Quantum Criticality at the Large-Dimensional Limit: Three-Body Coulomb Systems

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ABSTRACT: We present quantum phase transitions and critical phenomena at the large-dimension (D) limit for three-body *ABA* Coulomb systems with charges (Q, q, Q) and masses (M, m, M). The Hamiltonian depends linearly on two parameters $\lambda = |Q/q|$ and $\kappa = [1 + (m/M)]^{-1}$. The system exhibits critical points with mean field critical exponents $(\alpha = 0, \beta = \frac{1}{2}, \delta = 3, \gamma = 1)$. We calculate the critical curve $\lambda_c(\kappa)$ through which all systems undergo a continuous-phase transition from the symmetrical configuration, the two like particles have the same distance from the reference particle, to the unsymmetrical phase. The critical curve at $D \to \infty$ limit is a convex function of κ and very similar to the one obtained at $D = 3$ with variational calculations. We also calculated the line of zero angular correlation in the mass polarization term, which separates the symmetrical phase to an atom-like region and a molecule-like region. Int J Quantum Chem 85: 307–314, 2001

Key words: *ABA* Coulomb system; Hamiltonian; reference particle; zero angular correlation; atom-like region; molecule-like region

Introduction

Quantum phase transitions are zero temperature phase transitions tuned by parameters in the Hamiltonian [1, 2]. Examples from condensed matter physics include the magnetic transitions of cuprates, superconductor–insulator transitions in alloys, and the quantum–Hall transitions [2, 3]. For two-electron atoms, the parameter that tunes the phase transition is the nuclear charge, Z. As the nuclear charge reaches a critical value $Z_c \simeq 0.911$, which is the minimum charge necessary to bind two electrons, one of the electrons jumps, in a first-order phase transition, to infinity with zero kinetic energy [4]. For three-electron atoms, a second-order phase transition [5] occurs at $Z_c \simeq 2.0$. The estimation of critical nuclear charge for N-electron atoms shows that, at most, only one electron can be added to a free atom in the gas phase [6]. The study of quantum phase transitions and critical phenomena is of increasing interest in the field of atomic and molecular physics. This is motivated by the recent experimental searches for the smallest stable multiply charged anions [7, 8], experimental and theoretical work on the stability of atoms and molecules in external fields [9, 10], the study of selectively break-

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ing chemical bonds in polyatomic molecules [9], controlling electronic properties of materials [11], and phase transitions of finite clusters [12].

Symmetry breaking, critical phenomena, and phase transitions at large-dimension (D) limits for many different models continue to be a subject of great interest [6, 13]. This is motived by the fact that as we treat real physical problems, exact treatments are seldom realizable, and so one has to rely on approximate methods. The large-D model and its $1/D$ expansion scheme have proven to be efficient in dealing with a diverse class of the problems [14, 15].

Symmetry breaking of electronic structure configurations at the large-D limit has been recently shown to be completely analogous to the standard phase transitions and critical phenomena in statistical mechanics [16]. For N-electron atoms [17] at the large-D limit, the symmetry breaking is shown to be a "first-order" phase transition. For the special case of two-electron atoms, the first-order transition shows a triple point where three phases with different symmetries exist. Treatment of the Hartree–Fock solution reveals a different kind of symmetry breaking where a "second-order" transition exists. The Hartree–Fock two-electron atom in a weak external electric field exhibits a critical point with mean field critical exponents [16] ($\beta = \frac{1}{2}$, $\alpha = 0_{\text{dis}}$, $\delta = 3$, and $\gamma = 1$).

Symmetry breaking of the molecular electronic structure configurations at the large-dimension limit shows similar phase transitions. For the Hartree–Fock hydrogen molecule at the large-D limit [18], for example, the phase diagram in the internuclear distance–nuclear charge plane shows three different stable phases with a bicritical point where the two continuous transition lines join a first-order transition line.

The stability of three-body Coulomb systems is an old but very important problem that has been treated in many particular cases [19–23]. Recently [24, 25] using the finite size scaling method we have shown that ABA Coulomb systems with charges (Q, q, Q) and masses (M, m, M) exhibit quantum phase transitions and critical phenomena. They undergo a first-order transition from the stable phase of ABA to the unstable breakup phase of $AB + A$ as their masses and charges vary. We also accurately calculate the transition line that separates the two phases. For any combination of the three particles of the form ABA, one can read directly from the phase diagram if the system is stable or unstable. Moreover, the transition line has a minimum at $\kappa_m = 0.35$, which leads to a new proposed classification of the ABA systems to either molecule-like systems or atom-like systems.

In this study, we generalize the three-body Hamiltonian to D-dimensional space and study the symmetry breaking at the large-D limit as a function of both parameters $\lambda = |Q/q|$ and $\kappa = [1 + (m/M)]^{-1}$. This large-D model is simple, has an analytical solution for the critical curve $\lambda_c(\kappa)$, which separates the symmetrical configuration from the unsymmetrical one, and yet contains a great deal of similarity to that obtained numerically using variational calculations at $D = 3$ with large basis sets [25]. We also show that the symmetry breaking of three-body structure configurations for the ABA systems in a weak electric field at the large-D limit is described as standard phase transitions. This symmetry breaking, which leads to dissociation or ionization, is completely analogous to phase transitions and critical phenomena in statistical mechanics. This analogy is shown by allowing the Coulomb strength parameter λ to play a role analogous to temperature in statistical mechanics. The symmetry breaking is shown to be a "continuous" phase transition with mean field critical exponents ($\beta = \frac{1}{2}$, $\alpha = 0$, $\delta = 3$, and $\gamma = 1$) for $\kappa_t \leq \kappa \leq 1.0$ and a first-order transition for $0 \leq \kappa \leq \kappa_t$, where $\kappa_t = 0.07$ is a tricritical point.

Large-D Hamiltonian for Three-Body Coulombic Systems

For three-body Coulombic systems with charges (Q_1, Q_2, Q_3) and masses (M_1, M_2, M_3), the Hamiltonian (atomic units are applied unless otherwise specified) is given by [24]

$$H = -\frac{1}{2\mu_1}\nabla_1^2 - \frac{1}{2\mu_2}\nabla_2^2 - \frac{1}{M_1}\nabla_1 \cdot \nabla_2 + \frac{Q_1Q_2}{r_1} + \frac{Q_1Q_3}{r_2} + \frac{Q_2Q_3}{r_{12}}, \quad (1)$$

where the reference particle is the particle with mass M_1 and charge Q_1, r_1 and r_2 are the relative coordinates of M_2 and M_3, $r_{12} = r_1 - r_2$, and μ_1, μ_2 are the reduced masses $\mu_i = M_1M_i/(M_1 + M_i)$.

In this study, we consider three-body ABA Coulombic systems with charges (Q, q, Q) and masses (M, m, M). Without loss of generality, we assume that $Q/|Q| = -q/|q|$, which may lead to a bound Coulombic system depending on the charges and masses of the particles. The correspond-

ing Hamiltonian reads

$$H = -\frac{1}{2\mu_0}\nabla_1^2 - \frac{1}{2\mu_0}\nabla_2^2 - \frac{1}{m}\nabla_1\cdot\nabla_2 + \frac{qQ}{r_1} + \frac{qQ}{r_2} + \frac{Q^2}{r_{12}}, \quad (2)$$

where the reduced mass $\mu_0 = mM/(m+M)$.

Herschbach [26] generalized this Hamiltonian to D-dimensional space in the case of infinite mass approximation, $m \to \infty$. Let us generalize the additional term, the mass polarization term, to the D-dimensional space. In the D-dimensional space, the Laplacian operator is defined by $\nabla^2 = \sum_{i=1}^{D}(\partial^2/\partial x_i^2)$ in terms of Cartesian coordinates x_i ($i = 1, 2, \ldots, D$). For the ground state with total angular momentum $L = 0$, the motion takes place on a plane spanned by the three particles, and the eigenfunction depends only on three variables and can be represented in polar coordinates $\Psi = \Psi(r_1, r_2, \theta)$. The radial coordinate is the radius of a D-dimensional sphere where $r_1 = x_1 i + x_2 j + \cdots + x_D k$ and $r_2 = y_1 i + y_2 j + \cdots + y_D k$. The Jacobian factor [14] is given by $J_D = (r_1 r_2)^{D-1}\sin^{D-2}\theta$. If we now introduce $\Psi = J_D^{-1/2}\Phi$ and carry out the calculations, the mass polarization term has the following form:

$$\begin{aligned}-\frac{1}{m}\nabla_1\cdot\nabla_2\,\Phi &= -\frac{1}{m}\left\{\cos\theta\frac{\partial^2}{\partial r_1\,\partial r_2} - \frac{\sin\theta}{r_2}\frac{\partial^2}{\partial r_1\,\partial\theta} - \frac{\sin\theta}{r_1}\frac{\partial^2}{\partial r_2\,\partial\theta}\right.\\ &\quad - \frac{\cos\theta}{2r_2}\frac{\partial}{\partial r_1} - \frac{\cos\theta}{2r_1}\frac{\partial}{\partial r_2} + \frac{\sin\theta}{r_1 r_2}\frac{\partial}{\partial\theta} - \frac{\cos\theta}{r_1 r_2}\frac{\partial^2}{\partial\theta^2}\\ &\quad \left. + \frac{1}{r_1 r_2}\left[\frac{\cos\theta}{4} + \left(\left(\frac{D-3}{2}\right)^2 - \frac{1}{4}\right)\frac{\cos\theta}{\sin^2\theta}\right]\right\}\Phi. \end{aligned} \quad (3)$$

Assembling the different terms gives the Schrödinger equation for the probability amplitude as $[T_1 + T_2 + T_{12} + U + V]\Phi = E_D\Phi$ where derivatives appear only in T_i ($i = 1, 2$) [26]

$$T_i = -\frac{1}{2\mu_0}\left[\frac{\partial^2}{\partial r_i^2} + \frac{1}{r_i^2}\frac{\partial^2}{\partial\theta^2}\right]; \quad (4)$$

and T_{12} from Eq. (3)

$$\begin{aligned}T_{12} = -\frac{1}{m}\left[\cos\theta\left(\frac{\partial^2}{\partial r_1\,\partial r_2} - \frac{1}{2r_2}\frac{\partial}{\partial r_1} - \frac{1}{2r_1}\frac{\partial}{\partial r_2}\right.\right.\\ \left.\left. - \frac{1}{r_1 r_2}\frac{\partial^2}{\partial\theta^2}\right)\\ - \sin\theta\left(-\frac{1}{r_2}\frac{\partial^2}{\partial r_1\,\partial\theta} - \frac{1}{r_1}\frac{\partial^2}{\partial r_2\,\partial\theta} + \frac{1}{r_1 r_2}\frac{\partial}{\partial\theta}\right)\Bigg].\end{aligned} \quad (5)$$

The dimension dependence appears only in the centrifugal term

$$U = \frac{1}{2\mu_0}\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right)\left[-\frac{1}{4} + \frac{(D-2)(D-4)}{4}\frac{1}{\sin^2\theta}\right] - \frac{1}{mr_1 r_2}\left[\frac{\cos\theta}{4} + \left(\left(\frac{D-3}{2}\right)^2 - \frac{1}{4}\right)\frac{\cos\theta}{\sin^2\theta}\right] \quad (6)$$

and V is the Coulombic potential.

Finally at $D \to \infty$, any scheme that scales the radial distances as D^2 in such a way as to cancel the D-dependence of the centrifugal potential will give an effective Hamiltonian H_∞^0, which determines the motion of the three particles on a surface $\{\Sigma : r_1, r_2, \theta\}$. Using the scaling transformation $fr \longrightarrow r$ and energy $H_\infty^0/f|qQ| \longrightarrow H_\infty^0$ with scaling factor $f = \mu_0|qQ|/(\Lambda^2 - \frac{1}{4})$, $\Lambda = (D-3)/2$, the scaled Hamiltonian is given by

$$H_\infty^0 = \frac{1}{2\sin^2\theta}\left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) - \frac{\kappa}{r_1 r_2}\frac{\cos\theta}{\sin^2\theta} - \frac{1}{r_1} - \frac{1}{r_2} + \frac{\lambda}{r_{12}}, \quad (7)$$

where $r_{12} = (r_1^2 + r_2^2 - 2r_1 r_2\cos\theta)^{1/2}$. The scaled Hamiltonian depends linearly on $\lambda = |Q/q|$ and $\kappa = 1/(1 + m/M)$.

For finite κ, the mass-polarization term depends on the angular-correlation factor $\cos\theta$. In the Hartree–Fock (HF) approximation at $D \to \infty$, the wave function lacks any explicit dependence on the angle θ; hence the angle becomes fixed at 90°and $\cos\theta = 0$. In this approximation the Hamiltonian becomes κ-independent and the correlation is purely radial due to $r_{12} = (r_1^2 + r_2^2)^{1/2}$. Here we will treat the general case where $\cos\theta \neq 0$ and the Hamiltonian includes both the radial and the angular correlations. Minimizing the H_∞^0 with respect to (r_1, r_2, θ) gives the large-D approximation of the ground-state energy. The results are in complete agreement with the one obtained by Rost using molecular Jacobian coordinates [27]. One can improve this calculations through the $1/D$ expansion [28, 29], but our main focus in this study is the symmetry breaking at the large-D limit and its analogy to critical phenomena and phase transition in statistical mechanics.

Symmetry Breaking

Symmetry breaking phenomena are well documented at the large-D limit for electronic structure configurations of atoms and simple molecules

[14, 26, 30–33]. Recently [6], we have shown that symmetry breaking of the configurations at the large-D limit for HF two-electron atoms and two-center molecules is completely analogous to standard phase transitions. This analogy was shown by allowing the nuclear charge for atoms and the inverse internuclear distance for molecules to play a role analogous to temperature in statistical mechanics [16].

In this section, we consider symmetry breaking of the large-D limit configuration for the three-body Coulombic systems as a function of λ and κ. Minimizing $H^0_\infty(r_1, r_2, \eta = \cos\theta)$ over $0 \le r_1, r_2 \le \infty$, and $0 \le \theta \le \pi$ shows that there is one symmetrical solution with $r_1 = r_2 = r_m$ and one unsymmetrical solution $r_1 \neq r_2$.

For the symmetrical solution the two equal particles have equal distance from the reference particle. This distance is given by

$$r_m = \frac{1+\kappa}{(1+\eta)^2}, \tag{8}$$

and the scaled energy becomes

$$E_\infty = -\frac{(1+\eta)^3(\kappa\eta - 1)}{(1+\kappa)^2(\eta - 1)}, \tag{9}$$

where η is determined by

$$\lambda = \frac{4[\kappa(1+\eta^2) - 2\eta]}{(1+\kappa)[2(1-\eta)]^{1/2}}. \tag{10}$$

Note that in the infinite-mass approximation for the reference particle, such as for two-electron atoms, the above equations reduce to Herschbach's equations [26] $1/r_m = (1+\eta)^2$ and $E_\infty = -(1+\eta)^3/(1-\eta)$ with $\eta = \frac{1}{64}[-\lambda^2 - \lambda(\lambda^2+128)^{1/2}]$.

By investigating the eigenvalues of the Hessian matrix, we find that the symmetry breaking takes place when the angular factor η satisfying the following equation:

$$3(1+\kappa)\eta^2 - 2(3+\kappa)\eta - (1-3\kappa) = 0, \tag{11}$$

which gives an analytic solution for $\eta_c = (3 + \kappa - 2c)/3(1+\kappa)$ with $c = (3 - 2\kappa^2)^{1/2}$. Now the critical value for λ is readily available using η_c:

$$\lambda_c = \frac{4}{3c}\left(\frac{1+\kappa}{\kappa + c}\right)^{1/2}\left[\kappa^3 + \kappa^2(9-2c) + 3\kappa + 6c - 9\right]. \tag{12}$$

In Figure 1, we compare the critical curve λ_c as a function of κ obtained at $D \to \infty$ with the one obtained at $D = 3$ using large basis set calculations (20,336 basis functions) with Laguerre polynomials [25]. Note the similarity between the two curves;

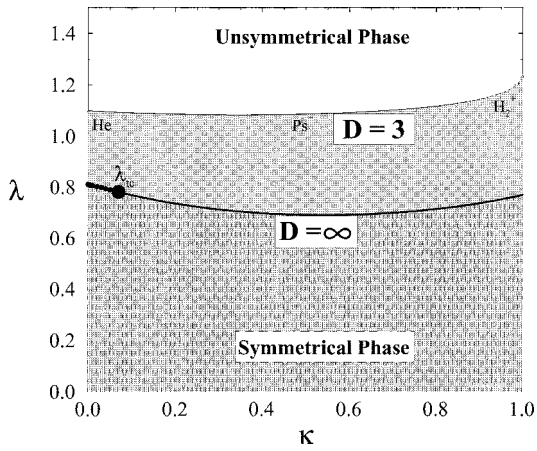

FIGURE 1. Comparison of the critical curve $\lambda_c(\kappa)$ at $D = 3$ and $D = \infty$. Note that $\kappa = 0$ corresponds to the He atom, $\kappa = \frac{1}{2}$ to Ps^- and $\kappa = 1$ to H_2^+. The solid line at $D = \infty$ corresponds to a continuous-phase transition from the symmetrical phase to the unsymmetrical phase. The dotted line is a first-order line that meets the continuous line at a tricritical point λ_{tc}.

both are convex functions with one minimum. At the large-D limit, there is a minimum at $\kappa_m = 3(12 - 21^{1/2})/41 \approx 0.5427$ while at $D = 3$, the minimum is at $\kappa_m \approx 0.35$. This critical curve separates the $(\lambda - \kappa)$-plane into a symmetrical phase (bound region at $D = 3$) for $\lambda < \lambda_c$, and an unsymmetrical phase (breakup region at $D = 3$) for $\lambda > \lambda_c$.

In the bound region, the curve $\lambda_{\eta=0}$ ($\eta = \cos\theta = 0$) where the mass polarization term in Eq. (7) is zero, divides the symmetrical phase into two regions as shown in Figure 2. In region I, $\eta < 0$, and for region II, $\eta > 0$ as shown in the lower part of Figure 2. So we may apply the angular correlation factor to distinguish between atom-like systems if $\kappa < \kappa_{\eta=0} = \frac{1}{3}$ and molecule-like systems if $\kappa > \kappa_{\eta=0}$. This proposed classification of atom-like and molecule-like systems is of great importance in exploring the resonance spectrum and dynamics of three particles where there is neither an obvious point of reference as the heavy nucleus in H^- nor a line of reference as the internuclear axis in H_2^+. Rost and Wintgen [34] have shown that the resonance spectrum of positronium negative ion Ps^- ($\kappa = 0.5$) can be understood and classified with the molecule H_2^+ quantum numbers by treating the interelectron axis of Ps^- as an adiabatic parameter. Our phase diagram at the large-D limit shows that for $\kappa > \frac{1}{3}$ the system belongs to the molecule-like region.

Furthermore one can introduce an external weak static electric field to break the symmetry of Eq. (7).

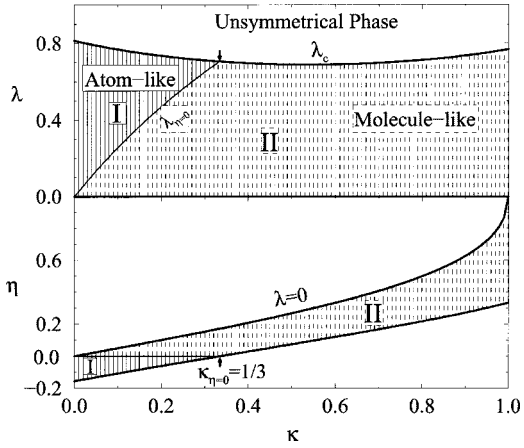

FIGURE 2. Stability diagram in the $(\lambda - \kappa)$ plane is shown in the upper part with the zero angular correlation line $\lambda_{\eta=0}$ separating the symmetrical phase into atom-like region I and molecule-like region II. In the lower part the angular correlation factor $\eta = \cos\theta$ is shown as a function of κ with the two regions I and II bounded by the curve $\lambda = 0$ and $\lambda = \lambda_c$. Note the atom-like region I has a negative domain while the molecule-like region II is positive.

With the presence of an external electric field $\mathcal{E}$ the Hamiltonian reads

$$H_\infty = H_\infty^0 - \mathcal{E}(r_1 - r_2). \tag{13}$$

The direction of the electric field is chosen in order to preserve the symmetry of the Hamiltonian $H_\infty(r_1, r_2, \mathcal{E}) = H_\infty(r_2, r_1, -\mathcal{E})$.

At $\mathcal{E} \neq 0$ there exists only one unsymmetrical solution. The deviation from the symmetrical solution can be expressed by introducing a new parameter s such that $r_1 = r$ and $r_2 = (1 - s)r$ with $0 \leq s \leq 1$.

The total symmetrical solution with $r_1 = r_2 = r_m$ at $\mathcal{E} = 0$ is obtained by taking $s = 0$. For $\mathcal{E} \neq 0$ minimizing energy about r, s, and $\eta = \cos\theta$ gives the following equation:

$$\lambda(\kappa, s, \eta) = r_{12}^{3/2} \frac{s_0}{\eta_0} \frac{(s^2 - 2s + 2)\eta + \kappa(s-1)(\eta^2 + 1)}{s^2 + s\eta_0 + \kappa(s-1)\eta_0 - \eta + 1}, \tag{14}$$

where

$$s_0 = -\frac{2 - 2s + s^2}{(s-2)(s-1)^2}, \qquad \eta_0 = \eta - 1,$$
$$r_{12} = s^2 + 2s(\eta - 1) - 2\eta + 2,$$

and

$$r(\kappa, s, \eta) = \frac{s^2 + s\eta_0 + \kappa(s-1)\eta_0 - \eta + 1}{s_0(s-1)^3(\eta - 1)(\eta + 1)^2}, \tag{15}$$

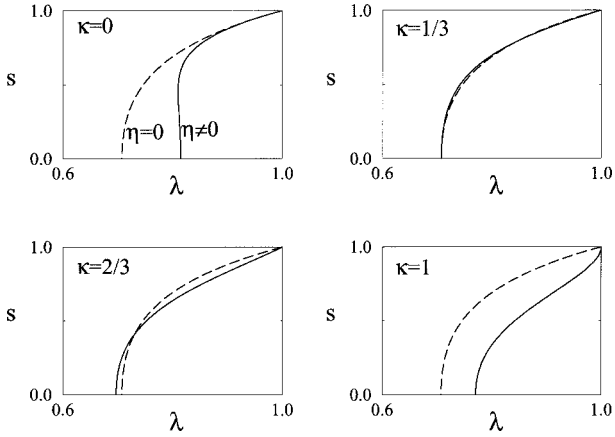

FIGURE 3. Asymmetry parameter s as a function of the Coulombic parameter λ for $\kappa = 0, \frac{1}{3}, \frac{2}{3}$, and 1.0. The solid curves with $\eta \neq 0$ and the dashed curves with $\eta = 0$.

and for

$$E_\infty = H_\infty(\kappa, s, \eta); \qquad \mathcal{E} = \mathcal{E}(\kappa, s, \eta). \tag{16}$$

Explicit expressions are given in Appendix A.

For external filed $\mathcal{E} = 0$, we show in Figure 3 the asymmetry parameter s as a function of the parameter λ for different values of κ. The parameter $s = 0$ for all $\lambda < \lambda_c$, which means we have the symmetrical solution, but once the system reaches λ_c the symmetry breaking occurs. Figure 4 shows the behavior of the asymmetry parameter as a function of the external field $\mathcal{E}$ for different values of κ. The behavior of the asymmetry parameter s is completely analogous

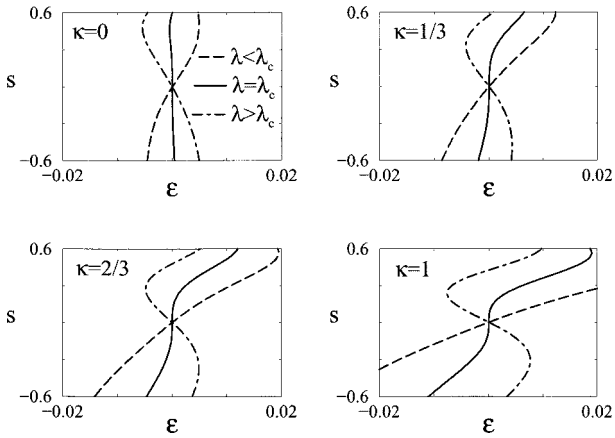

FIGURE 4. Asymmetry parameter s as a function of the external electric field $\mathcal{E}$ for three different values of $\lambda = \lambda_c - 0.05 < \lambda_c$ (dashed line), $\lambda = \lambda_c$ (solid line), and $\lambda = \lambda_c + 0.05 > \lambda_c$ (dot-dashed line) at $\kappa = 0, \frac{1}{3}, \frac{2}{3}$, and 1.0.

to figures representing the behavior of magnetization as a function of temperature in the mean field theory.

Mapping to Critical Phenomena

In statistical mechanics of quantum systems, the quantities of interest are the partition function of the system $Z(\beta) = \mathrm{Tr}\, e^{-\beta H}$ and the expectation values of an arbitrary operator A, $\langle A \rangle = [1/Z(\beta)]\,\mathrm{Tr}(Ae^{-\beta H})$, where H is the Hamiltonian of the system and β is the inverse of temperature $\beta = 1/kT$. Upon taking the limit $T \to 0$, the free energy $F = -(1/\beta)\ln Z(\beta)$ becomes the ground-state energy, and the various thermal averages become ground-state expectation values [6]. Now a mapping between symmetry breaking for three-body Coulombic systems and critical phenomena in statistical mechanics is readily given by

$$\begin{aligned}
\text{Coulomb strength } \lambda &\Longleftrightarrow \text{Temperature } T,\\
\text{Asymmetry } s &\Longleftrightarrow \text{Ordering parameter } m,\\
\text{External field } \mathcal{E} &\Longleftrightarrow \text{Ordering field } h,\\
\text{Ground state energy } E_\infty(\lambda,\mathcal{E}) &\Longleftrightarrow \text{Free energy } f(T,h),\\
\text{Stability limit point } \lambda_c &\Longleftrightarrow \text{Critical point } T_c.
\end{aligned}$$

Using this scheme of mapping between the two problems, one can define the four critical exponents $(\alpha, \beta, \delta, \gamma)$ in the following way:

$$-\frac{\partial^2 E_\infty}{\partial \lambda^2}(\mathcal{E}=0,\lambda)\Big|_{\lambda\to\lambda_c^-} \sim |\lambda_c - \lambda|^{-\alpha}, \tag{17}$$

$$s(\mathcal{E}=0,\lambda)\Big|_{\lambda\to\lambda_c^-} \sim |\lambda_c - \lambda|^{\beta}, \tag{18}$$

$$\mathcal{E}(\lambda_c, s)\Big|_{s\to 0} \sim |s|^{\delta}, \tag{19}$$

$$\frac{\partial s}{\partial \mathcal{E}}(\mathcal{E}=0,\lambda)\Big|_{\lambda\to\lambda_c^-} \sim |\lambda_c - \lambda|^{-\gamma}. \tag{20}$$

To obtain the critical exponents we start with Eq. (16) at $\mathcal{E} = 0$, which gives $\eta = \eta(\kappa, s)$:

$$\begin{aligned}
\eta = \big(&-s^4 + 5s^3 - 2\kappa s^2 - 11s^2 + 4\kappa s + 12s\\
&+ f - 2\kappa - 6\big)\\
&\times \big(2(\kappa+1)(s-1)(s^2-3s+3)\big)^{-1},
\end{aligned} \tag{21}$$

where $f = (2-s)(f_1 + \kappa^2 f_2)^{1/2}$, $f_1 = (s^2-3s+3)(s^4 - 3s^3 + 7s^2 - 8s + 4)$, and $f_2 = -4(s-1)^2(s^2-2s+2)$ with the restriction that $s \le 1$ and $0 \le \kappa \le 1$.

Taking the asymptotic limit of Eq. (14), $s \to 0$, we find that $\lambda_c - \lambda \sim s^2$, which gives the critical exponent $\beta = \frac{1}{2}$. In order to obtain the critical exponent α, we have to expand energy E_∞ in Eq. (16) as a function of $(\lambda_c - \lambda)$ in order to get its second derivative at $\mathcal{E} = 0$. Unfortunately, we could not have an explicit expression for $s = s(\lambda)$ from Eq. (14). We have to find an approximate solution $s = s(\lambda)$ from $\lambda = \lambda(s)$ at $s \to 0$ and then put the solution into an s sequence of energy. We noted that the energy sequence does not include s^1 terms and for the real solution of equation $c_2 s^2 + c_3 s^3 - (\lambda - \lambda_c) = 0$, the s^3 terms in the sequence are canceled. For the real solution of equation $c_2 s^2 + c_3 s^3 + c_4 s^4 - (\lambda - \lambda_c) = 0$ at $s \le 1$ the s^3 terms are canceled too, and we get an approximate expansion of E_∞ which is exact up to s^4 or $(\lambda_c - \lambda)^2$. Here c_2, c_3, and c_4 are functions of the parameter κ from Eq. (14). Using $\partial^2 E_\infty/\partial\lambda^2$ at $\mathcal{E} = 0$ and comparing it to Eq. (17) we finally identify $\alpha = 0$. We evaluate $\delta = 3$ and $\gamma = 1$ without approximations.

The continuous-phase transition discussed above and the related mean field critical exponents are valid over the range $\kappa_t = 0.07 < \kappa \le 1.0$, where $\kappa_t = 0.07$. This special point, κ_t, where the second-order line meets the first-order line over $[0, \kappa_t)$ in Figure 1 is called a tricritical point. Our further calculations of E_∞ at $\mathcal{E} = 0$ show that over $0 \le \kappa \le \kappa_t$ there are two local minima at $s_1 \ne 0$ and $s_2 \ne 0$ with a maximum at $s = 0$, and over $\kappa_t \le \kappa \le 1.0$ there is only one global minimum at $s = 0$. As κ increases to κ_t, two local minima merge into a global minimum at $s = 0$, and the energy transition takes place between the symmetrical and the unsymmetrical regions as shown in Figure 1.

Concluding Remarks

We have shown that there is a universal behavior of all *ABA* Coulomb systems at the large-dimension limit. They exhibit a continuous quantum phase transition as the parameter λ varies. The critical line, $\lambda_c(\kappa)$, between the symmetrical and the unsymmetrical phases is analytically calculated using the large-D model Hamiltonian. The critical line is a convex function of the mass parameter κ and has a minimum at $\kappa_m \simeq 0.5$. The transition line is a second-order line over the range $\kappa_t \le \kappa \le 1.0$ and a first-order line over the range $0 \le \kappa \le \kappa_t$ where the point $\kappa_t = 0.07$ is a tricritical point. It is interesting to note that the *ABA* Coulomb systems exhibit a first-order quantum phase transition at $D = 3$ as the parameter λ varies. This suggests that there is a transition crossover as the physical dimension varies between $D = \infty$ and $D = 3$ over $\kappa_t \le \kappa \le 1.0$.

The line with the zero angular correlation ($\eta = 0$) crosses the critical line at $\kappa = \frac{1}{3}$ and separates the symmetrical phase into two regions: atom-like and molecule-like regions. One is of negative η, which includes the helium atom, and the other has a positive η and covers the hydrogen molecule ion. This finding is very similar to the proposed classification of the three-body Coulombic systems at $D = 3$: molecule-like systems with $\kappa > \kappa_m = 0.35$ and atom-like systems with $\kappa < \kappa_m$. This might be a powerful result in understanding the dynamics and resonances of *ABA* three-body Coulombic systems.

Appendix A

The explicit expressions for the energy and the external fields at the large-D limit as a function of parameters s, κ, and η in Eq. (16) are given by

$$E_\infty = \frac{(2 - 2s + s^2)(1 + \eta)^2 h_0}{2(-1 + s)h_1^2}, \tag{22}$$

where h_0 is a polynomial in s:

$$h_0 = c_0 + c_1 s + c_2 s^2 + c_3 s^3 + c_4 s^4 + c_5 s^5 + c_6 s^6$$

with coefficient

$$\begin{aligned}
c_0 &= 4(-1 + \kappa\eta)\left(-1 + \eta^2\right),\\
c_1 &= -12(-1 + \kappa\eta)\left(-1 + \eta^2\right),\\
c_2 &= 2\left(2\left(5 + 6\eta - 7\eta^2\right) + \kappa\left(-6 - 3\eta - 6\eta^2 + 7\eta^3\right)\right),\\
c_3 &= -4\left(5 + 12\eta - 9\eta^2 + 2\kappa\left(-3 + \eta - 3\eta^2 + \eta^3\right)\right),\\
c_4 &= 9 + 44\eta - 21\eta^2 + 2\kappa\left(-8 + 3\eta - 8\eta^2 + \eta^3\right),\\
c_5 &= -1 - 20\eta + 5\eta^2 + 4\kappa\left(1 + \eta^2\right),\\
c_6 &= 4\eta,
\end{aligned}$$

and h_1 is given by

$$\begin{aligned}
h_1 = (-2 + s)\big(1 + s^2 + \kappa(-1 + s)(-1 + \eta)\\
+ s(-1 + \eta) - \eta\big).
\end{aligned}$$

The external field has the following form:

$$\begin{aligned}
\mathcal{E} = s\left(2 - 2s + s^2\right)^2(-1 + \eta)(1 + \eta)^4 e_0\\
\times\big((-2 + s)^3\big(1 + s^2 + \kappa(-1 + s)(-1 + \eta)\\
+ s(-1 + \eta) - \eta\big)^3\big)^{-1},
\end{aligned} \tag{23}$$

where

$$\begin{aligned}
e_0 &= 1 + 6\eta - 3\eta^2 + e_1 + e_2,\\
e_1 &= s^4\eta + s^3(-5 + \eta)\eta + s^2\left(1 + 11\eta - 4\eta^2\right)\\
&\quad + 2s\left(-1 - 6\eta + 3\eta^2\right),\\
e_2 &= \kappa(-1 + s)\big(3 - 2\eta + 3\eta^2\\
&\quad + s\left(-3 + 2\eta - 3\eta^2\right) + s^2\left(1 + \eta^2\right)\big),
\end{aligned}$$

where η is given by Eq. (21), $s \le 1$ and $0 \le \kappa \le 1$.

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