{\rm rl}\rangle/E_{\rm rl}$ (solid), calculated for $N = 6$ from Eqs. (4a)–(4c), respectively. The markers represent the values determined from MCTDHF.

In the second part of our analysis, we will show that Eq. (2) has important ramifications for the experimental characterization and theoretical calculation of many-body eigenstates and observables of harmonically trapped quantum particles. We start by expressing the kinetic, trap, and repulsive energies as functions of ω_b. This is possible by using Eq. (2) together with the quantum virial theorem ($2\langle\hat{T}\rangle = 2\langle\hat{U}\rangle - \alpha\lambda\langle\hat{V}\rangle$) and yields

$$\frac{\lambda\langle\hat{V}\rangle}{E_{\rm rl}} = \frac{2(4-\omega_b^2)}{(2-\alpha)(2\alpha+4-\omega_b^2)} \tag{4a}$$

$$\frac{\langle\hat{T}_{\rm rl}\rangle}{E_{\rm rl}} = \frac{\alpha(\omega_b^2-\alpha-2)}{(2-\alpha)(2\alpha+4-\omega_b^2)} \tag{4b}$$

$$\frac{\langle\hat{U}_{\rm rl}\rangle}{E_{\rm rl}} = \frac{\alpha}{(2\alpha+4-\omega_b^2)}, \tag{4c}$$

where $E_{\rm rl} = \langle 0|\hat{H}_{\rm rl}|0\rangle$ with $|0\rangle$ the ground state of $\hat{H}$; all expectation values in Eq. (4) are taken with respect to $|0\rangle$. Equation (4) are valid when $\sigma \ll 1$. From the above expressions together with the analytical solution for the corresponding c.m. contributions, the total kinetic, potential trap, and repulsive energies can be obtained. In Fig. 2, Eq. (4) for $N = 6$ are compared with the MCTDHF results; the $N = 2 - 4$ calculations display similar results. Fairly good agreement is achieved with the small discrepancies for larger λ occurring as a result of neglecting the shielding parameter in Eq. (2). Thus, experimental measurement of ω_b in conjunction with Eq. (4) gives information about the state of the interacting trapped quantum system and presents a useful experimental tool. For $\lambda = 0 \to \infty$, the normalized relative kinetic energy varies in a range $\langle\hat{T}_{\rm rl}\rangle/E_{\rm rl} = 1/2 \to 0$; its value is an indicator of the state of the quantum system. For $\langle\hat{T}_{\rm rl}\rangle/E_{\rm rl} \approx 1/2$, 1/4, 0 the quantum system is weakly interacting, metal-like, or in a state of Wigner crystallization, respectively. In Fig. 2 we see that for $\lambda \approx 10$ the kinetic energy is frozen out nearly completely and the system is close to a mesoscopic crystal [26]. Similar conclusions can also be drawn from $\lambda\langle\hat{V}\rangle/E_{\rm rl}$. Note that the above relations are valid for an arbitrary number of trapped particles N [18]. We are not aware of other methods to determine the internal status of the quantum system of trapped particles, in particular, in the strongly correlated limit $\lambda \gg 1$. Direct experimental measurement is not possible; for systems with larger N, theoretical calculation is extremely challenging and often not feasible.

Another important consequence of Eq. (2) is that it can be used to derive an approximate Hamiltonian with quadratic electron repulsion. The resulting Hamiltonian depends only on ω_b. As quadratic Hamiltonians can be solved analytically [29,30], any observable or measure of harmonically trapped quantum particles can be obtained as a function of ω_b.

In what follows we denote the exact, quadratic, and interaction free Hamiltonians by $\hat{H}$, $\hat{H}_{\rm q}$, and $\hat{H}^{(0)} = \hat{H}(\lambda = 0)$ with eigenstates $|j\rangle$, $|j_{\rm q}\rangle$, and $|j^{(0)}\rangle$, and energies E_j, ε_j, and $E_j^{(0)}$, respectively. Our derivation starts from the quadratic Hamiltonian $\hat{H}_q = \hat{T} + \hat{U} + \kappa\hat{U}_{\rm rl}$ where the Coulomb repulsion has been replaced by $\hat{V}_q = \kappa\hat{U}_{\rm rl}$, motivated by Eq. (2). The parameter κ could be determined by requiring maximum overlap between ground states of the exact and quadratic Hamiltonian, $\langle 0|0_q(\kappa = \kappa_m)\rangle = \max$. This is not practical, as the exact ground state is usually unknown. However, we expect that any observable $\hat{O}$ approximately fulfills $\langle 0|\hat{O}|0\rangle \simeq \langle 0_q(\kappa_m)|\hat{O}|0_q(\kappa_m)\rangle$. As a result, a reasonable approximation of $\kappa_{\rm m}$ can also be

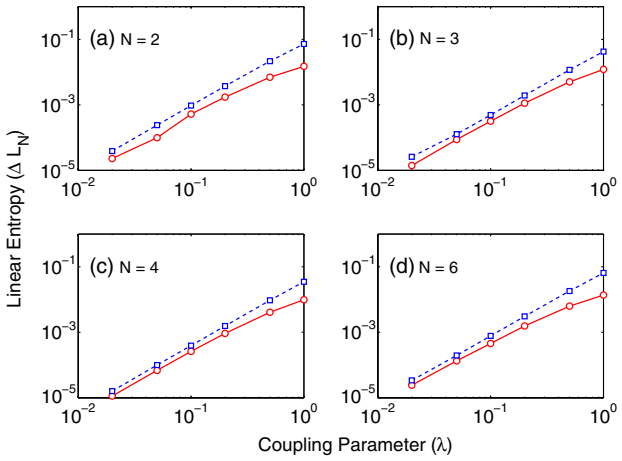

FIG. 3 (color online). Linear entropy [ΔL_N from Eq. (7)] vs λ for different N values calculated by MCTDHF (squares) and by using Eq. (7) derived from $\hat{H}_q$ (circles).

extracted from expectation values. We anticipate slight variations of κ_m in dependence on the investigated properties of the wave function, as will be confirmed in Fig. 3. Here relations (4a)–(4c) for $\langle 0|\hat{T}, \hat{U}, \hat{V}|0\rangle$ are used. The respective expectation values for the quadratic Hamiltonian can be determined from its analytical solution [29]; comparison of the two expressions yields κ_m.

We follow here a simpler but less general argument to determine κ_m that relies on perturbation theory in λ and is valid only for $\lambda < 1$. By using the virial theorem, expectation values of the exact and quadratic Hamiltonian can be expressed as $E_0 = \langle 0|\hat{H}|0\rangle = \langle 0|2\hat{U} - (2-\alpha)\lambda\hat{V}/2|0\rangle$ and $\varepsilon_0 = \langle 0_q|\hat{H}_q|0_q\rangle = \langle 0_q|2\hat{U} + 2\kappa\hat{U}_{rl}|0_q\rangle$. The ground state energies to first order in electron repulsion are given by $E_0 = E_0^{(0)} + (\alpha/2)\langle 0^{(0)}|\lambda\hat{V}|0^{(0)}\rangle$ and $\varepsilon_0 = E_0^{(0)} + \langle 0^{(0)}|\kappa\hat{U}_{rl}|0^{(0)}\rangle$. Inserting the energies in the above expressions and keeping only first-order terms in the electron repulsion yields $2\langle 0|\hat{U}|0\rangle = E_0^{(0)} + (\alpha/2)\langle 0^{(0)}|\lambda\hat{V}|0^{(0)}\rangle$ and $2\langle 0_q|\hat{U}|0_q\rangle = E_0^{(0)} - \langle 0^{(0)}|\kappa\hat{U}_{rl}|0^{(0)}\rangle$. After replacing $\lambda\hat{V}$ by using relation (2), one finds that equality of these two expressions is satisfied when

$$\kappa_m = -\frac{4-\omega_b^2}{2-\alpha}. \tag{5}$$

Finally, $\hat{U}$ can be replaced by using $\hat{H} = \hat{T} + \hat{U} + \lambda\hat{V}$, yielding expressions for $\langle 0|\hat{T}, \hat{V}|0\rangle$ and $\langle 0_q|\hat{T}, \hat{V}|0_q\rangle$, for which equality also holds for κ_m given in Eq. (5).

The final quadratic Hamiltonian $\hat{H}_q$ can be written as

$$\hat{H}_q = \hat{T} + \Omega_q^2\hat{U} + \hat{V}_q \tag{6}$$

with $\Omega_q^2 = 1 + \kappa_m(N-1)/N$ and $\hat{V}_q = -(\kappa_m/2N)\sum_{i\neq j}\hat{x}_i \cdot \hat{x}_j$. Part of the quadratic repulsion term U_{rl} contributes to and therefore has been pulled into the harmonic trap potential. The exact solutions of $\hat{H}_q$ [29] are spinless, and it is not trivial to derive anticommuting, fermionic solutions with a given pure spin eigenstate. Therefore, and for consistency with the $\mathcal{O}(\lambda)$ validity of Eq. (5), the ground state $|0_q\rangle$ is determined here by first-order perturbation theory. We then use this ground state to calculate the linear entropy $L_N = 1 - N\sum_i \mu_i^2$ of the N-electron system, where the μ_i's are the eigenvalues of the one-body density matrix. The one-body density matrix can still be obtained analytically and has to be diagonalized numerically. As a result, we obtain the simple expression

$$\Delta L_N(\lambda) = L_N(\lambda) - L_N(0) \simeq K_N g^2 \tag{7}$$

with $g = \kappa_m/2N$; in the case of Coulomb interaction, $K_2 = 0.25$, $K_3 = 0.22$, $K_4 = 0.14$, and $K_6 = 0.14$; $L_4(0) = 1/4$ and $L_N(0) = 0$ for $N = 2, 3, 6$.

In Fig. 3 the linear entropy is compared to the exact numerical results as a function of λ. Up to $\lambda = 0.5$, our analytical relation predicts the correct functional form of the linear entropy; however, it consistently underestimates L_N by a constant factor of $\mathcal{O}(2)$, meaning that κ_m is about a factor $\sqrt{2}$ too small. This was expected, as κ_m was determined as the best approximation to the kinetic and potential energy of $\hat{H}$. Nonetheless, our expression for L_N provides a reasonable approximation for the linear entropy for $\lambda \lesssim 1$. Furthermore, it provides a means by which the linear entropy can be determined by an experimentally measurable parameter.

In summary, we have presented analytical and numerical MCTDHF results for the breathing frequency $\omega_b(\lambda)$ of trapped quantum particles covering the whole range from weak (Fermi gas) to strong (Wigner crystal) coupling. Furthermore, we have shown that knowledge of $\omega_b(\lambda)$—e.g. obtained in an experiment—gives direct access to key ground state properties of the system, including the mean kinetic, potential, and interaction energy. Moreover, from the energy contributions one immediately has access to the equation of state (via differentiation with respect to λ) or the chemical potential (by considering the total energy for different particle numbers). As an interesting theoretical result we demonstrated how to use the breathing frequency to—approximately—map the complex trapped system with power-law interaction to an effective harmonically interacting one which can be solved exactly. While our numerical simulations were performed for electrons in quantum dots, all analytical expressions are valid for any quantum system with a power-law pair interaction; this includes dipole interacting cold quantum gases.

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