

The N -body problem and the $1/d$ expansion

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The family of trajectories of the bound states of a cluster of N identical particles (atoms, molecules, etc.) is studied by the method of the $1/d$ expansion (d is the dimensionality of space). In particular, the critical values of the coupling constant that correspond to the formation of a new bound state as the potential deepens are calculated. Approximate formulas are obtained for the critical coupling constants of inert-gas microclusters.

1. INTRODUCTION

The problem of the spectrum of the bound states of a system of identical particles interacting through a short-range potential has a number of applications in the physics of the nucleus and the physics of the condensed state. In the present paper we consider the case of a central pair interaction $U(r)$ —a case that bears a direct relation to atomic and molecular clusters.

Besides being of interest in its own right, the study of clusters also has importance for an understanding of the process of the gradual formation of the properties of a condensed medium as the number of particles in the cluster increases. In addition, the spectroscopy of clusters provides additional information on the character of the interaction of particles that cannot be obtained from data on two-particle processes.

Recently experimentalists have paid considerable attention to inert-gas clusters,^{1–4} for which an approximate formula for the binding energies will be obtained in the present paper.

The problem, in the framework of the method developed here is solved in three stages. First we calculate the spectrum of the critical coupling constants λ_c , i.e., those values of λ for which the spectra of the Hamiltonians with potentials $(\lambda + 0)U$ and $(\lambda - 0)U$ differ by one bound state. Then, for each value of λ_c , we find the spectrum of the bound states and, finally, construct the family of trajectories $\mathcal{E}(\{n_k\}, \lambda)$ in the “energy–coupling constant” plane for the levels with the set of quantum numbers $\{n_k\}$. The intersection of the trajectories with the straight line $\lambda = \lambda_{ph}$ (where λ_{ph} is the physical value of the coupling constant) gives the spectrum of the excited states (both bound states and resonances) of the cluster. In addition, in those cases when the pair potential is too weak for a two-particle bound state to exist (as is the case, e.g., for helium atoms), our method makes it possible to determine the threshold number of particles N_c above which a bound state exists in a cluster.

It should be noted that the quantum problem is extremely complicated even for three or four particles, because of the abundance of bound states, resonances, and decay channels. Progress in the N -body problem has been associated mainly with scattering theory,⁵ if we have in mind methods that do not use model approximations. In particular, such theorem-type statements as the Efimov effect and the Thomas theorem^{6–8} were obtained in the framework of scattering theory. In a number of papers^{9–11} the critical coupling constants of the ground state of a three-particle and a four-particle cluster have been calculated in the case of separable

potentials, and estimates have also been made for local short-range potentials.

However, using scattering theory alone, up to now no one has succeeded in obtaining (approximate) analytical formulas for the energy-level spectrum in the many-particle problem. Our aim is to obtain such formulas for the case of identical particles and a broad class of short-range potentials. In addition, the proposed method (unlike variational and quasiclassical methods) makes it possible to investigate the spectrum as a whole.

The main idea of the method is as follows. We place N identical (structureless) particles in d -dimensional Euclidean space. In the limit $d \rightarrow \infty$ the system “crystallizes” (the fluctuations are of order $\langle(\Delta r^2)\rangle \sim d^{-1}$) about the completely symmetrical configuration of a regular simplex (a triangle for $N = 3$, and a tetrahedron for $N = 4$). It can be shown that the limiting problem is exactly solvable. The system is completely localized in configuration space, and this makes it possible to calculate the asymptotic value of λ_c from the static configuration:

$$\lambda_c \sim \frac{d^2}{2N|U(a_0)|a_0^2}, \quad d \rightarrow \infty. \quad (1)$$

Henceforth we shall call quantities calculated in the static limit “classical”, meaning by this only the following: We neglect fluctuations on the background of the static configuration. It should be stressed that the limit $d \rightarrow \infty$ has nothing in common with the quasiclassical approximation. (In fact, the static effective potential contains terms of order $\hbar^2 d^2$.) Superposed on the equilibrium symmetric configuration there are quantum fluctuations, which, in the harmonic approximation, lead to corrections $\sim d^1$ to the asymptotic formula (1). Allowance for anharmonic effects gives corrections $\sim d^0, d^{-1}$, etc. Thus, an asymptotic perturbation theory in the parameter $1/d$ can be constructed.

In Secs. 2–4 we calculate λ_c , in Sec. 5 we discuss the question of the selection of the states that have symmetry compatible with the statistics of the particles, in Sec. 6 we consider the problem of the bound-state spectrum, and in Sec. 7 we give the results for Lennard-Jones clusters (in particular, for inert gases).

2. EFFECTIVE HAMILTONIAN OF THE s -SECTOR

We turn to the formulation of the method of the $1/d$ expansion for application to the problem of calculating the spectrum of λ_c . We shall consider a system of N identical particles with mass M (for definiteness, we temporarily assume them to be bosons with spin zero), placed in d -dimen-

sional Euclidean space ($d \geq N - 1$) and interacting via a central pair potential $U(r)$ that decreases faster than $1/r^2$ at infinity. In such a potential there is only a finite number of bound two-particle states. The potential $U(r)$ has, possibly, a singular core [$U(r) \sim 1/r^{2+\nu}$, $\nu > 0$, $r \rightarrow 0$], but not an absolutely hard core, and is an analytic function on the positive semi-axis. In addition, we require that the function $r^2 U(r)$ have precisely one nondegenerate local minimum at $r \neq 0, \infty$, this (as will be seen from the following) being necessary for the existence and uniqueness of a symmetric equilibrium configuration of a cluster in the limit $d \rightarrow \infty$.

The Schrödinger equation (in the system of units with $\hbar = M = 1$) for the critical coupling constant λ_c and the wavefunctions ψ_c at the localization threshold has the form

$$-\frac{1}{2} \sum_{A=1}^N \sum_{a=1}^d \frac{\partial^2 \psi_c}{\partial u_{Aa}^2} + \lambda_c \sum_{A < B} U(r_{AB}) \psi_c = 0, \quad (2)$$

where u_{Aa} ($A = 1, \dots, N$; $a = 1, \dots, d$) are the coordinates of the particles, and $r_{AB} = |\mathbf{u}_A - \mathbf{u}_B|$.

We now confine ourselves to considering states with zero total orbital angular momentum, i.e., to the s -sector. In this sector there are (for $d \geq N - 1$) only $\frac{1}{2}N(N - 1)$ dynamical variables—namely, the internal coordinates r_{AB} of the cluster. To eliminate the nonphysical degrees of freedom (the Euler angles describing the orientation of the cluster, and the coordinates of the center of mass of the cluster), in (2) we go over to the cluster internal coordinates and the conjugate momenta p_{AB} . At the same time we replace the wavefunction using the rule $\varphi_c = \psi_c J^{1/2}$, where J is the Jacobian of the transformation to the internal coordinates, with the aim of disposing of the terms linear in the momenta. We obtain the equation

$$H_{eff,c} \varphi_c = 0, \quad H_{eff,c} = T + V_{eff,c}, \quad (3)$$

$$T = \sum_{A < B} p_{AB}^2 + \sum_A \sum_{B < C}^{(A)} \frac{r_{AB}^2 + r_{AC}^2 - r_{BC}^2}{2r_{AB}r_{AC}} p_{AB} p_{AC},$$

where $\Sigma^{(A)}$ denotes that the index A is omitted in the summation. The effective potential $V_{eff,c}$ consists of the “centrifugal potential” W and a sum V_c of pair potentials:

$$V_{eff,c} = W + V_c, \quad W = \frac{\alpha}{2} \Gamma^{-1} \sum_A \Gamma^{(A)},$$

$$V_c = \lambda_c \sum_{A < B} U(r_{AB}), \quad \alpha = \frac{1}{4} (d-1)(d-2N+1), \quad (3')$$

where $\Gamma = \det(\gamma_{AB})$ is the Gram determinant of the N -particle system, $\gamma_{AB} = \mathbf{u}_{AN} \cdot \mathbf{u}_{BN}$, and $\Gamma^{(A)}$ is the Gram determinant of the subsystem obtained by throwing away the particle with label A . The boundary conditions on φ_c correspond to localized states on the threshold of binding.

We consider the $d \rightarrow \infty$ limit of Eq. (3). The system is at the effective-potential minimum corresponding to the symmetric configuration, which is determined by a single parameter—namely the equilibrium interparticle spacing a . We expand $V_{eff,c}$ about a , setting $r_{AB} = a + x_{AB}$. The condition for vanishing of the coefficient of $\sum_{A < B} x_{AB}$ gives

$$-4\alpha/Na^3 + \lambda_c U'(a) = 0. \quad (4)$$

The asymptotic value of λ_c is found from the condition for

vanishing of the effective potential at the minimum:

$$V_{eff,c}(a) = \frac{1}{2} N(N-1) \lambda_c U(a) + \alpha(N-1)/a^2. \quad (5)$$

As a result, we obtain the relation (1), in which a_0 is equal to the value of the equilibrium interparticle spacing in the leading order in $1/d$ and is determined from (4):

$$\frac{d}{dr} [r^2 U(r)] |_{r=a_0} = 0. \quad (4')$$

The relations (1) and (4') give the asymptotic value of the threshold coupling constant, corresponding to the “classical” limit. We, however, shall be interested in the value of λ_c at a physical value of d ($d_{ph} = 2$ or 3). We shall seek an expression for λ_c in the form of an asymptotic series in powers of $1/d$:

$$\lambda_c^{(p+1)} \sim \lambda_2 d^2 + \lambda_1 d + \lambda_0 + \sum_{h=1}^p \lambda_{-h} d^{-h} + O(d^{-p-1}). \quad (6)$$

Truncating the expansion (6) at the first term corresponds to the “classical” approximation, while truncating it at the second corresponds to the harmonic approximation. Taking the third term into account means calculating the correction from the cubic and quartic anharmonicities in the first non-vanishing order. An analogous expansion also holds for the equilibrium interparticle spacing a :

$$a^{(p)} \sim a_0 + \sum_{h=1}^p a_{-h} d^{-h} + O(d^{-p-1}). \quad (7)$$

To find the spectrum of λ_c to terms $\sim d^{-p}$ it is necessary to expand the effective Hamiltonian $H_{eff,c}$ to anharmonicities of degree $2p + 4$ and to calculate by perturbation theory its spectrum, which will have a $1/d$ structure analogous to (6):

$$\mathcal{E}_c \sim \mathcal{E}_2 d^2 + \mathcal{E}_1 d + \mathcal{E}_0 + \sum_{h=1}^p \mathcal{E}_{-h} d^{-h} + O(d^{-p-1}). \quad (8)$$

Setting in (8) $\mathcal{E}_k(\{n_M\}) = 0$ ($k = 2, 1, \dots, -p$), we obtain a recursive chain of equations for the coefficients $\lambda_l(\{n_M\})$ ($l = 2, 1, \dots, -p$) in the asymptotic expansion (6).

3. ASYMPTOTIC SYMMETRY OF THE CLUSTER: THE NORMAL MODES

We shall consider the quantum dynamics superposed on the classical equilibrium configuration. In the asymptotic limit $d \rightarrow \infty$ the problem becomes exactly solvable owing to the symmetry of the Hamiltonian (3) and the wavefunctions under the group of permutations of the particles, which is isomorphic to the symmetric group S_N (we recall that we have temporarily confined ourselves to considering bosons with spin zero).

In the asymptotic limit the quantum fluctuations are harmonic, and the problem reduces to that of a harmonic oscillator with $\frac{1}{2}N(N - 1)$ degrees of freedom and an additional symmetry. Small displacements x_{AB} from the equilibrium configuration transform according to a $\frac{1}{2}N(N - 1)$ -dimensional representation of S_N , equal to the direct sum of three irreducible representations—namely, a one-dimensional representation (N), an $(N - 1)$ -dimensional representation ($N - 1, 1$), and a $\frac{1}{2}N(N - 3)$ -dimensional representation ($N - 2, 2$), which we designate as the scalar (s),

vector (v), and tensor (t) representations, respectively. Thus, the vibrational spectrum of the cluster is classified using three irreducible representations, and has three different normal modes Ω_s , Ω_v , and Ω_t .

The correction to the classical energy (5) on account of harmonic oscillations about the equilibrium configuration is given by the following obvious expression:

$$\mathcal{E}_{\text{harm}} = \sum_{\gamma=s,v,t} (K_\gamma + D_\gamma/2) \Omega_\gamma, \quad (9)$$

where D_γ are the dimensionalities of the irreducible representations, and K_γ are the principal quantum numbers of the three S_N -invariant "spherical" oscillators.

To determine the normal-mode frequencies Ω_γ we bring the part of the effective Hamiltonian that is quadratic in the operators p_{AB} and x_{CD} into diagonal form:

$$H_2 = \frac{\pi_0^2}{2M_s} + \frac{M_s \Omega_s^2 \xi_0^2}{2} + \frac{1}{2M_v} \sum_{k=2}^N \pi_k^2 + \frac{M_v \Omega_v^2}{2} \sum_{k=2}^N \xi_k^2 + \frac{1}{2M_t} \sum_{l=4}^N \sum_{k=2}^{l-1} \pi_{kl}^2 + \frac{M_t \Omega_t^2}{2} \sum_{l=4}^N \sum_{k=2}^{l-1} \xi_{kl}^2, \quad (10)$$

where ξ_0 , ξ_k , and ξ_{kl} are normal coordinates, and π_0 , π_k , and π_{kl} are the conjugate momenta, corresponding to the scalar, vector, and tensor types of oscillation of the cluster. The normal coordinates are constructed from the internal coordinates x_{AB} of the cluster as follows:

$$\begin{aligned} \xi_0 &= \left(\frac{2}{N(N-1)} \right)^{1/2} \sum_{A < B} x_{AB}, \\ \xi_k &= [k(k-1)(N-2)]^{-1/2} \left[\sum_{p=1}^{k-1} x_p - (k-1)x_k \right], \\ k &= 2, \dots, N, \\ \xi_{kl} &= [k(k-1)(l-2)(l-3)]^{-1/2} \left[\sum_{m=1}^{k-1} y_{ml} - (k-1)y_{kl} \right], \\ k &= 2, \dots, l-1; \quad l=4, \dots, N, \end{aligned} \quad (11)$$

where

$$x_A = \sum_B^{(A)} x_{AB}, \quad y_{mk} = \sum_{A=1}^{k-1}^{(m)} x_{mA} - (k-3)x_{mk}, \\ m=1, \dots, k-1.$$

Similarly, π_0 , π_k , and π_{kl} can be expressed in terms of p_{AB} . It is easy to convince oneself that the normal coordinates and momenta determined by Eq. (11) are canonically conjugate. After substitution of (11) into (10) and identification with the quadratic part of the Hamiltonian (3) we find the following expressions for the normal modes Ω_γ and masses M_γ of the vibrational excitations of the cluster:

$$\begin{aligned} \Omega_s &= \left(\frac{12\alpha}{a^4} + \lambda N U''(a) \right)^{1/2}, \quad M_s = \frac{1}{N}; \\ \Omega_v &= \left(\frac{14\alpha}{a^4} + \frac{\lambda N}{2} U''(a) \right)^{1/2}, \quad M_v = \frac{2}{N}; \end{aligned} \quad (12)$$

$$\Omega_t = \left(\frac{(16-4N^{-1})\alpha}{a^4} + \lambda U''(a) \right)^{1/2}, \quad M_t=1.$$

To calculate λ_c to terms $\sim d^1$ we equate to zero the coefficients \mathcal{E}_2 and \mathcal{E}_1 in the expansion (8), where \mathcal{E}_2 is determined by the minimum of the effective potential and is the leading (in $1/d$) term of the "classical" part of the energy, while \mathcal{E}_1 contains both the harmonic part of the energy (9) (in leading order in $1/d$) and a correction to the "classical" part of the energy (in the next-to-leading order). As a result, we find

$$\begin{aligned} \lambda_2 &= \frac{1}{2N|U(a_0)|a_0^2}, \\ \lambda_1 &= \frac{1}{|U(a_0)|} \left(-\frac{1}{a_0^2} + \frac{2}{N(N-1)} \mathcal{E}_{\text{harm},1} \right), \end{aligned} \quad (13)$$

where

$$\mathcal{E}_{\text{harm},1} = \sum_{\gamma=s,v,t} (K_\gamma + D_\gamma/2) \omega_\gamma$$

is the leading (in $1/d$) term of the harmonic part of the energy.

We give an explicit expression for the leading coefficients ω_γ in the $1/d$ expansion of the frequencies $\Omega_\gamma \sim \omega_\gamma d + \Omega_{\gamma,0} + \dots$:

$$\begin{aligned} \omega_s &= \left(\frac{3}{a_0^4} + \frac{U''(a_0)}{2|U(a_0)|a_0^2} \right)^{1/2}, \\ \omega_v &= \left(\frac{7}{2a_0^4} + \frac{U''(a_0)}{4|U(a_0)|a_0^2} \right)^{1/2}, \\ \omega_t &= \left(\frac{4-N^{-1}}{a_0^4} + \frac{U''(a_0)}{2N|U(a_0)|a_0^2} \right)^{1/2}. \end{aligned} \quad (12')$$

The expression $\lambda_2 d^2 + \lambda_1 d$ corresponds to the exact quantum solution, for the existence of which it is necessary that all frequencies be positive (to leading order in $1/d$), i.e., that $\omega_\gamma > 0$ ($\gamma = s, v, t$). As can be seen without difficulty, the positivity of ω_γ follows from the condition imposed on the potential U at the beginning of Sec. 2 [the function $r^2 U(r)$ has a single nondegenerate minimum]. Thus, an exact quantum solution exists for this class of potentials. For $N = 3$ and $N = 4$ this solution is also unique (provided that the minimum of $r^2 U(r)$ is unique).

We now shift the expansion parameter d , using the formula

$$\tilde{d}(\{n_\kappa\}) = d + \delta(\{n_\kappa\}), \quad \delta(\{n_\kappa\}) = -N + 2a_0^2 \mathcal{E}_{\text{harm},1} / (N-1). \quad (14)$$

Then, to within terms $\sim O(d^0)$, the expression $\lambda_2 d^2 + \lambda_1 d$ is equivalent to $\lambda_2 \tilde{d}^2$, i.e., the shift (14) makes it possible to interpret the quantum corrections as an effective renormalization of the dimensionality $d \rightarrow \tilde{d}$. As will be seen from the following, the renormalization (14) is necessary for the elimination of structures (in higher orders of perturbation theory in the parameter $1/d$) that diverge in the quasiclassical limit (i.e., at large values of the vibrational quantum numbers), and corresponds to a certain special way of resumming the perturbation-theory series. This renormalization, for the class of potentials $U_\mu(r) = r^{-2\mu-2} - 2r^{-\mu-2}$,

which are exactly solvable for $N = 2$, leads to the result that the renormalized classical value of λ_c (for $N = 2$) coincides with the exact value for all values of K_s .

We note that in a number of papers on the $1/d$ expansion a shift of the expansion parameter is used to improve the convergence of the perturbation-theory series.¹²⁻¹⁴ For the two-body problem the shifted $1/d$ expansion can be interpreted as a $1/n$ expansion (where n is the principal or radial quantum number).¹⁵

The spectrum of λ_c in the harmonic approximation is strongly degenerate. In fact, it follows from (13) that λ_c depends only on the three principal quantum numbers

$$K_s = n_0, \quad K_v = \sum_{k=2}^n n_k, \quad K_t = \sum_{l=1}^n \sum_{k=2}^{l-1} n_{kl}.$$

In the classical limit, i.e., for $n_0, n_k, n_{kl} \rightarrow \infty$, we have multi-dimensional classical degeneracy, implying coincidence of the frequencies in the sectors corresponding to purely vector or tensor oscillations. Allowing for the corrections to λ_c that arise from the anharmonicities lifts the continuous (in the classical limit) degeneracy and leaves only "accidental" discrete degeneracy.

4. PERTURBATION THEORY IN THE PARAMETER $1/d$

We turn now to the analysis of the general structure of the corrections to the asymptotic formula $\lambda_c \sim \lambda_2 \bar{d}^2$ that arise on account of the anharmonic terms in $H_{\text{eff},c}$. The scale of the quantum fluctuations in the harmonic approximation, as we have seen, is as follows: $\langle x_{AB}^2 \rangle \sim d^{-1}$, $\langle p_{AB}^2 \rangle \sim d(d \rightarrow \infty)$. In the harmonic approximation each of the three terms T , W , and V_c of the effective Hamiltonian (3) is of order d . Thus, the anharmonic terms of degree $k + 2$ in (3) are of order $d^{1-k/2}$.

We shall regard the anharmonic part H_{anh} of the operator $H_{\text{eff},c}$ as a perturbation. In the f th order of perturbation theory (in the anharmonicity) structures arise that contain in the numerator a product of f matrix elements of the operator H_{anh} , and in the denominator a product of $f - 1$ linear combinations of normal-mode frequencies. We shall estimate in leading order in $1/d$ the contribution of the structure containing anharmonic terms of degrees $k_j + 2$ ($j = 1, \dots, f$) in the dynamical variables. The numerator is of order $d^{f-k/2}$, where

$$k = \sum_{j=1}^f k_j,$$

while the denominator is of order d^{f-1} ; consequently, the contribution of the structure under consideration is $O(d^{1-k/2})$. Thus, the correction of order d^{-s} contains structures with different f and $\{k_j\}$, satisfying the condition $k = 2s + 2$. The total number of different structures giving a contribution of order d^{-s} to λ_c is equal to the number of partitions of the number $2s + 2$ into natural numbers. The function $p(k)$ increases rapidly with increase of k (e.g., $p(10) = 42$, and $p(100) = 190,569,292$), and this leads to a sharp increase in the size of the calculations as each successive correction is taken into account. We shall enumerate the partitions for the first three corrections, using the standard notation ($1^s 2^g \dots$), indicating that the partition contains

precisely g_1 ones, g_2 twos, etc., with

$$\sum_{j \geq 1} g_j j = k.$$

For $s = 0$ there are two partitions: (2) and (1²), corresponding to allowance for the quartic anharmonicity in first order and for the cubic anharmonicity in second order; for $s = 1$ there are five partitions: (4), (13), (2²), (1²2), and (1⁴); for $s = 2$ there are already eleven partitions: (6), (15), (24), (1²4), (3²), (123), (1³3), (2³), (1²2²), (1⁴2), (1⁶).

The multiple (in the classical sense) degeneracy of the spectrum of λ_c that obtains in the harmonic approximation is lifted by the $O(d^0)$ terms. There remains only the "accidental" degeneracy with a multiplicity not greater than a certain value fixed for each value of N (equal to 2 for $N = 3$, and 3 for $N = 4$).

To calculate λ_c to order $\sim d^0$ we need (besides a more exact calculation of the "classical" and "harmonic" parts of the energy) to solve the secular equation in a layer with fixed principal quantum numbers K_γ (i.e., in the subspace of the states belonging to one value of λ_c in the harmonic approximation):

$$\det(KP(\{K_\gamma\}) - \varepsilon P(\{K_\gamma\})) = 0 \quad (15)$$

with effective Hamiltonian K . The operator K has the form

$$K = \sum_{\{K_\gamma\}} P(\{K_\gamma\}) \left(H_c - H_s \sum_{\{K_\gamma'\}} \frac{P(\{K_\gamma'\})}{\mathcal{E}_{\text{harm}}(\{K_\gamma'\}) - \mathcal{E}_{\text{harm}}(\{K_\gamma\})} H_s \right) \times P(\{K_\gamma\}), \quad (16)$$

where $P(\{K_\gamma\})$ is the projection operator on to the $\{K_\gamma\}$ -layer, $\mathcal{E}_{\text{harm}}(\{K_\gamma\})$ is the value of the energy of the degenerate level with quantum numbers K_γ in the harmonic approximation, and H_3 and H_4 are the cubic and quartic terms of H_{anh} . Here, since we are interested in the correction of order d^0 , it is sufficient to calculate the spectrum of ε in leading order. To determine the splitting of the harmonic spectrum of $\lambda_c^{(0)}(\{K_\gamma\})$ in the $\{K_\gamma\}$ -layer, it is necessary to equate successively to zero all the values of \mathcal{E} , calculated with allowance for ε , in the given $\{K_\gamma\}$ -layer.

The problem of the diagonalization of the Hamiltonian K is rather complicated since the scalar, vector, and tensor degrees of freedom are strongly mixed on account of the anharmonicity. In the limit $K_\gamma \rightarrow \infty$ the problem of the diagonalization of the operator (16) becomes purely classical, and for its solution it is convenient to make use of a representation of the Hamiltonian in terms of action-angle variables. We shall regard n_0, n_k , and n_{kl} as continuous variables of the action type and introduce phases φ_0, φ_k , and φ_{kl} conjugate to them. Representing the matrix elements of (16) in trigonometric form, we obtain the classical effective Hamiltonian in a phase space of dimensionality $N(N - 1)$.

The terms of the perturbation-theory series in the parameter $1/d$ for λ_c have the structure n_M^{s+2}/d^s ($s = -2, -1, 0, 1, 2, \dots$) in the classical limit $n_M \rightarrow \infty$, whereas, obviously, the correct quasiclassical asymptotic form for λ_c should be of order n_M^2 for $n_M \rightarrow \infty$. To eliminate terms with a pathological increase in the quasiclassical limit we must renormalize d by the rule (14). It is not difficult to show that with such a renormalization of the expansion pa-

parameter the sum of any number of terms of the perturbation-theory series has the correct quasiclassical asymptotic form.

Three degrees of freedom do not participate in the dynamics for $N \geq 4$. The action variables K_s , K_v , and K_t are integrals of the motion for the classical analog of the Hamiltonian (16): $\{K_\gamma, K\}_{PB} = 0$, while the corresponding phases

$$\chi_s = \varphi_0, \quad \chi_v = \frac{1}{N-1} \sum_{k=2}^N \varphi_k, \quad \chi_t = \frac{2}{N(N-3)} \sum_{l=4}^N \sum_{k=2}^{l-1} \varphi_{kl}$$

are cyclic variables. For the asymptotic calculation of the spectrum of the Hamiltonian (16) we must apply the Maslov technique of multidimensional quasiclassical quantization. The main complication lies in the fact that four integrals are insufficient for integration of the problem (for $N > 4$), and also in the nontriviality of the topology of the subspace $K = \text{const}$.

In this respect the three-particle problem is somewhat distinct. For this problem the number of integrals of the motion at the level of the effective Hamiltonian (16) coincides with the number of degrees of freedom and the corresponding dynamical system is exactly integrable (the dynamics is one-dimensional).

We shall discuss the dynamical symmetry of the problem. As we have seen, the spectrum of the Hamiltonian (10) is multiply degenerate. This fact is a consequence of a non-commutative invariance algebra A_{inv} isomorphic to $su(D_v) \oplus su(D_t)$. The dynamical symmetry makes it possible to obtain a representation of the effective Hamiltonian (16) in the form of a quadratic form on the algebra A_{inv} . In a number of special cases such Hamiltonians admit exact integrability.

For example, for a three-particle cluster we have $A_{\text{inv}} \approx su(2)$, and the spectrum of the Hamiltonian K has the form

$$\varepsilon = k_{vv} k_v^2 + k_{vs} K_v K_s + k_{ss} K_s^2 + l L_v^2 + k_v K_v + k_s K_s + k_0,$$

where the coefficients k and l are expressed in terms of the derivatives $U^{(p)}(a_0)$ ($p = 0, 1, \dots, 4$) and, in view of their cumbersome form, are not given here; $L_v^2 = L_{23}^2$, where $L_{23} = \xi_2 \pi_3 - \xi_3 \pi_2$ is the "orbital angular momentum" of the vector excitations of the cluster.

For bosons with spin zero, only states with L_v a multiple of three are physically admissible. We note also the distinctive "supersymmetry" of the problem, which manifests itself in the fact that the spectrum of K for bosons with spin zero coincides with that for fermions with spin 1/2 and total spin 3/2. (The ground state of the Bose cluster does not have a super-partner.)

Thus, the three-particle problem is integrable in the first three orders in $1/d$.

5. SPIN, STATISTICS, AND SYMMETRY

The entire preceding analysis pertained, in fact, to "boltzmannons"—particles that are identical, but distinguishable in principle. We turn now to the question of the selection of the admissible states for particles possessing a given spin and statistics (including, possibly, parastatistics).

We shall consider the subspace $L(\{K_\gamma\})$ of the unperturbed wavefunctions with a fixed set of principal quantum numbers. The space $L(\{K_\gamma\})$ is isomorphic to the space of the representation

$\text{Symm} \{(N)^{K_s}(N-1, 1)^{K_v}(N-2, 2)^{K_t}\}$.

(In fact, the excitations of a cluster have boson statistics, and this requires symmetrization of the inner product of the corresponding set of one-particle representations.) By virtue of the invariance of the Hamiltonian (10) under the group S_N each subspace $L(\{K_\gamma\})$ decomposes into a direct sum of invariant (under S_N) subspaces $L^{(\mu)}(\{K_\gamma\})$, isomorphic to the direct sum of several complexes of the spaces $L^{(\mu)}$ of irreducible representation (μ). Some of the subspaces $L^{(\mu)}(\{K_\gamma\})$ may turn out to be trivial.

Fixing the number of particles, the spin and the statistics, and also the multiplet state of the system, we obtain the set of representations (μ) that corresponds to the physically observable states. For identical bosons with spin zero the only admissible representation is the completely symmetric representation (N), while for identical fermions with spin 1/2 in the $(N+1)$ -plet state, only the completely antisymmetric representation (1^N) is admissible. Selecting the physically admissible states, we obtain the spectrum (of the critical constants or energies) corresponding to the given type of particle. We note that the ground state of a fermion cluster with maximum total spin lies substantially above the ground state of the boson cluster. We shall illustrate this remark using the examples of three particles with spins $\frac{1}{2}$ and with spins 0, respectively. The space $L^{(1^3)}(K_s, K_v)$ is trivial for $K_v = 0, 1, 2$, and one-dimensional for $K_v = 3$. Thus, the ground state of the fermion cluster is shifted by an amount of order $3\tilde{d}\omega_v$ relative to the ground state of the boson cluster.

Thus, in the harmonic approximation one selects the (degenerate) levels satisfying certain symmetry requirements that follow from the statistics of the particles. However, not all states corresponding to a given level have the required symmetry. It is necessary to distinguish the physically admissible states and, only for these, solve the secular equation (15). To this end we shall expand the Hamiltonian (16) as a sum of irreducible operators:

$$K = \sum_{\{K_\gamma\}} \sum_{\mu} K P^{(\mu)}(\{K_\gamma\}). \quad (17)$$

Each level corresponding to the subspace $L^{(\mu)} = \oplus_{\{K_\gamma\}} L^{(\mu)}(\{K_\gamma\})$ is degenerate with multiplicity $\dim(\mu)$, which can be determined using the well known hook rule. This degeneracy is preserved, by virtue of the selection rules of Ref. 16, in all orders of perturbation theory. However, it has no physical meaning, since the Hamiltonian does not depend on the spin variables. In fact, the complete wavefunction is a superposition of coordinate wavefunctions corresponding to different components of the representation (μ) with coefficients equal to the spin wavefunctions, which are chosen in such a way that the complete wavefunction has the required symmetry.

6. TRAJECTORIES OF THE BOUND STATES IN THE "ENERGY-COUPLED CONSTANT" PLANE

We turn now to the calculation of the energy of the bound states. For simplicity we confine ourselves to the harmonic approximation. We first find the spectrum of the lev-

els for a threshold value of the coupling constant. The spectrum has a universal form and is a superposition of three equal-spacing spectra with frequencies that depend linearly on the quantum numbers $K_\gamma^{(0)}$ parametrizing the threshold:

$$\mathcal{E}(\{K_\tau\}, \{K_\tau^{(0)}\}) = \mathcal{E}(\{K_\tau^{(0)}\}) (\mathcal{E}_{\text{harm},1}(\{K_\tau\}) - \mathcal{E}_{\text{harm},1}(\{K_\tau^{(0)}\})), \quad (18)$$

where the first argument of \mathcal{E} denotes the set of quantum numbers of the (degenerate, in the harmonic approximation) level, and the second argument denotes the set of quantum numbers parametrizing the threshold at which the spectrum is calculated. Despite the fact that in the definition of $\mathcal{E}(\{K_\tau\}, \{K_\tau^{(0)}\})$ the arguments (the quantum numbers of the level and of the threshold) appear asymmetrically, the formula (18) possesses a well defined symmetry under interchange of the arguments of \mathcal{E} :

$$\mathcal{E}(\{K_\tau\}, \{K_\tau'\}) - \mathcal{E}(\{K_\tau'\}, \{K_\tau\}) = N(N-1) |U(a_0)| (\lambda_c(\{K_\tau\}) - \lambda_c(\{K_\tau'\})). \quad (19)$$

Using the formula (18), we now find the trajectories of the bound levels in the "energy-coupling constant" plane.

In constructing the trajectories we shall digress from questions associated with the particle statistics. We shall consider the part of the trajectory of a bound state with quantum numbers K_γ abutting the threshold $\lambda_c(\{K_\gamma\})$. For a value λ_{ph} differing little from the threshold value, the following approximate formula is valid:

$$\mathcal{E}(\{K_\tau\}) \approx -\frac{N(N-1)}{2} |U(a_0)| \left[\Delta\lambda + \frac{(\Delta\lambda)^2}{4\lambda_c(\{K_\tau\})} \right] + O((\Delta\lambda)^3), \quad (20)$$

where $\Delta\lambda = \lambda_{\text{ph}} - \lambda_c(\{K_\gamma\})$. We note that with increase of K_γ the relative contribution of the second term in the right-hand side of (20) decreases rapidly (at a fixed $\Delta\lambda$). The formula (20) is, in essence, the analytic continuation of (18) from a discrete set of threshold spectral values to arbitrary λ . In the opposite limiting case $\Delta\lambda \gg \lambda_c(\{K_\gamma\})$, we have

$$\mathcal{E}(\{K_\tau\}) \approx -N(N-1) |U(a_0)| \Delta\lambda. \quad (21)$$

We see that as $\Delta\lambda$ varies from zero to infinity the slope of the trajectories is doubled. (Of course, all of this applies only to the harmonic approximation.) We note that to obtain more-exact quantitative values for the energies of the bound states it is necessary to go beyond the harmonic approximation.

7. THE LENNARD-JONES POTENTIAL

We now apply the formulas obtained above to the Lennard-Jones potential

$$U(r) = 4\epsilon [(\sigma/r)^{12} - (\sigma/r)^6].$$

(The parameters ϵ and σ for the inert gases are given in, e.g., Ref. 17.) From the condition $r^2 U(r)|_{r=a_0} = \min$ we find $a_0^2 = (5/2)^{1/3} \sigma^2$ and $U(a_0) = 24\epsilon/25$. Substituting the values obtained into (12'), we find

$$\omega_s = 2^{1/3} \cdot 5^{1/6} \hbar^2 / M\sigma^2, \quad \omega_v = 2^{1/3} \cdot 3^{1/6} \cdot 5^{-1/6} \hbar^2 / M\sigma^2, \quad \omega_t = (1+4/N)^{1/2} 2^{1/3} \cdot 5^{-1/6} \hbar^2 / M\sigma^2. \quad (22)$$

Setting $d = 3$, from (22) we find the values of the "effective dimensionality" \bar{d} for different N :

$$\bar{d} = \begin{cases} 1 + 4\sqrt{5}(K_s + 1/2), & N = 2 \\ 2\sqrt{5}(K_s + 1/2) + 2\sqrt{3}(K_v + 1), & N = 3. \\ -1 + 2/3[2\sqrt{5}(K_s + 1/2) + 2\sqrt{3}(K_v + 3/2) + 2\sqrt{2}(K_t + 1)], & N = 4 \end{cases} \quad (23)$$

Using the parameters of the interatomic potentials (see Ref. 17), we obtain the spectrum of the critical coupling constants for inert-gas clusters in the harmonic approximation. For example, for ${}^4\text{He}_N$ clusters in the ground state we have [substituting (22) into (13)] the following values for the critical coupling constants:

$$\lambda_c(N=2) = 1.03, \quad \lambda_c(N=3) = 0.75, \quad \lambda_c(N=4) = 0.60, \quad (24)$$

which are in qualitative agreement with the results obtained by other methods (see, e.g., Refs. 3 and 4).

For a quantitative comparison of the method of the $1/d$ expansion with other methods it is necessary to calculate the next (in $1/d$) corrections in the perturbation-theory series.

8. CONCLUSION

Thus, as we see, the method of the $1/d$ expansion makes it possible to obtain the spectra of the critical coupling constants and bound-state energies of microclusters ($N \leq 4$). We note that this method is also suitable for calculating the energies of resonances decaying as a result of tunneling through the barrier in the effective potential.

For clusters with a larger number of particles the method of the $1/d$ expansion can be applied to calculate λ_c and the binding energy of the ground state of the cluster. We note, however, that the accuracy of this method worsens as N increases.

To improve the accuracy of the $1/d$ expansion we can employ interpolation using the limiting value $\lambda_c(N = \infty)$ calculated by other methods (e.g., by means of a cluster expansion). For example, in Ref. 18 it was shown that the potential

$$U_\mu(r) = \frac{1}{r^{2\mu+2}} - \frac{2}{r^{\mu+2}}$$

admits an exact solution in the limit $N \rightarrow \infty$: $\lambda_c = \frac{1}{4}(\mu - d + 2)^2$ for $\mu > d - 2$. Interpolating the $1/d$ expansion with the exact solution, we can obtain a formula which gives a sufficiently good approximation for all $N \geq 2$.

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